



wwPDB X-ray Structure Validation Summary Report ⓘ

Apr 18, 2026 – 06:32 PM UTC

PDB ID : 8E5Z / pdb_00008e5z
Title : Crystal structure of SARS-CoV-2 3CL protease in complex with a dimethyl sulfonyl benzene inhibitor
Authors : Lovell, S.; Liu, L.; Battaile, K.P.; Miller, M.J.; Groutas, W.C.
Deposited on : 2022-08-22
Resolution : 1.80 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

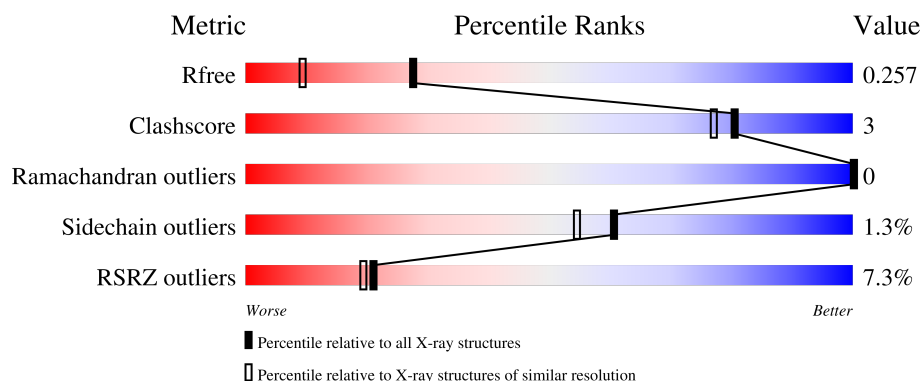
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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

Mol	Chain	Length	Quality of chain
1	A	309	10% 91% 6% .
1	B	309	4% 89% 8% .

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4777 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.

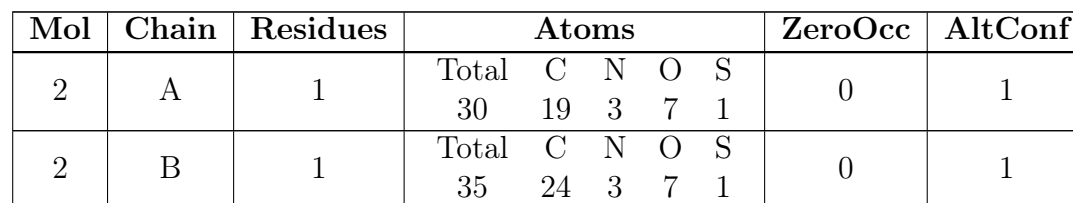
- Molecule 1 is a protein called 3C-like proteinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	300	Total	C	N	O	S	0	0	0
			2241	1421	376	423	21			
1	B	299	Total	C	N	O	S	0	0	0
			2241	1422	372	425	22			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	SER	-	expression tag	UNP P0DTD1
A	-2	ASN	-	expression tag	UNP P0DTD1
A	-1	ILE	-	expression tag	UNP P0DTD1
A	0	GLY	-	expression tag	UNP P0DTD1
B	-3	SER	-	expression tag	UNP P0DTD1
B	-2	ASN	-	expression tag	UNP P0DTD1
B	-1	ILE	-	expression tag	UNP P0DTD1
B	0	GLY	-	expression tag	UNP P0DTD1

- Molecule 2 is (1R,2S)-2-[(N-{[2-(benzenesulfonyl)-2-methylpropoxy]carbonyl}-L-leucyl)amino]-1-hydroxy-3-[(3S)-2-oxopyrrolidin-3-yl]propane-1-sulfonic acid (CCD ID: WJB) (formula: C₂₄H₃₇N₃O₁₀S₂).



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- The chemical structure of Uridine-5'-phosphate (UMP) is shown with atom labels. The pyrimidine ring is labeled with N1, C2, N3, C4, C5, C6, and N7. The ribose sugar is labeled with C1', C2', C3', C4', and C5'. The phosphate group is labeled with P1, O1, O2, and O3. The uracil base is labeled with N9, C10, C11, C12, C13, and C14. The ribose sugar is labeled with C15, C16, C17, C18, and C19. The phosphate group is labeled with P2, O4, O5, and O6. The uracil base is labeled with N10, C11, C12, C13, C14, and C15. The ribose sugar is labeled with C16, C17, C18, and C19. The phosphate group is labeled with P3, O7, O8, and O9. The uracil base is labeled with N11, C12, C13, C14, C15, and C16. The ribose sugar is labeled with C17, C18, C19, and C20. The phosphate group is labeled with P4, O10, O11, and O12. The uracil base is labeled with N12, C13, C14, C15, C16, and C17. The ribose sugar is labeled with C18, C19, C20, and C21. The phosphate group is labeled with P5, O13, O14, and O15. The uracil base is labeled with N13, C14, C15, C16, C17, and C18. The ribose sugar is labeled with C19, C20, C21, and C22. The phosphate group is labeled with P6, O16, O17, and O18. The uracil base is labeled with N14, C15, C16, C17, C18, and C19. The ribose sugar is labeled with C20, C21, C22, and C23. The phosphate group is labeled with P7, O19, O20, and O21. The uracil base is labeled with N15, C16, C17, C18, C19, and C20. The ribose sugar is labeled with C21, C22, C23, and C24. The phosphate group is labeled with P8, O22, O23, and O24. The uracil base is labeled with N16, C17, C18, C19, C20, and C21. The ribose sugar is labeled with C22, C23, C24, and C25. The phosphate group is labeled with P9, O25, O26, and O27. The uracil base is labeled with N17, C18, C19, C20, C21, and C22. The ribose sugar is labeled with C23, C24, C25, and C26. The phosphate group is labeled with P10, O28, O29, and O30. The uracil base is labeled with N18, C19, C20, C21, C22, and C23. The ribose sugar is labeled with C24, C25, C26, and C27. The phosphate group is labeled with P11, O31, O32, and O33. The uracil base is labeled with N19, C20, C21, C22, C23, and C24. The ribose sugar is labeled with C25, C26, C27, and C28. The phosphate group is labeled with P12, O34, O35, and O36. The uracil base is labeled with N20, C21, C22, C23, C24, and C25. The ribose sugar is labeled with C26, C27, C28, and C29. The phosphate group is labeled with P13, O37, O38, and O39. The uracil base is labeled with N21, C22, C23, C24, C25, and C26. The ribose sugar is labeled with C27, C28, C29, and C30. The phosphate group is labeled with P14, O40, O41, and O42. The uracil base is labeled with N22, C23, C24, C25, C26, and C27. The ribose sugar is labeled with C28, C29, C30, and C31. The phosphate group is labeled with P15, O43, O44, and O45. The uracil base is labeled with N23, C24, C25, C26, C27, and C28. The ribose sugar is labeled with C29, C30, C31, and C32. The phosphate group is labeled with P16, O46, O47, and O48. The uracil base is labeled with N24, C25, C26, C27, C28, and C29. The ribose sugar is labeled with C30, C31, C32, and C33. The phosphate group is labeled with P17, O49, O50, and O51. The uracil base is labeled with N25, C26, C27, C28, C29, and C30. The ribose sugar is labeled with C31, C32, C33, and C34. The phosphate group is labeled with P18, O52, O53, and O54. The uracil base is labeled with N26, C27, C28, C29, C30, and C31. The ribose sugar is labeled with C32, C33, C34, and C35. The phosphate group is labeled with P19, O55, O56, and O57. The uracil base is labeled with N27, C28, C29, C30, C31, and C32. The ribose sugar is labeled with C33, C34, C35, and C36. The phosphate group is labeled with P20, O58, O59, and O60. The uracil base is labeled with N28, C29, C30, C31, C32, and C33. The ribose sugar is labeled with C34, C35, C36, and C37. The phosphate group is labeled with P21, O61, O62, and O63. The uracil base is labeled with N29, C30, C31, C32, C33, and C34. The ribose sugar is labeled with C35, C36, C37, and C38. The phosphate group is labeled with P22, O64, O65, and O66. The uracil base is labeled with N30, C31, C32, C33, C34, and C35. The ribose sugar is labeled with C36, C37, C38, and C39. The phosphate group is labeled with P23, O67, O68, and O69. The uracil base is labeled with N31, C32, C33, C34, C35, and C36. The ribose sugar is labeled with C37, C38, C39, and C40. The phosphate group is labeled with P24, O70, O71, and O72. The uracil base is labeled with N32, C33, C34, C35, C36, and C37. The ribose sugar is labeled with C38, C39, C40, and C41. The phosphate group is labeled with P25, O73, O74, and O75. The uracil base is labeled with N33, C34, C35, C36, C37, and C38. The ribose sugar is labeled with C39, C40, C41, and C42. The phosphate group is labeled with P26, O76, O77, and O78. The uracil base is labeled with N34, C35, C36, C37, C38, and C39. The ribose sugar is labeled with C40, C41, C42, and C43. The phosphate group is labeled with P27, O79, O80, and O81. The uracil base is labeled with N35, C36, C37, C38, C39, and C40. The ribose sugar is labeled with C41, C42, C43, and C44. The phosphate group is labeled with P28, O82, O83, and O84. The uracil base is labeled with N36, C37, C38, C39, C40, and C41. The ribose sugar is labeled with C42, C43, C44, and C45. The phosphate group is labeled with P29, O85, O86, and O87. The uracil base is labeled with N37, C38, C39, C40, C41, and C42. The ribose sugar is labeled with C43, C44, C45, and C46. The phosphate group is labeled with P30, O88, O89, and O90. The uracil base is labeled with N38, C39, C40, C41, C42, and C43. The ribose sugar is labeled with C44, C45, C46, and C47. The phosphate group is labeled with P31, O91, O92, and O93. The uracil base is labeled with N39, C40, C41, C42, C43, and C44. The ribose sugar is labeled with C45, C46, C47, and C48. The phosphate group is labeled with P32, O94, O95, and O96. The uracil base is labeled with N40, C41, C42, C43, C44, and C45. The ribose sugar is labeled with C46, C47, C48, and C49. The phosphate group is labeled with P33, O97, O98, and O99. The uracil base is labeled with N41, C42, C43, C44, C45, and C46. The ribose sugar is labeled with C47, C48, C49, and C50. The phosphate group is labeled with P34, O100, O101, and O102. The uracil base is labeled with N42, C43, C44, C45, C46, and C47. The ribose sugar is labeled with C48, C49, C50, and C51. The phosphate group is labeled with P35, O103, O104, and O105. The uracil base is labeled with N43, C44, C45, C46, C47, and C48. The ribose sugar is labeled with C49, C50, C51, and C52. The phosphate group is labeled with P36, O106, O107, and O108. The uracil base is labeled with N44, C45, C46, C47, C48, and C49. The ribose sugar is labeled with C50, C51, C52, and C53. The phosphate group is labeled with P37, O109, O110, and O111. The uracil base is labeled with N45, C46, C47, C48, C49, and C50. The ribose sugar is labeled with C51, C52, C53, and C54. The phosphate group is labeled with P38, O112, O113, and O114. The uracil base is labeled with N46, C47, C48, C49, C50, and C51. The ribose sugar is labeled with C52, C53, C54, and C55. The phosphate group is labeled with P39, O115, O116, and O117. The uracil base is labeled with N47, C48, C49, C50, C51, and C52. The ribose sugar is labeled with C53, C54, C55, and C56. The phosphate group is labeled with P40, O118, O119, and O120. The uracil base is labeled with N48, C49, C50, C51, C52, and C53. The ribose sugar is labeled with C54, C55, C56, and C57. The phosphate group is labeled with P41, O121, O122, and O123. The uracil base is labeled with N49, C50, C51, C52, C53, and C54. The ribose sugar is labeled with C55, C56, C57, and C58. The phosphate group is labeled with P42, O124, O125, and O126. The uracil base is labeled with N50, C51, C52, C53, C54, and C55. The ribose sugar is labeled with C56, C57, C58, and C59. The phosphate group is labeled with P43, O127, O128, and O129. The uracil base is labeled with N51, C52, C53, C54, C55, and C56. The ribose sugar is labeled with C57, C58, C59, and C60. The phosphate group is labeled with P44, O130, O131, and O132. The uracil base is labeled with N52, C53, C54, C55, C56, and C57. The ribose sugar is labeled with C58, C59, C60, and C61. The phosphate group is labeled with P45, O133, O134, and O135. The uracil base is labeled with N53, C54, C55, C56, C57, and C58. The ribose sugar is labeled with C59, C60, C61, and C62. The phosphate group is labeled with P46, O136, O137, and O138. The uracil base is labeled with N54, C55, C56, C57, C58, and C59. The ribose sugar is labeled with C60, C61, C62, and C63. The phosphate group is labeled with P47, O139, O140, and O141. The uracil base is labeled with N55, C56, C57, C58, C59, and C60. The ribose sugar is labeled with C61, C62, C63, and C64. The phosphate group is labeled with P48, O142, O143, and O144. The uracil base is labeled with N56, C57, C58, C59, C60, and C61. The ribose sugar is labeled with C62, C63, C64, and C65. The phosphate group is labeled with P49, O145, O146, and O147. The uracil base is labeled with N57, C58, C59, C60, C61, and C62. The ribose sugar is labeled with C63, C64, C65, and C66. The phosphate group is labeled with P50, O148, O149, and O150. The uracil base is labeled with N58, C59, C6

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	1
			30	19	3	7	1		



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	S	0	1
			35	24	3	7	1		

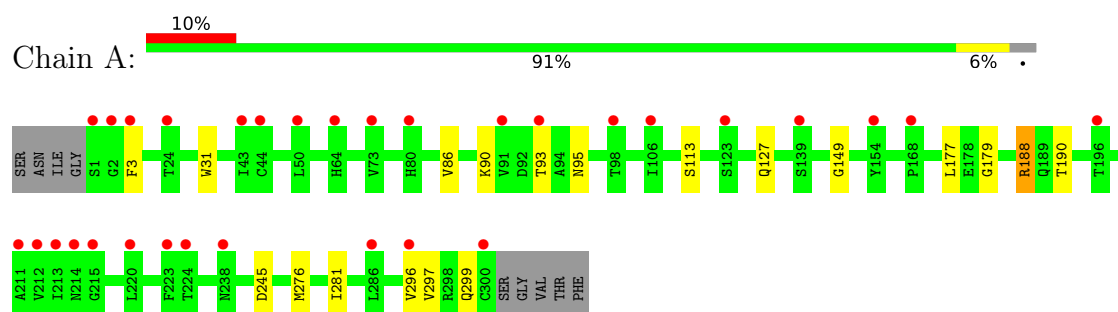
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	72	Total	O	0	0
			72	72		
4	B	93	Total	O	0	0
			93	93		

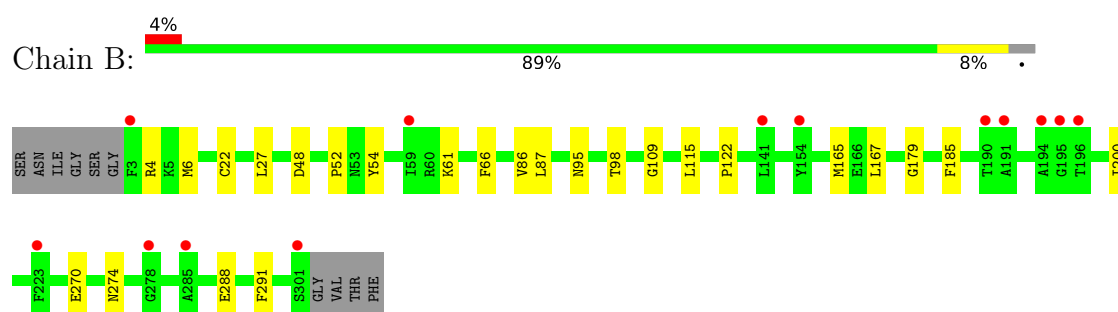
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: 3C-like proteinase



- Molecule 1: 3C-like proteinase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	54.69Å 98.35Å 58.33Å 90.00° 107.22° 90.00°	Depositor
Resolution (Å)	33.36 – 1.80 33.36 – 1.80	Depositor EDS
% Data completeness (in resolution range)	97.5 (33.36-1.80) 97.5 (33.36-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.58 (at 1.79Å)	Xtriage
Refinement program	PHENIX 1.20RC2_4402	Depositor
R, R_{free}	0.195 , 0.253 0.202 , 0.257	Depositor DCC
R_{free} test set	2637 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	27.6	Xtriage
Anisotropy	0.418	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 41.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	4777	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.93% 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: WJB, UQO

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	0.44	0/2290	0.61	0/3123
1	B	0.46	0/2290	0.64	0/3124
All	All	0.45	0/4580	0.62	0/6247

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2241	0	2132	11	0
1	B	2241	0	2130	13	0
2	A	30	0	0	0	0
2	B	35	0	0	0	0
3	A	30	0	0	0	0
3	B	35	0	0	0	0
4	A	72	0	0	1	0
4	B	93	0	0	1	0
All	All	4777	0	4262	23	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 3.

The worst 5 of 23 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:86:VAL:HG13	1:A:179:GLY:HA2	1.74	0.68
1:B:86:VAL:HG13	1:B:179:GLY:HA2	1.75	0.68
1:B:115:LEU:HD11	1:B:122:PRO:HB3	1.85	0.58
1:B:109:GLY:HA2	1:B:200:ILE:HD13	1.88	0.56
1:B:22:CYS:SG	1:B:61:LYS:NZ	2.73	0.56

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	298/309 (96%)	289 (97%)	9 (3%)	0	100	100
1	B	297/309 (96%)	288 (97%)	9 (3%)	0	100	100
All	All	595/618 (96%)	577 (97%)	18 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	237/265 (89%)	233 (98%)	4 (2%)	53	45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	239/265 (90%)	237 (99%)	2 (1%)	73	70
All	All	476/530 (90%)	470 (99%)	6 (1%)	61	54

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	297	VAL
1	B	27	LEU
1	B	165	MET
1	A	93	THR
1	A	90	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	119	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the

expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	UQO	B	402[B]	1	34,36,40	1.66	4 (11%)	41,51,59	2.60	11 (26%)
2	WJB	B	401[A]	1	34,36,40	1.65	5 (14%)	41,51,59	2.55	11 (26%)
3	UQO	A	402[B]	1	28,30,40	1.72	6 (21%)	35,43,59	2.18	9 (25%)
2	WJB	A	401[A]	1	28,30,40	1.63	5 (17%)	35,43,59	2.35	9 (25%)

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	UQO	B	402[B]	1	-	4/42/53/61	0/2/2/2
2	WJB	B	401[A]	1	-	2/42/53/61	0/2/2/2
3	UQO	A	402[B]	1	-	4/33/47/61	0/1/1/2
2	WJB	A	401[A]	1	-	4/33/47/61	0/1/1/2

The worst 5 of 20 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401[A]	WJB	C17-N18	5.54	1.39	1.33
3	A	402[B]	UQO	C17-N18	5.46	1.39	1.33
2	B	401[A]	WJB	C17-N18	5.44	1.39	1.33
3	B	402[B]	UQO	C17-N18	5.42	1.39	1.33
2	B	401[A]	WJB	C28-S27	-4.03	1.71	1.76

The worst 5 of 40 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	402[B]	UQO	O04-C03-C02	8.49	120.56	107.79
3	A	402[B]	UQO	O04-C03-C02	8.20	120.11	107.79
2	B	401[A]	WJB	O04-C03-C02	8.01	119.84	107.79
2	A	401[A]	WJB	O04-C03-C02	6.59	117.70	107.79
2	A	401[A]	WJB	C26-C02-S27	-6.58	102.79	108.25

There are no chirality outliers.

5 of 14 torsion outliers are listed below:

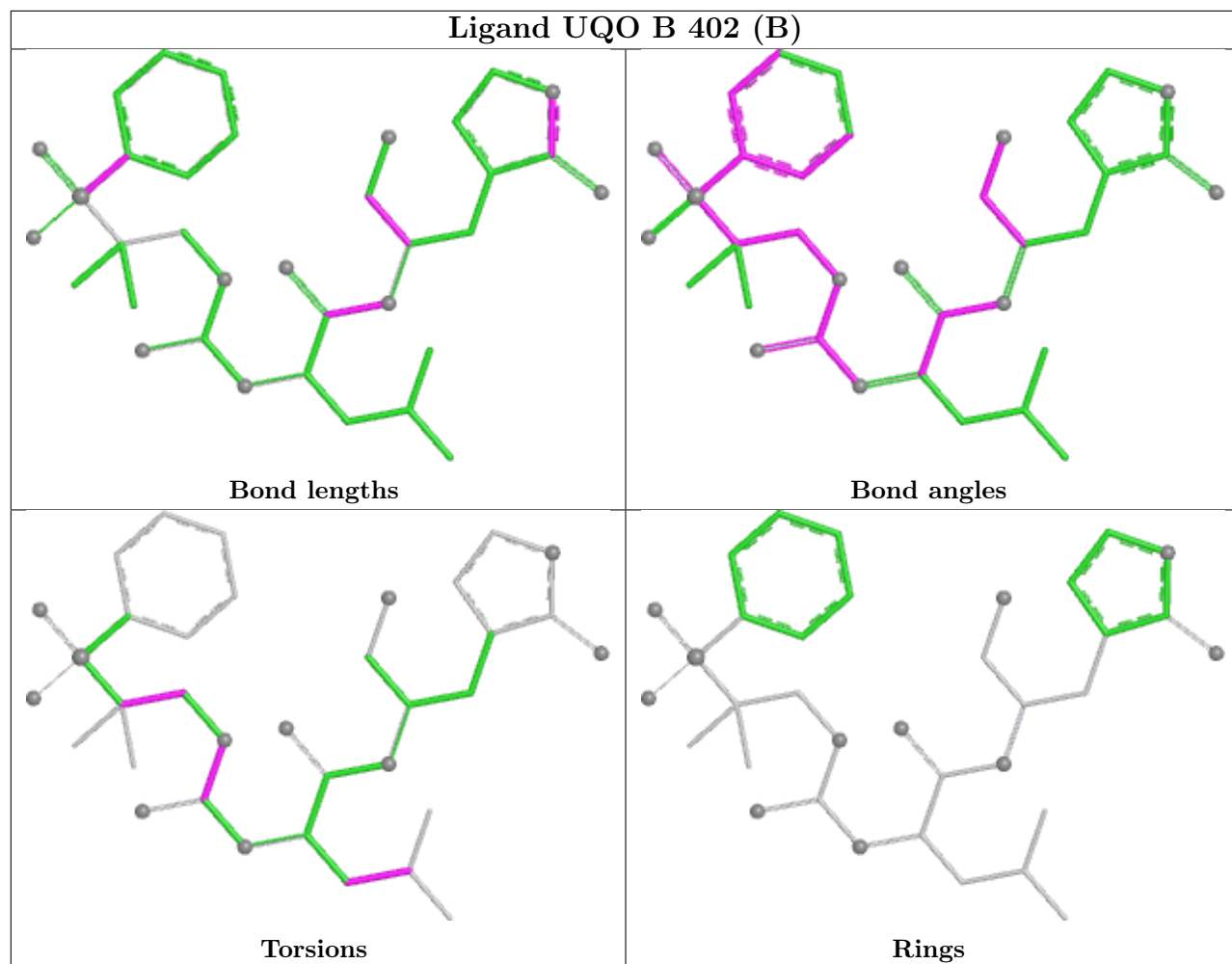
Mol	Chain	Res	Type	Atoms
2	A	401[A]	WJB	C26-C02-C03-O04
2	A	401[A]	WJB	C01-C02-C03-O04
2	A	401[A]	WJB	N06-C05-O04-C03
3	A	402[B]	UQO	C26-C02-C03-O04
3	A	402[B]	UQO	C01-C02-C03-O04

There are no ring outliers.

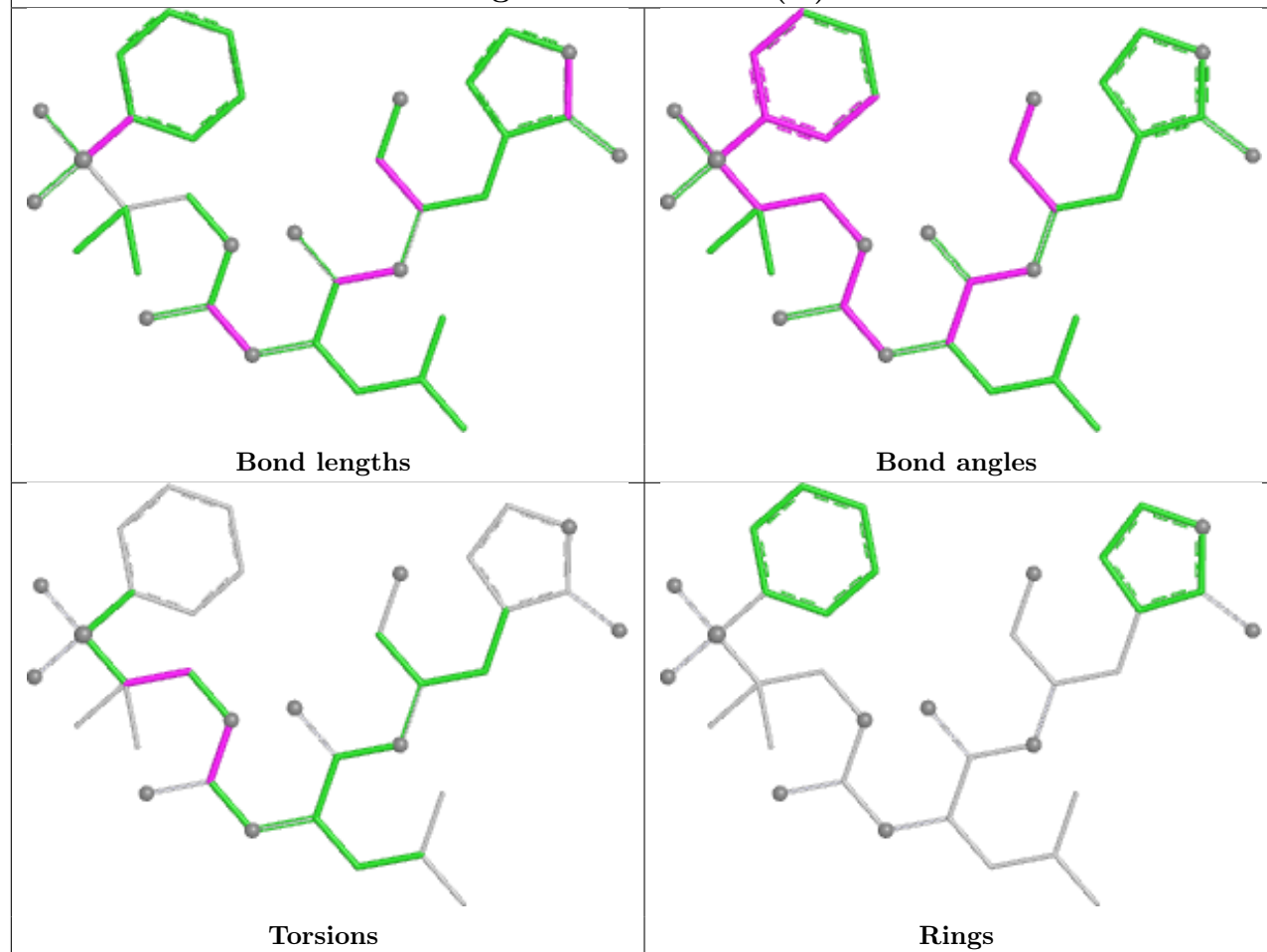
No monomer is involved in short contacts.

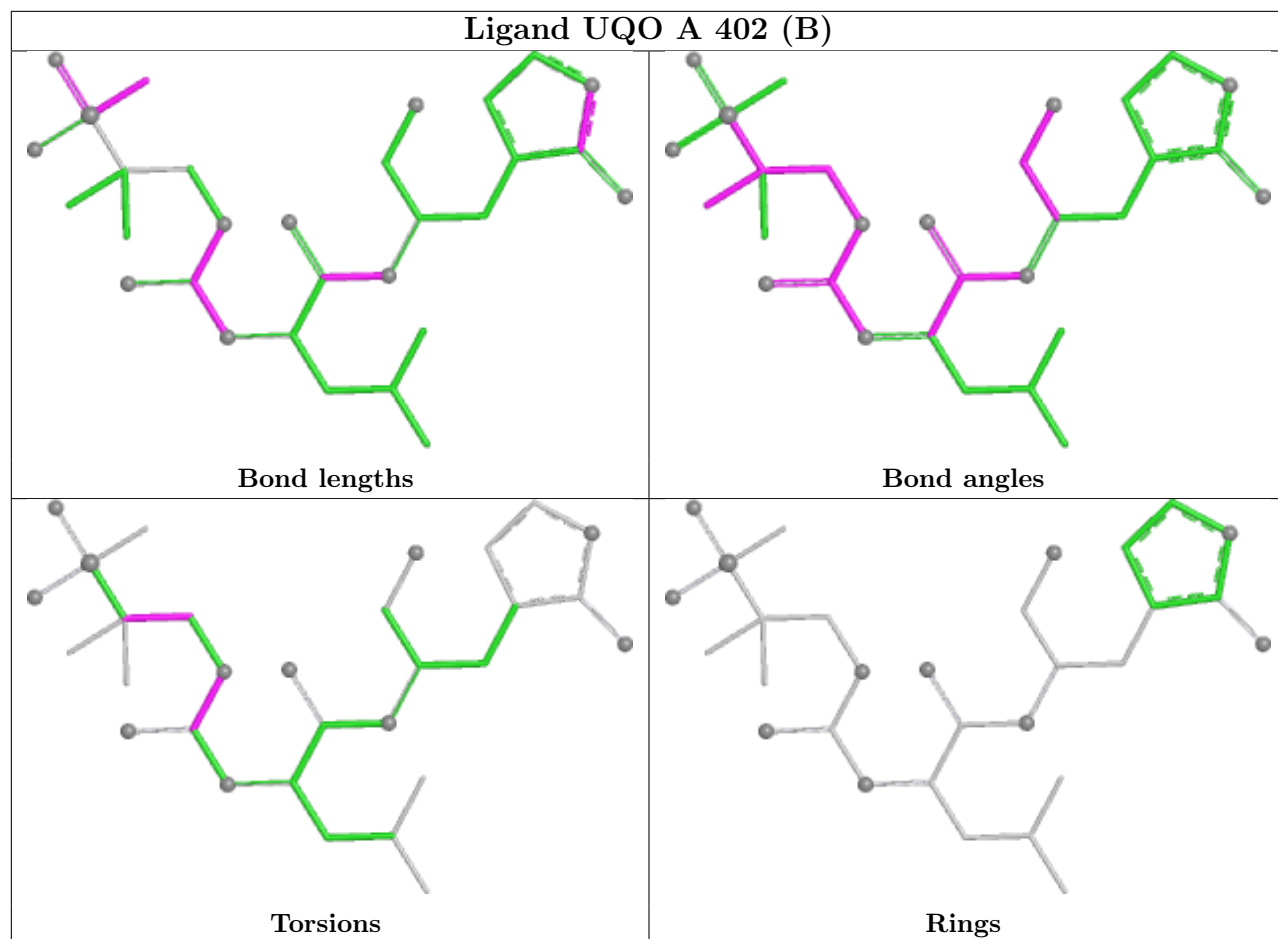
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

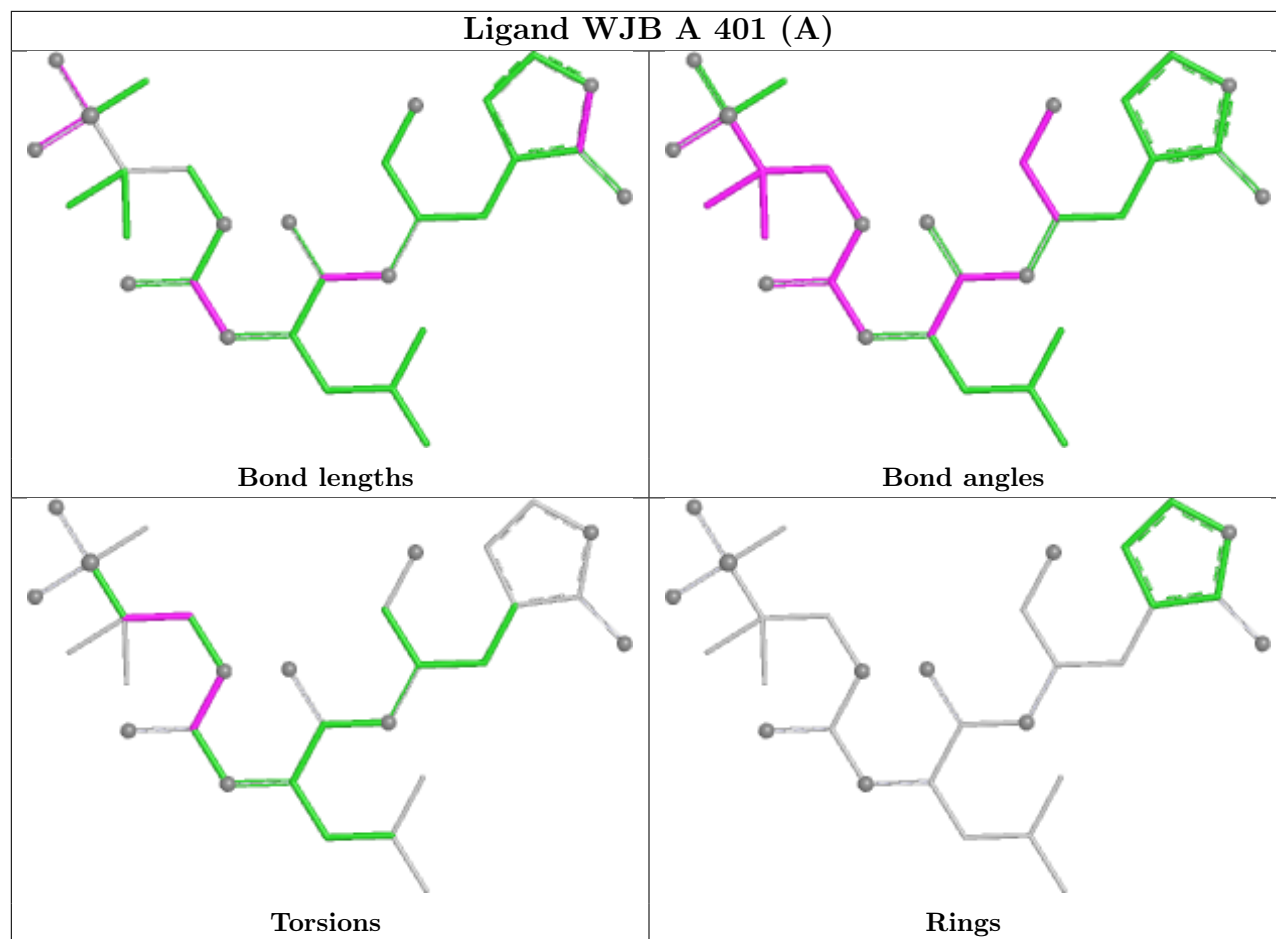
Ligand UQO B 402 (B)



Ligand WJB B 401 (A)







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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	300/309 (97%)	0.89	31 (10%) 12 10	26, 43, 63, 85	0
1	B	299/309 (96%)	0.62	13 (4%) 40 39	26, 36, 59, 70	0
All	All	599/618 (96%)	0.76	44 (7%) 21 19	26, 39, 61, 85	0

The worst 5 of 44 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	223	PHE	3.6
1	A	154	TYR	3.3
1	B	223	PHE	3.1
1	A	3	PHE	3.0
1	A	24	THR	2.9

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

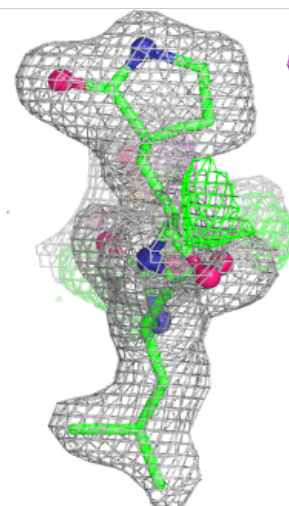
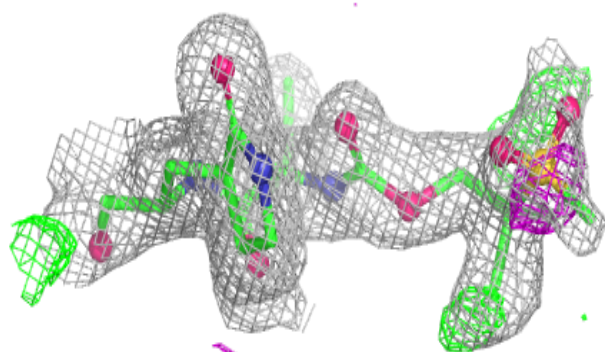
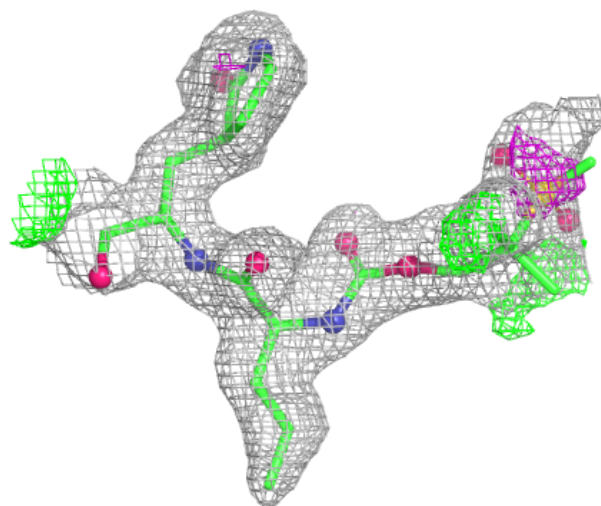
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	WJB	A	401[A]	30/39	0.83	0.16	29,38,62,75	30
3	UQO	A	402[B]	30/39	0.84	0.15	21,38,62,79	30
2	WJB	B	401[A]	35/39	0.88	0.13	30,41,54,55	35
3	UQO	B	402[B]	35/39	0.88	0.13	26,41,54,55	35

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.

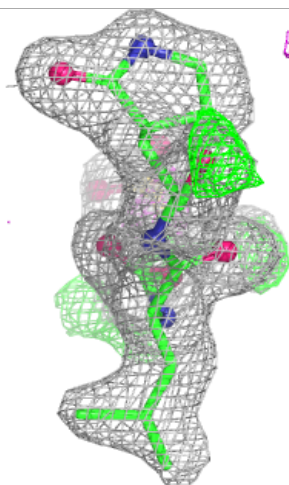
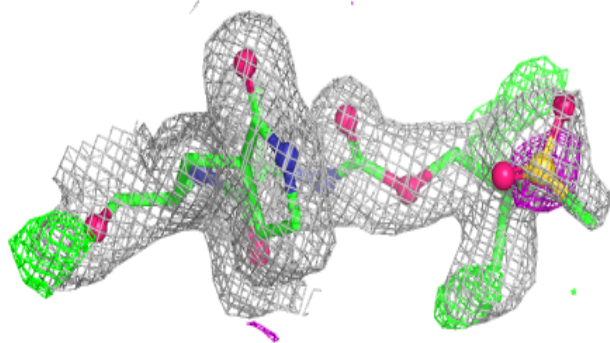
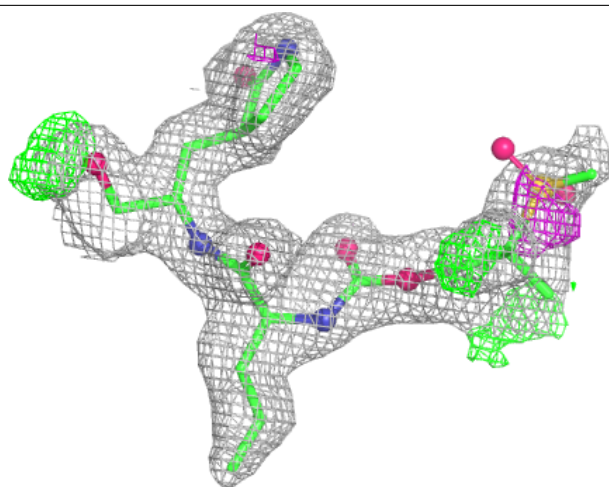
Electron density around WJB A 401 (A):

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



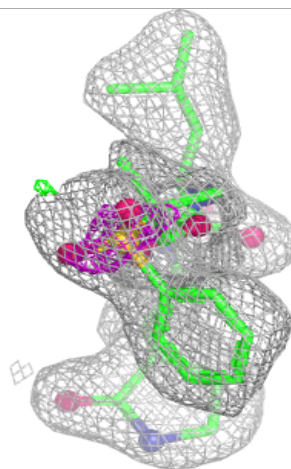
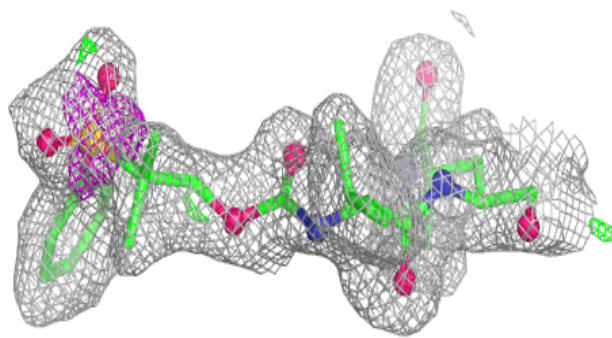
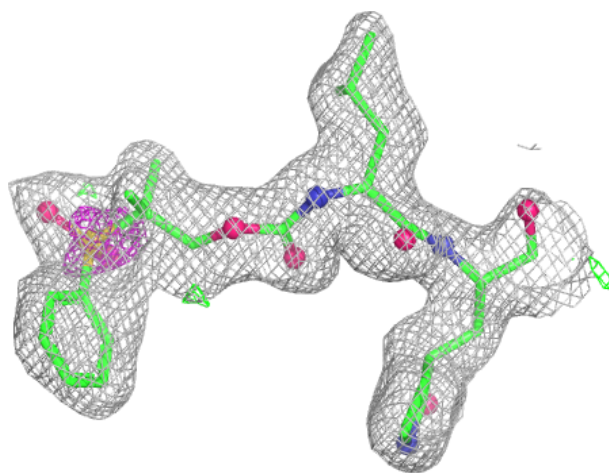
Electron density around UQO A 402 (B):

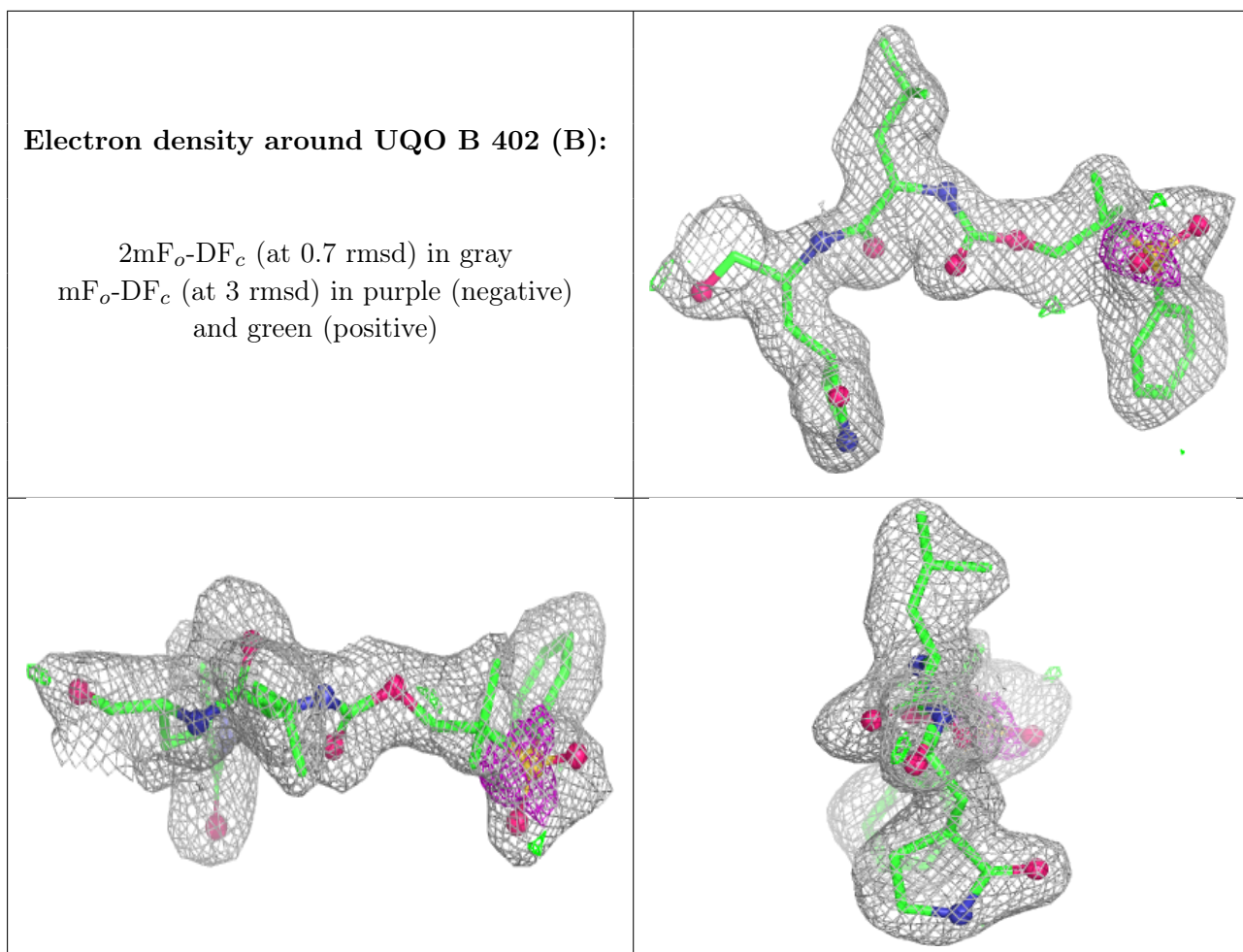
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around WJB B 401 (A):

$2mF_o-DF_c$ (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.