



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 01:54 PM UTC

PDB ID : 6X0T / pdb_00006x0t
Title : Structure of human plasma factor XIIa in complex with (2S)-1-(N,3-dicyclohexyl-D-alanyl)-4-[(4R,5S)-4-methyl-5-phenyl-4,5-dihydro-1,3-oxazol-2-yl]-N-[(thiophen-2-yl)methyl]piperazine-2-carboxamide (compound 8h)
Authors : Orth, P.
Deposited on : 2020-05-17
Resolution : 1.39 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

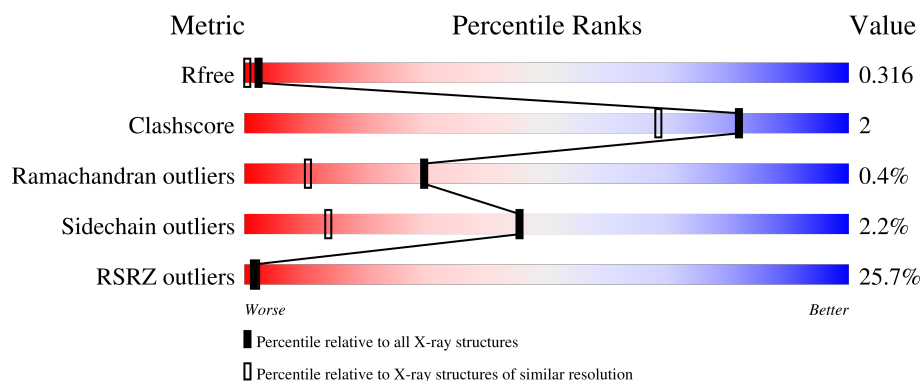
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.39 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	4403 (1.40-1.36)
Clashscore	190562	4528 (1.40-1.36)
Ramachandran outliers	187476	4459 (1.40-1.36)
Sidechain outliers	187428	4458 (1.40-1.36)
RSRZ outliers	180081	4399 (1.40-1.36)

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	259	25% 83% 10% 7%
1	B	259	25% 81% 10% 8%
1	C	259	21% 85% 8% 7%

2 Entry composition [i](#)

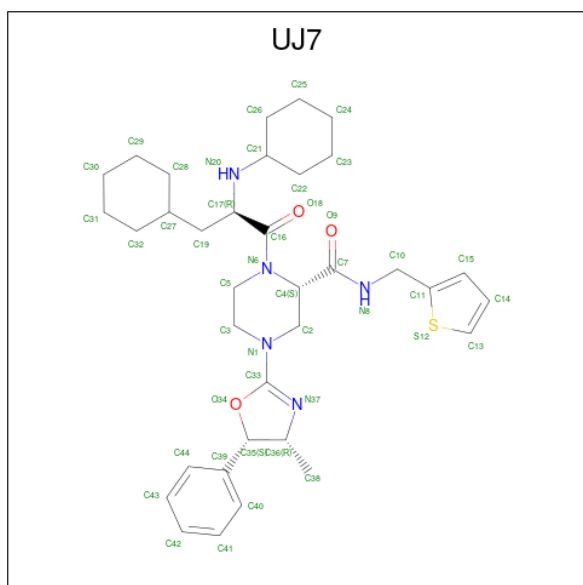
There are 4 unique types of molecules in this entry. The entry contains 5816 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Coagulation factor XII.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	241	Total	C	N	O	S	0	0	0
			1796	1132	319	330	15			
1	B	238	Total	C	N	O	S	0	0	0
			1784	1125	317	327	15			
1	C	240	Total	C	N	O	S	0	0	0
			1796	1131	316	334	15			

- Molecule 2 is (2S)-1-(N,3-dicyclohexyl-D-alanyl)-4-[(4R,5S)-4-methyl-5-phenyl-4,5-dihydro-1,3-oxazol-2-yl]-N-[(thiophen-2-yl)methyl]piperazine-2-carboxamide (CCD ID: UJ7) (formula: C₃₅H₄₉N₅O₃S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			44	35	5	3	1		
2	B	1	Total	C	N	O	S	0	0
			44	35	5	3	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	S	0	0
			44	35	5	3	1		

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

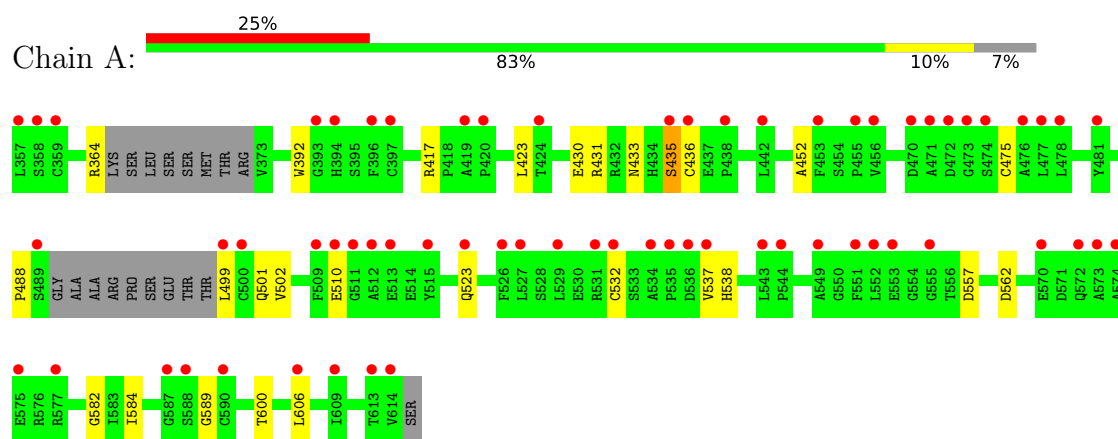
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	93	Total	O	0	0
			93	93		
4	B	105	Total	O	0	0
			105	105		
4	C	105	Total	O	0	0
			105	105		

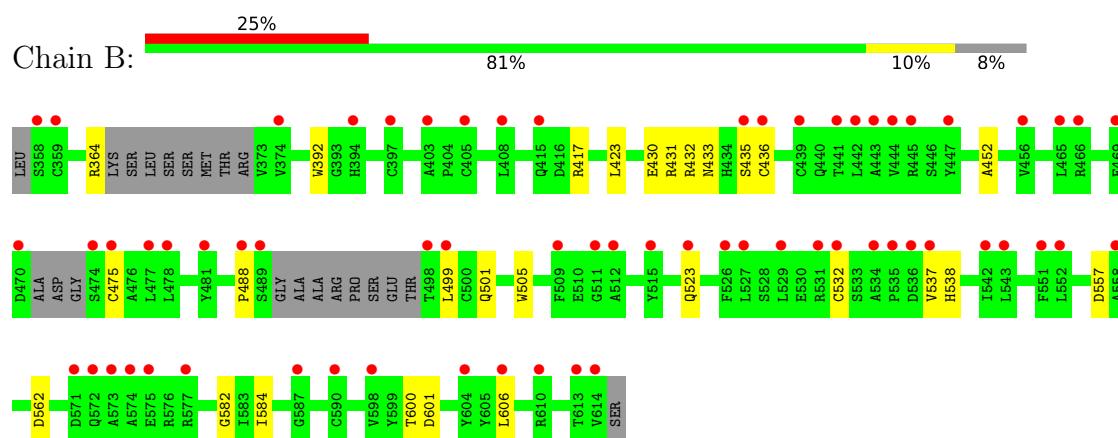
3 Residue-property plots [i](#)

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.

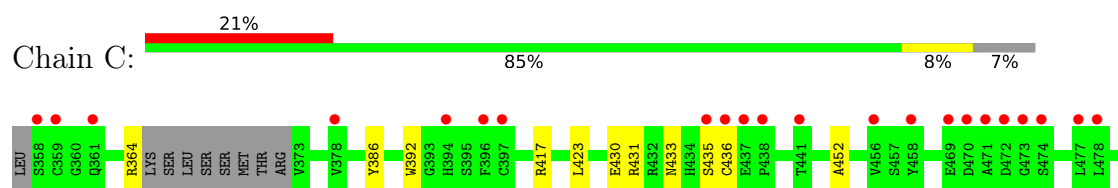
• Molecule 1: Coagulation factor XII

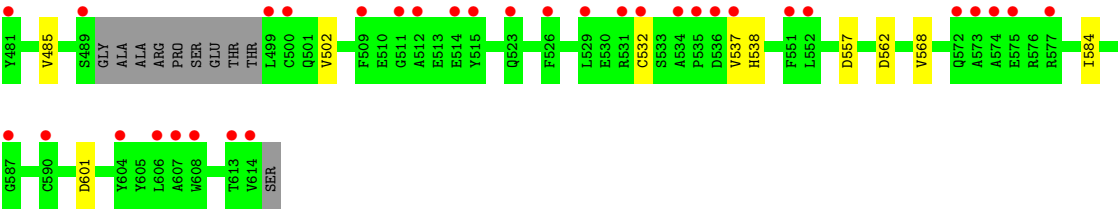


• Molecule 1: Coagulation factor XII



• Molecule 1: Coagulation factor XII





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	77.12Å 133.41Å 88.86Å 90.00° 104.40° 90.00°	Depositor
Resolution (Å)	47.26 – 1.39 47.26 – 1.39	Depositor EDS
% Data completeness (in resolution range)	63.5 (47.26-1.39) 63.5 (47.26-1.39)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.46 (at 1.39Å)	Xtriage
Refinement program	BUSTER 2.11.7 (6-FEB-2020)	Depositor
R, R_{free}	0.289 , 0.311 0.290 , 0.316	Depositor DCC
R_{free} test set	2229 reflections (2.01%)	wwPDB-VP
Wilson B-factor (Å ²)	13.7	Xtriage
Anisotropy	0.344	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 27.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	5816	wwPDB-VP
Average B, all atoms (Å ²)	10.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.84% 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: SO4, UJ7

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	0.72	1/1841 (0.1%)	0.97	3/2510 (0.1%)
1	B	0.74	1/1828 (0.1%)	0.98	4/2491 (0.2%)
1	C	0.73	0/1841	0.98	4/2510 (0.2%)
All	All	0.73	2/5510 (0.0%)	0.98	11/7511 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	475	CYS	CA-C	6.11	1.55	1.52
1	B	475	CYS	CA-C	6.10	1.55	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	430	GLU	N-CA-C	-6.37	103.40	112.13
1	B	430	GLU	N-CA-C	-6.29	103.69	112.12
1	C	430	GLU	N-CA-C	-6.15	103.70	112.13
1	B	601	ASP	CA-CB-CG	5.66	118.26	112.60
1	B	557	ASP	CA-CB-CG	5.55	118.15	112.60
1	A	557	ASP	CA-CB-CG	5.42	118.02	112.60
1	C	557	ASP	CA-CB-CG	5.39	117.99	112.60
1	C	601	ASP	CA-CB-CG	5.24	117.84	112.60
1	B	435	SER	N-CA-C	-5.17	103.21	110.50
1	A	435	SER	N-CA-C	-5.01	103.07	110.48
1	C	435	SER	N-CA-C	-5.00	103.08	110.48

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	1796	0	1696	10	0
1	B	1784	0	1692	10	0
1	C	1796	0	1695	9	0
2	A	44	0	0	0	0
2	B	44	0	0	0	0
2	C	44	0	0	0	0
3	A	5	0	0	0	0
4	A	93	0	0	0	0
4	B	105	0	0	0	0
4	C	105	0	0	0	0
All	All	5816	0	5083	26	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 2.

All (26) 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:431:ARG:HH21	1:A:433:ASN:HD21	1.29	0.81
1:B:501:GLN:HE21	1:B:523:GLN:NE2	1.84	0.74
1:C:431:ARG:HH21	1:C:433:ASN:HD21	1.49	0.59
1:B:431:ARG:HH21	1:B:433:ASN:HD21	1.51	0.58
1:B:488:PRO:HD2	1:B:606:LEU:HD21	1.96	0.47
1:A:488:PRO:HD2	1:A:606:LEU:HD21	1.98	0.45
1:A:502:VAL:HG23	1:A:584:ILE:HD11	1.98	0.45
1:C:392:TRP:HB3	1:C:423:LEU:HD23	1.99	0.45
1:C:431:ARG:HH21	1:C:433:ASN:ND2	2.13	0.45
1:A:510:GLU:OE1	1:A:589:GLY:HA2	2.17	0.44
1:C:502:VAL:HG23	1:C:584:ILE:HD11	1.99	0.44
1:A:582:GLY:HA2	1:A:600:THR:O	2.18	0.43
1:B:392:TRP:HB3	1:B:423:LEU:HD23	2.00	0.43
1:B:432:ARG:HG3	1:B:505:TRP:CD1	2.53	0.43
1:B:582:GLY:HA2	1:B:600:THR:O	2.18	0.43
1:B:562:ASP:HB3	1:B:584:ILE:HD13	2.01	0.42
1:C:562:ASP:HB3	1:C:584:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:TRP:HB3	1:A:423:LEU:HD23	2.01	0.42
1:A:562:ASP:HB3	1:A:584:ILE:HD13	2.01	0.42
1:C:532:CYS:SG	1:C:538:HIS:HD2	2.43	0.42
1:A:417:ARG:CZ	1:C:452:ALA:HB2	2.50	0.41
1:A:532:CYS:SG	1:A:538:HIS:HD2	2.44	0.41
1:A:452:ALA:HB2	1:B:417:ARG:CZ	2.52	0.40
1:B:452:ALA:HB2	1:C:417:ARG:CZ	2.51	0.40
1:B:532:CYS:SG	1:B:538:HIS:HD2	2.43	0.40
1:C:386:TYR:CG	1:C:485:VAL:HB	2.56	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	235/259 (91%)	227 (97%)	7 (3%)	1 (0%)	30	10
1	B	230/259 (89%)	222 (96%)	7 (3%)	1 (0%)	30	10
1	C	234/259 (90%)	226 (97%)	7 (3%)	1 (0%)	30	10
All	All	699/777 (90%)	675 (97%)	21 (3%)	3 (0%)	30	10

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	537	VAL
1	B	537	VAL
1	C	537	VAL

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	184/207 (89%)	178 (97%)	6 (3%)	33	6
1	B	185/207 (89%)	182 (98%)	3 (2%)	55	22
1	C	186/207 (90%)	183 (98%)	3 (2%)	55	22
All	All	555/621 (89%)	543 (98%)	12 (2%)	45	14

All (12) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	364	ARG
1	A	435	SER
1	A	436	CYS
1	A	499	LEU
1	A	501	GLN
1	A	523	GLN
1	B	364	ARG
1	B	436	CYS
1	B	499	LEU
1	C	364	ARG
1	C	436	CYS
1	C	568	VAL

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

Mol	Chain	Res	Type
1	A	429	GLN
1	A	508	GLN
1	A	523	GLN
1	B	429	GLN
1	B	508	GLN
1	B	523	GLN
1	C	508	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](#)

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	$\# Z > 2$
2	UJ7	C	701	-	48,49,49	0.81	2 (4%)	58,67,67	1.70	6 (10%)
2	UJ7	A	701	-	48,49,49	0.88	3 (6%)	58,67,67	1.69	3 (5%)
3	SO4	A	702	-	4,4,4	0.31	0	6,6,6	0.57	0
2	UJ7	B	701	-	48,49,49	0.80	1 (2%)	58,67,67	1.64	6 (10%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UJ7	C	701	-	-	1/33/74/74	0/6/6/6
2	UJ7	A	701	-	-	1/33/74/74	0/6/6/6
2	UJ7	B	701	-	-	1/33/74/74	0/6/6/6

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	701	UJ7	C16-N6	2.25	1.39	1.34
2	B	701	UJ7	O34-C35	-2.21	1.43	1.46
2	A	701	UJ7	C36-N37	-2.20	1.44	1.48
2	A	701	UJ7	C36-C35	-2.17	1.52	1.55
2	C	701	UJ7	C36-N37	-2.12	1.44	1.48
2	C	701	UJ7	O34-C35	-2.05	1.43	1.46

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	UJ7	O34-C33-N37	-8.55	113.36	117.78
2	B	701	UJ7	O34-C33-N37	-7.99	113.65	117.78
2	C	701	UJ7	O34-C33-N37	-7.51	113.89	117.78
2	C	701	UJ7	O34-C35-C36	6.96	107.90	102.83
2	A	701	UJ7	O34-C35-C36	5.96	107.17	102.83
2	B	701	UJ7	O34-C35-C36	5.30	106.69	102.83
2	C	701	UJ7	C3-N1-C2	4.41	121.57	113.07
2	B	701	UJ7	C3-N1-C2	4.12	121.01	113.07
2	A	701	UJ7	C3-N1-C2	3.83	120.45	113.07
2	B	701	UJ7	C7-C4-N6	-2.73	104.58	111.21
2	B	701	UJ7	C4-C7-N8	-2.31	111.00	115.99
2	C	701	UJ7	C5-N6-C4	2.30	120.58	115.81
2	C	701	UJ7	C7-C4-N6	-2.23	105.79	111.21
2	B	701	UJ7	C5-N6-C4	2.22	120.41	115.81
2	C	701	UJ7	C35-C36-N37	-2.22	100.29	103.91

There are no chirality outliers.

All (3) torsion outliers are listed below:

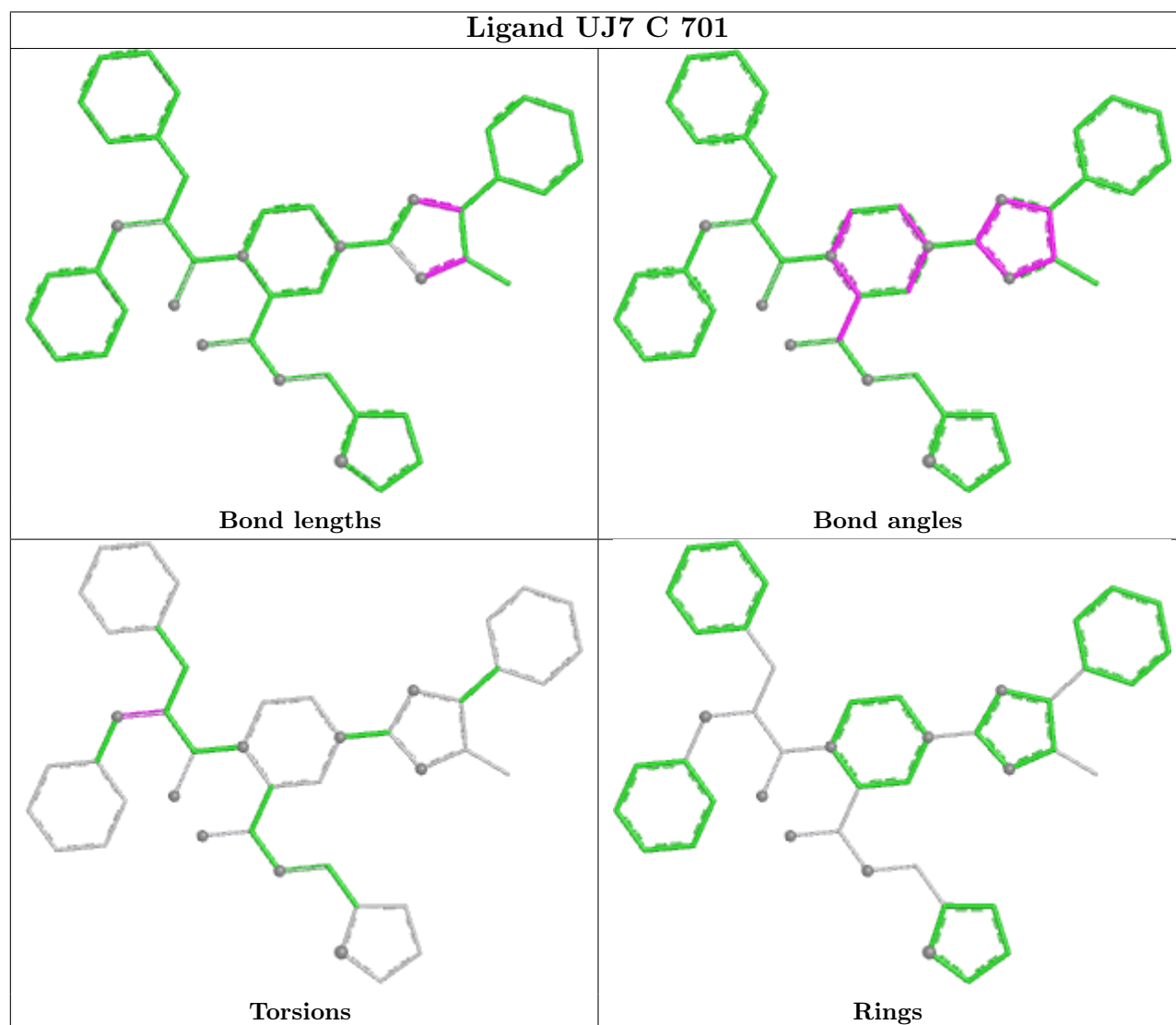
Mol	Chain	Res	Type	Atoms
2	A	701	UJ7	C16-C17-N20-C21
2	B	701	UJ7	C16-C17-N20-C21
2	C	701	UJ7	C16-C17-N20-C21

There are no ring outliers.

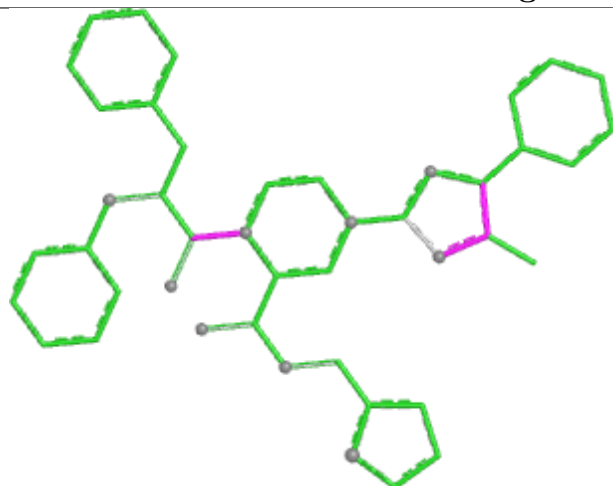
No monomer is involved in short contacts.

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

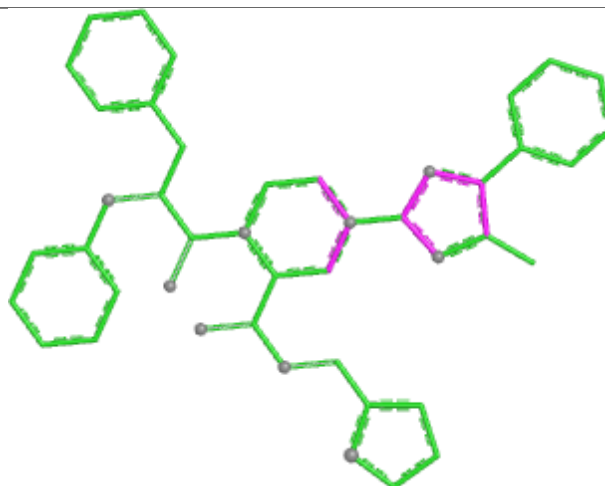
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified 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.



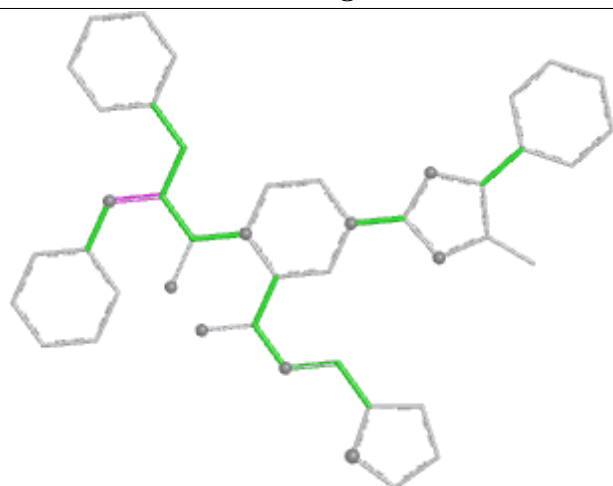
Ligand UJ7 A 701



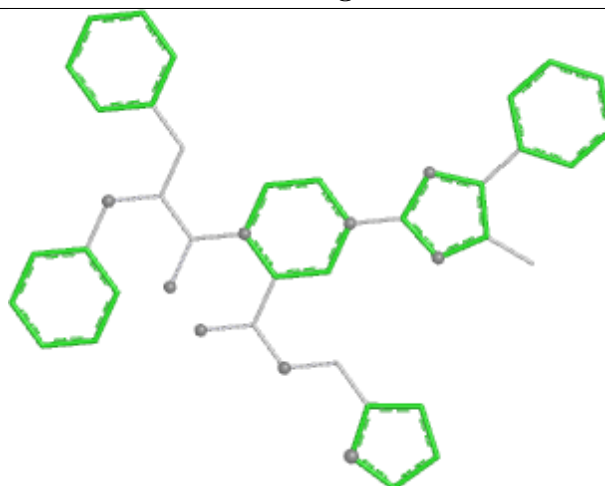
Bond lengths



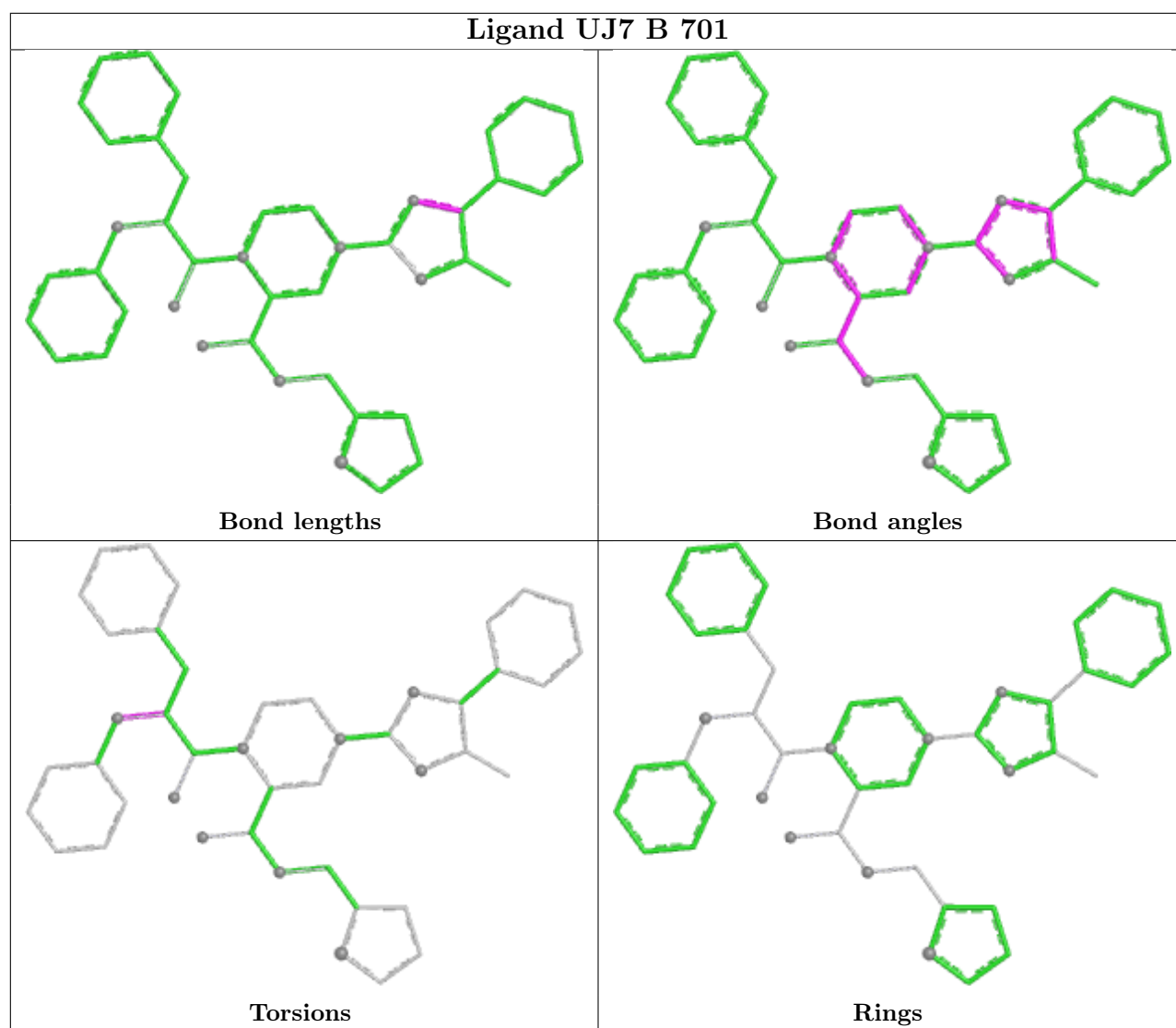
Bond angles



Torsions



Rings



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	241/259 (93%)	1.59	65 (26%) 1 2	3, 9, 22, 29	0
1	B	238/259 (91%)	1.61	65 (27%) 1 2	3, 9, 20, 28	0
1	C	240/259 (92%)	1.50	55 (22%) 2 2	3, 9, 21, 24	0
All	All	719/777 (92%)	1.56	185 (25%) 1 2	3, 9, 21, 29	0

All (185) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	357	LEU	10.9
1	B	614	VAL	8.7
1	C	499	LEU	7.0
1	B	498	THR	5.8
1	A	614	VAL	5.7
1	A	471	ALA	5.7
1	C	532	CYS	5.6
1	C	614	VAL	5.5
1	C	471	ALA	5.2
1	A	499	LEU	5.2
1	B	499	LEU	5.2
1	C	515	TYR	5.1
1	B	532	CYS	5.1
1	B	515	TYR	4.8
1	B	470	ASP	4.7
1	A	511	GLY	4.7
1	A	358	SER	4.6
1	B	358	SER	4.6
1	A	477	LEU	4.6
1	C	606	LEU	4.5
1	C	489	SER	4.5
1	A	473	GLY	4.5
1	A	435	SER	4.4

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Mol	Chain	Res	Type	RSRZ
1	C	529	LEU	4.4
1	B	478	LEU	4.3
1	B	526	PHE	4.1
1	A	472	ASP	4.1
1	A	512	ALA	4.1
1	B	573	ALA	4.1
1	A	532	CYS	4.1
1	A	515	TYR	4.1
1	B	489	SER	4.0
1	A	397	CYS	4.0
1	A	509	PHE	4.0
1	A	526	PHE	4.0
1	B	529	LEU	3.9
1	A	570	GLU	3.9
1	C	577	ARG	3.9
1	B	509	PHE	3.9
1	A	436	CYS	3.9
1	C	397	CYS	3.9
1	B	575	GLU	3.9
1	C	358	SER	3.9
1	B	610	ARG	3.9
1	B	531	ARG	3.8
1	B	536	ASP	3.8
1	C	477	LEU	3.8
1	B	397	CYS	3.8
1	B	551	PHE	3.8
1	C	575	GLU	3.8
1	B	474	SER	3.7
1	B	511	GLY	3.7
1	C	509	PHE	3.7
1	B	613	THR	3.7
1	C	394	HIS	3.6
1	B	537	VAL	3.6
1	A	531	ARG	3.6
1	C	478	LEU	3.5
1	C	472	ASP	3.5
1	C	435	SER	3.5
1	B	359	CYS	3.5
1	A	478	LEU	3.5
1	A	481	TYR	3.5
1	B	481	TYR	3.5
1	C	551	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	489	SER	3.5
1	B	436	CYS	3.4
1	C	470	ASP	3.4
1	A	513	GLU	3.4
1	A	396	PHE	3.4
1	A	500	CYS	3.4
1	C	590	CYS	3.4
1	C	481	TYR	3.3
1	A	470	ASP	3.3
1	A	394	HIS	3.3
1	B	394	HIS	3.3
1	A	536	ASP	3.2
1	B	527	LEU	3.2
1	C	573	ALA	3.2
1	B	606	LEU	3.2
1	C	552	LEU	3.2
1	A	535	PRO	3.1
1	A	573	ALA	3.1
1	A	574	ALA	3.1
1	C	436	CYS	3.1
1	C	456	VAL	3.0
1	B	534	ALA	3.0
1	A	527	LEU	3.0
1	A	590	CYS	3.0
1	C	535	PRO	2.9
1	A	529	LEU	2.9
1	C	531	ARG	2.9
1	B	439	CYS	2.9
1	C	396	PHE	2.9
1	B	552	LEU	2.9
1	C	574	ALA	2.9
1	A	551	PHE	2.8
1	A	577	ARG	2.8
1	B	477	LEU	2.8
1	C	512	ALA	2.8
1	C	534	ALA	2.8
1	A	609	ILE	2.8
1	B	558	ALA	2.8
1	A	613	THR	2.8
1	B	465	LEU	2.8
1	C	572	GLN	2.8
1	C	359	CYS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	543	LEU	2.7
1	A	552	LEU	2.7
1	A	575	GLU	2.7
1	B	469	GLU	2.7
1	C	500	CYS	2.7
1	A	393	GLY	2.7
1	C	438	PRO	2.7
1	B	435	SER	2.7
1	A	359	CYS	2.6
1	A	474	SER	2.6
1	A	534	ALA	2.6
1	B	443	ALA	2.6
1	C	437	GLU	2.6
1	C	536	ASP	2.6
1	B	512	ALA	2.6
1	C	613	THR	2.5
1	B	444	VAL	2.5
1	B	590	CYS	2.5
1	B	405	CYS	2.5
1	A	456	VAL	2.5
1	A	455	PRO	2.5
1	B	571	ASP	2.5
1	A	510	GLU	2.5
1	B	577	ARG	2.5
1	A	588	SER	2.4
1	C	526	PHE	2.4
1	B	574	ALA	2.4
1	A	606	LEU	2.4
1	B	415	GLN	2.4
1	B	542	ILE	2.4
1	C	458	TYR	2.4
1	C	523	GLN	2.4
1	A	476	ALA	2.4
1	C	473	GLY	2.3
1	B	445	ARG	2.3
1	B	447	TYR	2.3
1	A	537	VAL	2.3
1	B	523	GLN	2.3
1	C	361	GLN	2.3
1	A	544	PRO	2.3
1	B	535	PRO	2.3
1	A	549	ALA	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	608	TRP	2.3
1	C	474	SER	2.3
1	B	442	LEU	2.3
1	C	514	GLU	2.3
1	C	537	VAL	2.3
1	B	441	THR	2.2
1	B	572	GLN	2.2
1	A	420	PRO	2.2
1	B	543	LEU	2.2
1	B	466	ARG	2.2
1	A	553	GLU	2.2
1	A	442	LEU	2.1
1	A	572	GLN	2.1
1	B	475	CYS	2.1
1	B	374	VAL	2.1
1	A	587	GLY	2.1
1	B	403	ALA	2.1
1	C	604	TYR	2.1
1	B	456	VAL	2.1
1	B	587	GLY	2.1
1	A	424	THR	2.1
1	B	408	LEU	2.1
1	C	441	THR	2.1
1	A	523	GLN	2.1
1	C	469	GLU	2.1
1	A	453	PHE	2.1
1	A	438	PRO	2.1
1	B	488	PRO	2.1
1	C	511	GLY	2.0
1	A	419	ALA	2.0
1	C	607	ALA	2.0
1	B	604	TYR	2.0
1	A	555	GLY	2.0
1	B	598	VAL	2.0
1	C	378	VAL	2.0
1	C	587	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

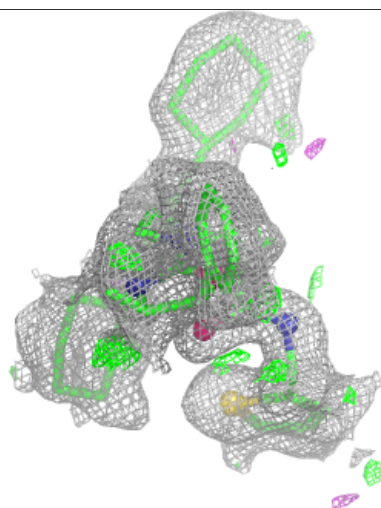
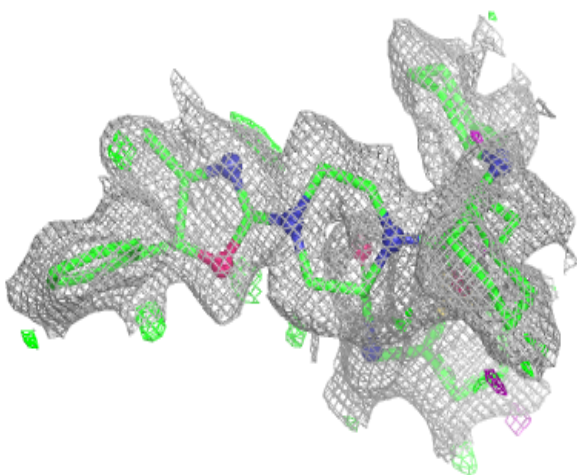
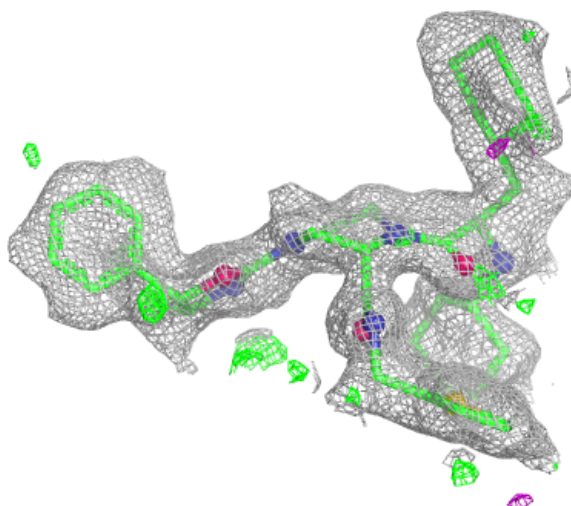
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	UJ7	C	701	44/44	0.85	0.13	9,11,16,16	0
2	UJ7	A	701	44/44	0.87	0.11	8,10,13,13	0
2	UJ7	B	701	44/44	0.88	0.11	7,12,14,14	0
3	SO4	A	702	5/5	0.96	0.08	8,8,9,9	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.

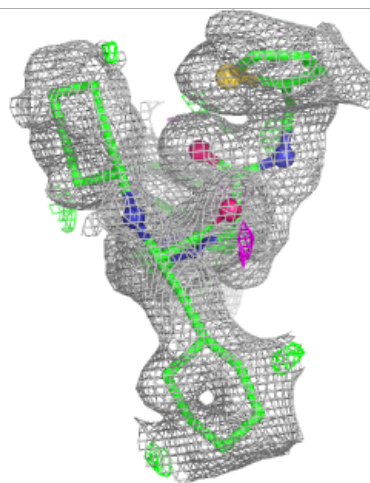
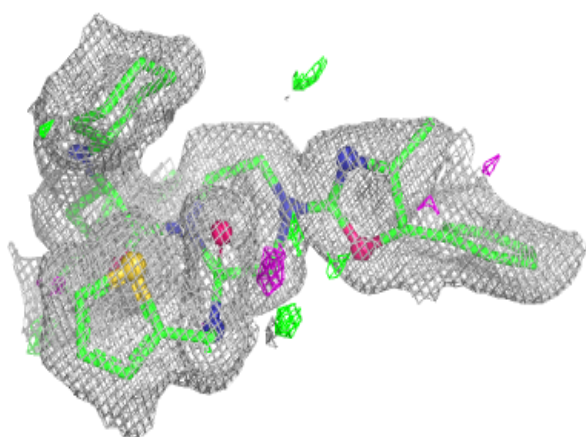
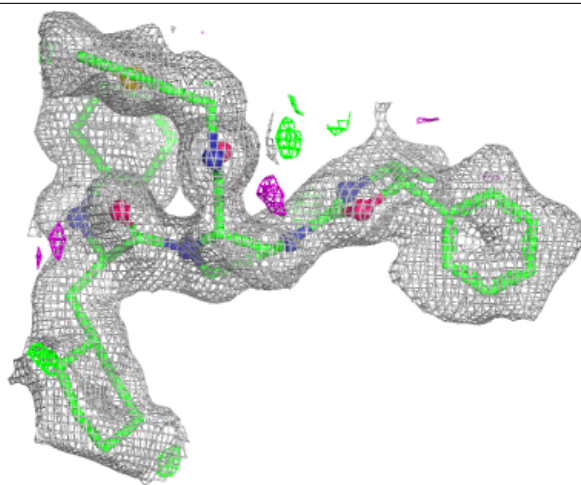
Electron density around UJ7 C 701:

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



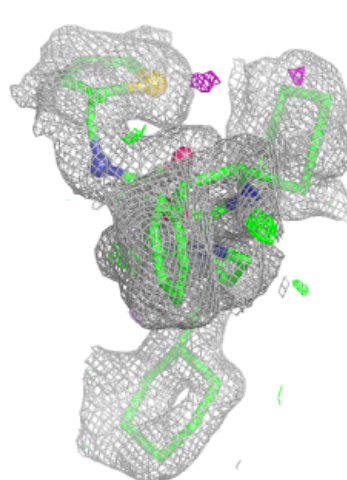
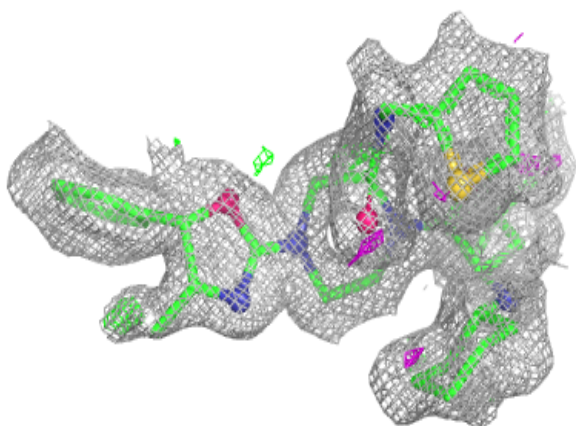
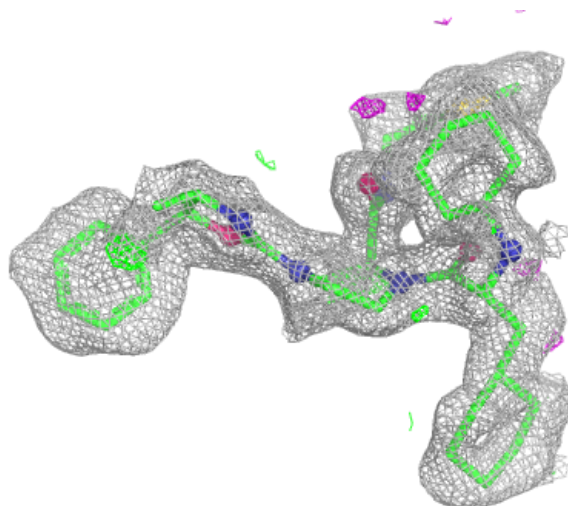
Electron density around UJ7 A 701:

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



Electron density around UJ7 B 701:

$2mF_o-DF_c$ (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.