



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 02:12 PM UTC

PDB ID : 4L7C / pdb_00004l7c
Title : Structure of keap1 kelch domain with 2-{[(1S)-2-{[(1R,2S)-2-(1H-tetrazol-5-yl)cyclohexyl]carbonyl}-1,2,3,4-tetrahydroisoquinolin-1-yl]methyl}-1H-isoindole-1,3(2H)-dione
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Deposited on : 2013-06-13
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)

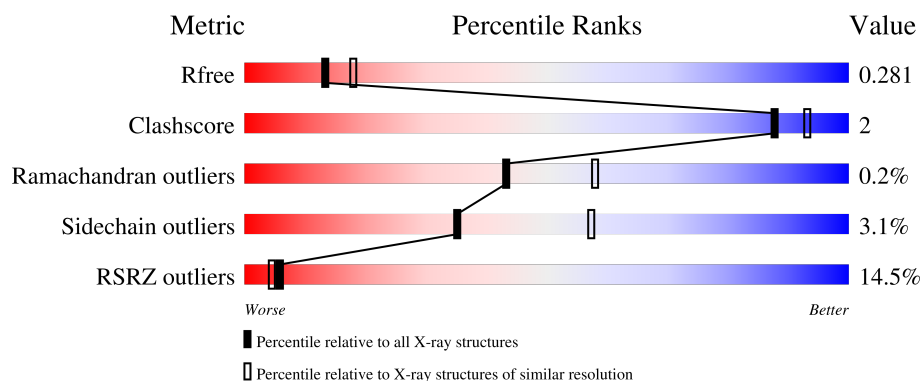
1 Overall quality at a glance

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	300	 6% 89% 6% 5%
1	B	300	 32% 90% 5% 5%
1	C	300	 4% 90% 5% 5%

Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7023 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 Kelch-like ECH-associated protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	286	Total	C	N	O	S	0	5	0
			2250	1396	407	432	15			
1	B	286	Total	C	N	O	S	0	2	0
			2221	1380	400	426	15			
1	C	286	Total	C	N	O	S	0	3	0
			2228	1384	401	428	15			

There are 36 discrepancies between the modelled and reference sequences:

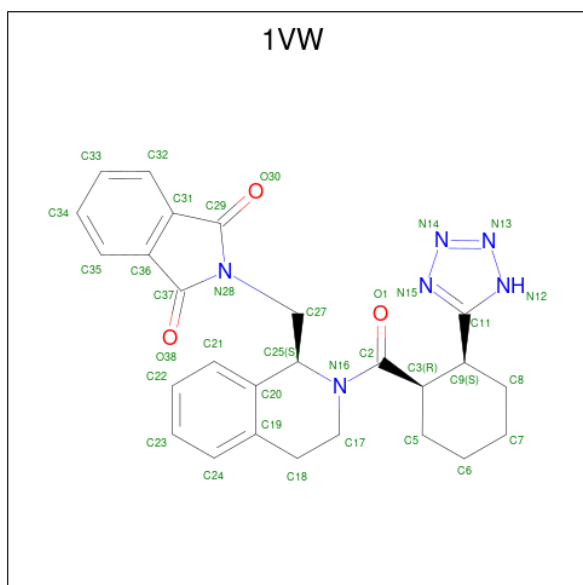
Chain	Residue	Modelled	Actual	Comment	Reference
A	318	MET	-	expression tag	UNP Q14145
A	319	GLY	-	expression tag	UNP Q14145
A	320	HIS	-	expression tag	UNP Q14145
A	354	ASP	ARG	engineered mutation	UNP Q14145
A	610	LEU	-	expression tag	UNP Q14145
A	611	GLU	-	expression tag	UNP Q14145
A	612	HIS	-	expression tag	UNP Q14145
A	613	HIS	-	expression tag	UNP Q14145
A	614	HIS	-	expression tag	UNP Q14145
A	615	HIS	-	expression tag	UNP Q14145
A	616	HIS	-	expression tag	UNP Q14145
A	617	HIS	-	expression tag	UNP Q14145
B	318	MET	-	expression tag	UNP Q14145
B	319	GLY	-	expression tag	UNP Q14145
B	320	HIS	-	expression tag	UNP Q14145
B	354	ASP	ARG	engineered mutation	UNP Q14145
B	610	LEU	-	expression tag	UNP Q14145
B	611	GLU	-	expression tag	UNP Q14145
B	612	HIS	-	expression tag	UNP Q14145
B	613	HIS	-	expression tag	UNP Q14145
B	614	HIS	-	expression tag	UNP Q14145
B	615	HIS	-	expression tag	UNP Q14145
B	616	HIS	-	expression tag	UNP Q14145

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Chain	Residue	Modelled	Actual	Comment	Reference
B	617	HIS	-	expression tag	UNP Q14145
C	318	MET	-	expression tag	UNP Q14145
C	319	GLY	-	expression tag	UNP Q14145
C	320	HIS	-	expression tag	UNP Q14145
C	354	ASP	ARG	engineered mutation	UNP Q14145
C	610	LEU	-	expression tag	UNP Q14145
C	611	GLU	-	expression tag	UNP Q14145
C	612	HIS	-	expression tag	UNP Q14145
C	613	HIS	-	expression tag	UNP Q14145
C	614	HIS	-	expression tag	UNP Q14145
C	615	HIS	-	expression tag	UNP Q14145
C	616	HIS	-	expression tag	UNP Q14145
C	617	HIS	-	expression tag	UNP Q14145

- Molecule 2 is 2-[[[(1S)-2-[[[(1R,2S)-2-(1H-tetrazol-5-yl)cyclohexyl]carbonyl]-1,2,3,4-tetrahydroisoquinolin-1-yl]methyl]-1H-isoindole-1,3(2H)-dione (CCD ID: 1VW) (formula: C₂₆H₂₆N₆O₃).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			35	26	6	3		
2	B	1	Total	C	N	O	0	0
			35	26	6	3		
2	C	1	Total	C	N	O	0	0
			35	26	6	3		

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

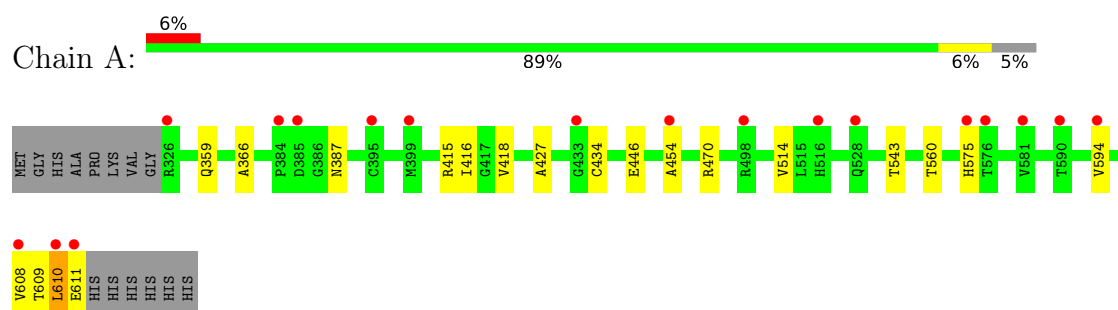
- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	82	Total O 82 82	0	0
4	B	30	Total O 30 30	0	0
4	C	87	Total O 87 87	0	0

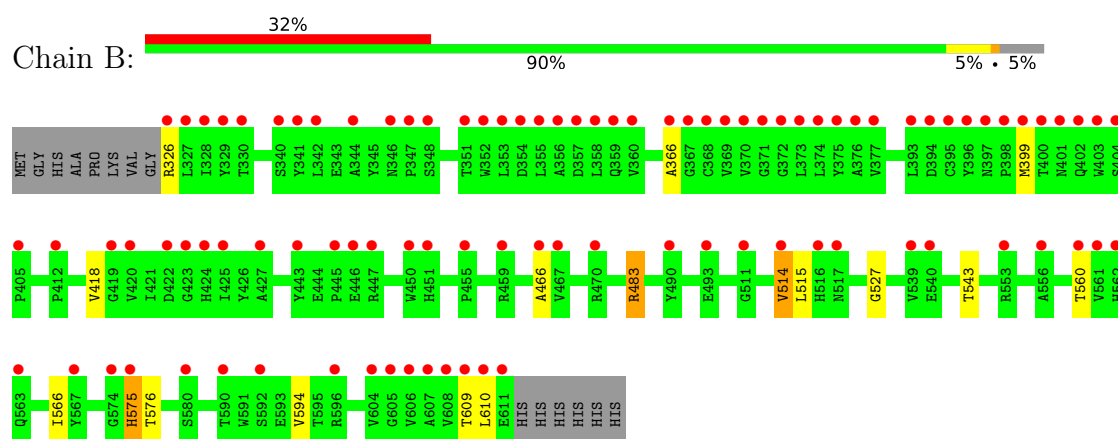
3 Residue-property plots [i](#)

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.

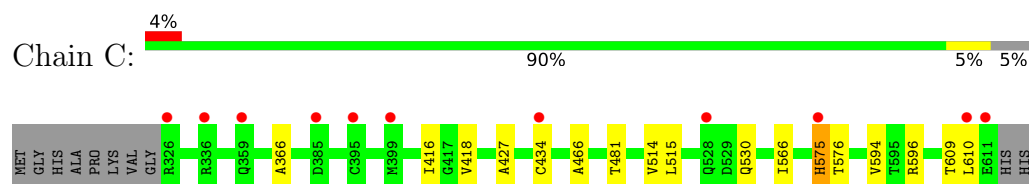
- Molecule 1: Kelch-like ECH-associated protein 1



- Molecule 1: Kelch-like ECH-associated protein 1



- Molecule 1: Kelch-like ECH-associated protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 2 ₁ 2 ₁ 2 ₁	Depositor
Cell constants a, b, c, α , β , γ	76.29Å 125.61Å 132.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.66 – 2.40 36.66 – 2.40	Depositor EDS
% Data completeness (in resolution range)	99.9 (36.66-2.40) 99.9 (36.66-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.74 (at 2.39Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.265 , 0.281 0.263 , 0.281	Depositor DCC
R_{free} test set	2573 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	40.8	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 13.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	7023	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.05% 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: ACT, 1VW

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	0.36	0/2303	0.58	0/3135
1	B	0.37	0/2274	0.59	0/3097
1	C	0.36	0/2284	0.59	0/3110
All	All	0.36	0/6861	0.59	0/9342

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 [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	2250	0	2130	14	0
1	B	2221	0	2107	8	0
1	C	2228	0	2111	6	0
2	A	35	0	26	0	0
2	B	35	0	26	0	0
2	C	35	0	26	0	0
3	A	4	0	3	0	0
3	B	8	0	6	0	0
3	C	8	0	6	0	0
4	A	82	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	30	0	0	0	0
4	C	87	0	0	0	0
All	All	7023	0	6441	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:470[B]:ARG:HH11	1:A:470[B]:ARG:HG3	0.96	1.12
1:A:470[B]:ARG:HH11	1:A:470[B]:ARG:CG	1.79	0.95
1:A:470[B]:ARG:HG3	1:A:470[B]:ARG:NH1	1.78	0.93
1:A:359[B]:GLN:HA	1:A:359[B]:GLN:OE1	1.77	0.82
1:C:466:ALA:HB1	1:C:514:VAL:HG23	1.86	0.56
1:B:466:ALA:HB1	1:B:514:VAL:HG23	1.89	0.54
1:A:366:ALA:HB1	1:A:418:VAL:HG22	1.89	0.53
1:A:387:ASN:HD22	1:A:387:ASN:N	2.07	0.53
1:A:470[B]:ARG:CG	1:A:470[B]:ARG:NH1	2.49	0.52
1:B:575:HIS:CD2	1:B:576:THR:HG23	2.44	0.52
1:A:446[B]:GLU:OE1	1:A:446[B]:GLU:N	2.26	0.51
1:B:527:GLY:HA3	1:C:481:THR:HG21	1.96	0.48
1:B:515:LEU:HD22	1:B:566:ILE:HG13	1.97	0.46
1:A:359[B]:GLN:OE1	1:A:359[B]:GLN:CA	2.59	0.46
1:A:454:ALA:HA	1:B:575:HIS:CE1	2.51	0.46
1:B:483:ARG:HD3	1:B:527:GLY:HA2	1.98	0.46
1:C:366:ALA:HB1	1:C:418:VAL:HG22	2.00	0.44
1:A:610:LEU:O	1:A:611:GLU:HB2	2.18	0.43
1:A:446[B]:GLU:H	1:A:446[B]:GLU:CD	2.21	0.43
1:C:575:HIS:ND1	1:C:576:THR:HG23	2.34	0.43
1:A:560:THR:OG1	1:A:608:VAL:HG23	2.19	0.42
1:C:515:LEU:HD22	1:C:566:ILE:HG13	2.01	0.42
1:C:416:ILE:HD11	1:C:427:ALA:HB1	2.01	0.41
1:A:416:ILE:HD11	1:A:427:ALA:HB1	2.02	0.41
1:B:399:MET:SD	1:B:399:MET:N	2.91	0.41
1:B:366:ALA:HB1	1:B:418:VAL:HG22	2.03	0.41

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	289/300 (96%)	280 (97%)	9 (3%)	0	100	100
1	B	286/300 (95%)	272 (95%)	13 (4%)	1 (0%)	36	50
1	C	287/300 (96%)	279 (97%)	7 (2%)	1 (0%)	36	50
All	All	862/900 (96%)	831 (96%)	29 (3%)	2 (0%)	43	58

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	575	HIS
1	C	575	HIS

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	238/244 (98%)	230 (97%)	8 (3%)	32	54
1	B	235/244 (96%)	226 (96%)	9 (4%)	29	49
1	C	236/244 (97%)	230 (98%)	6 (2%)	42	64
All	All	709/732 (97%)	686 (97%)	23 (3%)	35	56

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	415	ARG

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Mol	Chain	Res	Type
1	A	434	CYS
1	A	514	VAL
1	A	543	THR
1	A	575	HIS
1	A	594	VAL
1	A	609	THR
1	A	610	LEU
1	B	326	ARG
1	B	483	ARG
1	B	514	VAL
1	B	543[A]	THR
1	B	543[B]	THR
1	B	560	THR
1	B	594	VAL
1	B	609	THR
1	B	610	LEU
1	C	434	CYS
1	C	530	GLN
1	C	594	VAL
1	C	596	ARG
1	C	609	THR
1	C	610	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	387	ASN
1	A	528	GLN
1	B	359	GLN
1	B	387	ASN
1	B	414	ASN
1	B	451	HIS
1	B	562	HIS
1	B	575	HIS
1	C	451	HIS
1	C	528	GLN
1	C	530	GLN

5.3.3 RNA ⓘ

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](#)

8 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	ACT	B	703	-	3,3,3	0.82	0	3,3,3	0.73	0
2	1VW	B	701	-	38,40,40	1.42	4 (10%)	53,58,58	2.13	11 (20%)
2	1VW	C	701	-	38,40,40	1.44	4 (10%)	53,58,58	2.13	11 (20%)
3	ACT	C	702	-	3,3,3	0.82	0	3,3,3	0.73	0
3	ACT	C	703	-	3,3,3	0.81	0	3,3,3	0.75	0
3	ACT	B	702	-	3,3,3	0.81	0	3,3,3	0.77	0
3	ACT	A	702	-	3,3,3	0.81	0	3,3,3	0.73	0
2	1VW	A	701	-	38,40,40	1.43	5 (13%)	53,58,58	2.14	11 (20%)

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	1VW	A	701	-	-	2/15/56/56	0/6/6/6
2	1VW	C	701	-	-	2/15/56/56	0/6/6/6
2	1VW	B	701	-	-	2/15/56/56	0/6/6/6

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	701	1VW	C11-N15	4.68	1.36	1.32
2	A	701	1VW	C11-N15	4.58	1.36	1.32
2	B	701	1VW	C11-N15	4.57	1.36	1.32
2	C	701	1VW	C11-N12	-2.86	1.31	1.33
2	A	701	1VW	C11-N12	-2.75	1.31	1.33
2	B	701	1VW	C11-N12	-2.72	1.31	1.33
2	C	701	1VW	C2-N16	2.43	1.40	1.34
2	B	701	1VW	C2-N16	2.42	1.39	1.34
2	A	701	1VW	C2-N16	2.35	1.39	1.34
2	A	701	1VW	C25-N16	-2.17	1.45	1.47
2	A	701	1VW	C36-C37	-2.04	1.45	1.48
2	B	701	1VW	C36-C37	-2.03	1.45	1.48
2	C	701	1VW	C36-C37	-2.02	1.45	1.48

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	1VW	O30-C29-N28	7.13	132.01	124.79
2	B	701	1VW	O30-C29-N28	6.99	131.86	124.79
2	C	701	1VW	O30-C29-N28	6.94	131.81	124.79
2	C	701	1VW	O38-C37-N28	6.80	131.67	124.79
2	A	701	1VW	O38-C37-N28	6.68	131.55	124.79
2	B	701	1VW	O38-C37-N28	6.68	131.55	124.79
2	B	701	1VW	C11-N15-N14	6.57	110.23	105.82
2	A	701	1VW	C11-N15-N14	6.52	110.19	105.82
2	C	701	1VW	C11-N15-N14	6.45	110.15	105.82
2	C	701	1VW	N15-N14-N13	-4.91	104.65	110.50
2	B	701	1VW	N15-N14-N13	-4.89	104.66	110.50
2	A	701	1VW	N15-N14-N13	-4.81	104.76	110.50
2	C	701	1VW	N12-N13-N14	3.33	111.41	106.68
2	B	701	1VW	N12-N13-N14	3.29	111.36	106.68
2	A	701	1VW	N12-N13-N14	3.17	111.19	106.68
2	A	701	1VW	C31-C29-N28	-2.97	103.69	105.88
2	C	701	1VW	C31-C29-N28	-2.94	103.72	105.88
2	B	701	1VW	C31-C29-N28	-2.86	103.77	105.88
2	A	701	1VW	C36-C37-N28	-2.80	103.82	105.88
2	C	701	1VW	C36-C37-N28	-2.74	103.86	105.88
2	B	701	1VW	C36-C37-N28	-2.59	103.97	105.88
2	A	701	1VW	C37-N28-C29	2.44	114.10	112.02
2	C	701	1VW	C37-N28-C29	2.42	114.08	112.02
2	C	701	1VW	C11-N12-N13	-2.41	106.05	109.05
2	B	701	1VW	C11-N12-N13	-2.40	106.06	109.05
2	B	701	1VW	C37-N28-C29	2.27	113.96	112.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	1VW	C11-N12-N13	-2.26	106.23	109.05
2	A	701	1VW	O30-C29-C31	-2.25	124.30	128.66
2	B	701	1VW	O30-C29-C31	-2.21	124.37	128.66
2	C	701	1VW	O38-C37-C36	-2.17	124.46	128.66
2	C	701	1VW	O30-C29-C31	-2.16	124.47	128.66
2	B	701	1VW	O38-C37-C36	-2.16	124.48	128.66
2	A	701	1VW	O38-C37-C36	-2.08	124.63	128.66

There are no chirality outliers.

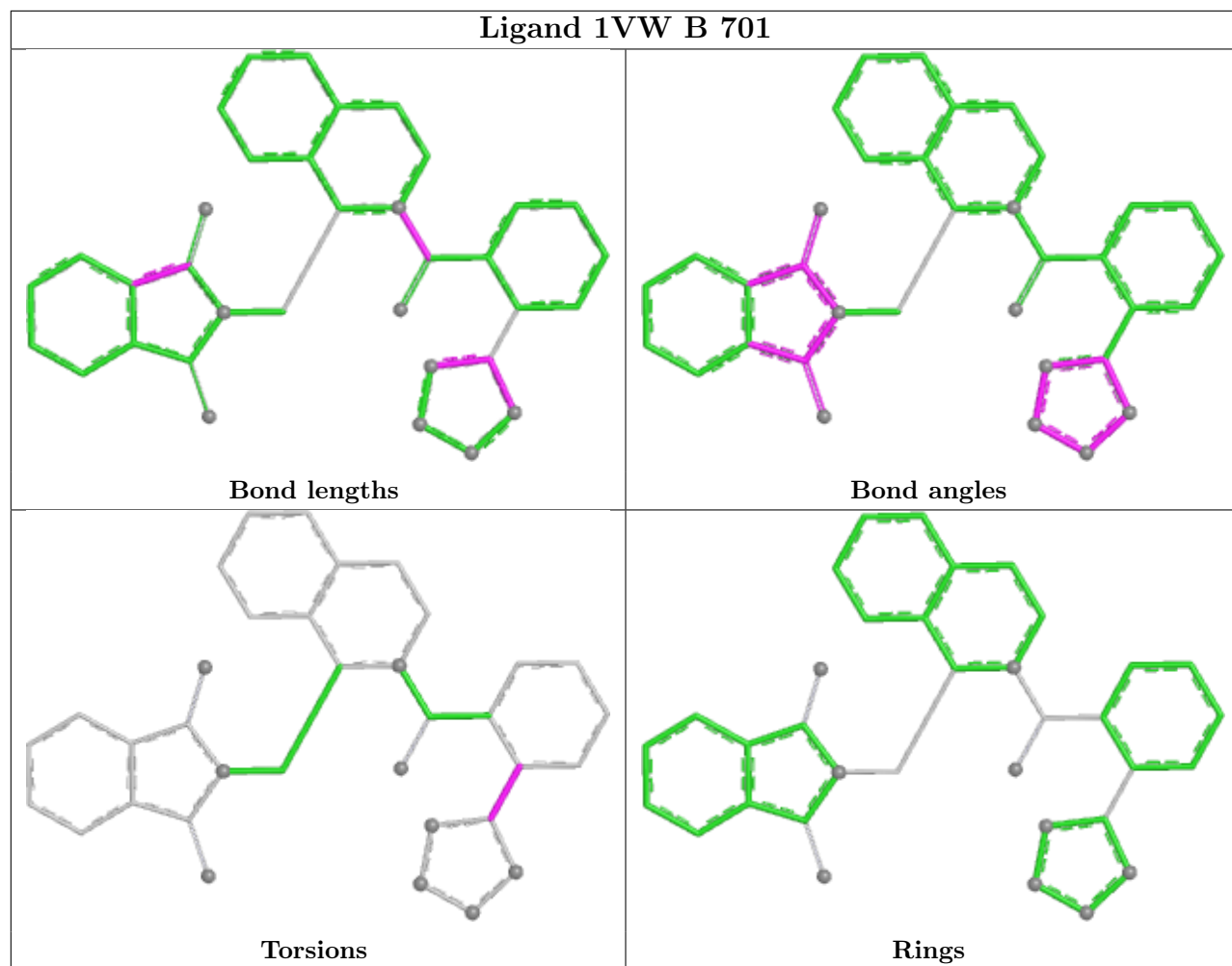
All (6) torsion outliers are listed below:

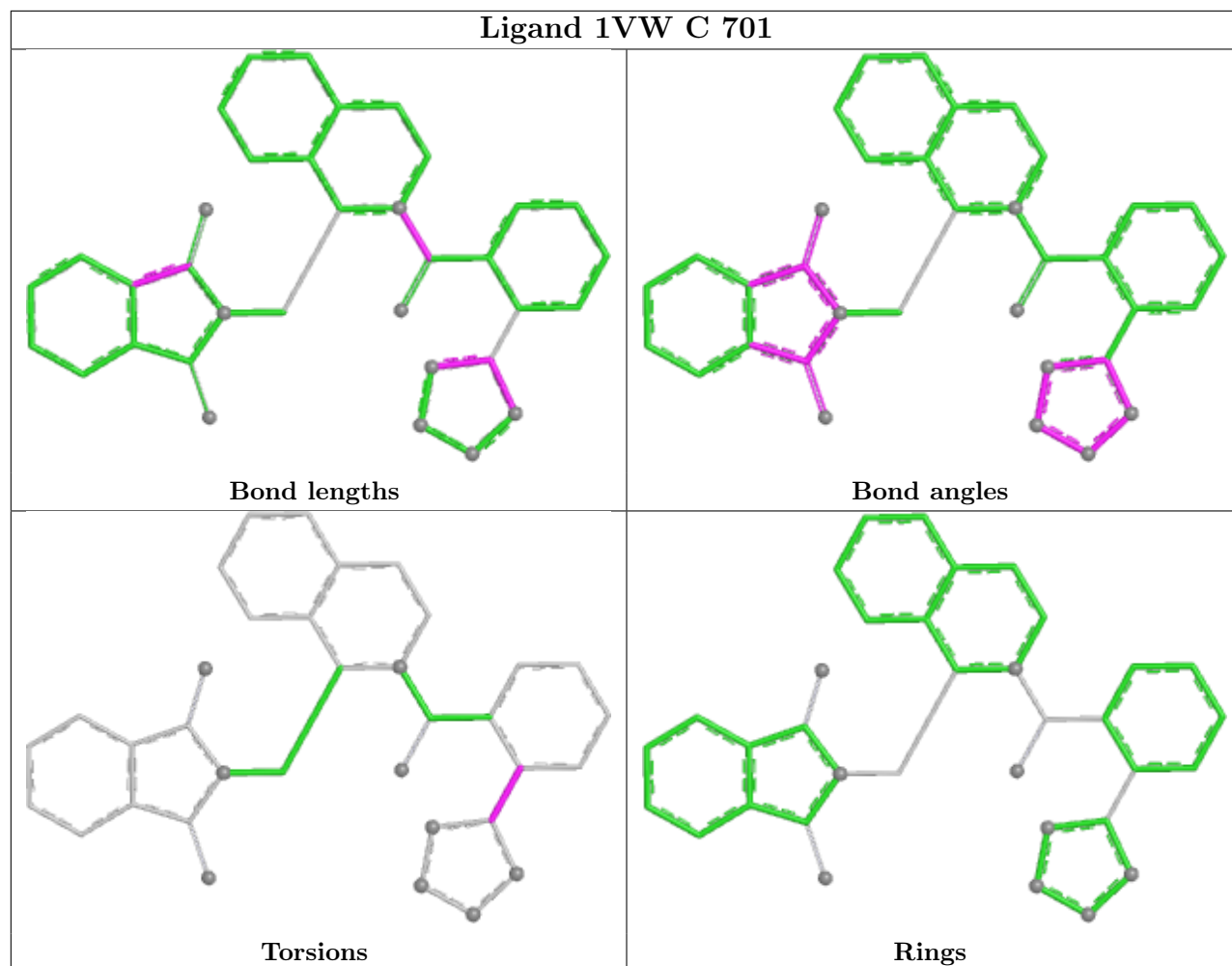
Mol	Chain	Res	Type	Atoms
2	A	701	1VW	N12-C11-C9-C8
2	A	701	1VW	N12-C11-C9-C3
2	B	701	1VW	N12-C11-C9-C8
2	B	701	1VW	N12-C11-C9-C3
2	C	701	1VW	N12-C11-C9-C8
2	C	701	1VW	N12-C11-C9-C3

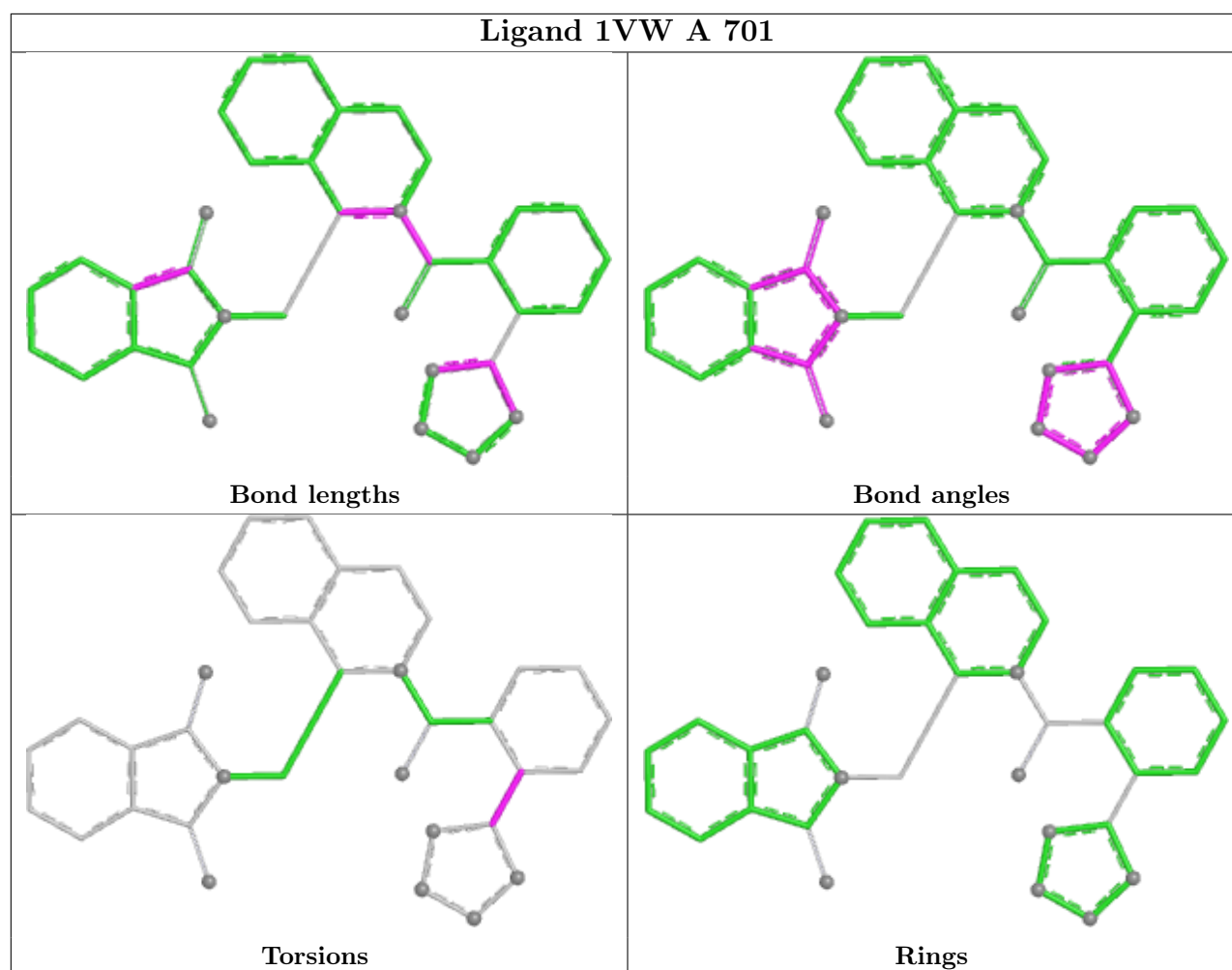
There are no ring outliers.

No monomer is involved in short contacts.

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	286/300 (95%)	0.60	18 (6%) 26 22	17, 38, 50, 58	5 (1%)
1	B	286/300 (95%)	1.77	95 (33%) 1 1	18, 56, 77, 86	2 (0%)
1	C	286/300 (95%)	0.39	11 (3%) 44 40	14, 35, 46, 53	3 (1%)
All	All	858/900 (95%)	0.92	124 (14%) 6 4	14, 40, 68, 86	10 (1%)

All (124) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	610	LEU	6.4
1	B	397	ASN	6.1
1	B	575	HIS	5.6
1	B	329	TYR	5.5
1	B	372	GLY	5.4
1	B	399	MET	5.3
1	B	371	GLY	5.2
1	B	356	ALA	4.9
1	B	607	ALA	4.9
1	A	326	ARG	4.9
1	B	611	GLU	4.6
1	B	368	CYS	4.6
1	B	326	ARG	4.6
1	B	398	PRO	4.3
1	A	575	HIS	4.2
1	B	396	TYR	4.1
1	B	373	LEU	4.1
1	B	366	ALA	4.1
1	B	327	LEU	4.1
1	B	539	VAL	4.1
1	B	608	VAL	4.1
1	B	375	TYR	4.1
1	A	611	GLU	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	553	ARG	4.0
1	B	402	GLN	4.0
1	B	405	PRO	4.0
1	B	374	LEU	3.9
1	B	605	GLY	3.9
1	A	608	VAL	3.9
1	B	344	ALA	3.8
1	B	400	THR	3.8
1	B	353	LEU	3.8
1	C	434	CYS	3.7
1	B	370	VAL	3.7
1	B	342	LEU	3.7
1	B	540	GLU	3.6
1	B	609	THR	3.6
1	B	606	VAL	3.5
1	B	352	TRP	3.5
1	A	590[A]	THR	3.4
1	B	395	CYS	3.4
1	B	328	ILE	3.4
1	B	354	ASP	3.3
1	B	340	SER	3.2
1	B	567	TYR	3.2
1	A	454	ALA	3.2
1	B	560	THR	3.2
1	B	419	GLY	3.1
1	B	355	LEU	3.1
1	B	393	LEU	3.1
1	B	420	VAL	3.1
1	A	385	ASP	3.0
1	B	403	TRP	3.0
1	C	326	ARG	3.0
1	B	377	VAL	3.0
1	B	445	PRO	3.0
1	B	341	TYR	2.9
1	B	369	VAL	2.8
1	C	395	CYS	2.8
1	B	367	GLY	2.8
1	C	575	HIS	2.8
1	B	360	VAL	2.7
1	B	556	ALA	2.7
1	B	517	ASN	2.7
1	B	427	ALA	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	528	GLN	2.7
1	B	516	HIS	2.7
1	B	404	SER	2.6
1	B	580	SER	2.6
1	B	561	VAL	2.6
1	B	423	GLY	2.6
1	B	574	GLY	2.6
1	B	443	TYR	2.6
1	C	359[A]	GLN	2.5
1	B	348	SER	2.5
1	B	425	ILE	2.5
1	B	446	GLU	2.5
1	A	610	LEU	2.5
1	B	514	VAL	2.5
1	B	394	ASP	2.5
1	B	401	ASN	2.5
1	B	596	ARG	2.5
1	B	470	ARG	2.5
1	C	336	ARG	2.5
1	B	376	ALA	2.5
1	A	498[A]	ARG	2.4
1	B	467	VAL	2.4
1	B	493	GLU	2.4
1	B	347	PRO	2.4
1	B	358	LEU	2.4
1	B	359	GLN	2.4
1	B	604	VAL	2.4
1	B	346	ASN	2.4
1	B	451	HIS	2.3
1	C	610	LEU	2.3
1	A	384	PRO	2.3
1	A	576	THR	2.3
1	B	459[A]	ARG	2.3
1	B	563	GLN	2.3
1	A	399	MET	2.3
1	B	450	TRP	2.3
1	B	490	TYR	2.3
1	C	611	GLU	2.2
1	A	594	VAL	2.2
1	A	395	CYS	2.2
1	B	592	SER	2.2
1	B	466	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	562	HIS	2.2
1	B	351	THR	2.2
1	B	590	THR	2.2
1	B	330	THR	2.2
1	C	399	MET	2.1
1	A	433	GLY	2.1
1	B	357	ASP	2.1
1	C	385	ASP	2.1
1	B	424	HIS	2.1
1	B	447	ARG	2.1
1	B	455	PRO	2.1
1	A	581	VAL	2.1
1	B	511	GLY	2.1
1	B	422	ASP	2.1
1	B	412	PRO	2.1
1	C	528	GLN	2.0
1	A	516	HIS	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	ACT	C	702	4/4	0.83	0.17	40,40,40,40	0
3	ACT	A	702	4/4	0.88	0.22	53,53,53,53	0
2	1VW	B	701	35/35	0.89	0.12	45,46,46,46	0
3	ACT	B	703	4/4	0.91	0.12	37,38,38,38	0
2	1VW	A	701	35/35	0.91	0.12	39,39,40,40	0
3	ACT	B	702	4/4	0.93	0.12	44,44,44,44	0

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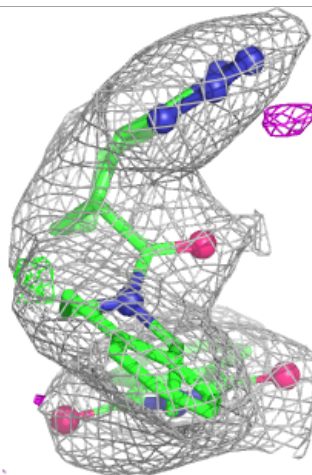
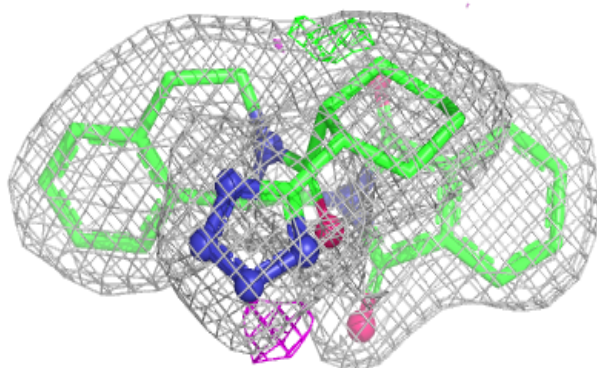
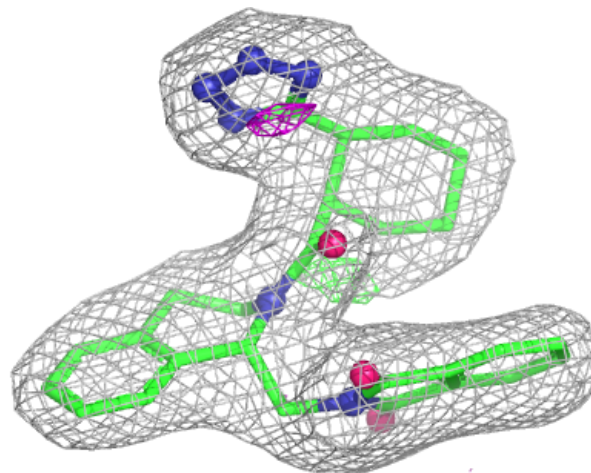
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	ACT	C	703	4/4	0.93	0.12	35,36,36,36	0
2	1VW	C	701	35/35	0.94	0.09	32,33,33,33	0

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.

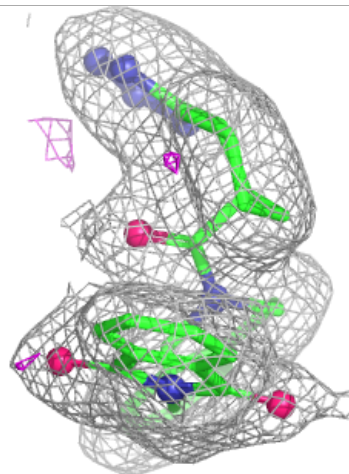
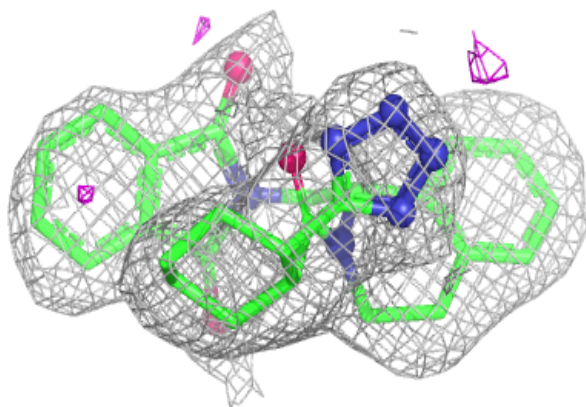
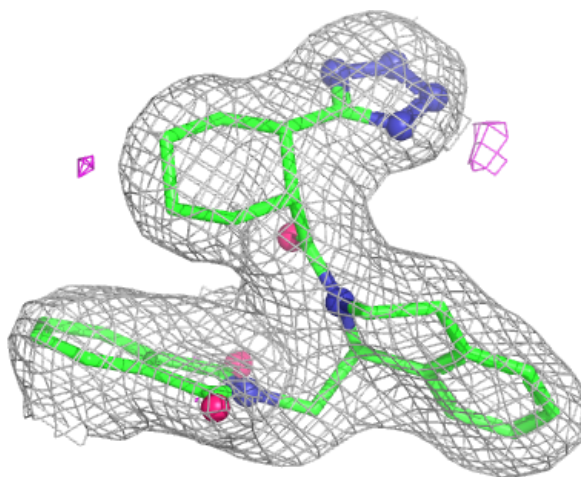
Electron density around 1VW B 701:

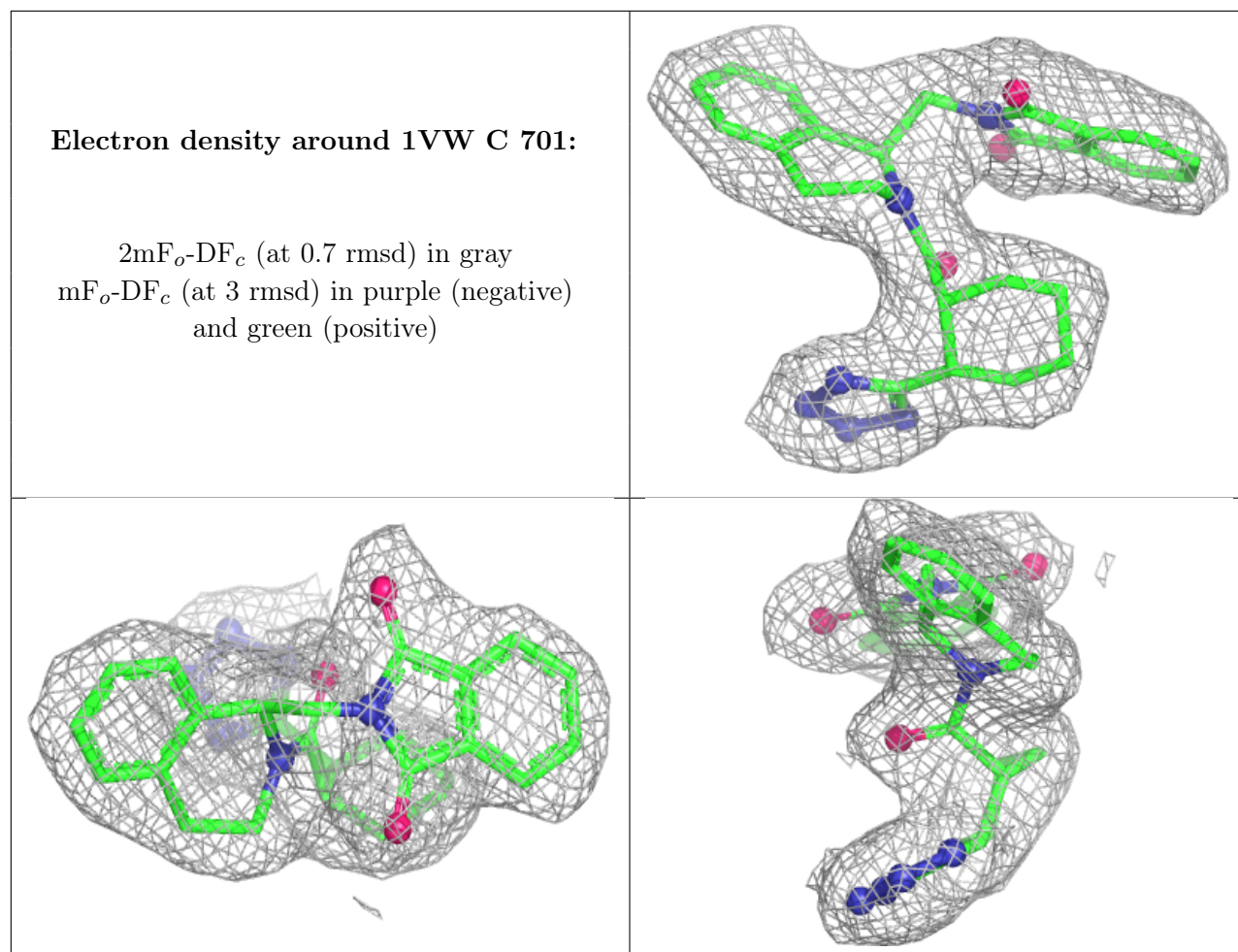
2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 1VW 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)





6.5 Other polymers [i](#)

There are no such residues in this entry.