



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 11:29 AM UTC

PDB ID : 5W2E / pdb_00005w2e
Title : HCV NS5B RNA-dependent RNA polymerase in complex with non-nucleoside inhibitor MK-8876
Authors : Lesburg, C.A.; Ummat, A.
Deposited on : 2017-06-06
Resolution : 2.80 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

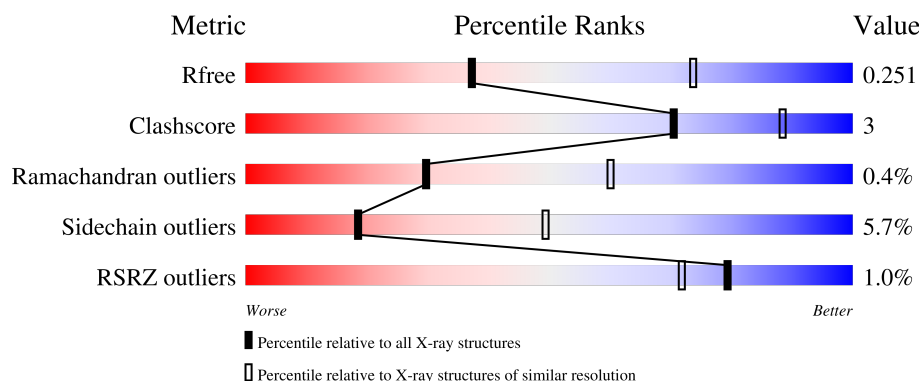
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (2.80-2.80)

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	576	% 81% 14% ..
1	B	576	% 83% 13% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9100 atoms, of which 48 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 Genome polyprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	559	Total	C	N	O	S	0	1	0
			4359	2752	772	805	30			
1	B	559	Total	C	N	O	S	0	0	0
			4346	2744	767	805	30			

There are 26 discrepancies between the modelled and reference sequences:

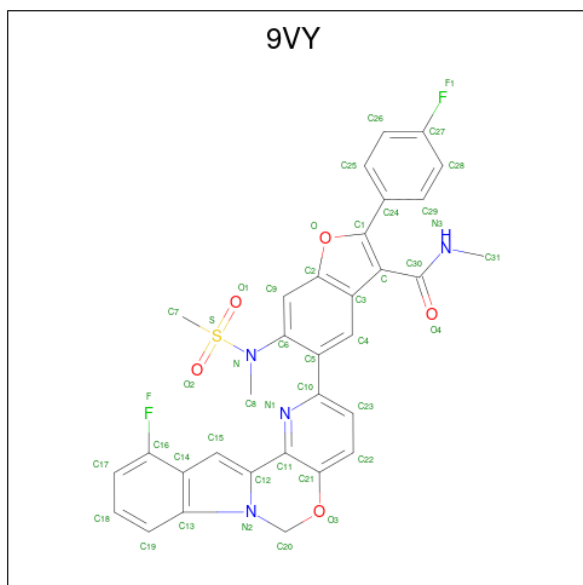
Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	ALA	-	expression tag	UNP P26663
A	-4	SER	-	expression tag	UNP P26663
A	-3	HIS	-	expression tag	UNP P26663
A	-2	HIS	-	expression tag	UNP P26663
A	-1	HIS	-	expression tag	UNP P26663
A	0	HIS	-	expression tag	UNP P26663
A	1	HIS	-	expression tag	UNP P26663
A	2	HIS	-	expression tag	UNP P26663
A	25	PRO	ALA	conflict	UNP P26663
A	46	SER	GLY	conflict	UNP P26663
A	329	VAL	THR	engineered mutation	UNP P26663
A	338	ALA	VAL	engineered mutation	UNP P26663
A	544	GLN	ARG	engineered mutation	UNP P26663
B	-5	ALA	-	expression tag	UNP P26663
B	-4	SER	-	expression tag	UNP P26663
B	-3	HIS	-	expression tag	UNP P26663
B	-2	HIS	-	expression tag	UNP P26663
B	-1	HIS	-	expression tag	UNP P26663
B	0	HIS	-	expression tag	UNP P26663
B	1	HIS	-	expression tag	UNP P26663
B	2	HIS	-	expression tag	UNP P26663
B	25	PRO	ALA	conflict	UNP P26663
B	46	SER	GLY	conflict	UNP P26663
B	329	VAL	THR	engineered mutation	UNP P26663
B	338	ALA	VAL	engineered mutation	UNP P26663

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Chain	Residue	Modelled	Actual	Comment	Reference
B	544	GLN	ARG	engineered mutation	UNP P26663

- Molecule 2 is 2-(4-fluorophenyl)-5-(11-fluoro-6H-pyrido[2',3':5,6][1,3]oxazino[3,4-a]indol-2-yl)-N-methyl-6-[methyl(methylsulfonyl)amino]-1-benzofuran-3-carboxamide (CCD ID: 9VY) (formula: C₃₂H₂₄F₂N₄O₅S).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
2	A	1	Total	C	F	H	N	O	S	0	0
			68	32	2	24	4	5	1		
2	B	1	Total	C	F	H	N	O	S	0	0
			68	32	2	24	4	5	1		

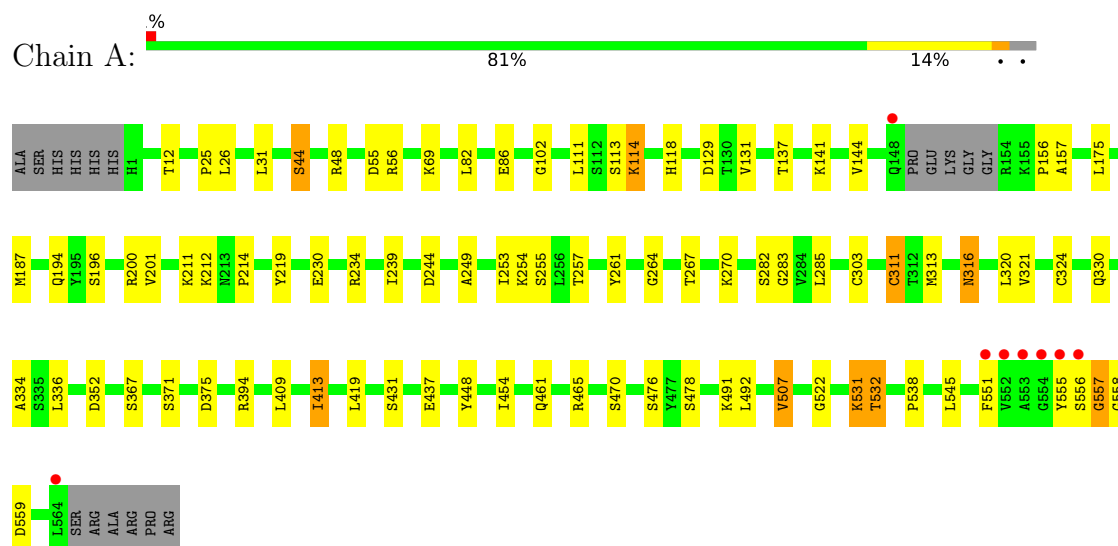
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	135	Total	O	0	0
			135	135		
3	B	124	Total	O	0	0
			124	124		

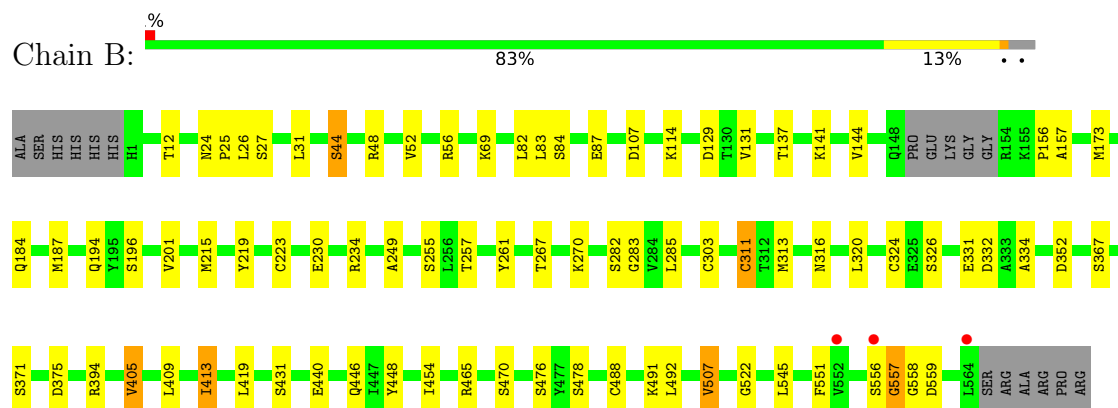
3 Residue-property plots [i](#)

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: Genome polyprotein



• Molecule 1: Genome polyprotein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.09Å 106.42Å 126.09Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	34.15 – 2.80 34.15 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (34.15-2.80) 99.9 (34.15-2.80)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.85 (at 2.82Å)	Xtriage
Refinement program	BUSTER 2.11.7	Depositor
R, R_{free}	0.181 , 0.239 0.191 , 0.251	Depositor DCC
R_{free} test set	1481 reflections (5.07%)	wwPDB-VP
Wilson B-factor (Å ²)	41.6	Xtriage
Anisotropy	0.698	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 69.4	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	0.95	EDS
Total number of atoms	9100	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 53.04 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 4.4637e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: 9VY

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	0.88	1/4459 (0.0%)	1.42	25/6052 (0.4%)
1	B	0.87	1/4442 (0.0%)	1.40	21/6030 (0.3%)
All	All	0.88	2/8901 (0.0%)	1.41	46/12082 (0.4%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	187	MET	SD-CE	-6.09	1.64	1.79
1	B	187	MET	SD-CE	-5.84	1.65	1.79

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	25	PRO	N-CA-CB	7.25	110.21	103.46
1	A	557	GLY	CA-C-N	7.15	128.04	120.03
1	A	557	GLY	C-N-CA	7.15	128.04	120.03
1	B	557	GLY	CA-C-N	6.94	127.80	120.03
1	B	557	GLY	C-N-CA	6.94	127.80	120.03
1	A	55	ASP	CA-CB-CG	6.67	119.27	112.60
1	A	129	ASP	CA-CB-CG	6.67	119.27	112.60
1	B	522	GLY	CA-C-N	6.41	128.87	120.28
1	B	522	GLY	C-N-CA	6.41	128.87	120.28
1	B	129	ASP	CA-CB-CG	6.36	118.96	112.60
1	A	330	GLN	CA-C-N	6.17	131.02	120.71
1	A	330	GLN	C-N-CA	6.17	131.02	120.71
1	B	25	PRO	N-CA-CB	6.10	109.66	103.25
1	B	559	ASP	CA-CB-CG	6.07	118.67	112.60
1	A	522	GLY	CA-C-N	6.06	128.72	120.54
1	A	522	GLY	C-N-CA	6.06	128.72	120.54
1	A	559	ASP	CA-CB-CG	6.04	118.64	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	244	ASP	CA-CB-CG	6.00	118.60	112.60
1	A	26	LEU	CA-C-N	5.89	128.98	120.79
1	A	26	LEU	C-N-CA	5.89	128.98	120.79
1	B	507	VAL	N-CA-CB	5.86	118.51	110.54
1	A	507	VAL	N-CA-CB	5.84	118.49	110.54
1	A	334	ALA	CA-C-N	5.83	128.37	120.38
1	A	334	ALA	C-N-CA	5.83	128.37	120.38
1	B	196	SER	N-CA-C	-5.83	101.64	110.39
1	B	375	ASP	CA-CB-CG	5.62	118.22	112.60
1	B	131	VAL	N-CA-C	5.61	116.38	111.56
1	A	375	ASP	CA-CB-CG	5.52	118.12	112.60
1	A	419	LEU	CA-C-N	5.47	128.06	120.29
1	A	419	LEU	C-N-CA	5.47	128.06	120.29
1	B	107	ASP	CA-C-N	5.44	127.62	120.60
1	B	107	ASP	C-N-CA	5.44	127.62	120.60
1	A	437	GLU	CB-CG-CD	5.41	121.79	112.60
1	B	419	LEU	CA-C-N	5.37	127.91	120.29
1	B	419	LEU	C-N-CA	5.37	127.91	120.29
1	A	196	SER	N-CA-C	-5.27	102.48	110.39
1	B	334	ALA	CA-C-N	5.25	127.31	120.28
1	B	334	ALA	C-N-CA	5.25	127.31	120.28
1	B	44	SER	CA-C-N	5.17	127.52	120.54
1	B	44	SER	C-N-CA	5.17	127.52	120.54
1	A	44	SER	CA-C-N	5.14	127.48	120.54
1	A	44	SER	C-N-CA	5.14	127.48	120.54
1	A	25	PRO	N-CA-C	-5.13	107.05	114.18
1	B	557	GLY	N-CA-C	-5.10	106.82	115.34
1	B	24	ASN	CA-CB-CG	5.10	117.70	112.60
1	A	239	ILE	N-CA-C	-5.01	105.96	110.82

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	4359	0	4369	32	0
1	B	4346	0	4351	29	0
2	A	44	24	0	1	0
2	B	44	24	0	0	0
3	A	135	0	0	1	0
3	B	124	0	0	2	0
All	All	9052	48	8720	60	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.

All (60) 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:B:48:ARG:HG3	1:B:157:ALA:O	1.83	0.79
1:A:48:ARG:HG3	1:A:157:ALA:O	1.83	0.79
1:B:44:SER:HB2	1:B:157:ALA:H	1.53	0.72
1:A:44:SER:HB2	1:A:157:ALA:H	1.54	0.70
1:A:219:TYR:HB3	1:A:320:LEU:HD23	1.74	0.69
1:A:230:GLU:O	1:A:234:ARG:HG3	1.93	0.68
1:B:219:TYR:HB3	1:B:320:LEU:HD23	1.75	0.67
1:B:230:GLU:O	1:B:234:ARG:HG3	1.95	0.66
1:A:200:ARG:NH1	1:A:316:ASN:HD21	1.96	0.64
1:A:264:GLY:HA3	3:A:716:HOH:O	1.99	0.63
1:B:283:GLY:HA2	1:B:557:GLY:HA3	1.81	0.62
1:A:283:GLY:HA2	1:A:557:GLY:HA3	1.81	0.62
1:A:531:LYS:H	1:A:531:LYS:HD3	1.65	0.61
1:B:215:MET:HB2	1:B:326:SER:HB2	1.86	0.57
1:A:285:LEU:HA	1:A:558:GLY:HA2	1.91	0.53
1:A:303:CYS:SG	1:A:313:MET:HE1	2.49	0.53
1:B:285:LEU:HA	1:B:558:GLY:HA2	1.92	0.51
1:B:303:CYS:SG	1:B:313:MET:HE1	2.50	0.51
1:A:538:PRO:HG2	1:B:270:LYS:HB3	1.96	0.48
1:A:321:VAL:HG21	2:A:601:9VY:C26	2.43	0.47
1:A:194:GLN:HA	1:A:551:PHE:O	2.14	0.47
1:A:44:SER:HB3	1:A:156:PRO:HA	1.96	0.47
1:B:44:SER:HB3	1:B:156:PRO:HA	1.96	0.47
1:B:194:GLN:HA	1:B:551:PHE:O	2.15	0.47
1:A:211:LYS:HB2	1:A:214:PRO:HB3	1.96	0.46
1:B:82:LEU:HD13	1:B:249:ALA:HB2	1.97	0.46
1:B:257:THR:HA	1:B:261:TYR:HB2	1.98	0.46
1:A:82:LEU:HD13	1:A:249:ALA:HB2	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:31:LEU:HD11	1:B:492:LEU:HD22	1.98	0.45
1:A:31:LEU:HD11	1:A:492:LEU:HD22	1.98	0.45
1:A:461:GLN:HG3	1:A:545:LEU:HD11	1.98	0.45
1:A:257:THR:HA	1:A:261:TYR:HB2	1.99	0.45
1:B:488:CYS:HB2	3:B:722:HOH:O	2.17	0.44
1:B:311:CYS:HB3	1:B:324:CYS:HB3	1.99	0.44
1:B:83:LEU:HB2	1:B:173:MET:HA	1.99	0.44
1:A:12:THR:HG21	1:A:270:LYS:HD2	1.99	0.43
1:B:12:THR:HG21	1:B:270:LYS:HD2	1.99	0.43
1:B:52:VAL:HG12	1:B:223:CYS:SG	2.59	0.43
1:B:184:GLN:HB2	3:B:728:HOH:O	2.18	0.43
1:A:114:LYS:O	1:A:118:HIS:HD2	2.02	0.42
1:A:413:ILE:HD13	1:A:454:ILE:HD13	2.01	0.42
1:B:144:VAL:HB	1:B:394:ARG:HG2	2.01	0.42
1:B:215:MET:HE2	1:B:332:ASP:HB3	2.02	0.42
1:B:413:ILE:HD13	1:B:454:ILE:HD13	2.02	0.42
1:A:409:LEU:O	1:A:413:ILE:HD12	2.20	0.42
1:B:409:LEU:O	1:B:413:ILE:HD12	2.20	0.41
1:A:144:VAL:HB	1:A:394:ARG:HG2	2.02	0.41
1:A:175:LEU:HD21	1:A:253:ILE:HG12	2.02	0.41
1:A:311:CYS:HB3	1:A:324:CYS:HB3	2.02	0.41
1:B:84:SER:OG	1:B:87:GLU:HG3	2.21	0.41
1:A:200:ARG:HH12	1:A:316:ASN:HD21	1.65	0.41
1:B:137:THR:HA	1:B:267:THR:O	2.21	0.41
1:B:313:MET:HE2	1:B:313:MET:HB3	1.91	0.41
1:A:102:GLY:O	1:A:114:LYS:HE3	2.20	0.41
1:A:531:LYS:HG2	1:A:532:THR:N	2.36	0.41
1:A:137:THR:HA	1:A:267:THR:O	2.21	0.41
1:A:555:TYR:HB3	1:A:558:GLY:HA3	2.02	0.41
1:B:405:VAL:HB	1:B:446:GLN:HB2	2.02	0.41
1:A:336:LEU:HA	1:A:336:LEU:HD12	1.73	0.41
1:B:44:SER:CB	1:B:157:ALA:H	2.30	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	556/576 (96%)	538 (97%)	16 (3%)	2 (0%)	30	60
1	B	555/576 (96%)	537 (97%)	16 (3%)	2 (0%)	30	60
All	All	1111/1152 (96%)	1075 (97%)	32 (3%)	4 (0%)	30	60

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	448	TYR
1	A	556	SER
1	B	448	TYR
1	B	556	SER

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	477/491 (97%)	449 (94%)	28 (6%)	18	48
1	B	475/491 (97%)	449 (94%)	26 (6%)	19	51
All	All	952/982 (97%)	898 (94%)	54 (6%)	18	49

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	56	ARG
1	A	69	LYS
1	A	86	GLU
1	A	111	LEU
1	A	113	SER
1	A	114	LYS
1	A	131	VAL
1	A	141	LYS

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Mol	Chain	Res	Type
1	A	201	VAL
1	A	212	LYS
1	A	254	LYS
1	A	255	SER
1	A	282	SER
1	A	311	CYS
1	A	316	ASN
1	A	352	ASP
1	A	367	SER
1	A	371	SER
1	A	413	ILE
1	A	431	SER
1	A	465	ARG
1	A	470	SER
1	A	476	SER
1	A	478	SER
1	A	491	LYS
1	A	507	VAL
1	A	531	LYS
1	A	532	THR
1	B	26	LEU
1	B	27	SER
1	B	56	ARG
1	B	69	LYS
1	B	114	LYS
1	B	141	LYS
1	B	201	VAL
1	B	255	SER
1	B	282	SER
1	B	311	CYS
1	B	316	ASN
1	B	331	GLU
1	B	352	ASP
1	B	367	SER
1	B	371	SER
1	B	405	VAL
1	B	413	ILE
1	B	431	SER
1	B	440	GLU
1	B	465	ARG
1	B	470	SER
1	B	476	SER

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Mol	Chain	Res	Type
1	B	478	SER
1	B	491	LYS
1	B	507	VAL
1	B	545	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	95	HIS
1	A	118	HIS
1	A	120	HIS
1	A	142	ASN
1	A	184	GLN
1	A	194	GLN
1	A	231	ASN
1	A	273	ASN
1	A	316	ASN
1	A	402	HIS
1	A	475	HIS
1	B	95	HIS
1	B	118	HIS
1	B	231	ASN
1	B	273	ASN
1	B	402	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

2 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	9VY	A	601	-	49,50,50	1.08	2 (4%)	61,77,77	1.30	4 (6%)
2	9VY	B	601	-	49,50,50	0.93	3 (6%)	61,77,77	1.31	4 (6%)

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	9VY	A	601	-	-	0/24/45/45	0/7/7/7
2	9VY	B	601	-	-	4/24/45/45	0/7/7/7

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	9VY	S-N	5.30	1.73	1.64
2	A	601	9VY	C12-N2	4.28	1.43	1.39
2	B	601	9VY	C12-N2	3.98	1.43	1.39
2	B	601	9VY	C6-N	-3.96	1.41	1.44
2	B	601	9VY	S-N	2.02	1.67	1.64

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	9VY	C8-N-S	5.88	126.67	118.23
2	B	601	9VY	C20-O3-C21	5.54	120.32	113.87
2	B	601	9VY	C5-C6-N	5.48	126.58	120.85
2	B	601	9VY	C8-N-S	4.80	125.13	118.23
2	A	601	9VY	C20-O3-C21	4.76	119.41	113.87
2	A	601	9VY	C5-C6-N	4.68	125.75	120.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	601	9VY	C14-C13-N2	-2.29	106.76	109.20
2	B	601	9VY	C14-C13-N2	-2.06	107.00	109.20

There are no chirality outliers.

All (4) torsion outliers are listed below:

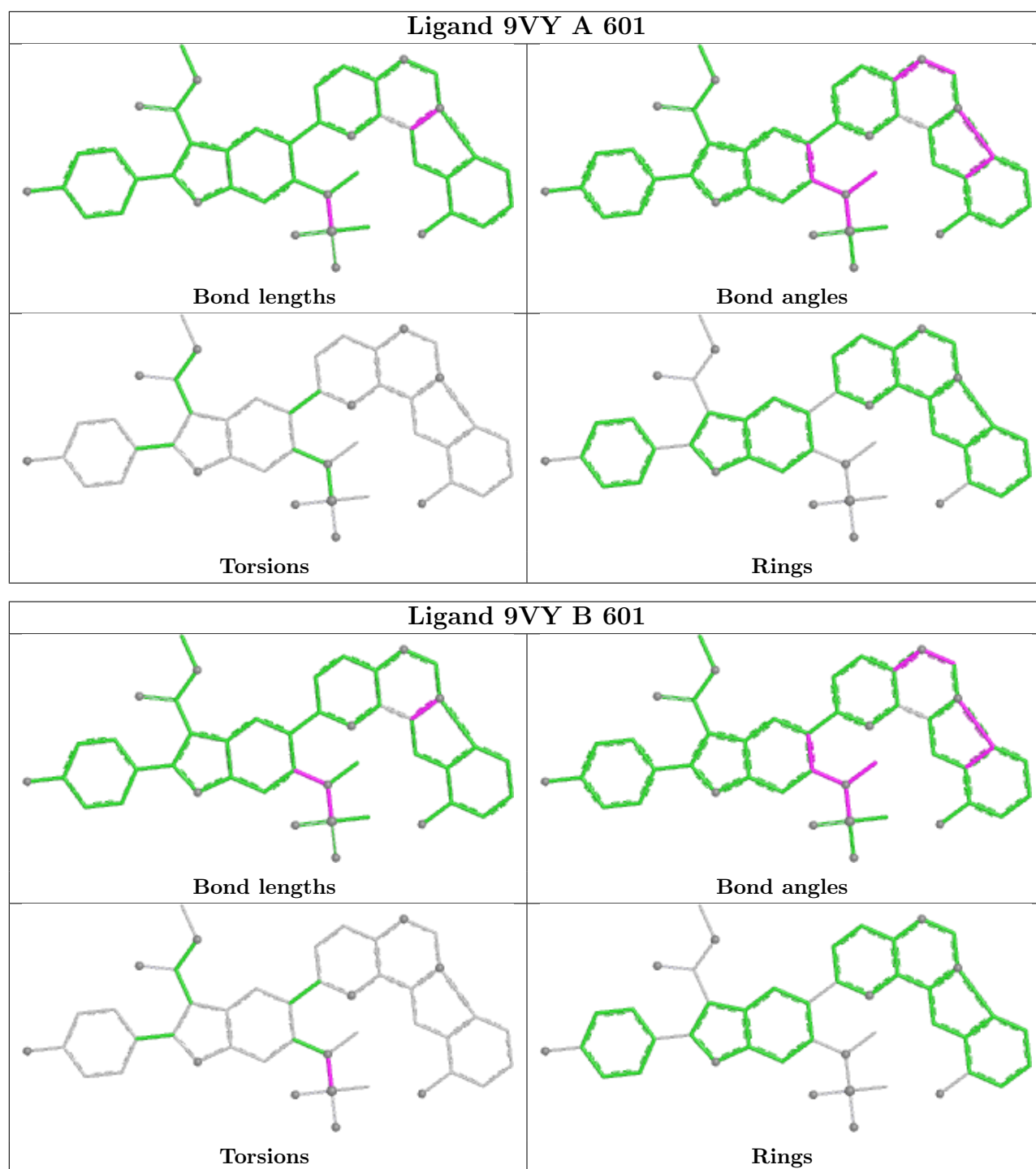
Mol	Chain	Res	Type	Atoms
2	B	601	9VY	C6-N-S-C7
2	B	601	9VY	C6-N-S-O1
2	B	601	9VY	C8-N-S-C7
2	B	601	9VY	C8-N-S-O1

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	9VY	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 [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	559/576 (97%)	-0.24	8 (1%) 73 64	20, 41, 73, 95	3 (0%)
1	B	559/576 (97%)	-0.21	3 (0%) 87 82	22, 45, 75, 99	1 (0%)
All	All	1118/1152 (97%)	-0.23	11 (0%) 79 72	20, 43, 74, 99	4 (0%)

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	552	VAL	4.5
1	B	556	SER	3.4
1	A	556	SER	3.0
1	B	552	VAL	2.7
1	A	553	ALA	2.6
1	A	554	GLY	2.5
1	A	551	PHE	2.3
1	A	148	GLN	2.3
1	B	564	LEU	2.3
1	A	564	LEU	2.2
1	A	555	TYR	2.1

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 ⓘ

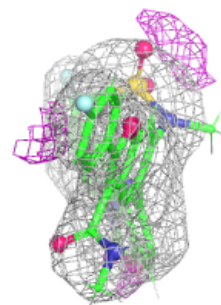
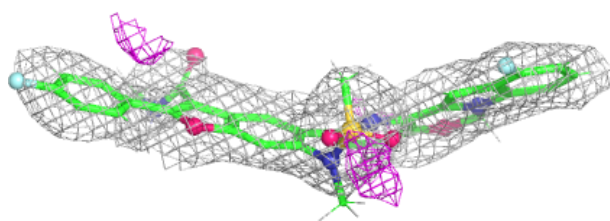
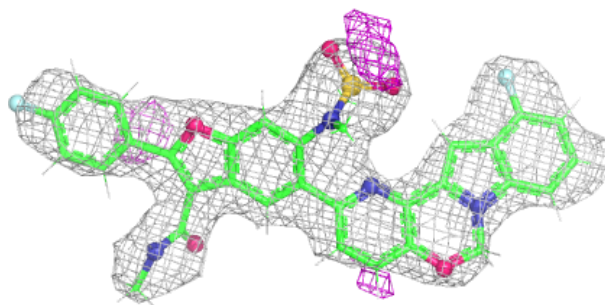
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	9VY	B	601	44/44	0.91	0.10	47,64,66,68	0
2	9VY	A	601	44/44	0.94	0.09	26,45,57,60	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.

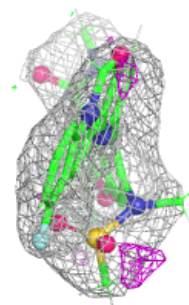
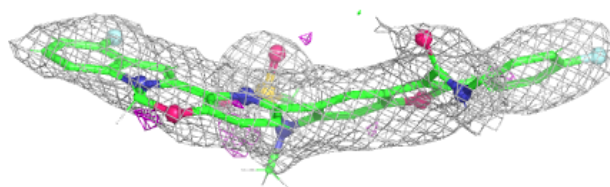
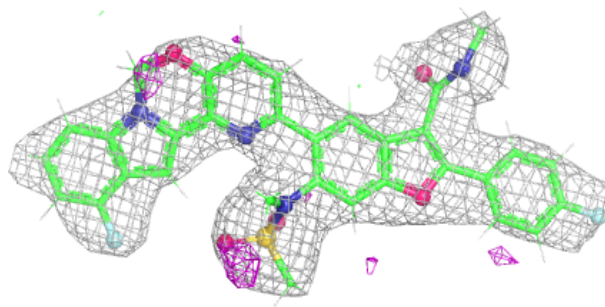
Electron density around 9VY B 601:

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 9VY A 601:

$2mF_o-DF_c$ (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.