



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 12:08 PM UTC

PDB ID : 4OK3 / pdb_00004ok3
Title : Crystal Structure of Hepatitis C Virus NS3 Helicase Inhibitor Co-complex with Compound 7 [[1-(3-chlorobenzyl)-1H-indol-3-yl]acetic acid]
Authors : Padyana, A.K.
Deposited on : 2014-01-21
Resolution : 2.30 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

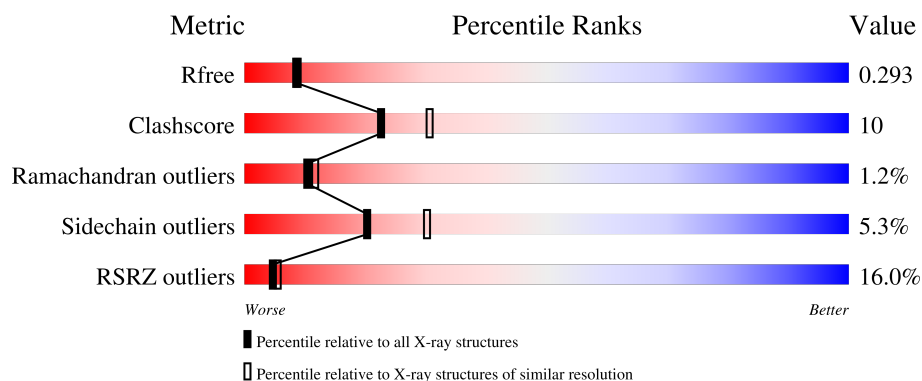
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	6319 (2.30-2.30)
Clashscore	190562	6919 (2.30-2.30)
Ramachandran outliers	187476	6854 (2.30-2.30)
Sidechain outliers	187428	6854 (2.30-2.30)
RSRZ outliers	180081	6325 (2.30-2.30)

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	464	16% 69% 20% 8%
1	B	464	13% 72% 14% 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6495 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 Serine protease NS3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	426	Total	C	N	O	S	0	1	0
			3203	2026	542	612	23			
1	B	420	Total	C	N	O	S	0	1	0
			3165	2008	531	604	22			

There are 30 discrepancies between the modelled and reference sequences:

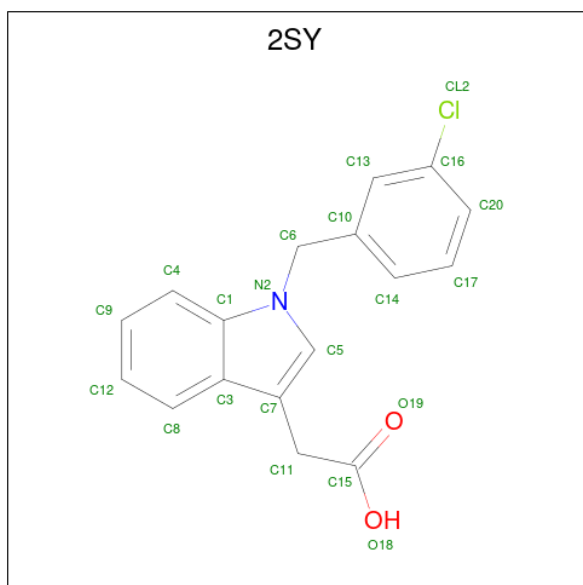
Chain	Residue	Modelled	Actual	Comment	Reference
A	167	MET	-	expression tag	UNP K4KA16
A	168	GLY	-	expression tag	UNP K4KA16
A	169	SER	-	expression tag	UNP K4KA16
A	170	SER	-	expression tag	UNP K4KA16
A	171	HIS	-	expression tag	UNP K4KA16
A	172	HIS	-	expression tag	UNP K4KA16
A	173	HIS	-	expression tag	UNP K4KA16
A	174	HIS	-	expression tag	UNP K4KA16
A	175	HIS	-	expression tag	UNP K4KA16
A	176	HIS	-	expression tag	UNP K4KA16
A	177	SER	-	expression tag	UNP K4KA16
A	178	SER	-	expression tag	UNP K4KA16
A	179	GLY	-	expression tag	UNP K4KA16
A	403	ASN	SER	conflict	UNP K4KA16
A	505	MET	THR	conflict	UNP K4KA16
B	167	MET	-	expression tag	UNP K4KA16
B	168	GLY	-	expression tag	UNP K4KA16
B	169	SER	-	expression tag	UNP K4KA16
B	170	SER	-	expression tag	UNP K4KA16
B	171	HIS	-	expression tag	UNP K4KA16
B	172	HIS	-	expression tag	UNP K4KA16
B	173	HIS	-	expression tag	UNP K4KA16
B	174	HIS	-	expression tag	UNP K4KA16
B	175	HIS	-	expression tag	UNP K4KA16
B	176	HIS	-	expression tag	UNP K4KA16

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Chain	Residue	Modelled	Actual	Comment	Reference
B	177	SER	-	expression tag	UNP K4KA16
B	178	SER	-	expression tag	UNP K4KA16
B	179	GLY	-	expression tag	UNP K4KA16
B	403	ASN	SER	conflict	UNP K4KA16
B	505	MET	THR	conflict	UNP K4KA16

- Molecule 2 is [1-(3-chlorobenzyl)-1H-indol-3-yl]acetic acid (CCD ID: 2SY) (formula: C₁₇H₁₄ClNO₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			21	17	1	1	2		

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	Ca	0	0
			2	2		

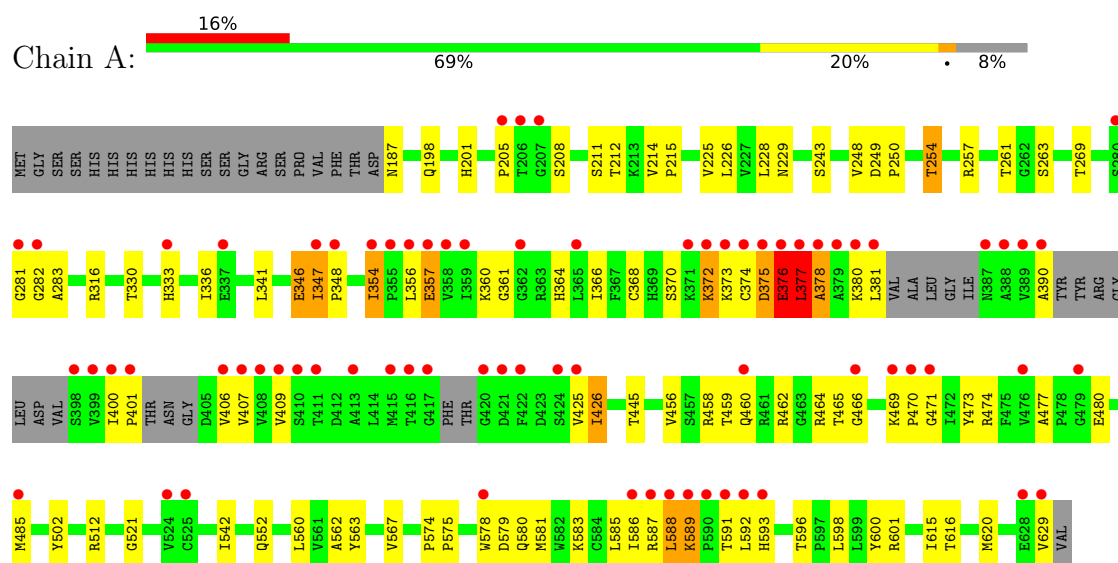
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	46	Total	O	0	0
			46	46		
4	B	58	Total	O	0	0
			58	58		

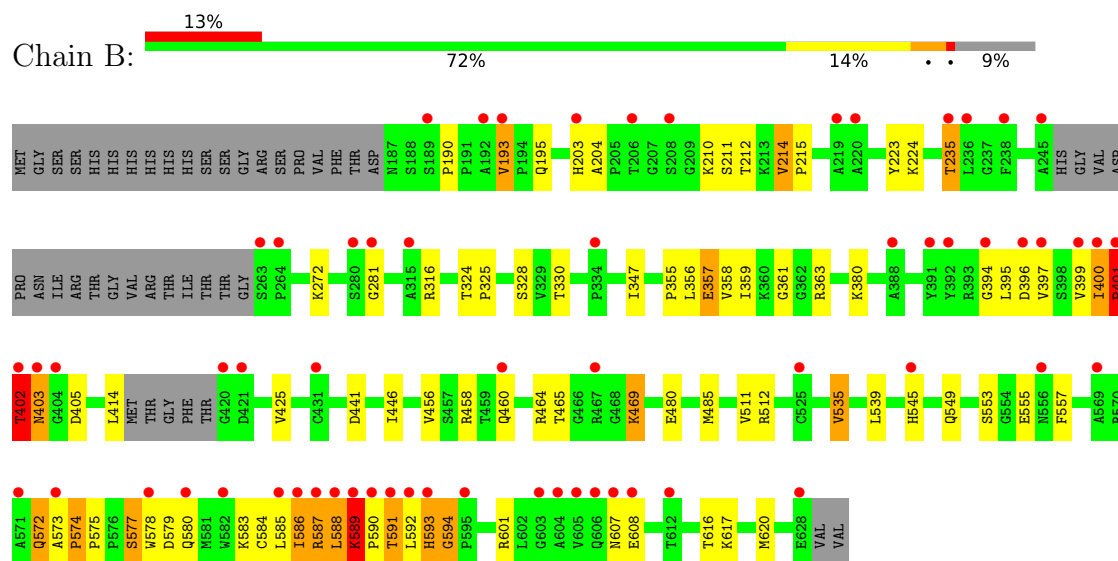
3 Residue-property plots

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

• Molecule 1: Serine protease NS3



• Molecule 1: Serine protease NS3



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	81.39Å 104.23Å 117.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	36.09 – 2.30 36.09 – 2.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (36.09-2.30) 93.1 (36.09-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.36 (at 2.29Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.232 , 0.292 0.240 , 0.293	Depositor DCC
R_{free} test set	2282 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	50.2	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 41.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.53$, $\langle L^2 \rangle = 0.37$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	6495	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.93% 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: 2SY, CA

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	0.62	0/3277	1.00	9/4471 (0.2%)
1	B	0.63	0/3241	1.02	16/4425 (0.4%)
All	All	0.62	0/6518	1.01	25/8896 (0.3%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	3
1	B	0	4
All	All	0	7

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	402	THR	N-CA-C	-9.84	98.30	110.41
1	A	376	GLU	N-CA-C	-9.69	100.38	112.88
1	A	589	LYS	CA-C-N	-8.26	111.13	119.56
1	A	589	LYS	C-N-CA	-8.26	111.13	119.56
1	A	377	LEU	N-CA-C	-7.40	103.35	112.38
1	B	580	GLN	N-CA-C	-6.77	104.76	113.16
1	B	587	ARG	N-CA-C	-6.40	103.54	112.25
1	B	589	LYS	CA-C-N	-6.21	112.45	119.28
1	B	589	LYS	C-N-CA	-6.21	112.45	119.28
1	B	460	GLN	CA-CB-CG	6.16	126.42	114.10
1	A	354	ILE	N-CA-C	6.07	114.83	107.61
1	B	574	PRO	CA-C-N	5.98	126.54	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	574	PRO	C-N-CA	5.98	126.54	120.38
1	B	190	PRO	CA-C-N	5.94	126.25	119.83
1	B	190	PRO	C-N-CA	5.94	126.25	119.83
1	B	594	GLY	CA-C-N	5.86	126.15	119.83
1	B	594	GLY	C-N-CA	5.86	126.15	119.83
1	B	401	PRO	N-CA-C	-5.50	107.64	114.68
1	A	263	SER	CA-C-N	-5.47	114.13	120.04
1	A	263	SER	C-N-CA	-5.47	114.13	120.04
1	B	214	VAL	CB-CA-C	-5.27	108.77	114.35
1	B	591	THR	N-CA-C	5.17	116.84	108.26
1	B	589	LYS	N-CA-C	5.12	121.12	109.81
1	A	333	HIS	CA-C-N	5.06	124.67	119.05
1	A	333	HIS	C-N-CA	5.06	124.67	119.05

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	375	ASP	Peptide
1	A	376	GLU	Peptide
1	A	377	LEU	Peptide
1	B	401	PRO	Peptide
1	B	402	THR	Peptide
1	B	579	ASP	Peptide
1	B	589	LYS	Peptide

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	3203	0	3162	79	0
1	B	3165	0	3122	54	0
2	A	21	0	13	1	0
3	A	2	0	0	0	0
4	A	46	0	0	0	0
4	B	58	0	0	2	0
All	All	6495	0	6297	133	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 10.

All (133) 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:378:ALA:C	1:A:380:LYS:H	1.87	0.81
1:A:400:ILE:HD12	1:A:401:PRO:HD2	1.60	0.81
1:B:616:THR:HG22	1:B:620:MET:HE2	1.65	0.79
1:A:460:GLN:HE21	1:A:464:ARG:HH21	1.33	0.76
1:A:616:THR:HG22	1:A:620:MET:HE2	1.66	0.75
1:B:441:ASP:O	1:B:601:ARG:NH1	2.21	0.73
1:A:376:GLU:HA	1:A:378:ALA:HA	1.73	0.70
1:B:617:LYS:HA	1:B:620:MET:HE3	1.73	0.70
1:A:370:SER:O	1:A:374:CYS:HB2	1.92	0.69
1:A:589:LYS:HD2	1:A:589:LYS:O	1.95	0.67
1:B:592:LEU:O	1:B:594:GLY:N	2.26	0.67
1:A:377:LEU:O	1:A:380:LYS:HB3	1.96	0.65
1:B:575:PRO:HG3	1:B:585:LEU:HD12	1.78	0.65
1:A:347:ILE:HG12	1:A:354:ILE:H	1.63	0.63
1:B:607:ASN:OD1	1:B:608:GLU:N	2.31	0.63
1:B:195:GLN:HA	1:B:316:ARG:HH21	1.63	0.62
1:B:195:GLN:HA	1:B:316:ARG:NH2	2.14	0.62
1:A:575:PRO:HG3	1:A:585:LEU:HD12	1.81	0.62
1:B:591:THR:HG23	1:B:593:HIS:H	1.64	0.62
1:A:375:ASP:OD1	1:A:380:LYS:HE3	2.00	0.61
1:A:187:ASN:HB3	1:A:201:HIS:O	2.01	0.60
1:A:368:CYS:HB2	1:A:374:CYS:HA	1.83	0.60
1:B:363:ARG:CZ	1:B:403:ASN:ND2	2.65	0.60
1:B:553:SER:OG	1:B:555:GLU:OE1	2.19	0.60
1:B:347:ILE:HD11	1:B:356:LEU:HD12	1.84	0.60
1:B:578:TRP:CZ2	1:B:588:LEU:HG	2.37	0.60
1:A:400:ILE:HG12	1:A:406:VAL:HG21	1.84	0.58
1:A:400:ILE:HD12	1:A:401:PRO:CD	2.32	0.56
1:A:373:LYS:HD3	1:A:376:GLU:HG2	1.88	0.56
1:A:458:ARG:NH2	1:A:477:ALA:O	2.39	0.56
1:B:363:ARG:NH2	1:B:400:ILE:O	2.37	0.56
1:B:574:PRO:HG2	1:B:607:ASN:ND2	2.20	0.56
1:A:377:LEU:HD23	1:A:409:VAL:HG11	1.88	0.55
1:B:212:THR:C	1:B:215:PRO:HD2	2.31	0.55
1:A:426:ILE:HD13	1:A:474:ARG:HB2	1.88	0.55
1:B:396:ASP:OD2	1:B:397:VAL:HG22	2.06	0.55
1:B:330:THR:HG21	1:B:458:ARG:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:572:GLN:C	1:B:591:THR:HG21	2.31	0.55
1:B:587:ARG:O	1:B:590:PRO:HD2	2.07	0.55
1:B:363:ARG:CZ	1:B:403:ASN:HD22	2.20	0.54
1:A:248:VAL:O	1:A:250:PRO:HD3	2.07	0.54
1:A:574:PRO:O	1:A:596:THR:OG1	2.19	0.53
1:B:361:GLY:HA2	1:B:405:ASP:OD2	2.09	0.53
1:A:281:GLY:O	1:A:283:ALA:N	2.39	0.53
1:A:341:LEU:CD1	1:A:474:ARG:HB3	2.40	0.52
1:A:445:THR:HG23	1:A:601:ARG:HB2	1.91	0.52
1:A:205:PRO:O	1:A:208:SER:HB3	2.10	0.52
1:B:572:GLN:O	1:B:591:THR:HG21	2.10	0.52
1:A:578:TRP:CH2	1:A:588:LEU:HD22	2.45	0.51
1:A:591:THR:C	1:A:593:HIS:H	2.19	0.51
1:B:572:GLN:HB2	1:B:591:THR:OG1	2.10	0.51
1:A:425:VAL:HG23	1:A:465:THR:HB	1.93	0.51
1:B:577:SER:OG	1:B:578:TRP:N	2.41	0.51
1:A:589:LYS:HA	1:A:592:LEU:HD23	1.93	0.50
1:A:376:GLU:CA	1:A:378:ALA:HA	2.42	0.50
1:B:402:THR:HG22	1:B:403:ASN:H	1.77	0.49
1:A:364:HIS:HB2	1:A:407:VAL:HG22	1.94	0.49
1:A:591:THR:O	1:A:593:HIS:N	2.45	0.49
1:A:502:TYR:OH	2:A:701:2SY:H1	2.12	0.49
1:B:414:LEU:C	1:B:464:ARG:HH12	2.20	0.49
1:A:378:ALA:O	1:A:380:LYS:HG2	2.13	0.49
1:A:380:LYS:HG3	1:A:381:LEU:N	2.27	0.49
1:A:346:GLU:OE1	1:A:346:GLU:N	2.45	0.48
1:B:330:THR:HG23	1:B:480:GLU:OE1	2.13	0.48
1:B:399:VAL:O	1:B:401:PRO:HD3	2.13	0.48
1:B:193:VAL:HG11	1:B:223:TYR:CE2	2.48	0.48
1:B:587:ARG:O	1:B:587:ARG:HG3	2.14	0.48
1:A:629:VAL:HA	4:B:702:HOH:O	2.12	0.48
1:A:563:TYR:HE2	1:A:615:ILE:HD13	1.78	0.48
1:A:560:LEU:O	1:A:600:TYR:OH	2.25	0.48
1:A:243:SER:OG	1:A:249:ASP:OD1	2.30	0.47
1:A:616:THR:HG22	1:A:620:MET:CE	2.42	0.47
1:B:574:PRO:HG2	1:B:607:ASN:HD21	1.79	0.47
1:B:545:HIS:O	1:B:549:GLN:HG3	2.14	0.47
1:A:380:LYS:HG3	1:A:381:LEU:H	1.78	0.47
1:A:560:LEU:HD22	1:A:600:TYR:CE2	2.49	0.47
1:B:324:THR:HG21	1:B:456:VAL:HG12	1.97	0.47
1:A:354:ILE:CD1	1:A:426:ILE:HG21	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:LYS:O	1:A:376:GLU:N	2.47	0.47
1:A:254:THR:HG22	1:A:257:ARG:O	2.15	0.47
1:A:378:ALA:C	1:A:380:LYS:N	2.62	0.46
1:A:346:GLU:HG3	1:A:356:LEU:HD23	1.97	0.46
1:A:354:ILE:HD11	1:A:426:ILE:HG21	1.96	0.46
1:A:330:THR:HG23	1:A:480:GLU:OE1	2.16	0.46
1:B:583:LYS:O	1:B:585:LEU:N	2.48	0.46
1:A:390:ALA:HA	1:A:409:VAL:O	2.15	0.46
1:A:229:ASN:O	1:A:269:THR:HA	2.16	0.45
1:B:210:LYS:H	1:B:235:THR:HG21	1.81	0.45
1:B:355:PRO:HG2	1:B:358:VAL:HG13	1.98	0.45
1:A:212:THR:C	1:A:215:PRO:HD2	2.42	0.45
1:A:341:LEU:HD11	1:A:474:ARG:HB3	1.99	0.45
1:A:377:LEU:HD23	1:A:409:VAL:CG1	2.47	0.45
1:A:591:THR:C	1:A:593:HIS:N	2.75	0.45
1:B:585:LEU:C	1:B:587:ARG:H	2.25	0.45
1:A:357:GLU:H	1:A:357:GLU:HG2	1.51	0.45
1:A:466:GLY:HA2	1:A:469:LYS:O	2.17	0.44
1:B:363:ARG:NH1	1:B:403:ASN:ND2	2.65	0.44
1:A:360:LYS:HA	1:A:361:GLY:HA2	1.60	0.44
1:A:589:LYS:HD2	1:A:589:LYS:C	2.42	0.44
1:B:591:THR:HG23	1:B:593:HIS:CG	2.52	0.44
1:B:535:VAL:O	1:B:539:LEU:HG	2.17	0.44
1:A:336:ILE:HA	1:A:471:GLY:O	2.17	0.44
1:A:376:GLU:O	1:A:376:GLU:HG3	2.18	0.43
1:A:249:ASP:O	1:A:261:THR:OG1	2.35	0.43
1:B:394:GLY:O	1:B:395:LEU:HD23	2.18	0.43
1:A:214:VAL:HB	1:A:215:PRO:HD3	2.01	0.43
1:A:583:LYS:O	1:A:586:ILE:HG12	2.19	0.43
1:A:460:GLN:NE2	1:A:464:ARG:HH21	2.09	0.43
1:A:542:ILE:HD11	1:A:562:ALA:HB3	2.00	0.43
1:B:400:ILE:HG23	1:B:402:THR:HB	2.01	0.43
1:A:426:ILE:HD13	1:A:474:ARG:HD2	2.01	0.42
1:B:203:HIS:ND1	1:B:204:ALA:O	2.50	0.42
1:B:397:VAL:O	1:B:397:VAL:HG23	2.20	0.42
1:B:601:ARG:HG3	4:B:716:HOH:O	2.20	0.42
1:A:462:ARG:HG3	1:A:473:TYR:CG	2.55	0.42
1:A:360:LYS:HE2	1:A:360:LYS:HB3	1.84	0.41
1:A:226:LEU:HD21	1:A:228:LEU:HD21	2.02	0.41
1:B:591:THR:CG2	1:B:593:HIS:H	2.33	0.41
1:B:358:VAL:HG23	1:B:359:ILE:HG23	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469:LYS:H	1:B:469:LYS:HG2	1.57	0.41
1:B:573:ALA:HA	1:B:591:THR:HG21	2.01	0.41
1:A:201:HIS:CE1	1:A:521:GLY:HA3	2.55	0.41
1:A:380:LYS:HG3	1:A:381:LEU:HG	2.01	0.41
1:B:357:GLU:H	1:B:357:GLU:HG3	1.40	0.41
1:B:425:VAL:HG23	1:B:465:THR:HB	2.03	0.41
1:B:446:ILE:HG21	1:B:557:PHE:CE2	2.56	0.41
1:A:575:PRO:HG3	1:A:585:LEU:CD1	2.50	0.41
1:A:579:ASP:OD1	1:A:580:GLN:N	2.54	0.41
1:A:376:GLU:C	1:A:378:ALA:N	2.79	0.41
1:A:347:ILE:HA	1:A:348:PRO:HD3	1.93	0.41
1:B:325:PRO:HD2	1:B:328:SER:OG	2.22	0.40
1:A:469:LYS:HA	1:A:470:PRO:HD3	1.99	0.40
1:A:366:ILE:HG12	1:A:426:ILE:HB	2.03	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	417/464 (90%)	392 (94%)	21 (5%)	4 (1%)	12	15
1	B	415/464 (89%)	390 (94%)	19 (5%)	6 (1%)	9	9
All	All	832/928 (90%)	782 (94%)	40 (5%)	10 (1%)	10	12

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	378	ALA
1	B	593	HIS
1	B	281	GLY
1	B	572	GLN

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Mol	Chain	Res	Type
1	A	282	GLY
1	B	584	CYS
1	A	372	LYS
1	A	581	MET
1	B	211	SER
1	B	586	ILE

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	351/382 (92%)	332 (95%)	19 (5%)	20	29
1	B	345/382 (90%)	327 (95%)	18 (5%)	21	31
All	All	696/764 (91%)	659 (95%)	37 (5%)	20	30

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	198	GLN
1	A	211	SER
1	A	225	VAL
1	A	254	THR
1	A	316	ARG
1	A	346	GLU
1	A	347	ILE
1	A	357	GLU
1	A	376	GLU
1	A	426	ILE
1	A	456	VAL
1	A	459	THR
1	A	485	MET
1	A	512	ARG
1	A	552	GLN
1	A	567	VAL
1	A	587	ARG

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Mol	Chain	Res	Type
1	A	588	LEU
1	A	598	LEU
1	B	193	VAL
1	B	214	VAL
1	B	224	LYS
1	B	235	THR
1	B	272	LYS
1	B	357	GLU
1	B	380	LYS
1	B	400	ILE
1	B	403	ASN
1	B	469	LYS
1	B	485	MET
1	B	511	VAL
1	B	512	ARG
1	B	535	VAL
1	B	577	SER
1	B	586	ILE
1	B	588	LEU
1	B	589	LYS

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

Mol	Chain	Res	Type
1	A	198	GLN
1	A	201	HIS
1	A	335	ASN
1	A	460	GLN
1	A	607	ASN
1	B	229	ASN
1	B	403	ASN
1	B	434	GLN
1	B	580	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](#)

Of 3 ligands modelled in this entry, 2 are monoatomic - leaving 1 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	2SY	A	701	-	23,23,23	0.74	0	32,32,32	1.41	5 (15%)

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	2SY	A	701	-	-	3/8/8/8	0/3/3/3

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	2SY	C10-C6-N2	3.78	118.53	112.78
2	A	701	2SY	C6-N2-C1	-2.94	121.90	126.13
2	A	701	2SY	C4-C1-C3	-2.26	119.43	121.95
2	A	701	2SY	C15-C11-C7	-2.22	111.52	114.93
2	A	701	2SY	C6-N2-C5	2.05	128.27	125.46

There are no chirality outliers.

All (3) torsion outliers are listed below:

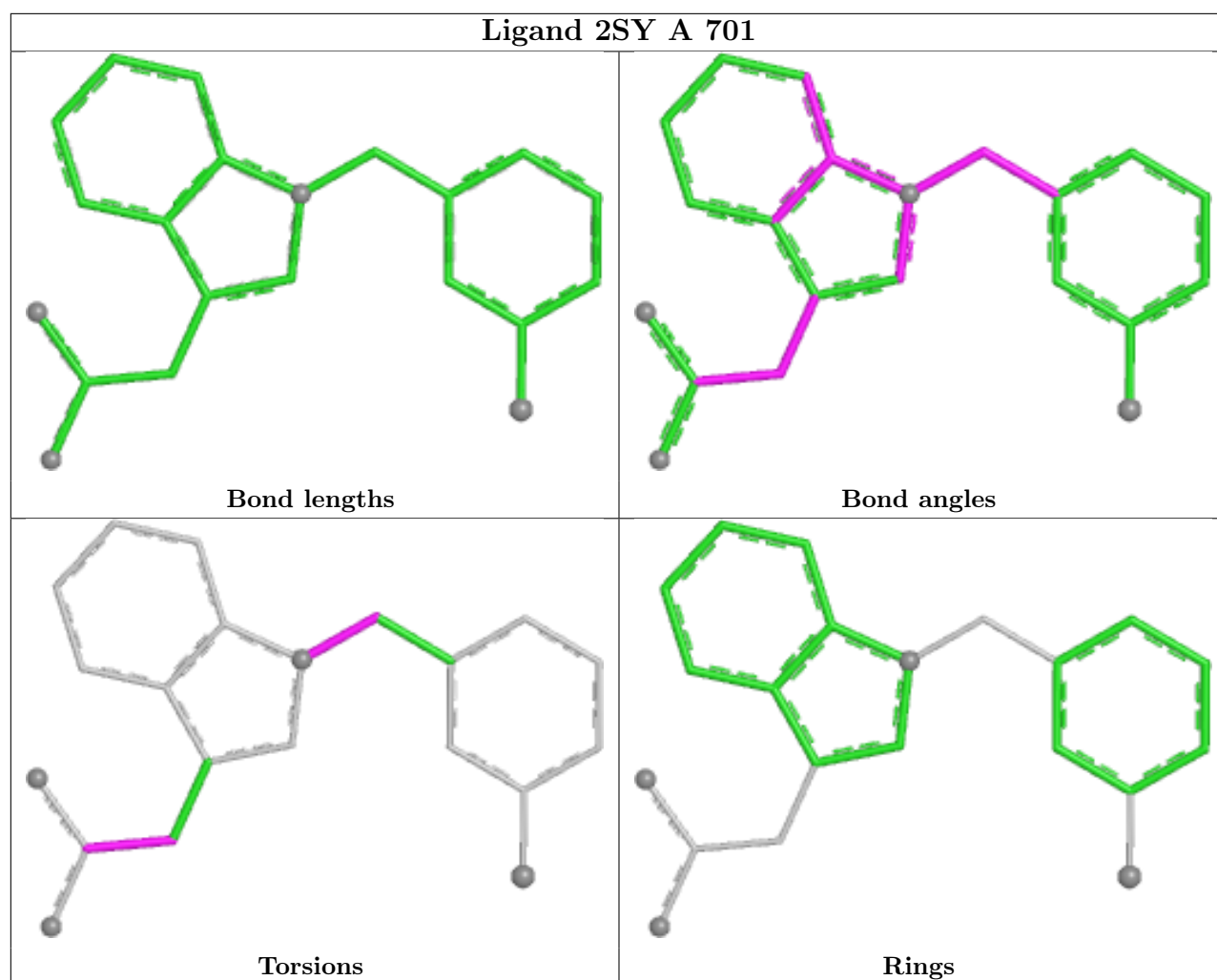
Mol	Chain	Res	Type	Atoms
2	A	701	2SY	C7-C11-C15-O18
2	A	701	2SY	C10-C6-N2-C5
2	A	701	2SY	C7-C11-C15-O19

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	701	2SY	1	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	426/464 (91%)	1.01	73 (17%) 4 5	43, 59, 96, 118	1 (0%)
1	B	420/464 (90%)	0.91	62 (14%) 5 6	37, 60, 94, 109	1 (0%)
All	All	846/928 (91%)	0.96	135 (15%) 5 5	37, 59, 95, 118	2 (0%)

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	379	ALA	8.3
1	A	525[A]	CYS	7.9
1	A	381	LEU	7.5
1	B	592	LEU	7.3
1	A	592	LEU	7.2
1	A	398	SER	6.3
1	A	629	VAL	5.9
1	A	420	GLY	5.7
1	A	417	GLY	5.1
1	A	389	VAL	5.1
1	A	524	VAL	5.0
1	B	590	PRO	4.9
1	A	400	ILE	4.8
1	A	399	VAL	4.8
1	A	354	ILE	4.7
1	A	377	LEU	4.7
1	A	206	THR	4.6
1	B	403	ASN	4.5
1	B	578	TRP	4.5
1	A	390	ALA	4.3
1	A	347	ILE	4.2
1	A	587	ARG	4.0
1	A	401	PRO	3.9
1	A	371	LYS	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	588	LEU	3.8
1	A	380	LYS	3.7
1	B	220	ALA	3.7
1	B	586	ILE	3.7
1	B	401	PRO	3.7
1	B	400	ILE	3.6
1	A	593	HIS	3.6
1	B	460	GLN	3.5
1	B	573	ALA	3.5
1	A	282	GLY	3.5
1	B	236	LEU	3.5
1	A	408	VAL	3.5
1	A	374	CYS	3.4
1	A	281	GLY	3.4
1	B	402	THR	3.3
1	B	397	VAL	3.3
1	A	591	THR	3.3
1	B	396	ASP	3.3
1	B	420	GLY	3.2
1	A	586	ILE	3.2
1	A	415	MET	3.2
1	B	605	VAL	3.2
1	A	589	LYS	3.2
1	B	208	SER	3.1
1	A	348	PRO	3.1
1	A	416	THR	3.1
1	A	421	ASP	3.1
1	B	281	GLY	3.1
1	B	235	THR	3.0
1	B	591	THR	3.0
1	B	280	SER	3.0
1	A	375	ASP	3.0
1	A	413	ALA	2.9
1	A	205	PRO	2.9
1	A	365	LEU	2.9
1	B	585	LEU	2.9
1	A	378	ALA	2.9
1	A	359	ILE	2.9
1	A	466	GLY	2.8
1	A	358	VAL	2.8
1	A	373	LYS	2.8
1	B	593	HIS	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	406	VAL	2.8
1	B	245	ALA	2.8
1	B	571	ALA	2.8
1	B	264	PRO	2.8
1	B	604	ALA	2.7
1	B	580	GLN	2.7
1	B	595	PRO	2.7
1	B	392	TYR	2.7
1	B	431[A]	CYS	2.7
1	A	425	VAL	2.7
1	A	410	SER	2.7
1	A	578	TRP	2.7
1	B	628	GLU	2.6
1	B	189	SER	2.6
1	A	356	LEU	2.6
1	B	467	ARG	2.6
1	A	207	GLY	2.6
1	A	471	GLY	2.6
1	B	219	ALA	2.6
1	B	394	GLY	2.6
1	A	280	SER	2.6
1	B	203	HIS	2.6
1	A	388	ALA	2.5
1	B	192	ALA	2.5
1	B	193	VAL	2.5
1	B	421	ASP	2.5
1	A	588	LEU	2.5
1	A	387	ASN	2.5
1	B	607	ASN	2.5
1	B	391	TYR	2.4
1	B	587	ARG	2.4
1	A	590	PRO	2.4
1	A	409	VAL	2.4
1	B	603	GLY	2.4
1	B	206	THR	2.4
1	B	612	THR	2.4
1	A	422	PHE	2.3
1	B	569	ALA	2.3
1	B	238	PHE	2.3
1	B	556	ASN	2.3
1	A	355	PRO	2.3
1	A	470	PRO	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	362	GLY	2.3
1	A	333	HIS	2.3
1	A	407	VAL	2.3
1	A	485	MET	2.3
1	B	582	TRP	2.3
1	B	545	HIS	2.3
1	B	606	GLN	2.3
1	A	628	GLU	2.2
1	B	263	SER	2.2
1	B	399	VAL	2.2
1	A	376	GLU	2.2
1	B	608	GLU	2.2
1	B	388	ALA	2.2
1	A	372	LYS	2.2
1	B	589	LYS	2.2
1	B	315	ALA	2.2
1	A	357	GLU	2.1
1	A	469	LYS	2.1
1	B	404	GLY	2.1
1	A	411	THR	2.1
1	A	337	GLU	2.1
1	A	476	VAL	2.1
1	A	424	SER	2.1
1	A	460	GLN	2.1
1	B	334	PRO	2.1
1	A	479	GLY	2.1
1	B	525	CYS	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.

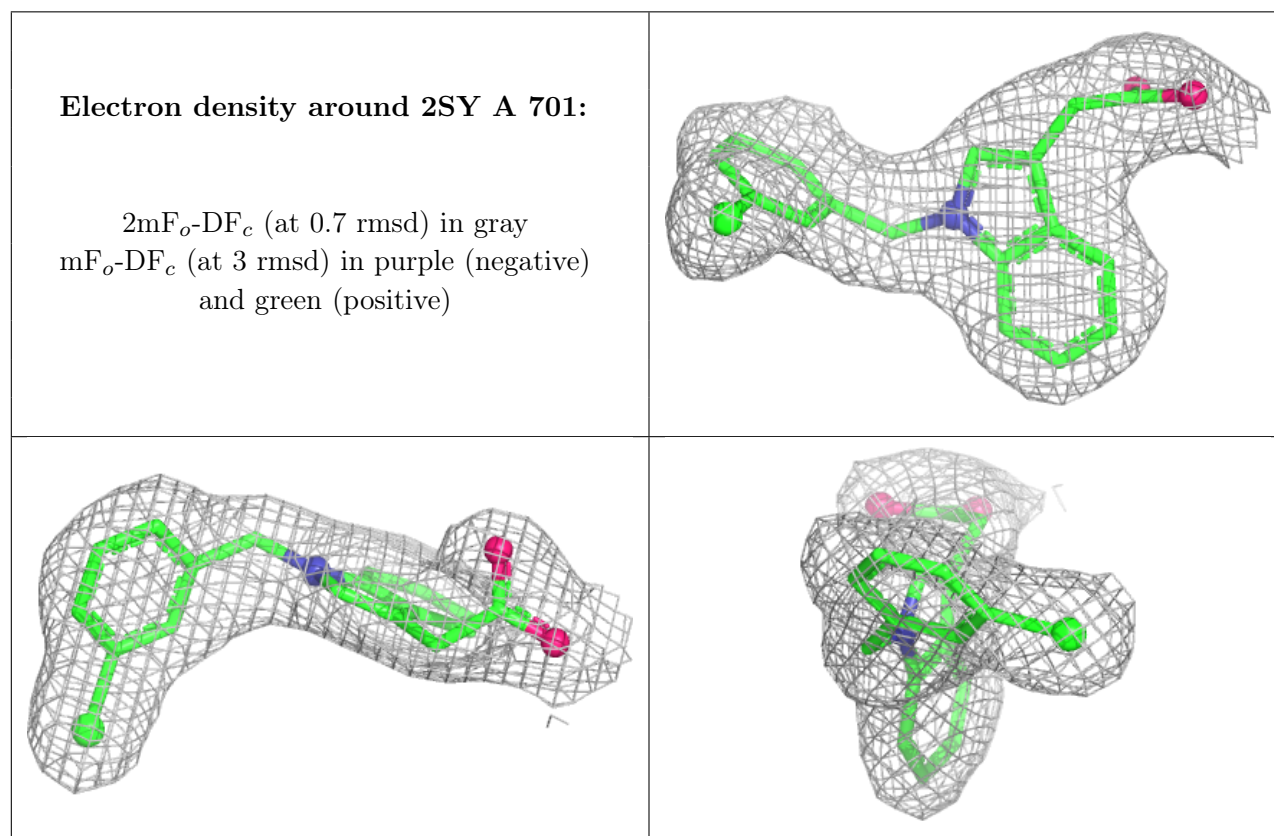
6.4 Ligands [i](#)

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
2	2SY	A	701	21/21	0.93	0.10	42,49,57,59	0
3	CA	A	703	1/1	0.93	0.07	76,76,76,76	0
3	CA	A	702	1/1	0.98	0.03	68,68,68,68	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.