



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:11 PM UTC

PDB ID : 4OJQ / pdb_00004ojq
Title : Crystal Structure of Hepatitis C Virus NS3 Helicase Inhibitor Co-complex with
Fragment 1 [(5-bromo-1H-indol-3-yl)acetic acid]
Authors : Padyana, A.K.
Deposited on : 2014-01-21
Resolution : 2.25 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

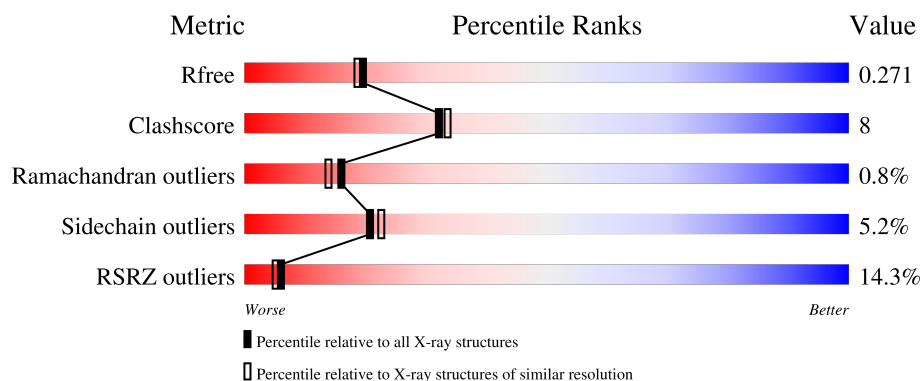
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.25 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	1898 (2.26-2.26)
Clashscore	190562	2005 (2.26-2.26)
Ramachandran outliers	187476	1965 (2.26-2.26)
Sidechain outliers	187428	1966 (2.26-2.26)
RSRZ outliers	180081	1898 (2.26-2.26)

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	17% 74% 18% 5%
1	B	464	10% 74% 14% 9%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6714 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	440	Total	C	N	O	S	0	4	0
			3337	2115	560	637	25			
1	B	420	Total	C	N	O	S	0	1	0
			3176	2018	532	603	23			

There are 30 discrepancies between the modelled and reference sequences:

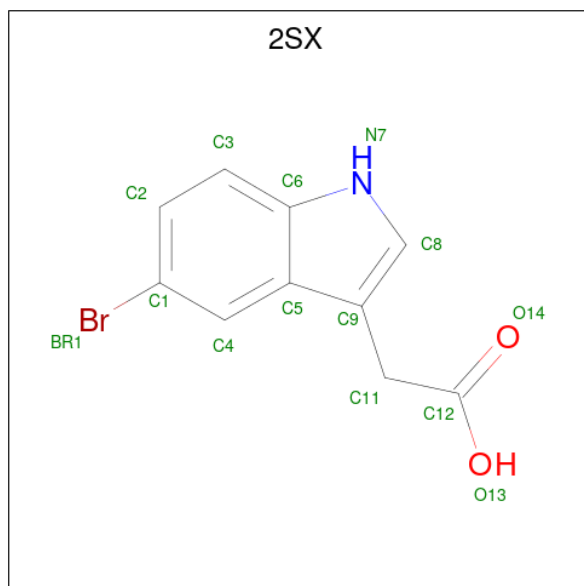
Chain	Residue	Modelled	Actual	Comment	Reference
A	167	MET	-	expression tag	UNP K4KA16
A	168	GLY	-	expression tag	UNP K4KA16
A	169	SER	-	expression tag	UNP K4KA16
A	170	SER	-	expression tag	UNP K4KA16
A	171	HIS	-	expression tag	UNP K4KA16
A	172	HIS	-	expression tag	UNP K4KA16
A	173	HIS	-	expression tag	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 (5-bromo-1H-indol-3-yl)acetic acid (CCD ID: 2SX) (formula: C₁₀H₈BrNO₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	Br	C	N	O	0	0
			14	1	10	1	2		

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

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

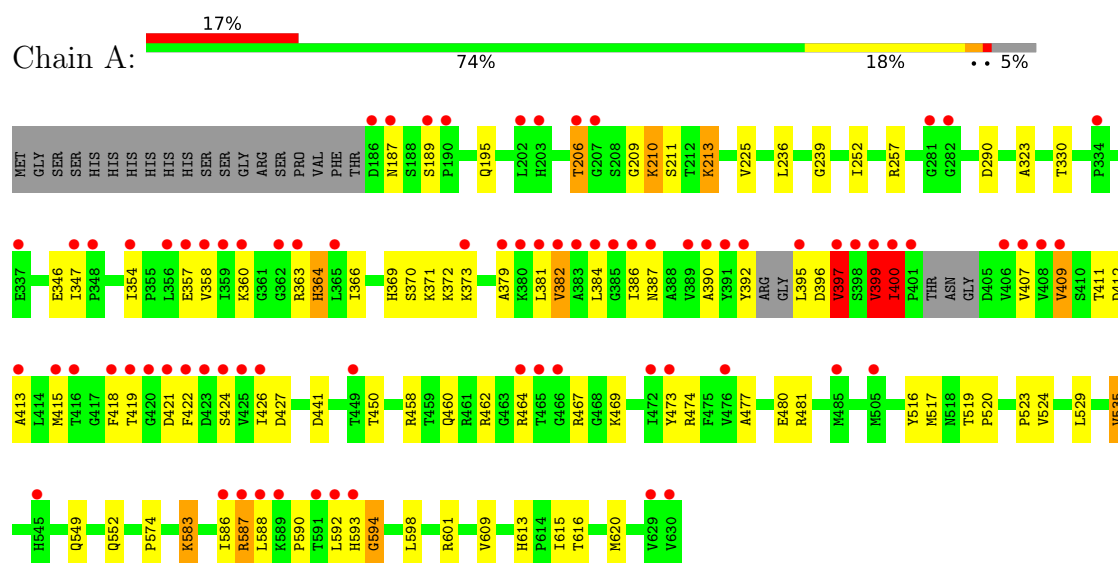
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	85	Total	O	0	0
			85	85		
4	B	100	Total	O	0	0
			100	100		

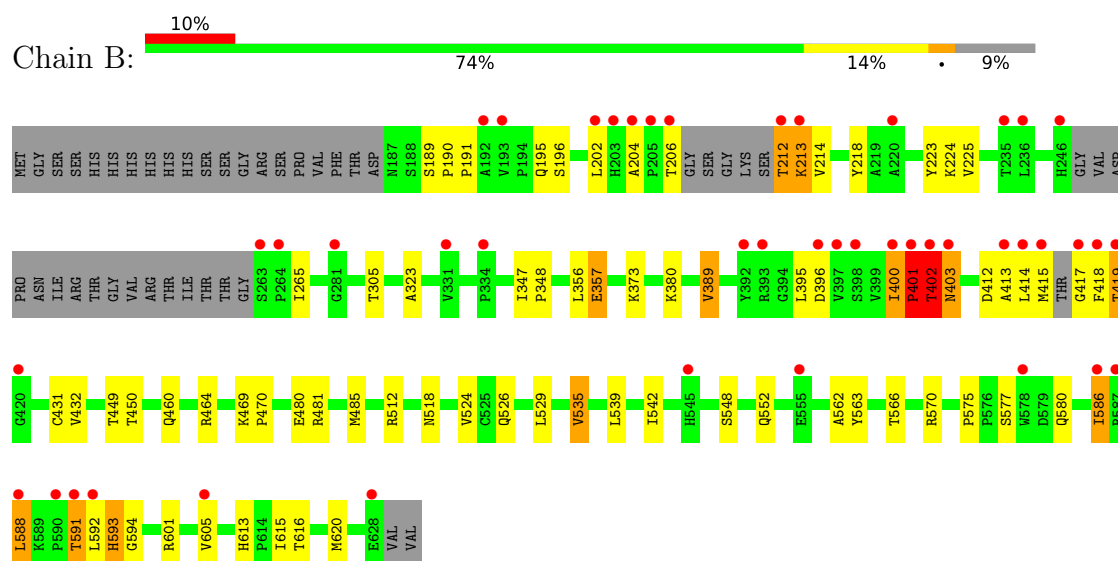
3 Residue-property plots [i](#)

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: 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	82.14Å 103.53Å 119.31Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.10 – 2.25 39.10 – 2.25	Depositor EDS
% Data completeness (in resolution range)	99.2 (39.10-2.25) 96.9 (39.10-2.25)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.34 (at 2.24Å)	Xtriage
Refinement program	PHENIX 1.8.4_1496	Depositor
R, R_{free}	0.217 , 0.270 0.221 , 0.271	Depositor DCC
R_{free} test set	2458 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	50.2	Xtriage
Anisotropy	0.398	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 42.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.52$, $\langle L^2 \rangle = 0.36$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6714	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.22% 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: CA, 2SX

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	0.58	1/3416 (0.0%)	0.94	8/4666 (0.2%)
1	B	0.57	1/3253 (0.0%)	0.93	6/4441 (0.1%)
All	All	0.58	2/6669 (0.0%)	0.94	14/9107 (0.2%)

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	2
1	B	0	1
All	All	0	3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	535	VAL	CA-CB	6.37	1.62	1.54
1	B	402	THR	CA-CB	5.77	1.63	1.53

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	400	ILE	CA-C-N	9.86	132.16	119.84
1	B	400	ILE	C-N-CA	9.86	132.16	119.84
1	A	399	VAL	N-CA-C	6.77	118.06	108.17
1	B	403	ASN	N-CA-C	-6.13	107.02	114.75
1	A	549	GLN	N-CA-C	-5.87	106.04	113.43
1	B	189	SER	CA-C-N	5.66	126.21	120.38
1	B	189	SER	C-N-CA	5.66	126.21	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	364	HIS	N-CA-C	5.56	118.26	108.75
1	A	594	GLY	CA-C-N	5.55	125.48	119.76
1	A	594	GLY	C-N-CA	5.55	125.48	119.76
1	A	400	ILE	N-CA-C	5.18	120.06	108.88
1	A	588	LEU	CA-CB-CG	5.14	134.31	116.30
1	A	415	MET	N-CA-C	5.13	116.78	109.14
1	B	396	ASP	N-CA-C	5.03	119.11	112.92

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	397	VAL	Peptide
1	A	399	VAL	Peptide
1	B	401	PRO	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	3337	0	3292	57	1
1	B	3176	0	3127	49	1
2	A	14	0	7	0	0
3	B	2	0	0	0	0
4	A	85	0	0	1	0
4	B	100	0	0	3	0
All	All	6714	0	6426	104	1

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 8.

All (104) 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:363:ARG:HG3	1:A:422:PHE:HA	1.55	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:402:THR:HG22	1:B:403:ASN:H	1.42	0.84
1:A:397:VAL:HG21	1:A:418:PHE:HE2	1.46	0.81
1:A:399:VAL:HG12	1:A:400:ILE:HB	1.68	0.75
1:B:417:GLY:N	4:B:1199:HOH:O	2.20	0.74
1:B:616:THR:HG22	1:B:620:MET:HE2	1.68	0.73
1:B:460:GLN:HE21	1:B:464:ARG:HH11	1.36	0.72
1:A:397:VAL:HG21	1:A:418:PHE:CE2	2.22	0.72
1:B:402:THR:CG2	1:B:403:ASN:H	2.03	0.72
1:A:381:LEU:HA	1:A:384:LEU:HB2	1.72	0.71
1:A:392:TYR:O	1:A:395:LEU:N	2.25	0.69
1:A:396:ASP:OD1	1:A:397:VAL:N	2.22	0.69
1:A:364:HIS:HB2	1:A:407:VAL:HG22	1.80	0.64
1:A:363:ARG:CZ	1:A:400:ILE:HD11	2.29	0.63
1:A:616:THR:HG22	1:A:620:MET:HE2	1.79	0.63
1:A:366:ILE:HG12	1:A:426:ILE:HB	1.81	0.62
1:B:389:VAL:HG21	1:B:400:ILE:HD13	1.81	0.61
1:A:411:THR:HG23	1:A:413:ALA:H	1.65	0.60
1:A:587:ARG:O	1:A:590:PRO:HD2	2.02	0.60
1:A:206:THR:HG23	1:A:323:ALA:HB2	1.84	0.59
1:A:481:ARG:HD3	1:B:485:MET:SD	2.43	0.59
1:A:363:ARG:NE	1:A:400:ILE:HD11	2.19	0.58
1:A:587:ARG:O	1:A:587:ARG:HG2	2.02	0.57
1:A:552:GLN:H	1:A:552:GLN:CD	2.13	0.57
1:B:348:PRO:HD2	1:B:380:LYS:HE2	1.86	0.57
1:B:460:GLN:NE2	1:B:464:ARG:HH11	2.02	0.56
1:B:347:ILE:HD11	1:B:356:LEU:HD13	1.88	0.56
1:A:381:LEU:HD13	1:A:386:ILE:HB	1.88	0.55
1:B:402:THR:CG2	1:B:403:ASN:N	2.69	0.55
1:B:432:VAL:HG22	1:B:450:THR:HG22	1.89	0.55
1:A:381:LEU:HB2	1:A:386:ILE:HD13	1.88	0.54
1:A:239:GLY:HA3	1:A:252:ILE:HD11	1.90	0.54
1:A:363:ARG:NH2	1:A:421:ASP:OD2	2.42	0.53
1:A:209:GLY:HA2	4:A:866:HOH:O	2.09	0.52
1:B:592:LEU:O	1:B:594:GLY:N	2.43	0.52
1:A:364:HIS:HD2	1:A:424:SER:OG	1.93	0.51
1:A:426:ILE:HG12	1:A:474:ARG:HB2	1.92	0.51
1:B:413:ALA:O	1:B:414:LEU:HB3	2.10	0.51
1:B:213:LYS:H	1:B:213:LYS:HD3	1.74	0.51
1:A:598:LEU:HD22	1:A:609:VAL:HG11	1.92	0.51
1:B:418:PHE:CG	1:B:419:THR:N	2.79	0.51
1:B:601:ARG:HH21	1:B:605:VAL:HB	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:517:MET:HE3	1:A:529:LEU:HD21	1.92	0.51
1:A:583:LYS:O	1:A:586:ILE:HG12	2.11	0.50
1:A:441:ASP:O	1:A:601:ARG:NH1	2.42	0.50
1:A:613:HIS:HE1	1:A:615:ILE:HD12	1.75	0.50
1:B:202:LEU:HD21	1:B:214:VAL:HG21	1.95	0.49
1:A:592:LEU:O	1:A:594:GLY:N	2.46	0.48
1:B:548:SER:O	1:B:552:GLN:HG3	2.14	0.48
1:A:400:ILE:HG21	1:A:419:THR:HG21	1.96	0.48
1:B:575:PRO:HB2	1:B:577:SER:O	2.14	0.47
1:A:411:THR:OG1	1:A:412:ASP:N	2.46	0.47
1:A:462:ARG:HG3	1:A:473:TYR:CG	2.50	0.47
1:A:613:HIS:CE1	1:A:615:ILE:HD12	2.50	0.46
1:A:236:LEU:HD23	1:A:252:ILE:HG21	1.96	0.46
1:A:379:ALA:HA	1:A:382:VAL:HG13	1.96	0.46
1:B:566:THR:O	1:B:570:ARG:HG3	2.16	0.46
1:A:464:ARG:HA	1:A:467:ARG:HH11	1.81	0.46
1:B:400:ILE:HA	1:B:401:PRO:HD2	1.45	0.46
1:A:213:LYS:HB2	1:A:213:LYS:HE3	1.55	0.45
1:A:330:THR:HG23	1:A:480:GLU:OE1	2.15	0.45
1:B:485:MET:HG3	1:B:524:VAL:HG23	1.96	0.45
1:A:206:THR:HG22	1:A:210:LYS:NZ	2.31	0.45
1:A:386:ILE:O	1:A:387:ASN:HB3	2.17	0.45
1:B:204:ALA:O	1:B:323:ALA:HA	2.17	0.45
1:B:373:LYS:NZ	4:B:1112:HOH:O	2.50	0.45
1:A:450:THR:O	1:B:526:GLN:NE2	2.47	0.45
1:A:347:ILE:HD12	1:A:354:ILE:O	2.17	0.44
1:B:542:ILE:HD11	1:B:562:ALA:HB3	1.99	0.44
1:B:591:THR:C	1:B:593:HIS:H	2.25	0.44
1:B:212:THR:OG1	1:B:213:LYS:N	2.49	0.44
1:A:427:ASP:OD2	1:A:473:TYR:OH	2.35	0.44
1:B:431:CYS:O	1:B:450:THR:HA	2.18	0.44
1:B:591:THR:O	1:B:593:HIS:N	2.50	0.44
1:B:412:ASP:O	1:B:415:MET:HE2	2.18	0.43
1:B:357:GLU:H	1:B:357:GLU:HG3	1.43	0.43
1:B:535:VAL:O	1:B:539:LEU:HG	2.18	0.43
1:A:519:THR:HA	1:A:520:PRO:HD3	1.85	0.43
1:A:552:GLN:CD	1:A:552:GLN:N	2.75	0.43
1:B:616:THR:O	1:B:620:MET:HG3	2.19	0.43
1:A:616:THR:HG22	1:A:620:MET:CE	2.47	0.43
1:A:458:ARG:NH2	1:A:477:ALA:O	2.51	0.43
1:B:518:ASN:ND2	4:B:1110:HOH:O	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:ALA:HA	1:A:409:VAL:O	2.19	0.42
1:B:563:TYR:HE2	1:B:615:ILE:HD13	1.83	0.42
1:A:366:ILE:O	1:A:409:VAL:HA	2.20	0.42
1:A:574:PRO:HG3	1:A:592:LEU:HA	2.01	0.42
1:B:469:LYS:HG2	1:B:470:PRO:N	2.34	0.42
1:B:613:HIS:CE1	1:B:615:ILE:HD12	2.54	0.42
1:B:380:LYS:HB3	1:B:380:LYS:HE3	1.77	0.42
1:B:591:THR:C	1:B:593:HIS:N	2.78	0.42
1:B:218:TYR:O	1:B:223:TYR:HB2	2.19	0.42
1:B:305:THR:OG1	1:B:512:ARG:HD3	2.20	0.42
1:A:469:LYS:HB3	1:A:469:LYS:HE3	1.67	0.42
1:B:415:MET:HG2	1:B:464:ARG:HH12	1.85	0.41
1:B:480:GLU:H	1:B:480:GLU:HG2	1.68	0.41
1:B:190:PRO:HA	1:B:191:PRO:HD3	1.83	0.41
1:A:187:ASN:HB3	1:A:189:SER:O	2.21	0.41
1:B:415:MET:HG2	1:B:464:ARG:NH1	2.36	0.41
1:A:369:HIS:CD2	1:A:370:SER:HB3	2.56	0.41
1:A:516:TYR:OH	1:A:523:PRO:HD2	2.22	0.40
1:B:225:VAL:HG22	1:B:265:ILE:HG12	2.03	0.40
1:B:586:ILE:O	1:B:588:LEU:N	2.54	0.40
1:A:210:LYS:NZ	1:A:290:ASP:OD1	2.42	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:257:ARG:NH1	1:B:195:GLN:O[3_545]	2.19	0.01

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	438/464 (94%)	412 (94%)	23 (5%)	3 (1%)	18	17
1	B	413/464 (89%)	388 (94%)	21 (5%)	4 (1%)	12	10
All	All	851/928 (92%)	800 (94%)	44 (5%)	7 (1%)	16	14

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	587	ARG
1	B	213	LYS
1	B	401	PRO
1	B	419	THR
1	B	593	HIS
1	A	593	HIS
1	A	400	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	366/382 (96%)	345 (94%)	21 (6%)	18	19
1	B	346/382 (91%)	330 (95%)	16 (5%)	24	28
All	All	712/764 (93%)	675 (95%)	37 (5%)	21	22

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

Mol	Chain	Res	Type
1	A	195	GLN
1	A	206	THR
1	A	210	LYS
1	A	211	SER
1	A	213	LYS
1	A	225	VAL
1	A	346	GLU
1	A	357	GLU
1	A	358	VAL

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Mol	Chain	Res	Type
1	A	360	LYS
1	A	371	LYS
1	A	372	LYS
1	A	373	LYS
1	A	382	VAL
1	A	397	VAL
1	A	399	VAL
1	A	409	VAL
1	A	460	GLN
1	A	524	VAL
1	A	535	VAL
1	A	583	LYS
1	B	196	SER
1	B	206	THR
1	B	212	THR
1	B	224	LYS
1	B	357	GLU
1	B	389	VAL
1	B	395	LEU
1	B	402	THR
1	B	449	THR
1	B	481	ARG
1	B	529	LEU
1	B	535	VAL
1	B	580	GLN
1	B	586	ILE
1	B	588	LEU
1	B	591	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	ASN
1	A	364	HIS
1	A	526	GLN
1	B	198	GLN
1	B	229	ASN
1	B	403	ASN
1	B	460	GLN
1	B	541	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 ⓘ

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	2SX	A	701	-	15,15,15	0.75	0	21,21,21	1.44	3 (14%)

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	2SX	A	701	-	-	4/4/4/4	0/2/2/2

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	2SX	C3-C6-C5	-3.52	118.78	122.19
2	A	701	2SX	BR1-C1-C2	2.48	122.68	119.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	701	2SX	C3-C6-N7	2.26	134.36	130.74

There are no chirality outliers.

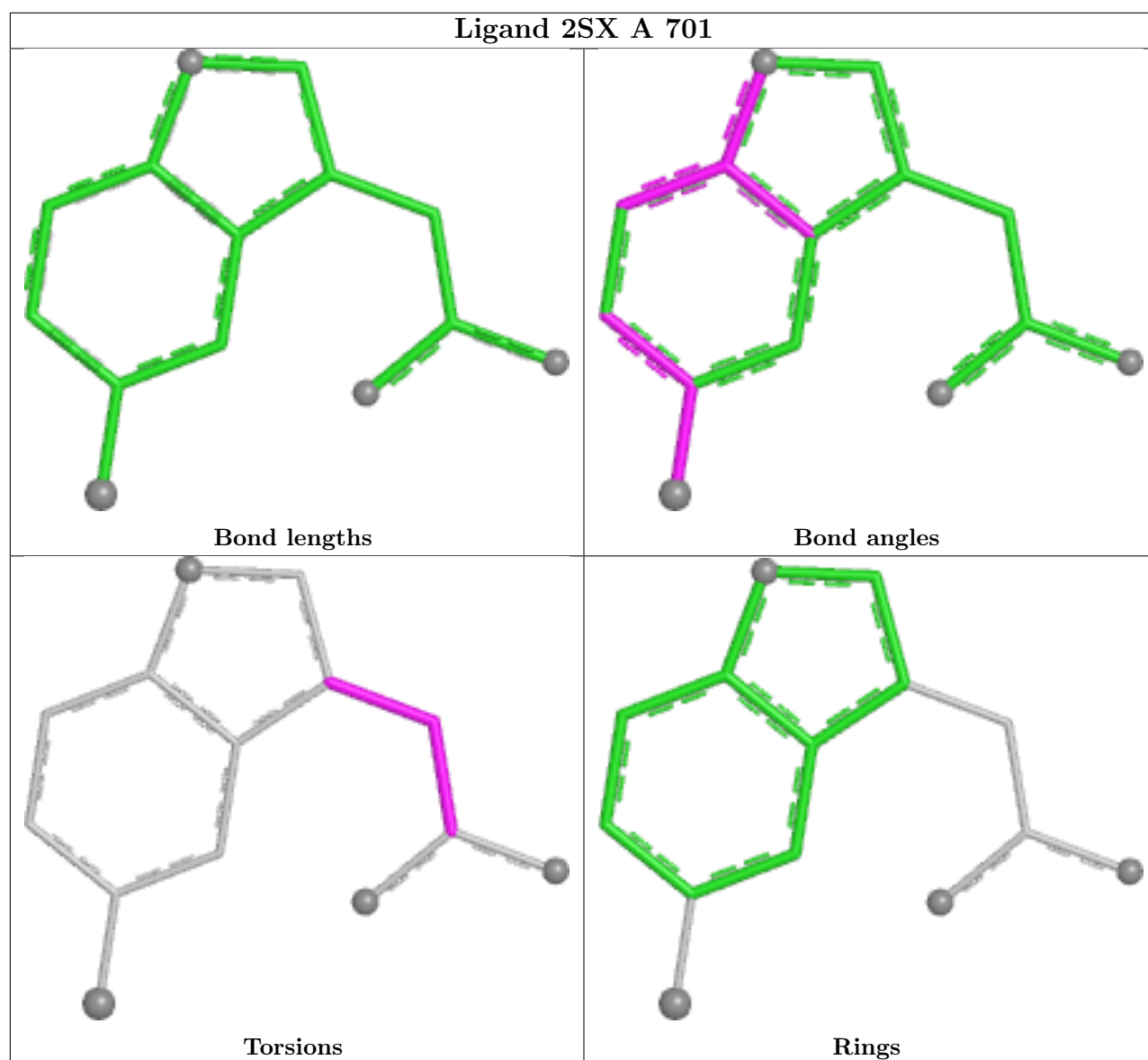
All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	701	2SX	C12-C11-C9-C5
2	A	701	2SX	C9-C11-C12-O13
2	A	701	2SX	C12-C11-C9-C8
2	A	701	2SX	C9-C11-C12-O14

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	440/464 (94%)	0.94	78 (17%) 4 3	24, 59, 98, 114	4 (0%)
1	B	420/464 (90%)	0.76	45 (10%) 11 10	25, 58, 94, 110	1 (0%)
All	All	860/928 (92%)	0.85	123 (14%) 6 5	24, 59, 97, 114	5 (0%)

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	420	GLY	5.9
1	B	592	LEU	5.8
1	A	592	LEU	5.0
1	A	382	VAL	5.0
1	A	418	PHE	4.6
1	B	401	PRO	4.5
1	A	401	PRO	4.2
1	B	236	LEU	4.2
1	B	402	THR	4.2
1	A	390	ALA	4.1
1	B	220	ALA	3.9
1	B	397	VAL	3.8
1	B	204	ALA	3.7
1	A	397	VAL	3.7
1	A	416	THR	3.6
1	B	628	GLU	3.6
1	A	391	TYR	3.6
1	B	588	LEU	3.6
1	A	593	HIS	3.5
1	B	281	GLY	3.4
1	B	591	THR	3.4
1	A	381	LEU	3.3
1	A	419	THR	3.3
1	A	392	TYR	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	386	ILE	3.2
1	A	358	VAL	3.2
1	A	406	VAL	3.2
1	B	212	THR	3.2
1	A	389	VAL	3.1
1	A	380	LYS	3.1
1	B	263	SER	3.1
1	B	264	PRO	3.1
1	A	354	ILE	3.0
1	B	206	THR	3.0
1	A	399	VAL	3.0
1	A	363	ARG	3.0
1	B	590	PRO	3.0
1	A	426	ILE	2.9
1	B	417	GLY	2.9
1	A	485[A]	MET	2.9
1	A	383	ALA	2.9
1	A	206	THR	2.9
1	A	282	GLY	2.8
1	A	629	VAL	2.8
1	B	419	THR	2.8
1	B	555	GLU	2.8
1	A	186	ASP	2.8
1	A	630	VAL	2.8
1	A	347	ILE	2.8
1	A	400	ILE	2.8
1	A	421	ASP	2.8
1	A	586	ILE	2.7
1	A	415	MET	2.7
1	A	587	ARG	2.7
1	B	331	VAL	2.7
1	A	356	LEU	2.7
1	B	578	TRP	2.7
1	B	413	ALA	2.6
1	A	591	THR	2.6
1	A	395	LEU	2.6
1	B	415	MET	2.6
1	B	586	ILE	2.6
1	A	379	ALA	2.6
1	A	423	ASP	2.5
1	A	187	ASN	2.5
1	A	362	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	360	LYS	2.5
1	A	337	GLU	2.5
1	A	398	SER	2.5
1	A	425	VAL	2.5
1	A	189	SER	2.4
1	A	359	ILE	2.4
1	B	418	PHE	2.4
1	B	403	ASN	2.4
1	A	348	PRO	2.4
1	A	408	VAL	2.4
1	A	422	PHE	2.4
1	A	472	ILE	2.4
1	B	400	ILE	2.4
1	B	605	VAL	2.4
1	B	205	PRO	2.3
1	A	384	LEU	2.3
1	B	545	HIS	2.3
1	A	281	GLY	2.3
1	A	505	MET	2.3
1	B	192	ALA	2.3
1	A	449	THR	2.3
1	A	203	HIS	2.3
1	A	545	HIS	2.3
1	A	409	VAL	2.3
1	B	334	PRO	2.3
1	B	393	ARG	2.3
1	B	587	ARG	2.3
1	A	588	LEU	2.2
1	B	193	VAL	2.3
1	A	334	PRO	2.2
1	A	385	GLY	2.2
1	A	413	ALA	2.2
1	B	398	SER	2.2
1	B	414	LEU	2.2
1	A	464	ARG	2.2
1	A	357	GLU	2.2
1	B	246	HIS	2.2
1	A	207	GLY	2.2
1	A	473	TYR	2.1
1	A	387	ASN	2.1
1	A	190	PRO	2.1
1	A	589	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	396	ASP	2.1
1	A	407	VAL	2.1
1	A	465	THR	2.1
1	B	202	LEU	2.1
1	B	392	TYR	2.1
1	B	203	HIS	2.1
1	A	476	VAL	2.1
1	B	420	GLY	2.1
1	A	373	LYS	2.0
1	A	424	SER	2.0
1	A	466	GLY	2.0
1	B	235	THR	2.0
1	A	202	LEU	2.0
1	A	365	LEU	2.0
1	B	213	LYS	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](#)

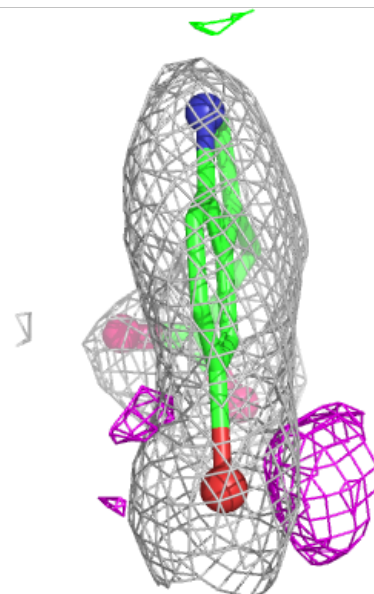
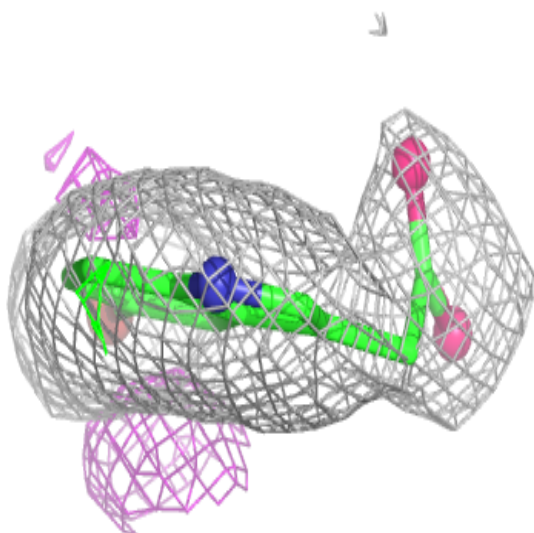
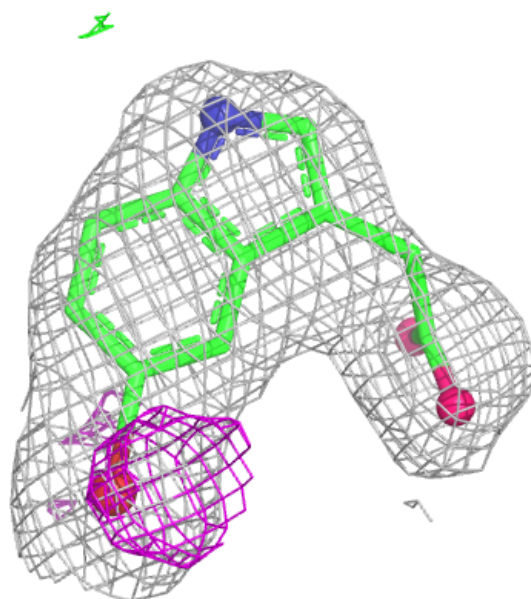
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CA	B	1001	1/1	0.82	0.11	76,76,76,76	0
2	2SX	A	701	14/14	0.89	0.12	55,61,68,115	0
3	CA	B	1002	1/1	0.96	0.06	81,81,81,81	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 2SX 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 ⓘ

There are no such residues in this entry.