



Full wwPDB X-ray Structure Validation Report ⓘ

Sep 24, 2025 – 12:07 PM EDT

PDB ID : 9DU0 / pdb_00009du0
Title : Crystal structure of the bromodomain of human BRM (SMARCA2) in complex with a SMARCA-BD binder
Authors : Wang, M.; Dou, Y.; Xu, C.
Deposited on : 2024-10-02
Resolution : 3.00 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 : 1.1.7 (2018)
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
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) : 2.46

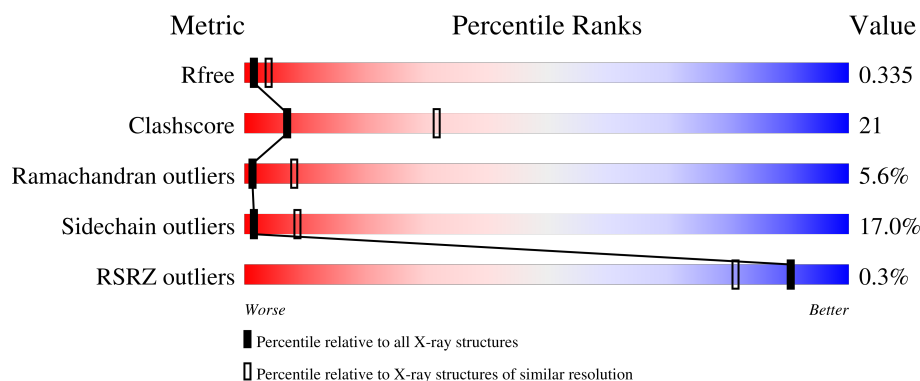
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	164625	2511 (3.00-3.00)
Clashscore	180529	2866 (3.00-3.00)
Ramachandran outliers	177936	2778 (3.00-3.00)
Sidechain outliers	177891	2781 (3.00-3.00)
RSRZ outliers	164620	2523 (3.00-3.00)

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	120	
1	B	120	
1	C	120	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 2890 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.

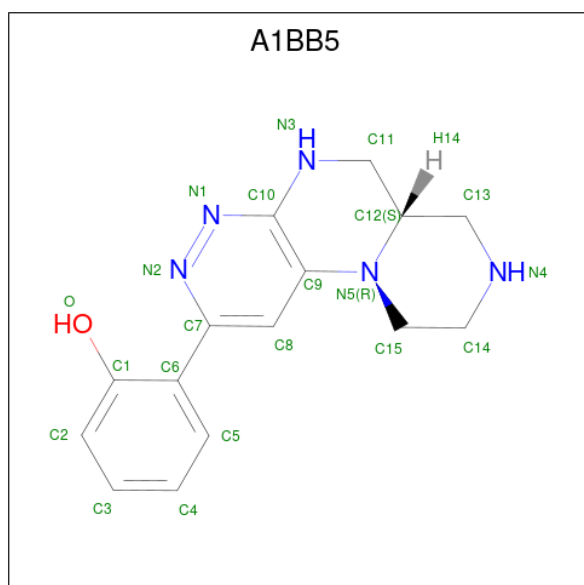
- Molecule 1 is a protein called Isoform Short of Probable global transcription activator SNF2L2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	115	Total	C	N	O	S	0	0	0
			944	601	166	174	3			
1	B	115	Total	C	N	O	S	0	0	0
			944	601	166	174	3			
1	C	115	Total	C	N	O	S	0	0	0
			944	601	166	174	3			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1372	SER	-	expression tag	UNP P51531
B	1372	SER	-	expression tag	UNP P51531
C	1372	SER	-	expression tag	UNP P51531

- Molecule 2 is (2P)-2-[(6aS,11R)-6,6a,7,8,9,10-hexahydro-5H-pyrazino[1',2':4,5]pyrazino[2,3-c]pyridazin-2-yl]phenol (CCD ID: A1BB5) (formula: C₁₅H₁₇N₅O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			21	15	5	1		
2	B	1	Total	C	N	O	0	0
			21	15	5	1		

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	B	1	Total	Zn	0	0
			1	1		
3	C	1	Total	Zn	0	0
			1	1		

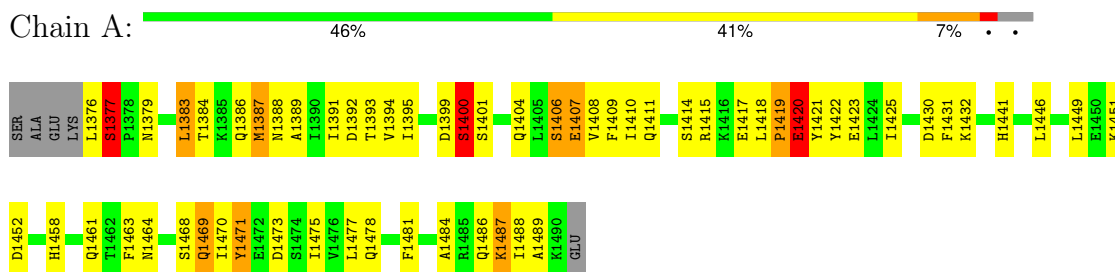
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	6	Total	O	0	0
			6	6		
4	B	2	Total	O	0	0
			2	2		
4	C	5	Total	O	0	0
			5	5		

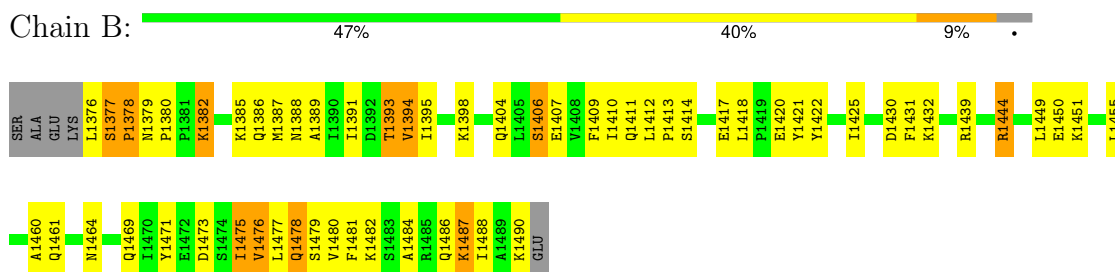
3 Residue-property plots

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.

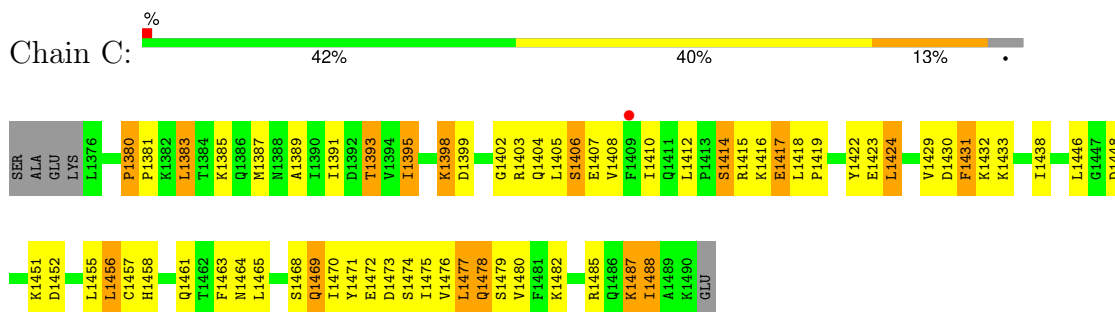
- Molecule 1: Isoform Short of Probable global transcription activator SNF2L2



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4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	64.56Å 64.56Å 89.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	47.40 – 3.00 47.40 – 3.00	Depositor EDS
% Data completeness (in resolution range)	87.5 (47.40-3.00) 87.5 (47.40-3.00)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.58 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.223 , 0.338 0.230 , 0.335	Depositor DCC
R_{free} test set	364 reflections (4.38%)	wwPDB-VP
Wilson B-factor (Å ²)	74.7	Xtriage
Anisotropy	0.004	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 63.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l 0.086 for h,-h-k,-l 0.051 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2890	wwPDB-VP
Average B, all atoms (Å ²)	89.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.02% 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: A1BB5, ZN

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	0.93	0/960	1.47	1/1289 (0.1%)
1	B	0.96	0/960	1.47	0/1289
1	C	1.00	0/960	1.59	1/1289 (0.1%)
All	All	0.96	0/2880	1.51	2/3867 (0.1%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1380	PRO	N-CA-C	5.92	117.93	110.70
1	A	1419	PRO	N-CA-C	-5.63	104.66	113.78

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	944	0	979	41	0
1	B	944	0	979	38	0
1	C	944	0	979	40	0
2	A	21	0	0	2	0
2	B	21	0	0	1	0
3	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	1	0	0	0	0
3	C	1	0	0	0	0
4	A	6	0	0	3	0
4	B	2	0	0	0	0
4	C	5	0	0	0	0
All	All	2890	0	2937	120	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 21.

All (120) 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:1461:GLN:HE22	1:A:1478:GLN:NE2	1.69	0.91
1:A:1441:HIS:NE2	4:A:1601:HOH:O	2.10	0.84
1:C:1380:PRO:HB2	1:C:1381:PRO:HD2	1.61	0.81
1:C:1395:ILE:O	1:C:1406:SER:OG	2.00	0.78
1:B:1461:GLN:NE2	1:B:1478:GLN:HE22	1.81	0.78
1:B:1404:GLN:O	1:B:1407:GLU:HG3	1.82	0.78
1:A:1411:GLN:HA	1:A:1430:ASP:OD2	1.83	0.77
1:B:1413:PRO:O	1:B:1422:TYR:OH	2.01	0.77
1:A:1409:PHE:O	1:A:1430:ASP:HB2	1.87	0.74
1:B:1395:ILE:O	1:B:1406:SER:OG	2.03	0.73
1:B:1379:ASN:OD1	1:B:1444:ARG:NH2	2.22	0.72
1:A:1395:ILE:O	1:A:1404:GLN:NE2	2.22	0.71
1:A:1461:GLN:HE22	1:A:1478:GLN:HE21	1.39	0.70
1:B:1377:SER:HB3	1:B:1378:PRO:HD2	1.72	0.69
1:A:1489:ALA:O	4:A:1602:HOH:O	2.10	0.68
1:C:1414:SER:OG	1:C:1417:GLU:HB2	1.95	0.66
1:C:1419:PRO:O	1:C:1423:GLU:HG3	1.97	0.65
1:A:1421:TYR:CE1	1:A:1425:ILE:HG13	2.32	0.64
1:C:1488:ILE:HG22	1:C:1488:ILE:O	1.97	0.64
1:B:1471:TYR:O	1:B:1475:ILE:HD12	1.98	0.63
1:B:1460:ALA:O	1:B:1464:ASN:ND2	2.21	0.62
1:B:1389:ALA:O	1:B:1393:THR:OG1	2.18	0.61
1:C:1395:ILE:O	1:C:1404:GLN:NE2	2.33	0.61
1:A:1386:GLN:O	1:A:1389:ALA:N	2.35	0.59
1:A:1388:ASN:O	1:A:1392:ASP:OD1	2.20	0.59
1:C:1410:ILE:HA	1:C:1431:PHE:HB2	1.84	0.59
1:B:1376:LEU:O	1:B:1444:ARG:NH1	2.36	0.59
1:B:1376:LEU:O	1:B:1376:LEU:HD12	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1471:TYR:CE1	1:C:1475:ILE:HD11	2.39	0.57
1:B:1377:SER:CB	1:B:1378:PRO:HD2	2.35	0.56
1:C:1477:LEU:O	1:C:1478:GLN:C	2.47	0.56
1:A:1475:ILE:HA	1:A:1478:GLN:NE2	2.20	0.55
1:C:1380:PRO:CB	1:C:1381:PRO:HD2	2.32	0.55
1:C:1395:ILE:HG22	1:C:1404:GLN:HE22	1.72	0.55
1:A:1415:ARG:HA	1:A:1422:TYR:CE2	2.42	0.54
1:B:1414:SER:OG	1:B:1417:GLU:N	2.40	0.54
1:C:1383:LEU:HD12	1:C:1387:MET:HE2	1.89	0.54
1:C:1464:ASN:ND2	1:C:1470:ILE:HG21	2.22	0.54
1:C:1404:GLN:HE21	1:C:1406:SER:CB	2.21	0.53
1:B:1431:PHE:O	1:B:1432:LYS:C	2.51	0.53
1:A:1418:LEU:O	1:A:1419:PRO:C	2.52	0.53
1:C:1389:ALA:O	1:C:1393:THR:OG1	2.26	0.53
1:A:1469:GLN:O	1:A:1473:ASP:OD1	2.27	0.52
1:C:1380:PRO:HB2	1:C:1381:PRO:CD	2.37	0.52
1:B:1481:PHE:C	1:B:1481:PHE:CD1	2.87	0.52
1:A:1451:LYS:HD3	1:A:1452:ASP:N	2.25	0.52
1:B:1461:GLN:HE22	1:B:1478:GLN:HE22	1.58	0.52
1:B:1421:TYR:CE1	1:B:1425:ILE:HG13	2.44	0.52
1:B:1409:PHE:O	1:B:1430:ASP:HB2	2.11	0.51
1:A:1487:LYS:HE2	1:A:1488:ILE:HD13	1.91	0.51
1:C:1455:LEU:O	1:C:1456:LEU:C	2.55	0.50
1:A:1399:ASP:O	1:A:1400:SER:C	2.54	0.49
1:B:1487:LYS:HG3	1:B:1488:ILE:HG13	1.93	0.49
1:C:1477:LEU:O	1:C:1480:VAL:N	2.46	0.49
1:B:1475:ILE:O	1:B:1478:GLN:HB2	2.12	0.49
1:C:1455:LEU:O	1:C:1458:HIS:HB3	2.13	0.49
1:C:1418:LEU:HD21	1:C:1463:PHE:CZ	2.48	0.48
1:A:1484:ALA:O	1:A:1487:LYS:HB3	2.13	0.48
1:C:1461:GLN:NE2	1:C:1474:SER:OG	2.46	0.48
1:C:1429:VAL:HG11	1:C:1455:LEU:HD23	1.96	0.48
1:A:1410:ILE:HA	1:A:1431:PHE:HB2	1.96	0.47
1:C:1395:ILE:HD13	1:C:1431:PHE:CD2	2.48	0.47
1:A:1446:LEU:O	1:A:1449:LEU:HB3	2.14	0.47
1:A:1414:SER:OG	1:A:1417:GLU:HB3	2.14	0.47
1:C:1412:LEU:HD12	1:C:1430:ASP:CG	2.39	0.47
1:A:1376:LEU:O	1:A:1377:SER:HB3	2.14	0.47
1:A:1458:HIS:CE1	4:A:1605:HOH:O	2.67	0.47
1:A:1475:ILE:HA	1:A:1478:GLN:HE21	1.79	0.47
1:A:1414:SER:OG	1:A:1417:GLU:CB	2.63	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1452:ASP:O	1:C:1455:LEU:HB3	2.14	0.46
1:C:1487:LYS:C	1:C:1487:LYS:HD2	2.40	0.46
1:B:1482:LYS:O	1:B:1486:GLN:HB2	2.15	0.46
1:A:1463:PHE:HD2	1:A:1464:ASN:ND2	2.13	0.46
1:B:1380:PRO:CB	1:B:1382:LYS:HE2	2.46	0.45
1:A:1399:ASP:O	1:A:1399:ASP:OD1	2.35	0.45
1:B:1377:SER:O	1:B:1378:PRO:C	2.59	0.45
1:B:1484:ALA:HA	1:B:1487:LYS:HE2	1.97	0.45
1:C:1380:PRO:HD2	1:C:1383:LEU:HD23	1.97	0.45
1:B:1477:LEU:O	1:B:1478:GLN:C	2.59	0.45
1:C:1403:ARG:CZ	1:C:1405:LEU:CD2	2.94	0.45
1:B:1412:LEU:HG	1:B:1430:ASP:HB3	1.98	0.45
1:A:1386:GLN:O	1:A:1387:MET:C	2.60	0.45
1:A:1451:LYS:HD3	1:A:1451:LYS:C	2.42	0.44
1:B:1380:PRO:HB3	1:B:1382:LYS:HE2	1.99	0.44
1:C:1446:LEU:HD13	1:C:1485:ARG:HG3	2.00	0.44
1:B:1461:GLN:HE21	1:B:1478:GLN:HE22	1.63	0.44
1:A:1477:LEU:O	1:A:1478:GLN:C	2.60	0.44
1:C:1403:ARG:NH1	1:C:1469:GLN:OE1	2.51	0.44
1:C:1404:GLN:HE21	1:C:1406:SER:HB2	1.82	0.44
1:C:1479:SER:O	1:C:1482:LYS:HB2	2.18	0.43
1:B:1409:PHE:HA	2:B:1501:A1BB5:C4	2.49	0.43
1:C:1475:ILE:O	1:C:1476:VAL:C	2.61	0.43
1:A:1468:SER:O	1:A:1469:GLN:C	2.61	0.43
1:A:1395:ILE:O	1:A:1406:SER:OG	2.27	0.43
1:A:1379:ASN:ND2	1:A:1441:HIS:HB3	2.34	0.42
1:B:1386:GLN:O	1:B:1387:MET:C	2.61	0.42
1:B:1455:LEU:HD12	1:B:1455:LEU:O	2.19	0.42
1:C:1412:LEU:N	1:C:1430:ASP:OD2	2.52	0.42
1:A:1481:PHE:CD1	1:A:1481:PHE:C	2.97	0.42
1:A:1471:TYR:CE1	1:A:1475:ILE:HD11	2.54	0.42
1:B:1418:LEU:HG	1:B:1421:TYR:HB2	2.02	0.42
1:B:1449:LEU:O	1:B:1450:GLU:C	2.62	0.42
1:A:1383:LEU:CD2	1:A:1387:MET:HE3	2.50	0.42
1:B:1476:VAL:O	1:B:1480:VAL:HG23	2.19	0.42
1:A:1420:GLU:O	1:A:1423:GLU:N	2.53	0.42
1:A:1420:GLU:O	1:A:1421:TYR:C	2.63	0.41
1:C:1398:LYS:HB2	1:C:1402:GLY:HA2	2.03	0.41
2:A:1501:A1BB5:O	2:A:1501:A1BB5:N2	2.53	0.41
1:A:1418:LEU:HD23	1:A:1421:TYR:HB2	2.03	0.41
1:C:1446:LEU:HD23	1:C:1446:LEU:HA	1.94	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1409:PHE:HA	2:A:1501:A1BB5:C4	2.51	0.41
1:B:1469:GLN:O	1:B:1473:ASP:OD2	2.39	0.41
1:C:1415:ARG:HA	1:C:1422:TYR:CE2	2.56	0.41
1:B:1394:VAL:O	1:B:1395:ILE:C	2.64	0.41
1:B:1484:ALA:O	1:B:1487:LYS:HG2	2.20	0.41
1:C:1416:LYS:O	1:C:1419:PRO:HD3	2.21	0.41
1:C:1468:SER:O	1:C:1469:GLN:C	2.63	0.41
1:A:1431:PHE:O	1:A:1432:LYS:C	2.64	0.40
1:B:1404:GLN:O	1:B:1407:GLU:CG	2.63	0.40
1:C:1479:SER:O	1:C:1482:LYS:N	2.55	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	113/120 (94%)	88 (78%)	16 (14%)	9 (8%)	1	3
1	B	113/120 (94%)	85 (75%)	23 (20%)	5 (4%)	2	12
1	C	113/120 (94%)	77 (68%)	31 (27%)	5 (4%)	2	12
All	All	339/360 (94%)	250 (74%)	70 (21%)	19 (6%)	1	8

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	1377	SER
1	A	1400	SER
1	C	1407	GLU
1	A	1420	GLU
1	A	1470	ILE
1	C	1399	ASP
1	C	1424	LEU

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Mol	Chain	Res	Type
1	C	1469	GLN
1	A	1387	MET
1	A	1407	GLU
1	A	1469	GLN
1	B	1378	PRO
1	B	1394	VAL
1	C	1478	GLN
1	A	1394	VAL
1	B	1388	ASN
1	B	1410	ILE
1	A	1471	TYR
1	B	1475	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	108/112 (96%)	95 (88%)	13 (12%)	4	18
1	B	108/112 (96%)	91 (84%)	17 (16%)	2	10
1	C	108/112 (96%)	83 (77%)	25 (23%)	0	3
All	All	324/336 (96%)	269 (83%)	55 (17%)	1	9

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1377	SER
1	A	1383	LEU
1	A	1384	THR
1	A	1391	ILE
1	A	1393	THR
1	A	1400	SER
1	A	1401	SER
1	A	1406	SER
1	A	1407	GLU
1	A	1408	VAL

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Mol	Chain	Res	Type
1	A	1420	GLU
1	A	1486	GLN
1	A	1487	LYS
1	B	1377	SER
1	B	1382	LYS
1	B	1385	LYS
1	B	1391	ILE
1	B	1393	THR
1	B	1398	LYS
1	B	1406	SER
1	B	1411	GLN
1	B	1420	GLU
1	B	1439	ARG
1	B	1444	ARG
1	B	1451	LYS
1	B	1476	VAL
1	B	1478	GLN
1	B	1479	SER
1	B	1487	LYS
1	B	1490	LYS
1	C	1383	LEU
1	C	1385	LYS
1	C	1391	ILE
1	C	1393	THR
1	C	1395	ILE
1	C	1398	LYS
1	C	1406	SER
1	C	1408	VAL
1	C	1414	SER
1	C	1417	GLU
1	C	1424	LEU
1	C	1431	PHE
1	C	1432	LYS
1	C	1433	LYS
1	C	1438	ILE
1	C	1448	ASP
1	C	1451	LYS
1	C	1456	LEU
1	C	1457	CYS
1	C	1465	LEU
1	C	1472	GLU
1	C	1473	ASP

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Mol	Chain	Res	Type
1	C	1477	LEU
1	C	1487	LYS
1	C	1488	ILE

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	1411	GLN
1	A	1464	ASN
1	A	1478	GLN
1	B	1386	GLN
1	B	1461	GLN
1	B	1478	GLN
1	B	1486	GLN
1	C	1386	GLN
1	C	1404	GLN
1	C	1461	GLN
1	C	1464	ASN

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 5 ligands modelled in this entry, 3 are monoatomic - leaving 2 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	A1BB5	B	1501	-	23,24,24	1.10	2 (8%)	22,34,34	2.07	6 (27%)
2	A1BB5	A	1501	-	23,24,24	0.87	1 (4%)	22,34,34	1.76	3 (13%)

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	A1BB5	B	1501	-	-	0/4/24/24	0/4/4/4
2	A1BB5	A	1501	-	-	0/4/24/24	0/4/4/4

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1501	A1BB5	N2-N1	-2.38	1.28	1.34
2	A	1501	A1BB5	N2-N1	-2.29	1.28	1.34
2	B	1501	A1BB5	C13-C12	2.13	1.54	1.52

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1501	A1BB5	C8-C7-N2	-6.17	116.99	121.61
2	A	1501	A1BB5	C15-N5-C12	-6.10	107.15	115.20
2	B	1501	A1BB5	C15-N5-C12	-3.88	110.09	115.20
2	B	1501	A1BB5	C8-C9-C10	-3.33	115.83	119.63
2	A	1501	A1BB5	C8-C9-C10	-3.06	116.14	119.63
2	B	1501	A1BB5	C7-N2-N1	2.81	124.16	119.93
2	A	1501	A1BB5	C8-C7-N2	-2.73	119.56	121.61
2	B	1501	A1BB5	C8-C9-N5	2.31	125.49	120.74
2	B	1501	A1BB5	C8-C7-C6	2.04	125.84	121.98

There are no chirality outliers.

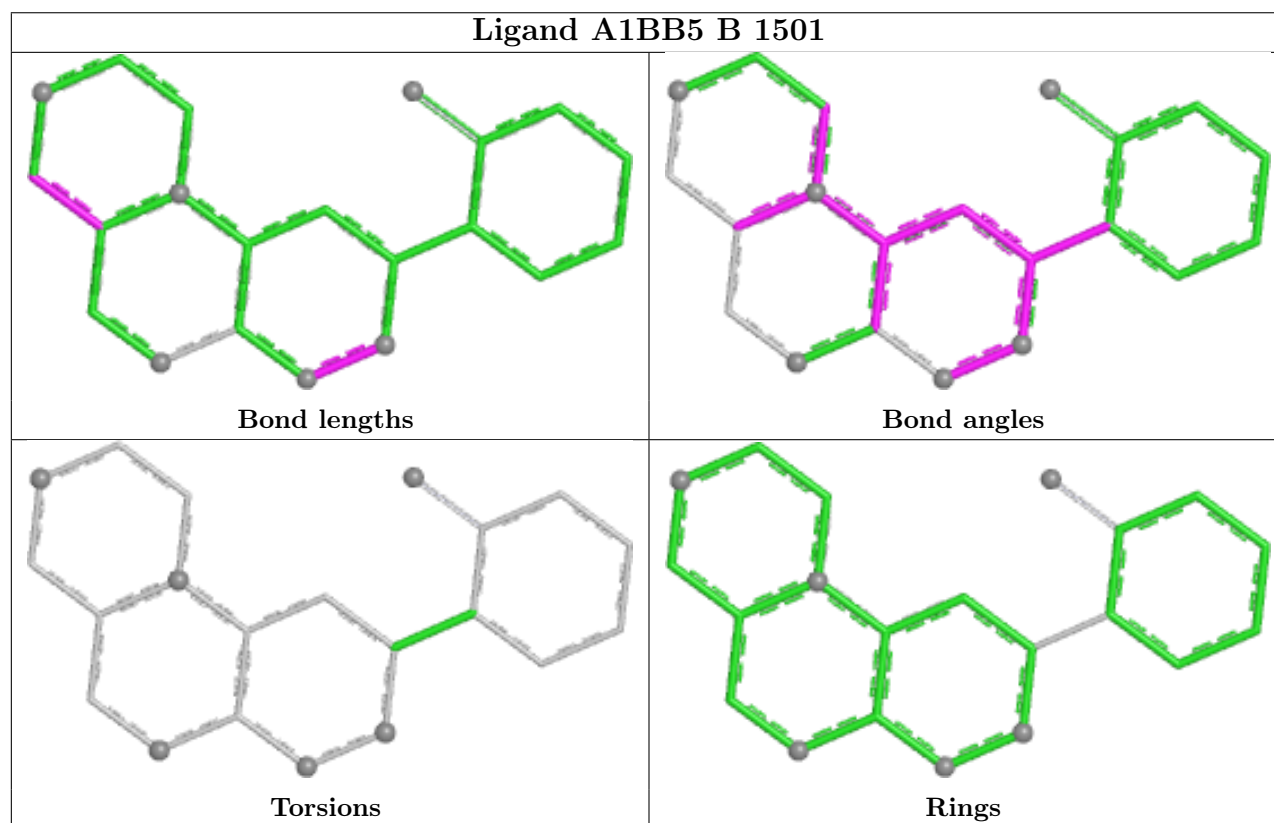
There are no torsion outliers.

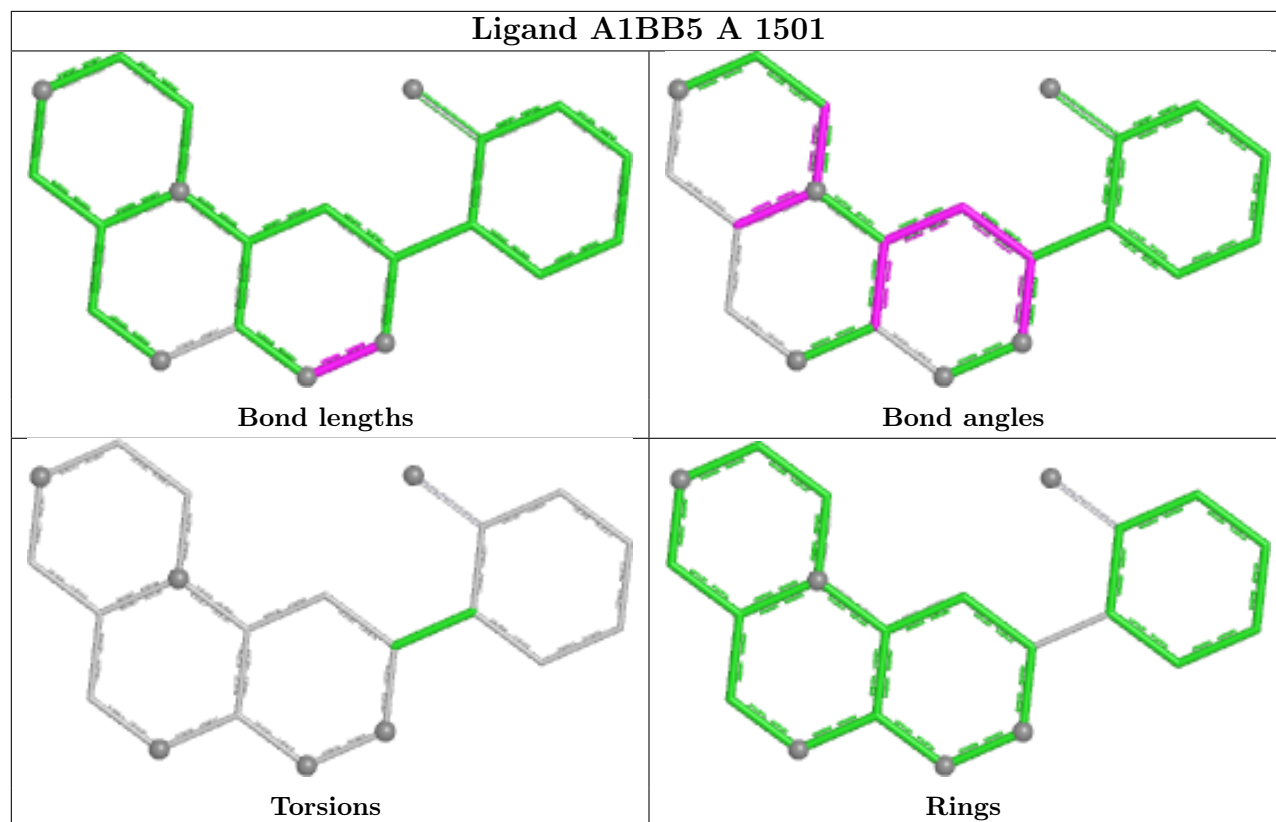
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1501	A1BB5	1	0
2	A	1501	A1BB5	2	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	115/120 (95%)	-0.68	0	100 100	47, 69, 100, 110	0
1	B	115/120 (95%)	-0.61	0	100 100	52, 78, 107, 144	0
1	C	115/120 (95%)	-0.37	1 (0%)	81 63	72, 112, 151, 169	0
All	All	345/360 (95%)	-0.55	1 (0%)	90 81	47, 84, 136, 169	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	1409	PHE	2.3

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	A1BB5	B	1501	21/21	0.92	0.07	88,91,94,96	0
2	A1BB5	A	1501	21/21	0.93	0.07	62,67,77,80	0

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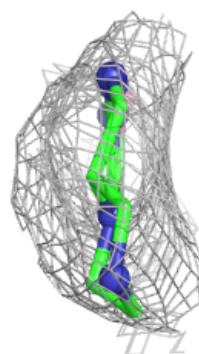
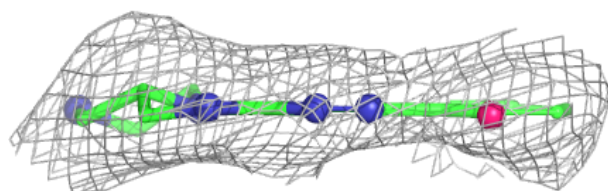
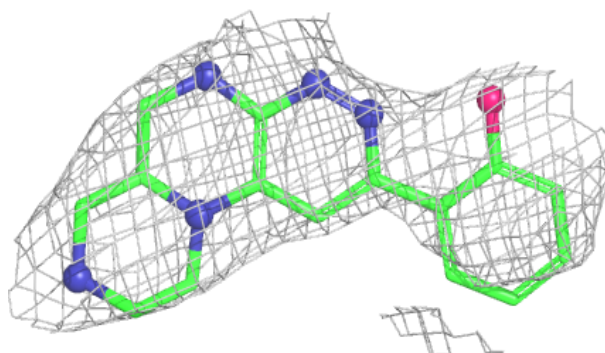
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	ZN	C	1501	1/1	0.95	0.07	120,120,120,120	0
3	ZN	A	1502	1/1	0.99	0.02	75,75,75,75	0
3	ZN	B	1502	1/1	1.00	0.04	74,74,74,74	0

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.

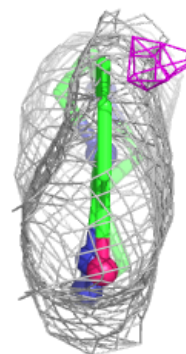
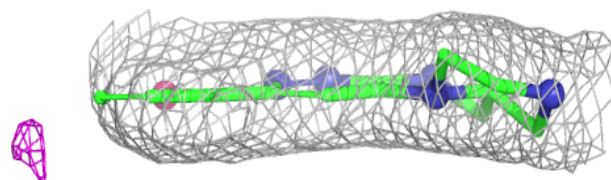
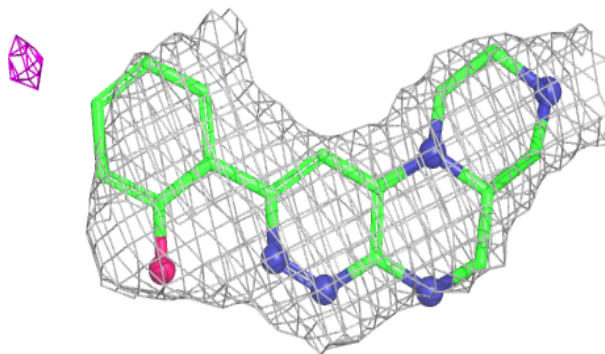
Electron density around A1BB5 B 1501:

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 A1BB5 A 1501:

$2mF_o-DF_c$ (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.