



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2026 – 11:57 PM UTC

PDB ID : 9N3Q / pdb_00009n3q
Title : Crystal structure of PRMT5:MEP50 in complex with MTA and oxamide compound 51
Authors : Whittington, D.A.
Deposited on : 2025-01-31
Resolution : 2.54 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

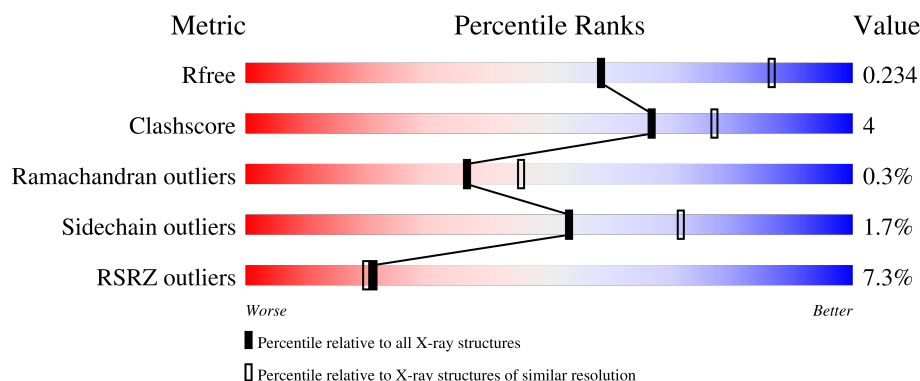
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.54 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	1091 (2.54-2.54)
Clashscore	190562	1120 (2.54-2.54)
Ramachandran outliers	187476	1106 (2.54-2.54)
Sidechain outliers	187428	1106 (2.54-2.54)
RSRZ outliers	180081	1091 (2.54-2.54)

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	645	6% 88% 9% .
1	C	645	6% 87% 9% .
2	B	350	7% 75% 10% . 15%
2	D	350	9% 73% 11% . 15%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 14850 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 Protein arginine N-methyltransferase 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	625	Total	C	N	O	S	0	0	0
			5061	3237	869	931	24			
1	C	624	Total	C	N	O	S	0	0	0
			5050	3231	865	930	24			

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP O14744
A	-6	ASP	-	expression tag	UNP O14744
A	-5	TYR	-	expression tag	UNP O14744
A	-4	LYS	-	expression tag	UNP O14744
A	-3	ASP	-	expression tag	UNP O14744
A	-2	ASP	-	expression tag	UNP O14744
A	-1	ASP	-	expression tag	UNP O14744
A	0	ASP	-	expression tag	UNP O14744
A	1	LYS	-	expression tag	UNP O14744
C	-7	MET	-	initiating methionine	UNP O14744
C	-6	ASP	-	expression tag	UNP O14744
C	-5	TYR	-	expression tag	UNP O14744
C	-4	LYS	-	expression tag	UNP O14744
C	-3	ASP	-	expression tag	UNP O14744
C	-2	ASP	-	expression tag	UNP O14744
C	-1	ASP	-	expression tag	UNP O14744
C	0	ASP	-	expression tag	UNP O14744
C	1	LYS	-	expression tag	UNP O14744

- Molecule 2 is a protein called Methylosome protein 50.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	299	Total	C	N	O	S	0	0	0
			2270	1426	388	444	12			

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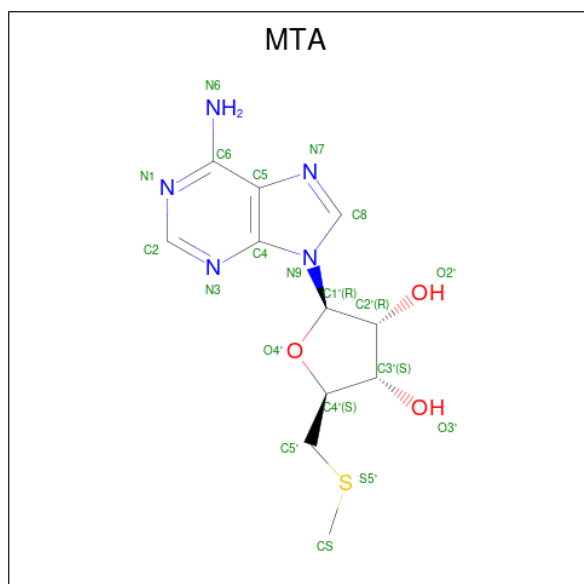
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	299	Total	C	N	O	S	0	0	0
			2270	1426	388	444	12			

There are 18 discrepancies between the modelled and reference sequences:

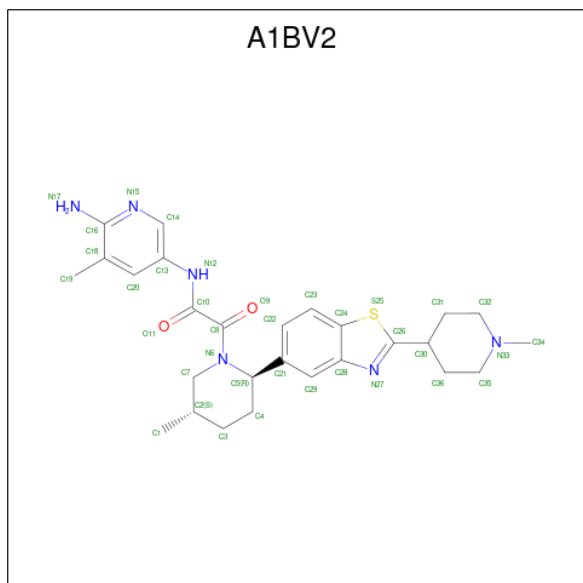
Chain	Residue	Modelled	Actual	Comment	Reference
B	-7	MET	-	initiating methionine	UNP Q9BQA1
B	-6	HIS	-	expression tag	UNP Q9BQA1
B	-5	HIS	-	expression tag	UNP Q9BQA1
B	-4	HIS	-	expression tag	UNP Q9BQA1
B	-3	HIS	-	expression tag	UNP Q9BQA1
B	-2	HIS	-	expression tag	UNP Q9BQA1
B	-1	HIS	-	expression tag	UNP Q9BQA1
B	0	HIS	-	expression tag	UNP Q9BQA1
B	1	HIS	-	expression tag	UNP Q9BQA1
D	-7	MET	-	initiating methionine	UNP Q9BQA1
D	-6	HIS	-	expression tag	UNP Q9BQA1
D	-5	HIS	-	expression tag	UNP Q9BQA1
D	-4	HIS	-	expression tag	UNP Q9BQA1
D	-3	HIS	-	expression tag	UNP Q9BQA1
D	-2	HIS	-	expression tag	UNP Q9BQA1
D	-1	HIS	-	expression tag	UNP Q9BQA1
D	0	HIS	-	expression tag	UNP Q9BQA1
D	1	HIS	-	expression tag	UNP Q9BQA1

- Molecule 3 is 5'-DEOXY-5'-METHYLTHIOADENOSINE (CCD ID: MTA) (formula: $C_{11}H_{15}N_5O_3S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	S	0	0
			20	11	5	3	1		
3	C	1	Total	C	N	O	S	0	0
			20	11	5	3	1		

- Molecule 4 is N-(6-amino-5-methylpyridin-3-yl)-2-[(2R,5S)-5-methyl-2-[2-(1-methylpiperidin-4-yl)-1,3-benzothiazol-5-yl]piperidin-1-yl]-2-oxoacetamide (CCD ID: A1BV2) (formula: C₂₇H₃₄N₆O₂S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	S	0	0
			36	27	6	2	1		
4	C	1	Total	C	N	O	S	0	0
			36	27	6	2	1		

- Molecule 5 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	O	0	0
			4	2	2		

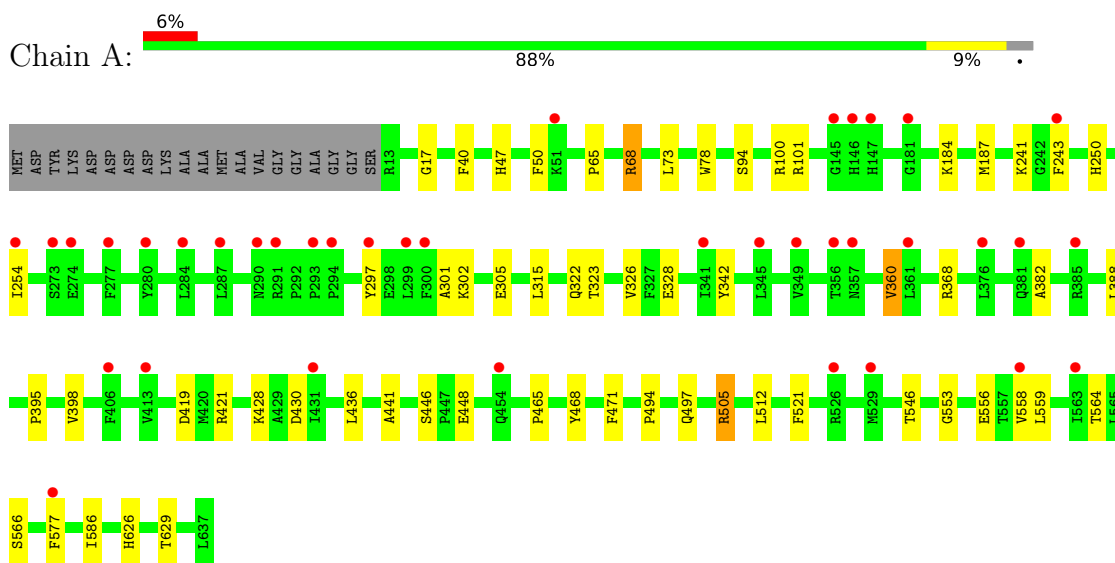
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	36	Total	O	0	0
			36	36		
6	B	2	Total	O	0	0
			2	2		
6	C	42	Total	O	0	0
			42	42		
6	D	3	Total	O	0	0
			3	3		

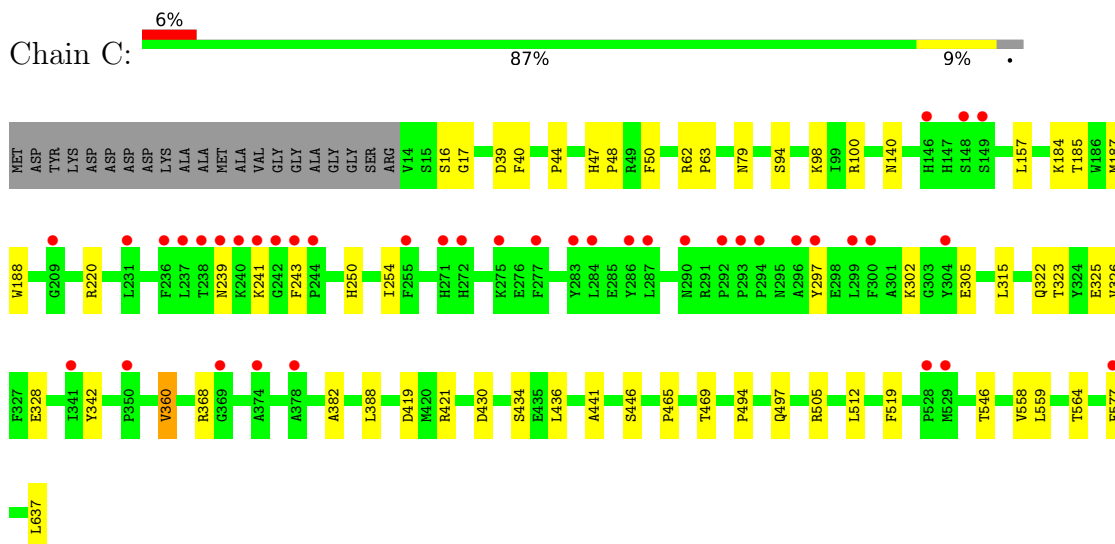
3 Residue-property plots [i](#)

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.

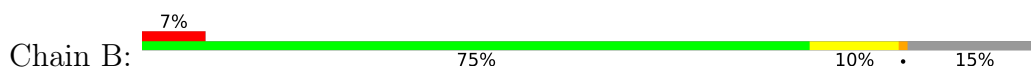
- Molecule 1: Protein arginine N-methyltransferase 5

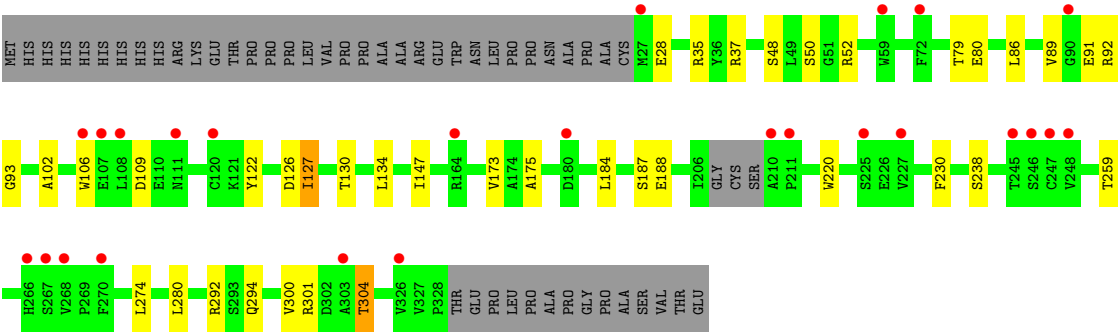


- Molecule 1: Protein arginine N-methyltransferase 5

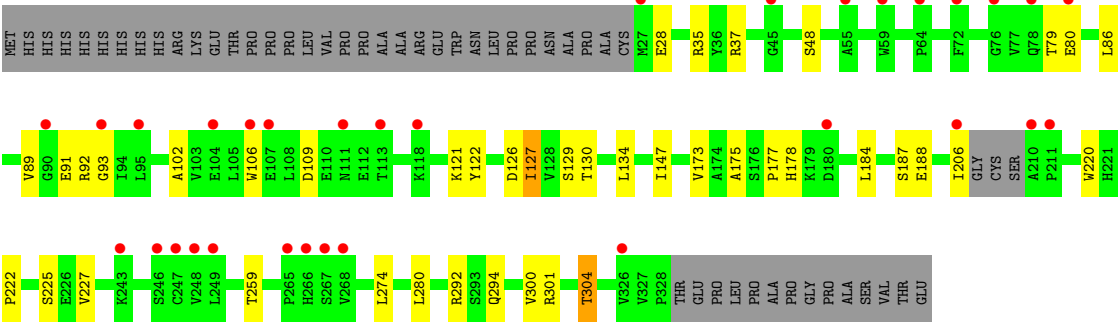


- Molecule 2: Methylosome protein 50





● Molecule 2: Methylosome protein 50



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	97.41Å 136.45Å 178.26Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.71 – 2.54 48.71 – 2.54	Depositor EDS
% Data completeness (in resolution range)	56.5 (48.71-2.54) 56.6 (48.71-2.54)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.26 (at 2.54Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487, REFMAC 5.8.0267	Depositor
R, R_{free}	0.232 , 0.267 (Not available) , 0.234	Depositor DCC
R_{free} test set	2161 reflections (2.72%)	wwPDB-VP
Wilson B-factor (Å ²)	39.1	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 28.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	14850	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 13.15% 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: MTA, A1BV2, EDO

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	0.14	0/5203	0.37	0/7078
1	C	0.14	0/5192	0.37	0/7064
2	B	0.13	0/2323	0.40	0/3171
2	D	0.13	0/2323	0.39	0/3171
All	All	0.13	0/15041	0.38	0/20484

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5061	0	4952	38	0
1	C	5050	0	4939	32	0
2	B	2270	0	2191	20	0
2	D	2270	0	2191	21	0
3	A	20	0	15	1	0
3	C	20	0	15	2	0
4	A	36	0	0	0	0
4	C	36	0	0	0	0
5	C	4	0	6	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	36	0	0	1	0
6	B	2	0	0	0	0
6	C	42	0	0	0	0
6	D	3	0	0	0	0
All	All	14850	0	14309	108	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 4.

All (108) 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:419:ASP:OD1	3:A:701:MTA:N6	2.27	0.68
1:C:360:VAL:HG13	1:C:430:ASP:H	1.58	0.67
2:D:126:ASP:OD1	2:D:127:ILE:N	2.28	0.66
1:A:360:VAL:HG13	1:A:430:ASP:H	1.62	0.65
2:B:126:ASP:OD1	2:B:127:ILE:N	2.29	0.65
2:D:35:ARG:NH1	2:D:86:LEU:O	2.34	0.61
1:A:68:ARG:NH1	2:B:52:ARG:O	2.34	0.60
1:A:297:TYR:HD1	1:A:577:PHE:HB3	1.67	0.58
2:B:35:ARG:NH1	2:B:86:LEU:O	2.35	0.58
1:A:558:VAL:HA	1:A:564:THR:HG22	1.86	0.58
2:D:274:LEU:HD23	2:D:300:VAL:HG12	1.86	0.57
1:C:558:VAL:HA	1:C:564:THR:HG22	1.88	0.56
1:C:360:VAL:HG13	1:C:430:ASP:N	2.20	0.56
1:C:250:HIS:O	1:C:254:ILE:HG12	2.06	0.55
2:B:102:ALA:HB2	2:B:122:TYR:CD1	2.42	0.54
1:C:465:PRO:HA	1:C:559:LEU:HA	1.87	0.54
1:A:360:VAL:HG13	1:A:430:ASP:N	2.23	0.54
2:B:274:LEU:HD23	2:B:300:VAL:HG12	1.88	0.54
2:D:102:ALA:HB2	2:D:122:TYR:CD1	2.42	0.54
2:D:134:LEU:HD23	2:D:175:ALA:HB1	1.90	0.54
1:A:250:HIS:O	1:A:254:ILE:HG12	2.07	0.54
2:B:134:LEU:HD23	2:B:175:ALA:HB1	1.90	0.53
2:D:35:ARG:HA	2:D:304:THR:HG21	1.89	0.53
2:B:35:ARG:HA	2:B:304:THR:HG21	1.91	0.53
1:A:465:PRO:HA	1:A:559:LEU:HA	1.92	0.51
1:C:241:LYS:HB2	1:C:243:PHE:HD1	1.76	0.51
2:B:89:VAL:HB	2:B:93:GLY:HA3	1.92	0.50
1:A:315:LEU:HD11	1:A:421:ARG:NH1	2.26	0.49
1:C:315:LEU:HD11	1:C:421:ARG:NH1	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:PRO:HB3	1:A:559:LEU:HD23	1.94	0.48
1:A:47:HIS:HB3	1:A:50:PHE:HB2	1.95	0.48
2:D:177:PRO:HG2	2:D:178:HIS:CD2	2.48	0.48
1:A:301:ALA:HB1	1:A:505:ARG:HD2	1.95	0.47
1:A:512:LEU:HD22	1:A:546:THR:HG21	1.97	0.47
1:C:421:ARG:NH2	1:C:637:LEU:OXT	2.43	0.47
2:D:130:THR:HG23	2:D:173:VAL:HG22	1.97	0.46
1:A:322:GLN:HE22	1:C:79:ASN:HD21	1.62	0.46
1:A:297:TYR:CD1	1:A:577:PHE:HB3	2.48	0.46
1:A:436:LEU:HB2	1:A:446:SER:HB2	1.97	0.46
1:C:302:LYS:HA	1:C:305:GLU:HG3	1.97	0.46
2:B:187:SER:OG	2:B:188:GLU:N	2.49	0.46
2:D:259:THR:HG21	2:D:301:ARG:NH2	2.31	0.46
1:C:239:ASN:OD1	1:C:243:PHE:HB2	2.16	0.45
2:B:130:THR:HG23	2:B:173:VAL:HG22	1.98	0.45
1:A:65:PRO:O	2:B:50:SER:OG	2.32	0.45
2:D:89:VAL:HB	2:D:93:GLY:HA3	1.97	0.45
2:B:28:GLU:CG	2:B:48:SER:HB3	2.47	0.45
2:B:259:THR:HG21	2:B:301:ARG:NH2	2.32	0.45
1:A:322:GLN:HE22	1:C:79:ASN:ND2	2.15	0.44
1:C:47:HIS:HB3	1:C:50:PHE:HB2	1.98	0.44
2:D:28:GLU:CG	2:D:48:SER:HB3	2.48	0.44
1:A:101:ARG:NH1	6:A:803:HOH:O	2.51	0.44
1:A:241:LYS:HD2	1:A:243:PHE:CE2	2.53	0.44
2:D:28:GLU:HG2	2:D:48:SER:HB3	2.00	0.44
1:A:342:TYR:CD2	1:A:382:ALA:HB2	2.53	0.43
1:C:323:THR:O	1:C:326:VAL:HG22	2.18	0.43
1:A:323:THR:O	1:A:326:VAL:HG22	2.18	0.43
2:D:187:SER:OG	2:D:188:GLU:N	2.51	0.43
2:B:37:ARG:HD2	2:B:91:GLU:HG3	1.99	0.43
1:A:360:VAL:HG11	1:A:428:LYS:O	2.18	0.43
1:C:342:TYR:CD2	1:C:382:ALA:HB2	2.53	0.43
1:A:448:GLU:OE1	1:A:448:GLU:N	2.48	0.43
2:B:280:LEU:O	2:B:292:ARG:HA	2.19	0.43
1:C:16:SER:N	1:C:39:ASP:OD2	2.48	0.43
1:C:465:PRO:HB3	1:C:559:LEU:HD23	2.00	0.43
2:D:37:ARG:HD2	2:D:91:GLU:HG3	2.00	0.43
1:A:494:PRO:O	1:A:497:GLN:NE2	2.48	0.43
2:D:178:HIS:NE2	2:D:222:PRO:O	2.52	0.43
1:C:328:GLU:OE2	1:C:368:ARG:HB2	2.19	0.43
1:A:328:GLU:OE1	1:A:368:ARG:NH1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:28:GLU:HG2	2:B:48:SER:HB3	2.00	0.42
1:A:395:PRO:HA	1:A:398:VAL:HB	2.01	0.42
1:A:471:PHE:O	1:A:553:GLY:HA2	2.19	0.42
1:C:436:LEU:HB2	1:C:446:SER:HB2	2.00	0.42
1:C:494:PRO:O	1:C:497:GLN:NE2	2.49	0.42
1:A:94:SER:O	1:A:100:ARG:HD3	2.20	0.42
1:A:302:LYS:HA	1:A:305:GLU:HG3	2.02	0.42
2:B:184:LEU:HG	2:B:220:TRP:CZ2	2.55	0.42
1:C:184:LYS:O	1:C:187:MET:HB3	2.19	0.42
1:C:469:THR:HA	1:C:519:PHE:O	2.20	0.42
1:A:73:LEU:HB2	1:A:78:TRP:CE2	2.55	0.42
1:C:419:ASP:OD1	3:C:701:MTA:N6	2.44	0.42
1:A:184:LYS:O	1:A:187:MET:HB3	2.19	0.41
2:B:92:ARG:NH2	2:B:109:ASP:O	2.50	0.41
1:C:94:SER:O	1:C:100:ARG:HD3	2.20	0.41
1:C:512:LEU:HD22	1:C:546:THR:HG21	2.02	0.41
1:C:17:GLY:HA2	1:C:40:PHE:O	2.20	0.41
2:D:121:LYS:HA	2:D:121:LYS:HD3	1.89	0.41
1:C:297:TYR:HD1	1:C:577:PHE:CD1	2.37	0.41
2:D:79:THR:HG22	2:D:106:TRP:CZ2	2.56	0.41
1:A:17:GLY:HA2	1:A:40:PHE:O	2.20	0.41
2:D:92:ARG:NH2	2:D:109:ASP:O	2.52	0.41
3:C:701:MTA:HCS2	3:C:701:MTA:H4'	1.91	0.41
1:C:185:THR:O	1:C:188:TRP:HB2	2.20	0.41
2:D:178:HIS:CD2	2:D:225:SER:HB3	2.56	0.41
1:A:586:ILE:HA	1:A:626:HIS:NE2	2.36	0.41
2:D:280:LEU:O	2:D:292:ARG:HA	2.21	0.41
1:A:497:GLN:H	1:A:497:GLN:CD	2.29	0.41
2:B:79:THR:HG22	2:B:106:TRP:CZ2	2.56	0.41
2:B:230:PHE:CE1	2:B:238:SER:HB2	2.56	0.41
1:C:44:PRO:HG3	1:C:48:PRO:HG3	2.03	0.41
1:C:62:ARG:HA	1:C:63:PRO:HD3	1.96	0.40
1:A:468:TYR:CE1	1:A:521:PHE:HB2	2.56	0.40
1:C:322:GLN:HA	1:C:325:GLU:HB3	2.04	0.40
1:A:328:GLU:OE2	1:A:368:ARG:HB2	2.21	0.40
1:A:556:GLU:HG2	1:A:566:SER:HB2	2.04	0.40
1:C:497:GLN:H	1:C:497:GLN:CD	2.29	0.40
2:D:184:LEU:HG	2:D:220:TRP:CZ2	2.56	0.40

There are no symmetry-related clashes.

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	615/645 (95%)	582 (95%)	32 (5%)	1 (0%)	43	56
1	C	622/645 (96%)	585 (94%)	36 (6%)	1 (0%)	43	56
2	B	295/350 (84%)	276 (94%)	17 (6%)	2 (1%)	18	25
2	D	295/350 (84%)	278 (94%)	15 (5%)	2 (1%)	18	25
All	All	1827/1990 (92%)	1721 (94%)	100 (6%)	6 (0%)	36	45

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	147	ILE
2	D	147	ILE
1	A	441	ALA
1	C	441	ALA
2	B	127	ILE
2	D	127	ILE

5.3.2 Protein sidechains [i](#)

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	352/570 (62%)	347 (99%)	5 (1%)	59	75
1	C	557/570 (98%)	549 (99%)	8 (1%)	59	75
2	B	149/298 (50%)	146 (98%)	3 (2%)	48	67
2	D	255/298 (86%)	249 (98%)	6 (2%)	43	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	1313/1736 (76%)	1291 (98%)	22 (2%)	53 72

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	68	ARG
1	A	360	VAL
1	A	388	LEU
1	A	505	ARG
1	A	629	THR
2	B	80	GLU
2	B	294	GLN
2	B	304	THR
1	C	98	LYS
1	C	140	ASN
1	C	157	LEU
1	C	220	ARG
1	C	360	VAL
1	C	388	LEU
1	C	434	SER
1	C	505	ARG
2	D	80	GLU
2	D	129	SER
2	D	206	ILE
2	D	227	VAL
2	D	294	GLN
2	D	304	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	263	GLN
1	A	322	GLN
2	B	111	ASN
1	C	215	ASN
1	C	263	GLN
1	C	270	ASN
1	C	322	GLN
1	C	359	GLN
1	C	525	ASN
2	D	111	ASN

5.3.3 RNA [i](#)

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](#)

5 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	$\# Z > 2$
4	A1BV2	A	702	-	40,40,40	1.03	4 (10%)	50,58,58	1.58	8 (16%)
5	EDO	C	703	-	3,3,3	0.45	0	2,2,2	0.46	0
4	A1BV2	C	702	-	40,40,40	1.02	4 (10%)	50,58,58	1.63	7 (14%)
3	MTA	A	701	-	22,22,22	0.55	0	32,32,32	0.53	0
3	MTA	C	701	-	22,22,22	0.55	0	32,32,32	0.53	0

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
4	A1BV2	A	702	-	-	3/20/43/43	0/5/5/5
5	EDO	C	703	-	-	1/1/1/1	-
4	A1BV2	C	702	-	-	3/20/43/43	0/5/5/5
3	MTA	A	701	-	-	0/7/23/23	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MTA	C	701	-	-	0/7/23/23	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	702	A1BV2	C8-C10	-3.34	1.49	1.53
4	C	702	A1BV2	C8-C10	-3.28	1.49	1.53
4	A	702	A1BV2	C26-S25	-2.95	1.70	1.75
4	C	702	A1BV2	C26-S25	-2.90	1.71	1.75
4	C	702	A1BV2	C28-N27	-2.28	1.35	1.39
4	A	702	A1BV2	C28-N27	-2.16	1.35	1.39
4	A	702	A1BV2	C16-N17	2.13	1.39	1.34
4	C	702	A1BV2	C16-N17	2.13	1.39	1.34

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	702	A1BV2	C13-C14-N15	-3.74	120.97	124.07
4	C	702	A1BV2	C8-C10-N12	3.67	118.74	112.28
4	A	702	A1BV2	S25-C26-N27	-3.63	111.67	116.24
4	C	702	A1BV2	S25-C26-N27	-3.62	111.69	116.24
4	C	702	A1BV2	C14-N15-C16	3.54	122.06	118.64
4	A	702	A1BV2	C14-N15-C16	3.53	122.05	118.64
4	C	702	A1BV2	C13-C14-N15	-3.48	121.19	124.07
4	A	702	A1BV2	C28-N27-C26	3.36	117.74	110.06
4	C	702	A1BV2	C28-N27-C26	3.34	117.70	110.06
4	A	702	A1BV2	O9-C8-C10	3.32	119.96	116.72
4	C	702	A1BV2	O9-C8-C10	3.28	119.92	116.72
4	A	702	A1BV2	C8-C10-N12	3.01	117.57	112.28
4	A	702	A1BV2	C24-S25-C26	2.95	90.81	88.91
4	C	702	A1BV2	C24-S25-C26	2.93	90.80	88.91
4	A	702	A1BV2	C24-C28-N27	-2.13	111.49	115.20

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	702	A1BV2	N12-C10-C8-O9
4	C	702	A1BV2	N12-C10-C8-O9
5	C	703	EDO	O1-C1-C2-O2
4	C	702	A1BV2	C22-C21-C5-C4

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Mol	Chain	Res	Type	Atoms
4	C	702	A1BV2	C29-C21-C5-C4
4	A	702	A1BV2	C29-C21-C5-C4
4	A	702	A1BV2	C22-C21-C5-C4

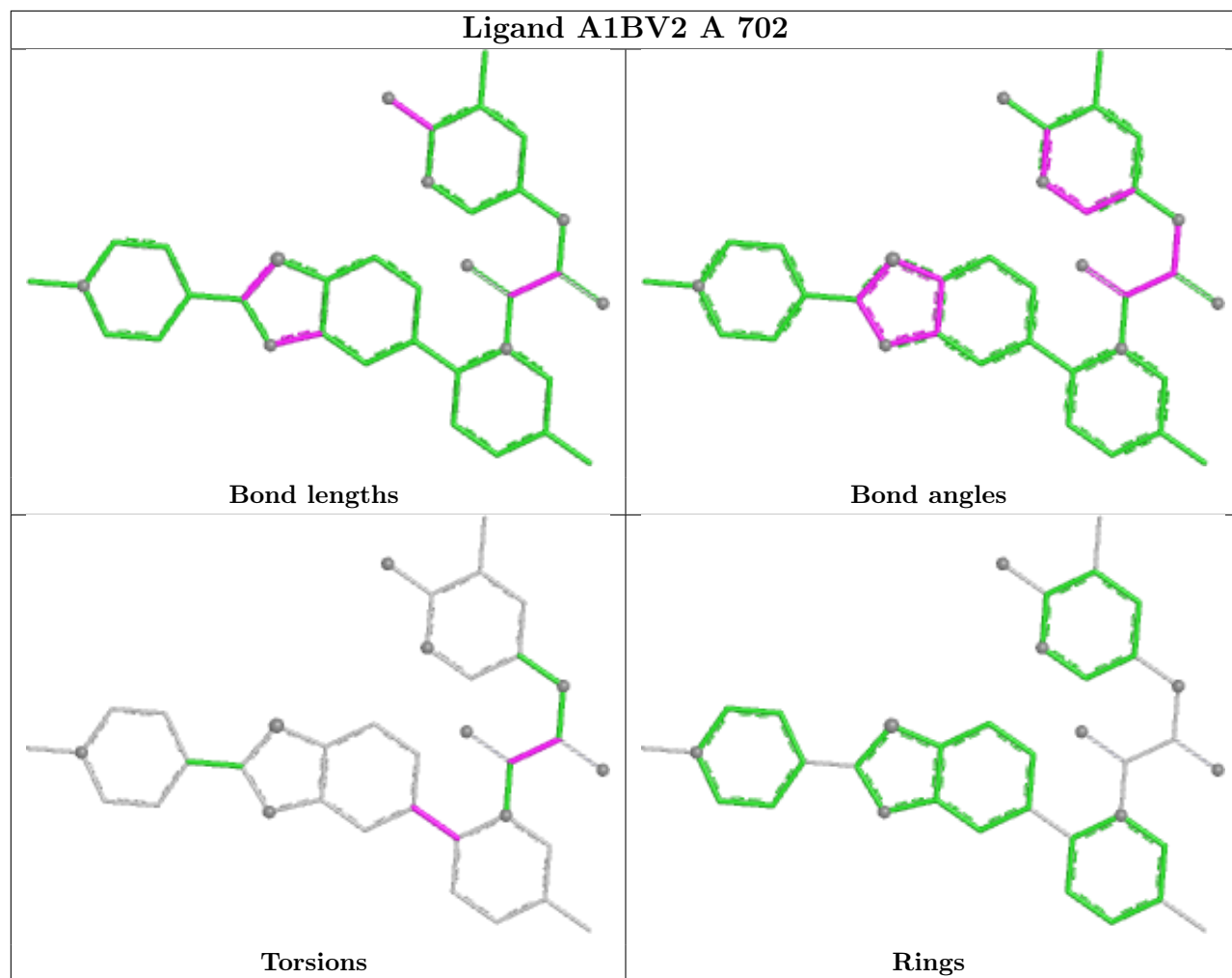
There are no ring outliers.

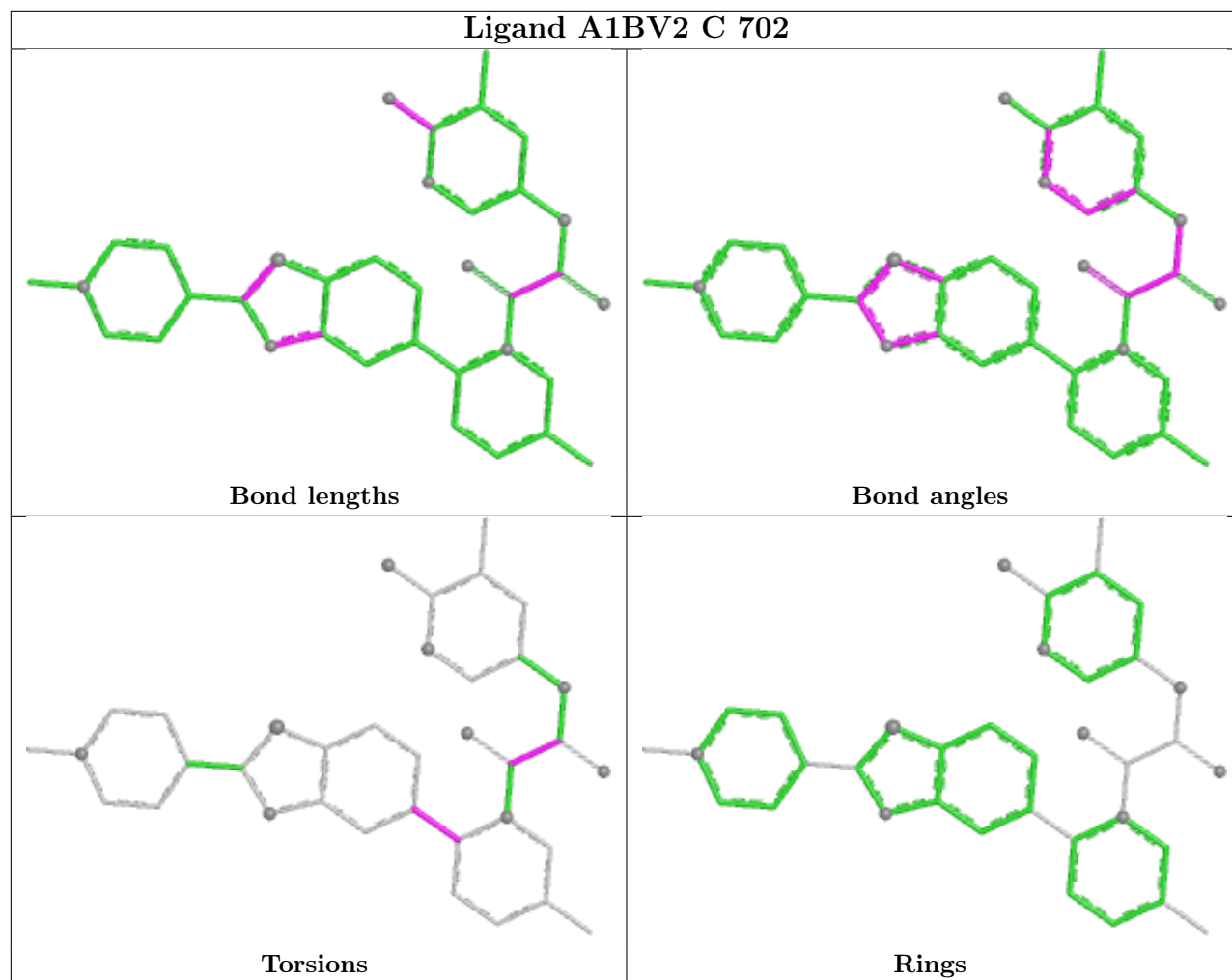
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	701	MTA	1	0
3	C	701	MTA	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.

Ligand A1BV2 A 702





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	625/645 (96%)	0.46	38 (6%)	27	26	11, 34, 85, 135	0
1	C	624/645 (96%)	0.43	40 (6%)	25	24	9, 31, 83, 141	0
2	B	299/350 (85%)	0.83	25 (8%)	17	16	36, 53, 87, 132	0
2	D	299/350 (85%)	0.81	32 (10%)	11	10	27, 49, 89, 122	0
All	All	1847/1990 (92%)	0.57	135 (7%)	21	20	9, 41, 86, 141	0

All (135) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	277	PHE	5.4
2	D	268	VAL	5.3
2	B	211	PRO	5.3
1	A	300	PHE	5.2
2	B	59	TRP	5.0
2	B	210	ALA	5.0
1	C	277	PHE	5.0
1	C	236	PHE	4.9
1	C	529	MET	4.9
2	D	210	ALA	4.7
1	C	286	TYR	4.4
1	A	299	LEU	4.4
1	A	294	PRO	4.2
1	C	341	ILE	4.2
2	D	64	PRO	4.1
1	C	294	PRO	4.1
2	B	27	MET	4.0
1	C	283	TYR	4.0
1	A	577	PHE	4.0
1	C	255	PHE	4.0
1	A	529	MET	4.0

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Mol	Chain	Res	Type	RSRZ
2	D	246	SER	3.9
1	A	297	TYR	3.8
1	C	292	PRO	3.8
1	C	297	TYR	3.6
2	B	225	SER	3.6
1	A	341	ILE	3.5
2	D	248	VAL	3.4
2	D	265	PRO	3.4
1	A	349	VAL	3.4
1	A	145	GLY	3.4
1	A	181	GLY	3.3
1	A	243	PHE	3.3
2	B	270	PHE	3.3
1	C	231	LEU	3.3
2	B	245	THR	3.3
1	C	293	PRO	3.2
2	D	59	TRP	3.2
1	C	272	HIS	3.2
1	C	244	PRO	3.1
1	A	381	GLN	3.0
1	C	296	ALA	3.0
2	D	266	HIS	3.0
2	D	27	MET	3.0
2	D	247	CYS	3.0
2	D	93	GLY	3.0
1	C	378	ALA	3.0
1	A	413	VAL	2.9
2	B	268	VAL	2.9
2	B	106	TRP	2.9
1	C	209	GLY	2.9
2	B	248	VAL	2.9
1	C	146	HIS	2.9
2	D	45	GLY	2.9
1	C	275	LYS	2.9
1	A	454	GLN	2.9
2	B	107	GLU	2.9
1	C	290	ASN	2.8
1	C	577	PHE	2.8
1	A	293	PRO	2.8
2	D	180	ASP	2.8
1	C	237	LEU	2.8
1	C	240	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	104	GLU	2.8
1	C	287	LEU	2.8
2	D	78	GLN	2.8
1	C	300	PHE	2.8
2	D	211	PRO	2.7
1	A	51	LYS	2.7
2	D	95	LEU	2.7
1	C	148	SER	2.7
1	A	146	HIS	2.6
1	A	361	LEU	2.6
2	B	108	LEU	2.6
2	D	249	LEU	2.6
1	A	357	ASN	2.6
1	C	284	LEU	2.6
2	B	247	CYS	2.6
1	C	149	SER	2.6
2	B	180	ASP	2.5
1	A	287	LEU	2.5
1	A	345	LEU	2.5
1	A	291	ARG	2.5
1	A	406	PHE	2.5
2	B	266	HIS	2.5
2	D	118	LYS	2.5
2	D	267	SER	2.5
2	D	76	GLY	2.5
2	B	90	GLY	2.4
2	D	243	LYS	2.4
1	A	284	LEU	2.4
2	D	55	ALA	2.4
1	A	273	SER	2.4
1	C	528	PRO	2.4
1	C	238	THR	2.4
1	A	558	VAL	2.4
2	D	326	VAL	2.4
1	C	242	GLY	2.3
1	A	376	LEU	2.3
1	C	243	PHE	2.3
1	C	241	LYS	2.3
2	B	72	PHE	2.3
1	C	304	TYR	2.3
1	C	374	ALA	2.2
1	A	274	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	D	72	PHE	2.2
2	D	111	ASN	2.2
1	C	369	GLY	2.2
2	D	113	THR	2.2
1	C	299	LEU	2.2
1	A	254	ILE	2.2
1	C	271	HIS	2.2
2	B	111	ASN	2.2
1	A	431	ILE	2.2
2	D	107	GLU	2.2
2	B	227	VAL	2.1
2	D	90	GLY	2.1
2	D	80	GLU	2.1
2	B	267	SER	2.1
2	D	206	ILE	2.1
2	B	164	ARG	2.1
1	C	350	PRO	2.1
1	A	290	ASN	2.1
1	A	385	ARG	2.1
2	B	326	VAL	2.0
1	A	526	ARG	2.0
2	B	303	ALA	2.0
1	C	239	ASN	2.0
1	A	356	THR	2.0
1	A	280	TYR	2.0
2	B	246	SER	2.0
1	A	147	HIS	2.0
2	B	120	CYS	2.0
1	A	563	ILE	2.0
2	D	106	TRP	2.0

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

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

6.3 Carbohydrates ⓘ

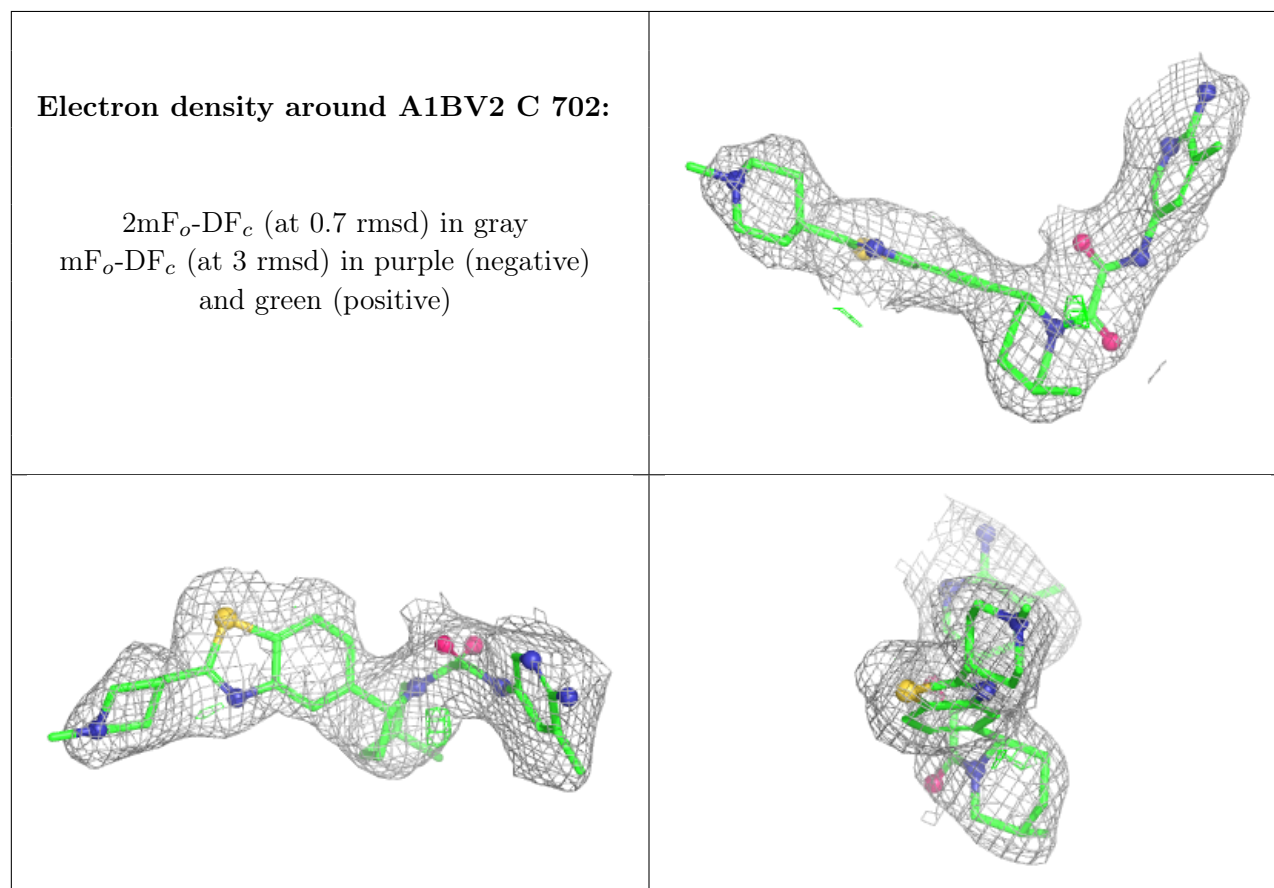
There are no oligosaccharides in this entry.

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.

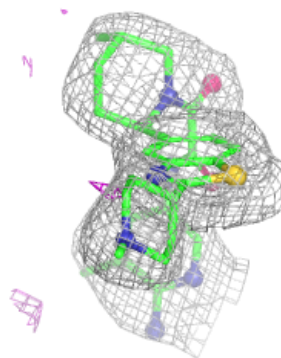
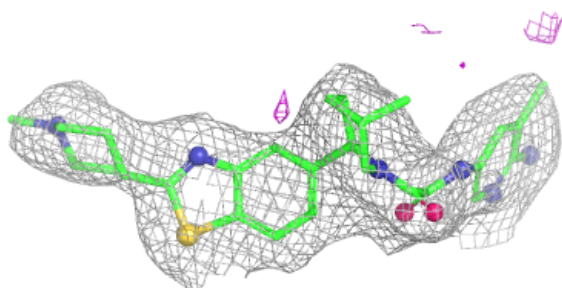
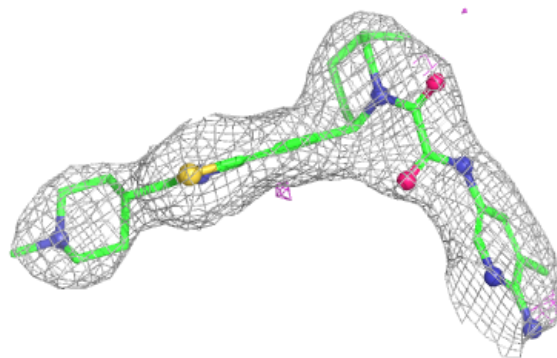
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	C	703	4/4	0.72	0.22	32,36,37,40	0
3	MTA	A	701	20/20	0.93	0.08	17,25,32,34	0
4	A1BV2	C	702	36/36	0.94	0.09	17,25,30,40	0
3	MTA	C	701	20/20	0.95	0.08	20,24,28,29	0
4	A1BV2	A	702	36/36	0.95	0.08	15,23,32,36	0

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 A1BV2 A 702:

$2mF_o-DF_c$ (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.