



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 4, 2025 – 04:26 PM EDT

PDB ID : 9BJ5 / pdb_00009bj5
Title : Crystal structure of the HEPN family member AbiV (P212121 space group)
Authors : Zhu, X.; Moineau, S.; Shi, R.
Deposited on : 2024-04-25
Resolution : 2.55 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 Phenix2.0rc1
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.45.1

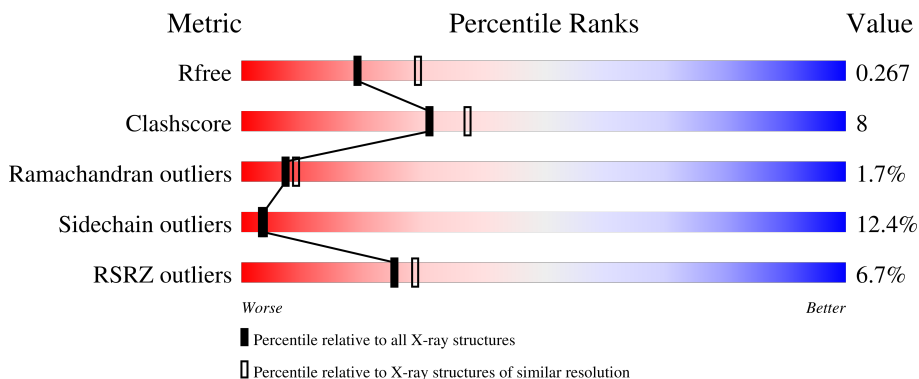
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.55 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	1004 (2.54-2.54)
Clashscore	180529	1055 (2.54-2.54)
Ramachandran outliers	177936	1048 (2.54-2.54)
Sidechain outliers	177891	1048 (2.54-2.54)
RSRZ outliers	164620	1004 (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	207	
1	D	207	
2	B	207	
3	C	207	

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 4823 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 AbiV family abortive infection protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	156	Total	C	N	O	S	0	0	0
			1219	778	186	251	4			
1	D	147	Total	C	N	O	S	0	0	0
			1156	735	177	239	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	202	HIS	-	expression tag	UNP Q9AGY3
A	203	HIS	-	expression tag	UNP Q9AGY3
A	204	HIS	-	expression tag	UNP Q9AGY3
A	205	HIS	-	expression tag	UNP Q9AGY3
A	206	HIS	-	expression tag	UNP Q9AGY3
A	207	HIS	-	expression tag	UNP Q9AGY3
D	202	HIS	-	expression tag	UNP Q9AGY3
D	203	HIS	-	expression tag	UNP Q9AGY3
D	204	HIS	-	expression tag	UNP Q9AGY3
D	205	HIS	-	expression tag	UNP Q9AGY3
D	206	HIS	-	expression tag	UNP Q9AGY3
D	207	HIS	-	expression tag	UNP Q9AGY3

- Molecule 2 is a protein called AbiV family abortive infection protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	150	Total	C	N	O	S	0	0	0
			1180	754	181	241	4			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	202	HIS	-	expression tag	UNP Q9AGY3
B	203	HIS	-	expression tag	UNP Q9AGY3

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Chain	Residue	Modelled	Actual	Comment	Reference
B	204	HIS	-	expression tag	UNP Q9AGY3
B	205	HIS	-	expression tag	UNP Q9AGY3
B	206	HIS	-	expression tag	UNP Q9AGY3
B	207	HIS	-	expression tag	UNP Q9AGY3

- Molecule 3 is a protein called AbiV family abortive infection protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	156	Total	C	N	O	S	0	0	0
			1227	784	187	251	5			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	202	HIS	-	expression tag	UNP Q9AGY3
C	203	HIS	-	expression tag	UNP Q9AGY3
C	204	HIS	-	expression tag	UNP Q9AGY3
C	205	HIS	-	expression tag	UNP Q9AGY3
C	206	HIS	-	expression tag	UNP Q9AGY3
C	207	HIS	-	expression tag	UNP Q9AGY3

- Molecule 4 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Na	0	0
			1	1		

- Molecule 5 is BROMIDE ION (CCD ID: BR) (formula: Br) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Br	0	0
			1	1		
5	B	1	Total	Br	0	0
			1	1		
5	D	1	Total	Br	0	0
			1	1		

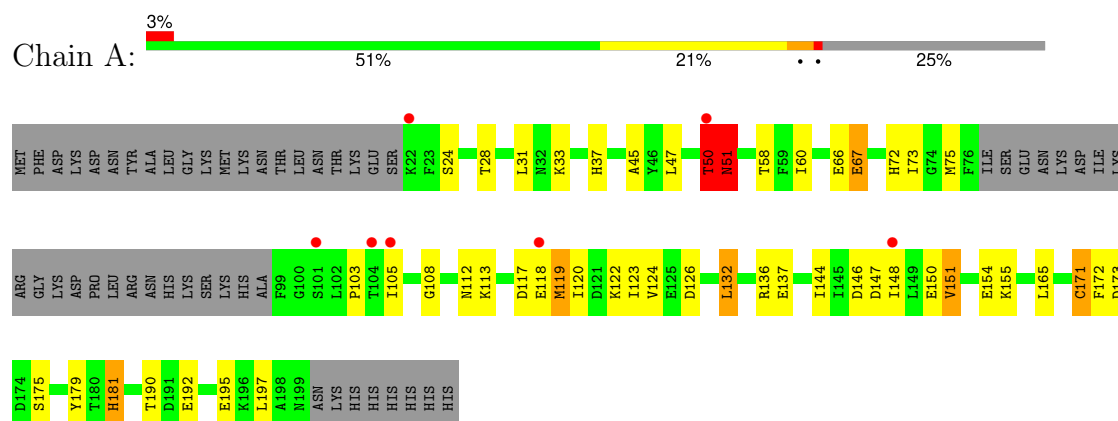
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	12	Total 12	O 12	0	0
6	B	4	Total 4	O 4	0	0
6	C	15	Total 15	O 15	0	0
6	D	6	Total 6	O 6	0	0

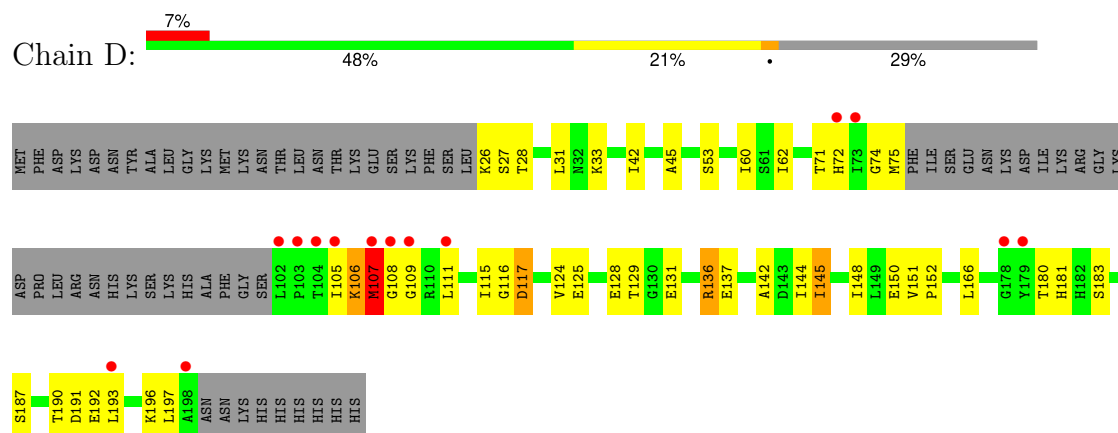
3 Residue-property plots [i](#)

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.

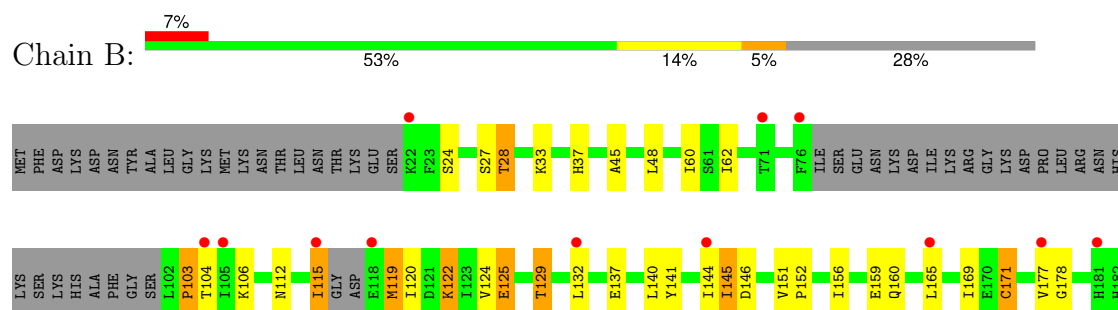
- Molecule 1: AbiV family abortive infection protein



- Molecule 1: AbiV family abortive infection protein



- Molecule 2: AbiV family abortive infection protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	73.69Å 79.17Å 136.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.31 – 2.55 42.31 – 2.55	Depositor EDS
% Data completeness (in resolution range)	99.7 (42.31-2.55) 99.7 (42.31-2.55)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.40 (at 2.54Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.219 , 0.267 0.222 , 0.267	Depositor DCC
R_{free} test set	1307 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	49.0	Xtriage
Anisotropy	0.702	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4823	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.75 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.9341e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MLY, NA, BR

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	1.22	1/1192 (0.1%)	1.64	14/1616 (0.9%)
1	D	1.23	0/1126	1.71	1/1525 (0.1%)
2	B	1.20	1/1151 (0.1%)	1.70	2/1557 (0.1%)
3	C	1.27	1/1211 (0.1%)	1.59	6/1638 (0.4%)
All	All	1.23	3/4680 (0.1%)	1.66	23/6336 (0.4%)

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	D	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	138	SER	C-O	-5.91	1.16	1.24
2	B	37	HIS	CE1-NE2	5.86	1.38	1.32
1	A	181	HIS	CE1-NE2	5.44	1.38	1.32

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	154	GLU	CB-CA-C	7.69	124.71	110.10
1	A	50	THR	CA-CB-OG1	-7.58	98.22	109.60
3	C	171	CYS	CB-CA-C	-6.97	99.66	110.81
1	A	51	ASN	CB-CA-C	6.54	123.44	110.42
2	B	190	THR	CA-CB-OG1	-6.45	99.93	109.60
2	B	28	THR	CB-CA-C	6.42	123.41	109.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	181	HIS	CA-CB-CG	-6.12	107.68	113.80
1	A	151	VAL	N-CA-CB	-5.93	102.91	111.21
1	A	33	LYS	N-CA-C	-5.71	104.97	111.14
1	A	108	GLY	CA-C-N	5.66	125.48	120.10
1	A	108	GLY	C-N-CA	5.66	125.48	120.10
1	A	51	ASN	CA-CB-CG	-5.64	106.96	112.60
1	A	173	ASP	N-CA-C	-5.64	105.05	111.14
3	C	169	ILE	CA-C-O	-5.45	115.40	121.17
3	C	169	ILE	O-C-N	5.38	127.18	121.91
1	A	175	SER	CA-C-O	-5.35	114.75	120.42
3	C	169	ILE	N-CA-C	-5.33	105.30	110.42
1	A	195	GLU	CB-CG-CD	5.32	121.64	112.60
1	A	171	CYS	CB-CA-C	-5.23	102.90	110.96
1	A	126	ASP	CA-CB-CG	5.11	117.71	112.60
1	D	142	ALA	CA-C-O	-5.06	116.19	121.55
1	A	67	GLU	CB-CA-C	5.03	120.51	109.99
3	C	109	GLY	CA-C-O	-5.02	116.48	121.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	116	GLY	Peptide

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	1219	0	1187	21	0
1	D	1156	0	1146	23	0
2	B	1180	0	1160	22	0
3	C	1227	0	1211	15	0
4	A	1	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	D	1	0	0	1	0
6	A	12	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	4	0	0	0	0
6	C	15	0	0	2	0
6	D	6	0	0	2	0
All	All	4823	0	4704	77	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 8.

All (77) 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:D:124:VAL:O	1:D:128:GLU:HG2	1.86	0.76
1:D:145:ILE:HG13	1:D:150:GLU:OE1	1.86	0.75
3:C:192:GLU:OE2	3:C:196:MLY:HH13	1.87	0.75
1:A:47:LEU:HD23	2:B:48:LEU:HD23	1.69	0.74
1:D:192:GLU:O	1:D:196:MLY:HG2	1.89	0.73
3:C:192:GLU:CD	3:C:196:MLY:HH13	2.14	0.72
1:D:26:LYS:N	6:D:401:HOH:O	2.27	0.67
1:D:107:MET:O	1:D:109:GLY:N	2.27	0.66
3:C:154:GLU:OE2	1:D:33:LYS:HE2	1.98	0.64
3:C:151:VAL:HG13	6:C:313:HOH:O	2.02	0.59
1:A:50:THR:C	1:A:51:ASN:O	2.43	0.58
2:B:177:VAL:HA	2:B:183:SER:HB2	1.85	0.58
3:C:103:PRO:HD3	3:C:171:CYS:SG	2.45	0.57
1:D:166:LEU:HD21	1:D:197:LEU:HB2	1.85	0.57
3:C:102:LEU:HG	3:C:167:TYR:OH	2.06	0.55
2:B:120:ILE:O	2:B:124:VAL:HG23	2.05	0.55
3:C:140:LEU:HA	6:C:303:HOH:O	2.06	0.55
1:D:106:LYS:HG2	1:D:107:MET:HG2	1.91	0.53
2:B:144:ILE:HD12	2:B:144:ILE:O	2.09	0.52
1:A:75:MET:HE1	1:A:179:TYR:CD2	2.44	0.52
2:B:178:GLY:HA2	2:B:184:PHE:CE2	2.45	0.52
1:D:45:ALA:HB2	1:D:60:ILE:HG22	1.92	0.51
2:B:140:LEU:HD23	2:B:141:TYR:CZ	2.46	0.51
1:A:37:HIS:CE1	2:B:152:PRO:HG2	2.46	0.51
1:D:144:ILE:O	1:D:144:ILE:HG13	2.10	0.50
1:A:150:GLU:OE1	1:A:155:MLY:HD3	2.11	0.50
3:C:75:MET:HE1	3:C:179:TYR:CD2	2.47	0.49
1:D:62:ILE:HB	1:D:136:ARG:HG3	1.94	0.49
2:B:125:GLU:O	2:B:129:THR:OG1	2.28	0.48
1:A:103:PRO:HD3	1:A:171:CYS:SG	2.55	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:45:ALA:HB2	2:B:60:ILE:HG22	1.96	0.47
1:A:45:ALA:HB2	1:A:60:ILE:CG2	2.45	0.47
1:D:180:THR:O	1:D:183:SER:OG	2.31	0.46
1:A:103:PRO:HG3	1:A:171:CYS:HA	1.97	0.46
2:B:112:ASN:OD1	2:B:120:ILE:HD12	2.16	0.46
2:B:119:MET:O	2:B:119:MET:HG3	2.15	0.46
1:D:166:LEU:HD21	1:D:197:LEU:CB	2.45	0.46
2:B:122:LYS:HA	2:B:122:LYS:HE2	1.98	0.46
1:D:111:LEU:O	1:D:115:ILE:HG12	2.16	0.46
1:A:118:GLU:O	1:A:119:MET:CB	2.64	0.46
2:B:103:PRO:HG3	2:B:171:CYS:HA	1.98	0.46
1:A:165:LEU:HD23	1:A:197:LEU:HD11	1.97	0.45
1:A:132:LEU:HD12	1:A:132:LEU:HA	1.87	0.45
1:A:75:MET:HE1	1:A:179:TYR:CG	2.53	0.44
3:C:75:MET:HE1	3:C:179:TYR:CE2	2.52	0.44
1:A:66:GLU:OE1	1:A:136:ARG:NH1	2.47	0.44
1:A:181:HIS:ND1	6:A:401:HOH:O	2.32	0.44
1:A:172:PHE:CE2	1:A:190:THR:HG21	2.53	0.44
3:C:37:HIS:CE1	1:D:152:PRO:HG2	2.52	0.43
3:C:132:LEU:HD23	3:C:132:LEU:HA	1.85	0.43
1:A:119:MET:HE2	1:A:123:ILE:HG13	2.00	0.43
2:B:145:ILE:HG22	2:B:145:ILE:O	2.18	0.43
2:B:115:ILE:HD12	2:B:119:MET:HG2	2.00	0.43
3:C:165:LEU:HD23	3:C:197:LEU:HD21	2.01	0.43
2:B:169:ILE:HG23	2:B:190:THR:HG23	2.01	0.42
1:D:187:SER:O	1:D:191:ASP:CG	2.62	0.42
2:B:122:LYS:HA	2:B:122:LYS:CE	2.49	0.42
1:A:120:ILE:O	1:A:124:VAL:HG23	2.18	0.42
3:C:72:HIS:HD2	3:C:101:SER:OG	2.02	0.42
3:C:197:LEU:HD12	3:C:197:LEU:HA	1.91	0.42
2:B:165:LEU:HD22	2:B:197:LEU:HD12	2.00	0.42
1:D:107:MET:N	1:D:107:MET:SD	2.93	0.42
1:A:112:ASN:ND2	1:A:117:ASP:OD2	2.53	0.42
1:A:119:MET:HE3	1:A:119:MET:HA	2.01	0.41
2:B:33:MLY:HH22	2:B:33:MLY:HD3	1.86	0.41
2:B:62:ILE:HG12	2:B:132:LEU:HD22	2.02	0.41
2:B:156:ILE:HA	2:B:160:GLN:OE1	2.21	0.41
2:B:178:GLY:HA2	2:B:184:PHE:CZ	2.55	0.41
1:D:31:LEU:HD13	1:D:75:MET:HE2	2.02	0.41
1:D:71:THR:O	1:D:74:GLY:N	2.53	0.41
3:C:102:LEU:HD12	3:C:102:LEU:HA	1.89	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:LEU:O	1:A:50:THR:HG22	2.21	0.41
1:D:181:HIS:HB2	5:D:301:BR:BR	2.75	0.41
1:A:72:HIS:O	1:A:75:MET:HG2	2.21	0.40
1:D:150:GLU:HA	6:D:402:HOH:O	2.20	0.40
1:D:192:GLU:O	1:D:196:MLY:CG	2.63	0.40
1:D:42:ILE:HG22	1:D:193:LEU:HD12	2.02	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	148/207 (72%)	137 (93%)	8 (5%)	3 (2%)	6	6
1	D	139/207 (67%)	129 (93%)	7 (5%)	3 (2%)	5	5
2	B	140/207 (68%)	132 (94%)	6 (4%)	2 (1%)	9	12
3	C	149/207 (72%)	143 (96%)	4 (3%)	2 (1%)	10	13
All	All	576/828 (70%)	541 (94%)	25 (4%)	10 (2%)	7	9

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	119	MET
1	D	108	GLY
1	D	117	ASP
3	C	101	SER
3	C	117	ASP
2	B	146	ASP
1	A	146	ASP
2	B	103	PRO

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Mol	Chain	Res	Type
1	D	107	MET

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	132/183 (72%)	115 (87%)	17 (13%)	3	3
1	D	127/183 (69%)	110 (87%)	17 (13%)	3	2
2	B	128/183 (70%)	111 (87%)	17 (13%)	3	2
3	C	136/184 (74%)	122 (90%)	14 (10%)	6	6
All	All	523/733 (71%)	458 (88%)	65 (12%)	4	3

All (65) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	SER
1	A	28	THR
1	A	31	LEU
1	A	50	THR
1	A	58	THR
1	A	67	GLU
1	A	73	ILE
1	A	105	ILE
1	A	113	LYS
1	A	122	LYS
1	A	132	LEU
1	A	137	GLU
1	A	144	ILE
1	A	147	ASP
1	A	148	ILE
1	A	151	VAL
1	A	192	GLU
2	B	24	SER
2	B	27	SER
2	B	28	THR

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Mol	Chain	Res	Type
2	B	104	THR
2	B	106	LYS
2	B	115	ILE
2	B	119	MET
2	B	122	LYS
2	B	125	GLU
2	B	129	THR
2	B	137	GLU
2	B	145	ILE
2	B	151	VAL
2	B	159	GLU
2	B	171	CYS
2	B	190	THR
2	B	197	LEU
3	C	24	SER
3	C	27	SER
3	C	52	GLU
3	C	101	SER
3	C	102	LEU
3	C	104	THR
3	C	107	MET
3	C	117	ASP
3	C	119	MET
3	C	132	LEU
3	C	137	GLU
3	C	144	ILE
3	C	151	VAL
3	C	185	GLU
1	D	27	SER
1	D	28	THR
1	D	53	SER
1	D	72	HIS
1	D	105	ILE
1	D	106	LYS
1	D	107	MET
1	D	117	ASP
1	D	125	GLU
1	D	129	THR
1	D	131	GLU
1	D	136	ARG
1	D	137	GLU
1	D	145	ILE

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Mol	Chain	Res	Type
1	D	148	ILE
1	D	151	VAL
1	D	190	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	HIS
1	A	112	ASN
3	C	72	HIS
3	C	182	HIS
1	D	72	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

15 non-standard protein/DNA/RNA residues are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	MLY	B	155	2	9,10,11	0.47	0	6,11,13	0.22	0
2	MLY	B	33	2	9,10,11	0.51	0	6,11,13	0.47	0
1	MLY	A	196	1	9,10,11	0.51	0	6,11,13	0.62	0
3	MLY	C	196	3	9,10,11	0.51	0	6,11,13	0.46	0
1	MLY	D	196	1	9,10,11	0.41	0	6,11,13	0.23	0
1	MLY	A	158	1	9,10,11	0.55	0	6,11,13	0.40	0
2	MLY	B	158	2	9,10,11	0.48	0	6,11,13	0.61	0
3	MLY	C	155	3	9,10,11	0.42	0	6,11,13	0.43	0
1	MLY	D	43	1	9,10,11	0.58	0	6,11,13	0.22	0
1	MLY	A	43	1	9,10,11	0.48	0	6,11,13	0.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	MLY	D	155	1	9,10,11	0.51	0	6,11,13	0.34	0
1	MLY	D	158	1	9,10,11	0.49	0	6,11,13	0.38	0
3	MLY	C	158	3	9,10,11	0.57	0	6,11,13	0.34	0
1	MLY	A	155	1	9,10,11	0.54	0	6,11,13	0.68	0
2	MLY	B	196	2	9,10,11	0.43	0	6,11,13	0.15	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
2	MLY	B	155	2	-	0/8/9/11	-
2	MLY	B	33	2	-	3/8/9/11	-
1	MLY	A	196	1	-	5/8/9/11	-
3	MLY	C	196	3	-	3/8/9/11	-
1	MLY	D	196	1	-	4/8/9/11	-
1	MLY	A	158	1	-	4/8/9/11	-
2	MLY	B	158	2	-	1/8/9/11	-
3	MLY	C	155	3	-	3/8/9/11	-
1	MLY	D	43	1	-	4/8/9/11	-
1	MLY	A	43	1	-	4/8/9/11	-
1	MLY	D	155	1	-	3/8/9/11	-
1	MLY	D	158	1	-	1/8/9/11	-
3	MLY	C	158	3	-	3/8/9/11	-
1	MLY	A	155	1	-	1/8/9/11	-
2	MLY	B	196	2	-	3/8/9/11	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (42) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	43	MLY	C-CA-CB-CG
2	B	33	MLY	C-CA-CB-CG
2	B	196	MLY	O-C-CA-CB
1	D	43	MLY	CD-CE-NZ-CH1

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Mol	Chain	Res	Type	Atoms
1	A	196	MLY	CD-CE-NZ-CH1
1	A	196	MLY	CD-CE-NZ-CH2
2	B	33	MLY	CD-CE-NZ-CH2
1	D	43	MLY	CD-CE-NZ-CH2
3	C	158	MLY	CG-CD-CE-NZ
1	A	43	MLY	CD-CE-NZ-CH2
3	C	196	MLY	CD-CE-NZ-CH2
1	D	155	MLY	CG-CD-CE-NZ
1	A	155	MLY	CA-CB-CG-CD
3	C	155	MLY	CD-CE-NZ-CH2
1	A	43	MLY	CA-CB-CG-CD
3	C	155	MLY	CA-CB-CG-CD
1	A	158	MLY	CG-CD-CE-NZ
2	B	196	MLY	CE-CD-CG-CB
1	D	196	MLY	CE-CD-CG-CB
1	A	196	MLY	CE-CD-CG-CB
1	A	158	MLY	CE-CD-CG-CB
3	C	155	MLY	CD-CE-NZ-CH1
1	D	155	MLY	CE-CD-CG-CB
1	D	43	MLY	CE-CD-CG-CB
2	B	33	MLY	CG-CD-CE-NZ
1	D	196	MLY	CD-CE-NZ-CH2
1	D	196	MLY	CA-CB-CG-CD
1	A	196	MLY	CA-CB-CG-CD
1	A	196	MLY	C-CA-CB-CG
2	B	158	MLY	C-CA-CB-CG
3	C	196	MLY	C-CA-CB-CG
1	D	43	MLY	C-CA-CB-CG
1	D	155	MLY	C-CA-CB-CG
1	D	196	MLY	CD-CE-NZ-CH1
3	C	158	MLY	CE-CD-CG-CB
3	C	196	MLY	CG-CD-CE-NZ
1	A	158	MLY	CA-CB-CG-CD
2	B	196	MLY	C-CA-CB-CG
1	D	158	MLY	CG-CD-CE-NZ
3	C	158	MLY	CD-CE-NZ-CH1
1	A	43	MLY	N-CA-CB-CG
1	A	158	MLY	CD-CE-NZ-CH1

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	33	MLY	1	0
3	C	196	MLY	2	0
1	D	196	MLY	2	0
1	A	155	MLY	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 4 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	152/207 (73%)	-0.05	7 (4%) 38 43	34, 50, 84, 122	0
1	D	143/207 (69%)	0.60	14 (9%) 14 18	46, 75, 117, 167	0
2	B	146/207 (70%)	0.56	14 (9%) 15 19	49, 76, 108, 136	0
3	C	153/207 (73%)	0.03	5 (3%) 49 55	35, 50, 95, 123	0
All	All	594/828 (71%)	0.28	40 (6%) 25 29	34, 63, 108, 167	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	103	PRO	4.8
1	D	102	LEU	4.7
1	D	108	GLY	4.5
1	D	198	ALA	4.3
2	B	198	ALA	4.0
2	B	181	HIS	4.0
3	C	77	ILE	3.8
2	B	71	THR	3.6
1	D	193	LEU	3.4
1	D	105	ILE	3.2
1	D	179	TYR	3.2
2	B	76	PHE	3.2
3	C	108	GLY	3.1
1	D	107	MET	2.9
3	C	24	SER	2.8
2	B	104	THR	2.8
1	A	50	THR	2.7
1	D	178	GLY	2.6
2	B	165	LEU	2.6
1	D	73	ILE	2.6
3	C	100	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	105	ILE	2.6
1	D	72	HIS	2.5
2	B	118	GLU	2.5
1	A	101	SER	2.5
2	B	105	ILE	2.5
1	A	118	GLU	2.3
1	D	111	LEU	2.3
2	B	132	LEU	2.3
1	A	22	LYS	2.3
2	B	115	ILE	2.2
2	B	22	LYS	2.2
3	C	99	PHE	2.2
1	D	109	GLY	2.1
1	D	104	THR	2.1
2	B	144	ILE	2.1
2	B	177	VAL	2.1
1	A	104	THR	2.0
1	A	148	ILE	2.0
2	B	197	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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	MLY	B	196	11/12	0.77	0.20	95,100,117,117	0
2	MLY	B	155	11/12	0.85	0.19	75,80,111,113	0
1	MLY	A	196	11/12	0.85	0.15	53,59,87,87	0
2	MLY	B	158	11/12	0.86	0.15	68,79,99,105	0
1	MLY	D	155	11/12	0.87	0.19	70,79,119,121	0
1	MLY	D	196	11/12	0.88	0.16	102,108,119,120	0
1	MLY	D	158	11/12	0.90	0.15	69,76,88,89	0
1	MLY	D	43	11/12	0.90	0.17	52,60,77,79	0
2	MLY	B	33	11/12	0.92	0.14	55,59,79,86	0
3	MLY	C	158	11/12	0.93	0.14	44,52,70,72	0
3	MLY	C	196	11/12	0.93	0.10	58,66,78,80	0
1	MLY	A	158	11/12	0.93	0.13	42,51,77,78	0
1	MLY	A	43	11/12	0.95	0.11	45,55,86,89	0
1	MLY	A	155	11/12	0.95	0.09	43,50,57,62	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MLY	C	155	11/12	0.95	0.09	46,56,63,65	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

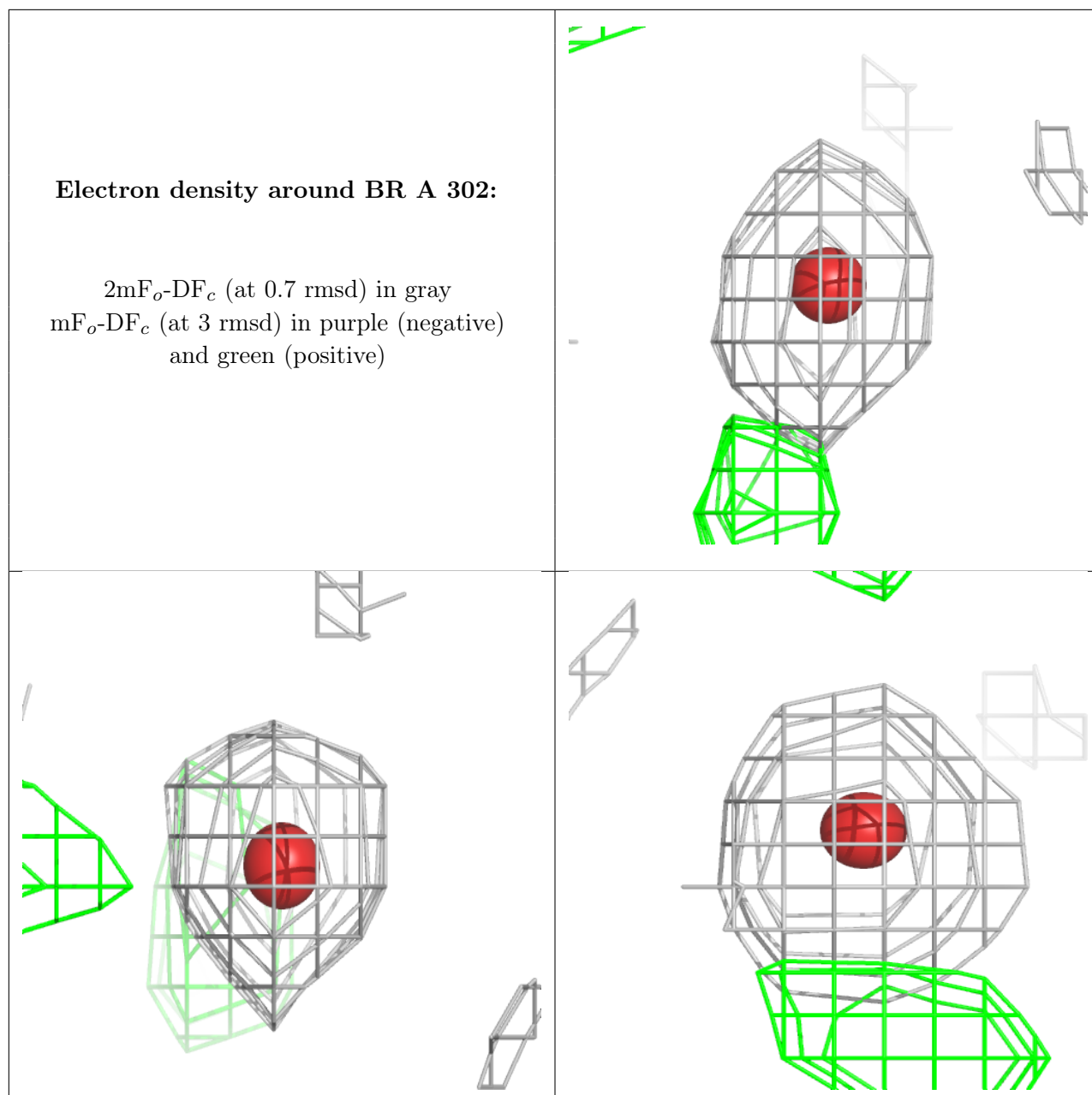
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	NA	A	301	1/1	0.92	0.16	43,43,43,43	0
5	BR	A	302	1/1	0.93	0.15	43,43,43,43	1
5	BR	D	301	1/1	0.94	0.06	52,52,52,52	1
5	BR	B	301	1/1	0.98	0.08	50,50,50,50	1

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.

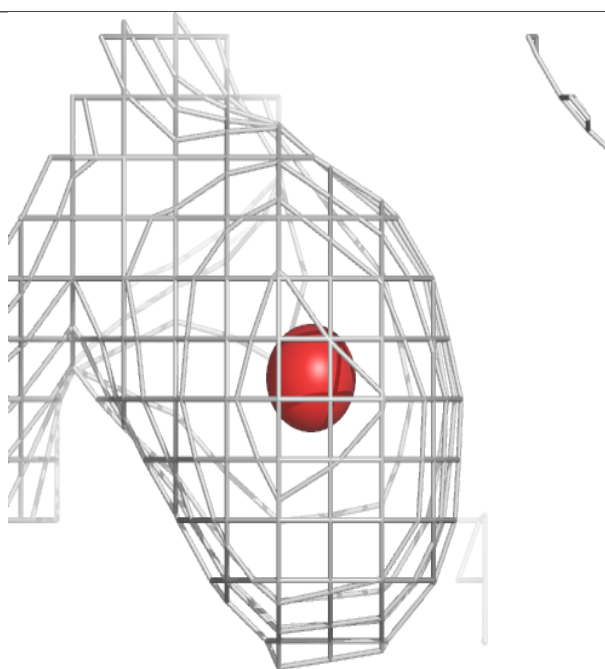
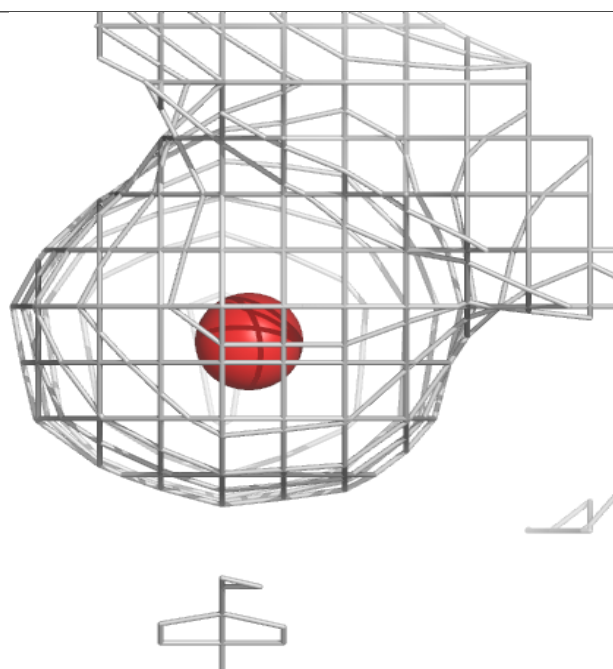
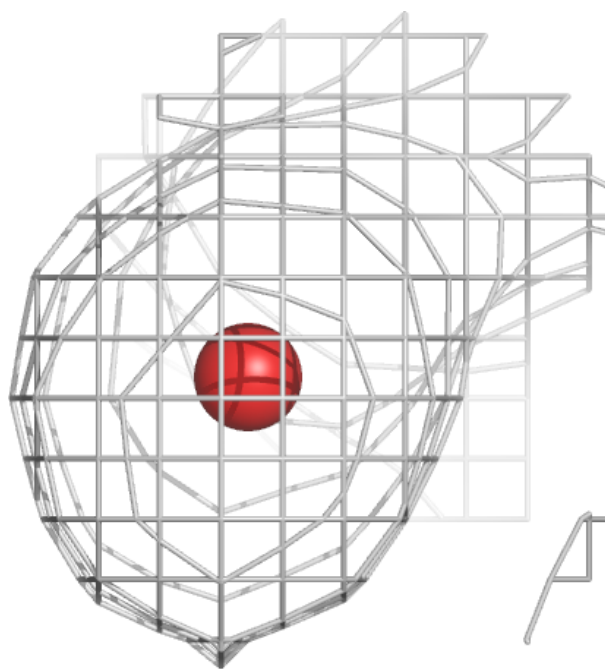
Electron density around BR A 302:

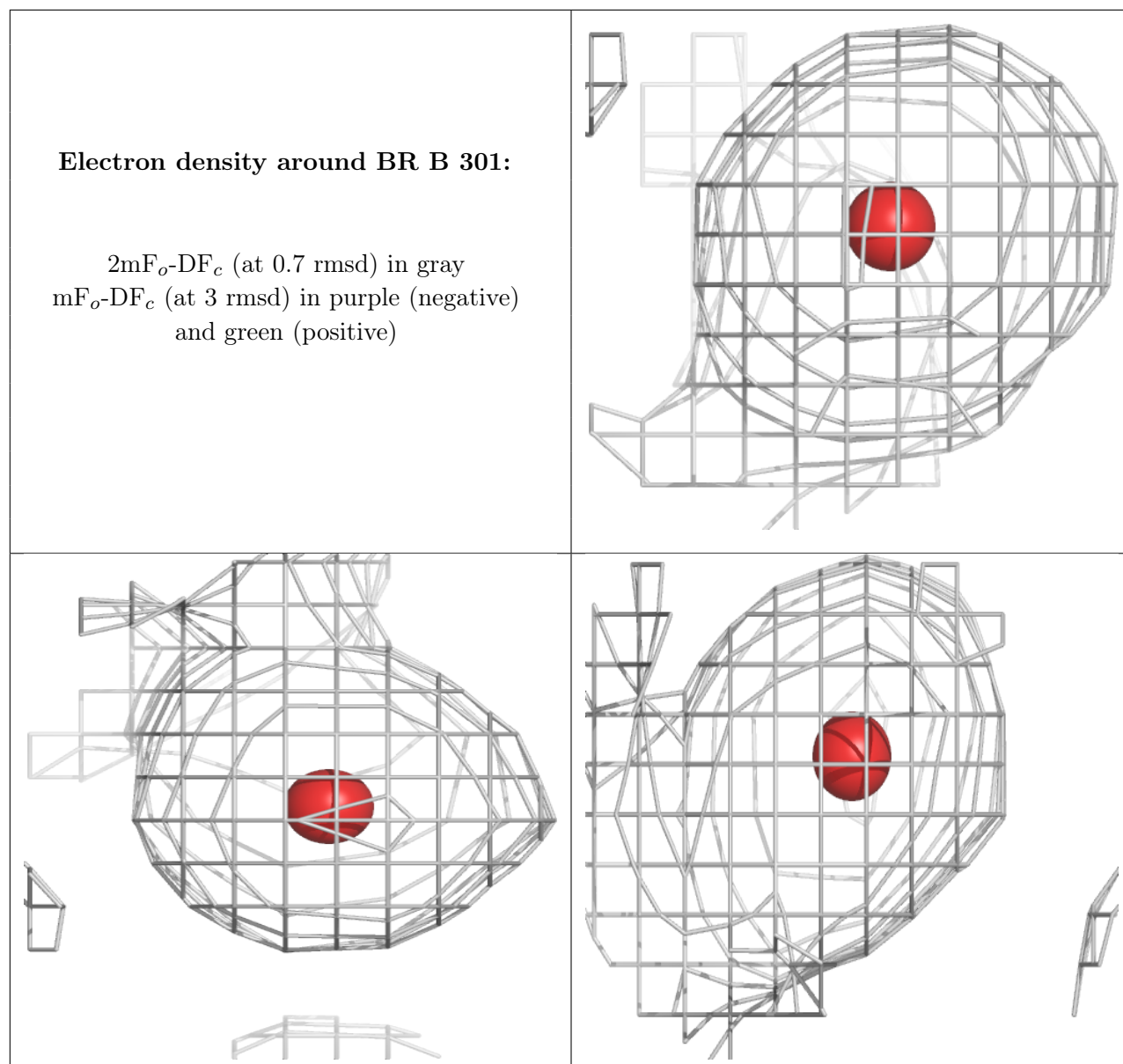
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around BR D 301:

$2mF_o-DF_c$ (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.