



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 06:42 AM UTC

PDB ID : 9N0V / pdb_00009n0v
Title : Crystal structure of the HIV capsid hexamer bound to the small molecule long-acting inhibitor, KFA-027
Authors : Dinh, T.T.; Kvaratskhelia, M.
Deposited on : 2025-01-24
Resolution : 2.98 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

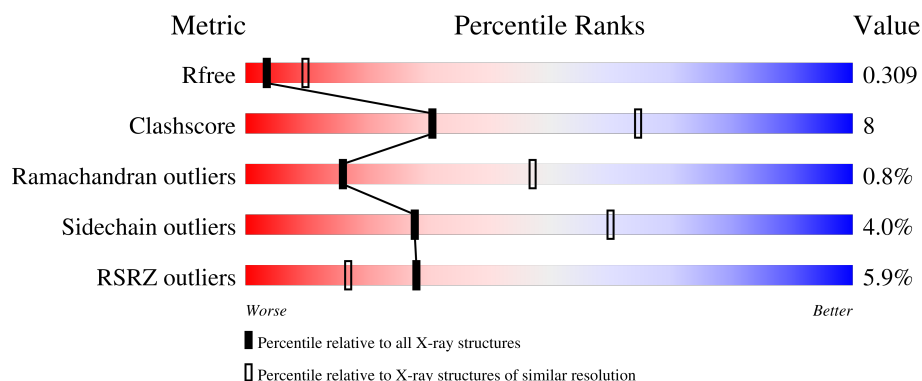
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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	220	5% 74% 25% .
1	B	220	4% 84% 15% .
1	C	220	8% 78% 20% .
1	D	220	7% 78% 20% .

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 14020 atoms, of which 6956 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 Capsid protein p24.

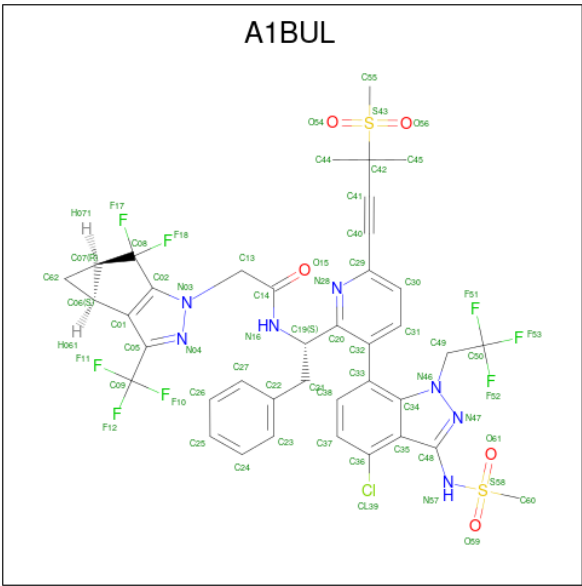
Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	220	Total	C	H	N	O	S	0	0	0
			3409	1071	1705	299	320	14			
1	B	220	Total	C	H	N	O	S	0	0	0
			3409	1071	1705	299	320	14			
1	C	220	Total	C	H	N	O	S	0	0	0
			3409	1071	1705	299	320	14			
1	D	220	Total	C	H	N	O	S	0	0	0
			3409	1071	1705	299	320	14			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	14	CYS	ALA	conflict	UNP P12497
A	45	CYS	GLU	conflict	UNP P12497
A	184	ALA	TRP	conflict	UNP P12497
A	185	ALA	MET	conflict	UNP P12497
B	14	CYS	ALA	conflict	UNP P12497
B	45	CYS	GLU	conflict	UNP P12497
B	184	ALA	TRP	conflict	UNP P12497
B	185	ALA	MET	conflict	UNP P12497
C	14	CYS	ALA	conflict	UNP P12497
C	45	CYS	GLU	conflict	UNP P12497
C	184	ALA	TRP	conflict	UNP P12497
C	185	ALA	MET	conflict	UNP P12497
D	14	CYS	ALA	conflict	UNP P12497
D	45	CYS	GLU	conflict	UNP P12497
D	184	ALA	TRP	conflict	UNP P12497
D	185	ALA	MET	conflict	UNP P12497

- Molecule 2 is N-[(1S)-1-[(3M)-3-[4-chloro-3-(methanesulfonamido)-1-(2,2,2-trifluoroethyl)-1H-indazol-7-yl]-6-[3-(methanesulfonyl)-3-methylbut-1-yn-1-yl]pyridin-2-yl]-2-phenylethyl]-2-[(3bS,4aR)-5,5-difluoro-3-(trifluoromethyl)-3b,4,4a,5-tetrahydro-1H-cyclopropa[3,4]cyclopenta[1,2-c]pyrazol-1-yl]acetamide (CCD ID: A1BUL) (formula: C₃₉H₃₄ClF₈N₇O₅S₂) (labeled

as "Ligand of Interest" by depositor).

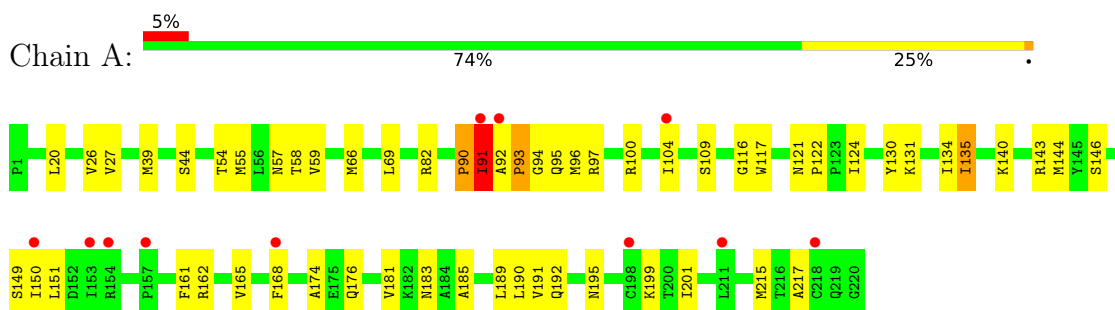


Mol	Chain	Residues	Atoms								ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	H	N	O	S	0	0
			96	39	1	8	34	7	5	2		
2	B	1	Total	C	Cl	F	H	N	O	S	0	0
			96	39	1	8	34	7	5	2		
2	C	1	Total	C	Cl	F	H	N	O	S	0	0
			96	39	1	8	34	7	5	2		
2	D	1	Total	C	Cl	F	H	N	O	S	0	0
			96	39	1	8	34	7	5	2		

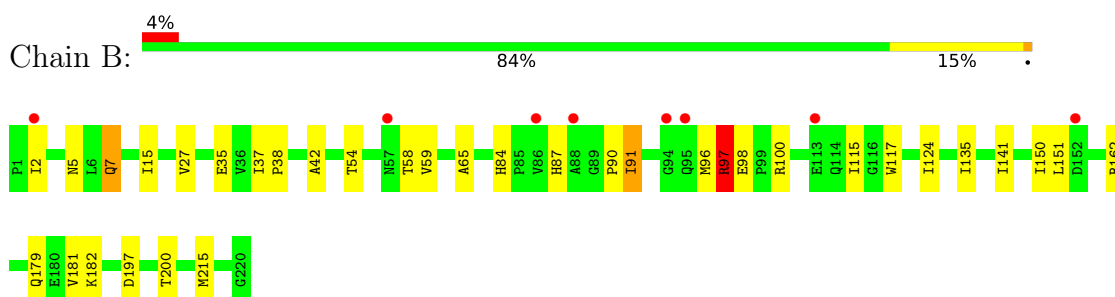
3 Residue-property plots [i](#)

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.

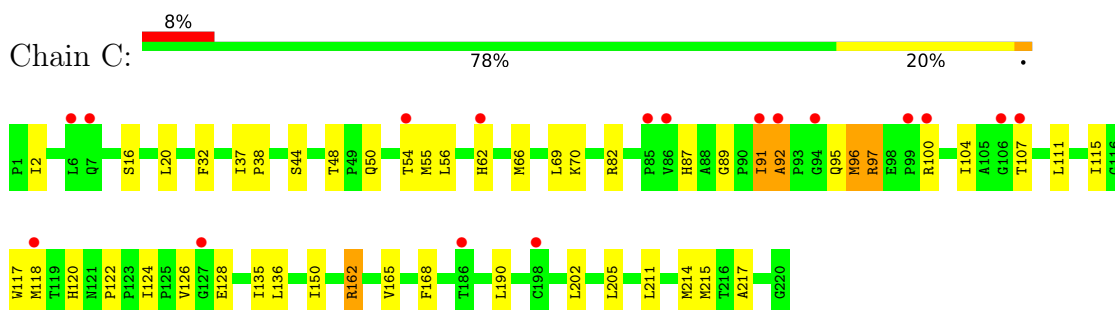
- Molecule 1: Capsid protein p24



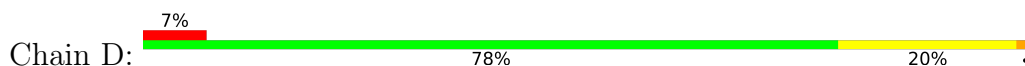
- Molecule 1: Capsid protein p24

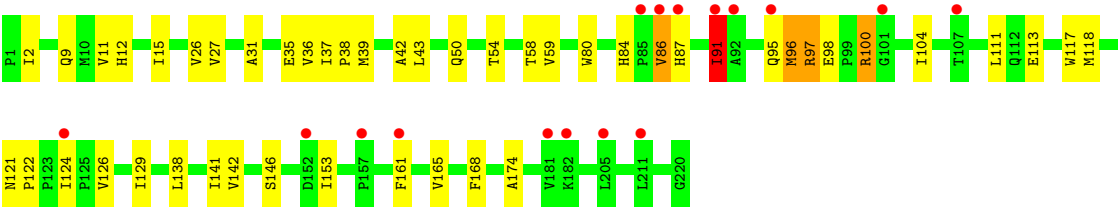


- Molecule 1: Capsid protein p24



- Molecule 1: Capsid protein p24





4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	153.32Å 153.32Å 112.33Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	42.88 – 2.98 42.88 – 2.98	Depositor EDS
% Data completeness (in resolution range)	99.6 (42.88-2.98) 99.6 (42.88-2.98)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.95Å)	Xtriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.274 , 0.309 0.274 , 0.309	Depositor DCC
R_{free} test set	1994 reflections (9.91%)	wwPDB-VP
Wilson B-factor (Å ²)	60.1	Xtriage
Anisotropy	0.347	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 18.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.049 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	14020	wwPDB-VP
Average B, all atoms (Å ²)	70.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.09% 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: A1BUL

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	0.20	0/1741	0.37	1/2366 (0.0%)
1	B	0.22	0/1741	0.38	1/2366 (0.0%)
1	C	0.25	0/1741	0.47	4/2366 (0.2%)
1	D	0.20	0/1741	0.38	1/2366 (0.0%)
All	All	0.22	0/6964	0.40	7/9464 (0.1%)

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
1	C	0	3
1	D	0	1
All	All	0	7

There are no bond length outliers.

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	91	ILE	CA-CB-CG2	8.23	124.49	110.50
1	C	96	MET	CB-CG-SD	7.67	135.70	112.70
1	C	97	ARG	CB-CG-CD	6.32	125.85	111.30
1	D	91	ILE	CA-CB-CG1	6.32	121.14	110.40
1	A	91	ILE	N-CA-C	5.74	115.85	106.72
1	C	97	ARG	CA-CB-CG	5.38	124.85	114.10
1	C	97	ARG	N-CA-CB	5.04	117.29	110.38

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	91	ILE	Mainchain
1	A	97	ARG	Sidechain
1	B	97	ARG	Sidechain
1	C	162	ARG	Sidechain
1	C	82	ARG	Sidechain
1	C	89	GLY	Peptide
1	D	100	ARG	Sidechain

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	1704	1705	1705	32	1
1	B	1704	1705	1705	23	1
1	C	1704	1705	1705	34	1
1	D	1704	1705	1705	32	1
2	A	62	34	0	1	0
2	B	62	34	0	0	0
2	C	62	34	0	1	0
2	D	62	34	0	1	0
All	All	7064	6956	6820	115	2

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 (115) 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:96:MET:HE2	1:A:117:TRP:N	1.98	0.79
1:D:37:ILE:HD11	1:D:142:VAL:HG21	1.70	0.73
1:C:87:HIS:CB	1:C:97:ARG:HD2	2.19	0.72
1:C:162:ARG:HE	1:C:215:MET:HE2	1.55	0.71
1:A:144:MET:HE1	1:B:215:MET:HE3	1.75	0.69
1:A:92:ALA:HB1	1:A:93:PRO:HD2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:91:ILE:O	1:C:91:ILE:HG22	1.94	0.66
1:B:84:HIS:O	1:B:100:ARG:NH2	2.31	0.64
1:D:84:HIS:O	1:D:100:ARG:NH2	2.32	0.63
1:D:100:ARG:HA	1:D:100:ARG:NE	2.14	0.62
1:D:100:ARG:HA	1:D:100:ARG:HE	1.65	0.61
1:A:92:ALA:HB1	1:A:93:PRO:CD	2.31	0.60
1:C:87:HIS:HB3	1:C:97:ARG:HD2	1.85	0.59
1:C:100:ARG:NE	1:C:100:ARG:HA	2.19	0.58
1:C:48:THR:HG22	1:C:118:MET:HE1	1.85	0.58
1:C:165:VAL:HG22	1:C:190:LEU:HD11	1.86	0.57
1:B:27:VAL:HG11	1:B:59:VAL:HG13	1.86	0.57
1:C:87:HIS:HB2	1:C:97:ARG:HD2	1.85	0.57
1:A:100:ARG:NE	1:A:100:ARG:HA	2.20	0.57
1:C:44:SER:HB3	1:C:55:MET:HE1	1.88	0.55
1:B:87:HIS:O	1:B:97:ARG:NH2	2.39	0.55
1:A:144:MET:HE3	1:B:162:ARG:NH2	2.22	0.54
1:C:66:MET:HA	1:C:66:MET:HE2	1.89	0.54
1:D:118:MET:HG2	1:D:126:VAL:HG22	1.88	0.54
1:B:5:ASN:ND2	1:B:7:GLN:OE1	2.41	0.54
1:C:50:GLN:OE1	1:C:111:LEU:HD22	2.07	0.54
1:D:96:MET:HE2	1:D:117:TRP:CG	2.44	0.53
1:D:153:ILE:HG21	1:D:168:PHE:HA	1.91	0.53
1:D:31:ALA:O	1:D:36:VAL:HG11	2.09	0.53
1:B:54:THR:O	1:B:58:THR:HG23	2.08	0.53
1:A:150:ILE:HG23	1:A:151:LEU:HD22	1.91	0.53
1:B:150:ILE:HG23	1:B:151:LEU:HD22	1.92	0.52
1:C:20:LEU:HD11	1:D:42:ALA:HB1	1.92	0.52
1:C:211:LEU:HD12	1:C:214:MET:HE3	1.93	0.51
1:B:96:MET:HE2	1:B:117:TRP:N	2.26	0.51
1:A:93:PRO:O	1:A:95:GLN:N	2.44	0.51
1:B:124:ILE:O	1:B:124:ILE:HG23	2.11	0.50
1:C:95:GLN:O	1:C:96:MET:SD	2.69	0.50
2:A:301:A1BUL:N16	2:A:301:A1BUL:F17	2.35	0.50
1:A:96:MET:HE2	1:A:116:GLY:C	2.35	0.50
1:C:2:ILE:HD11	1:C:115:ILE:HG12	1.94	0.49
1:C:20:LEU:HD11	1:D:42:ALA:CB	2.42	0.49
1:A:162:ARG:HA	1:A:215:MET:HE2	1.93	0.49
1:D:138:LEU:HD23	1:D:141:ILE:HD12	1.94	0.49
1:A:161:PHE:O	1:A:165:VAL:HG23	2.13	0.48
1:D:26:VAL:HG11	1:D:39:MET:HE2	1.95	0.48
1:B:37:ILE:HB	1:B:38:PRO:HD3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:2:ILE:HD13	1:D:12:HIS:HA	1.95	0.48
1:C:87:HIS:ND1	1:C:97:ARG:HD3	2.28	0.48
1:C:97:ARG:O	1:C:117:TRP:NE1	2.42	0.48
1:A:20:LEU:HD11	1:B:42:ALA:HB1	1.96	0.47
1:D:54:THR:O	1:D:58:THR:HG23	2.14	0.47
1:D:96:MET:HE2	1:D:117:TRP:CD2	2.50	0.47
1:A:191:VAL:HG22	1:A:199:LYS:HG3	1.96	0.47
1:B:100:ARG:NE	1:B:100:ARG:HA	2.30	0.47
1:A:66:MET:HE2	1:A:66:MET:HA	1.97	0.47
1:A:121:ASN:HB2	1:A:122:PRO:HD3	1.97	0.47
1:A:26:VAL:HG21	1:A:39:MET:HG3	1.97	0.47
1:A:54:THR:O	1:A:58:THR:HG23	2.15	0.46
1:A:146:SER:HB2	1:A:174:ALA:HB1	1.97	0.46
1:D:124:ILE:HG23	1:D:124:ILE:O	2.15	0.46
1:C:44:SER:CB	1:C:55:MET:HE1	2.45	0.46
1:C:91:ILE:O	1:C:92:ALA:O	2.32	0.46
1:A:201:ILE:CG2	1:A:217:ALA:HB1	2.45	0.46
1:C:205:LEU:HD11	1:C:217:ALA:CB	2.47	0.45
1:A:150:ILE:HD11	1:A:168:PHE:CE1	2.52	0.45
1:A:44:SER:CB	1:A:55:MET:HE1	2.46	0.45
1:D:146:SER:HB2	1:D:174:ALA:HB1	1.98	0.45
1:C:96:MET:HG2	1:C:120:HIS:NE2	2.32	0.45
1:B:35:GLU:C	1:B:38:PRO:HD2	2.43	0.44
1:A:20:LEU:HD11	1:B:42:ALA:CB	2.47	0.44
1:D:39:MET:HE3	1:D:43:LEU:HD11	1.98	0.44
1:B:2:ILE:HD11	1:B:115:ILE:HG12	2.00	0.44
1:C:124:ILE:HG23	1:C:124:ILE:O	2.17	0.44
1:D:86:VAL:HG22	1:D:97:ARG:CD	2.48	0.44
1:D:37:ILE:H	1:D:37:ILE:HD12	1.84	0.43
1:C:202:LEU:HA	1:C:205:LEU:HD12	1.99	0.43
1:A:57:ASN:HB3	1:B:38:PRO:CG	2.49	0.43
1:A:91:ILE:O	1:A:91:ILE:HG13	2.19	0.43
1:C:54:THR:HG21	1:D:42:ALA:HB2	2.00	0.43
1:B:15:ILE:O	1:B:15:ILE:HG23	2.18	0.43
1:D:87:HIS:H	1:D:97:ARG:HD3	1.83	0.43
1:A:27:VAL:HG11	1:A:59:VAL:HG13	2.01	0.43
1:A:185:ALA:HB1	1:A:189:LEU:HD12	1.99	0.43
1:D:37:ILE:HB	1:D:38:PRO:HD3	2.00	0.43
1:A:69:LEU:HD21	1:A:134:ILE:HG23	2.01	0.42
1:A:130:TYR:CE2	1:A:134:ILE:HD11	2.54	0.42
1:D:97:ARG:O	1:D:117:TRP:NE1	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:301:A1BUL:C40	2:D:301:A1BUL:O54	2.63	0.42
1:A:168:PHE:CD1	1:A:190:LEU:HD13	2.53	0.42
1:B:97:ARG:HG3	1:B:98:GLU:N	2.34	0.42
1:D:161:PHE:O	1:D:165:VAL:HG23	2.19	0.42
1:D:15:ILE:O	1:D:15:ILE:HG23	2.19	0.42
1:D:35:GLU:OE1	1:D:35:GLU:N	2.49	0.42
1:C:162:ARG:HH21	1:C:215:MET:HB3	1.85	0.42
1:C:190:LEU:HD23	1:C:214:MET:HE1	2.01	0.42
1:D:27:VAL:HG11	1:D:59:VAL:HG13	2.01	0.42
1:A:44:SER:HB3	1:A:55:MET:HE1	2.01	0.42
1:C:91:ILE:O	1:C:92:ALA:C	2.63	0.42
1:C:104:ILE:HG13	1:C:126:VAL:HG12	2.00	0.42
1:C:107:THR:HG23	2:C:301:A1BUL:F53	2.10	0.41
1:B:197:ASP:O	1:B:200:THR:HG22	2.20	0.41
1:D:80:TRP:CH2	1:D:129:ILE:HD13	2.55	0.41
1:B:37:ILE:CG2	1:B:135:ILE:HG23	2.50	0.41
1:B:65:ALA:HB1	1:B:141:ILE:HD13	2.01	0.41
1:D:96:MET:HE1	1:D:113:GLU:O	2.20	0.41
1:D:9:GLN:O	1:D:11:VAL:HG13	2.20	0.41
1:A:131:LYS:O	1:A:135:ILE:HD12	2.21	0.41
1:B:7:GLN:NE2	1:B:7:GLN:N	2.69	0.41
1:C:37:ILE:HB	1:C:38:PRO:HD3	2.03	0.41
1:C:56:LEU:HD22	1:C:69:LEU:CD2	2.50	0.40
1:C:150:ILE:HD11	1:C:168:PHE:CZ	2.56	0.40
1:C:32:PHE:HE2	1:C:62:HIS:HB3	1.86	0.40
1:D:50:GLN:OE1	1:D:111:LEU:HD22	2.21	0.40
1:A:140:LYS:HG3	1:A:143:ARG:HH22	1.85	0.40

All (2) 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:B:90:PRO:O	1:C:91:ILE:N[9_554]	2.07	0.13
1:A:90:PRO:O	1:D:91:ILE:N[9_554]	2.19	0.01

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	218/220 (99%)	210 (96%)	5 (2%)	3 (1%)	9	34
1	B	218/220 (99%)	206 (94%)	12 (6%)	0	100	100
1	C	218/220 (99%)	206 (94%)	9 (4%)	3 (1%)	9	34
1	D	218/220 (99%)	209 (96%)	8 (4%)	1 (0%)	24	58
All	All	872/880 (99%)	831 (95%)	34 (4%)	7 (1%)	16	47

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	90	PRO
1	A	93	PRO
1	C	122	PRO
1	C	92	ALA
1	C	91	ILE
1	D	122	PRO
1	A	94	GLY

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	186/186 (100%)	175 (94%)	11 (6%)	18	48
1	B	186/186 (100%)	180 (97%)	6 (3%)	34	65
1	C	186/186 (100%)	181 (97%)	5 (3%)	39	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	D	186/186 (100%)	178 (96%)	8 (4%)	26	58
All	All	744/744 (100%)	714 (96%)	30 (4%)	28	60

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	82	ARG
1	A	104	ILE
1	A	109	SER
1	A	124	ILE
1	A	135	ILE
1	A	149	SER
1	A	176	GLN
1	A	181	VAL
1	A	183	ASN
1	A	192	GLN
1	A	195	ASN
1	B	7	GLN
1	B	91	ILE
1	B	97	ARG
1	B	179	GLN
1	B	181	VAL
1	B	182	LYS
1	C	16	SER
1	C	70	LYS
1	C	128	GLU
1	C	135	ILE
1	C	136	LEU
1	D	86	VAL
1	D	91	ILE
1	D	95	GLN
1	D	96	MET
1	D	97	ARG
1	D	98	GLU
1	D	104	ILE
1	D	121	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	4	GLN

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Mol	Chain	Res	Type
1	A	114	GLN
1	A	139	ASN
1	A	176	GLN
1	B	4	GLN
1	B	120	HIS
1	B	179	GLN
1	C	121	ASN
1	C	176	GLN
1	C	219	GLN
1	D	192	GLN
1	D	219	GLN

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](#)

4 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	$\# Z > 2$
2	A1BUL	B	301	-	62,68,68	3.45	25 (40%)	78,110,110	6.45	25 (32%)
2	A1BUL	A	301	-	62,68,68	3.49	27 (43%)	78,110,110	6.37	32 (41%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	A1BUL	C	301	-	62,68,68	3.42	27 (43%)	78,110,110	6.62	27 (34%)
2	A1BUL	D	301	-	62,68,68	3.47	27 (43%)	78,110,110	6.56	28 (35%)

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	A1BUL	B	301	-	-	12/45/72/72	0/7/7/7
2	A1BUL	A	301	-	-	25/45/72/72	0/7/7/7
2	A1BUL	C	301	-	-	6/45/72/72	0/7/7/7
2	A1BUL	D	301	-	-	12/45/72/72	0/7/7/7

All (106) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	301	A1BUL	C02-C01	-12.53	1.21	1.37
2	B	301	A1BUL	C02-C01	-12.44	1.21	1.37
2	C	301	A1BUL	C02-C01	-12.43	1.21	1.37
2	D	301	A1BUL	C02-C01	-12.39	1.21	1.37
2	C	301	A1BUL	C01-C05	8.73	1.48	1.40
2	D	301	A1BUL	C01-C05	8.35	1.47	1.40
2	B	301	A1BUL	C01-C05	8.22	1.47	1.40
2	A	301	A1BUL	C01-C05	8.03	1.47	1.40
2	D	301	A1BUL	C14-N16	7.49	1.49	1.34
2	A	301	A1BUL	C42-C41	7.44	1.57	1.46
2	B	301	A1BUL	N03-N04	-7.36	1.23	1.36
2	A	301	A1BUL	C14-N16	7.32	1.49	1.34
2	D	301	A1BUL	N03-N04	-7.31	1.23	1.36
2	B	301	A1BUL	C14-N16	7.31	1.49	1.34
2	A	301	A1BUL	N03-N04	-7.16	1.24	1.36
2	C	301	A1BUL	N03-N04	-7.10	1.24	1.36
2	B	301	A1BUL	C42-C41	7.09	1.57	1.46
2	A	301	A1BUL	C55-S43	7.00	1.84	1.76
2	D	301	A1BUL	C42-C41	6.95	1.56	1.46
2	B	301	A1BUL	C55-S43	6.86	1.84	1.76
2	C	301	A1BUL	C14-N16	6.77	1.48	1.34
2	D	301	A1BUL	C55-S43	6.72	1.84	1.76
2	C	301	A1BUL	C42-C41	6.71	1.56	1.46
2	A	301	A1BUL	C05-N04	-6.53	1.22	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	A1BUL	C55-S43	6.52	1.84	1.76
2	D	301	A1BUL	C05-N04	-6.40	1.22	1.32
2	B	301	A1BUL	C05-N04	-6.39	1.22	1.32
2	A	301	A1BUL	C29-C40	6.28	1.56	1.44
2	C	301	A1BUL	C05-N04	-6.16	1.22	1.32
2	D	301	A1BUL	C29-C40	5.94	1.55	1.44
2	B	301	A1BUL	C29-C40	5.90	1.55	1.44
2	C	301	A1BUL	C29-C40	5.76	1.55	1.44
2	C	301	A1BUL	C06-C07	5.23	1.59	1.51
2	B	301	A1BUL	C06-C07	5.18	1.59	1.51
2	D	301	A1BUL	C06-C07	5.09	1.58	1.51
2	D	301	A1BUL	C02-N03	5.04	1.40	1.35
2	B	301	A1BUL	C02-N03	5.01	1.40	1.35
2	A	301	A1BUL	C06-C07	5.00	1.58	1.51
2	D	301	A1BUL	O56-S43	4.79	1.47	1.44
2	A	301	A1BUL	C62-C07	4.69	1.58	1.50
2	B	301	A1BUL	C62-C07	4.67	1.58	1.50
2	C	301	A1BUL	C62-C07	4.66	1.58	1.50
2	B	301	A1BUL	O56-S43	4.63	1.47	1.44
2	C	301	A1BUL	O56-S43	4.62	1.47	1.44
2	D	301	A1BUL	C62-C07	4.60	1.58	1.50
2	A	301	A1BUL	O56-S43	4.52	1.47	1.44
2	A	301	A1BUL	O54-S43	4.27	1.47	1.44
2	D	301	A1BUL	O54-S43	4.26	1.47	1.44
2	B	301	A1BUL	O54-S43	4.21	1.47	1.44
2	C	301	A1BUL	C02-N03	4.16	1.39	1.35
2	C	301	A1BUL	O54-S43	4.01	1.47	1.44
2	A	301	A1BUL	C02-N03	3.96	1.39	1.35
2	D	301	A1BUL	C60-S58	3.58	1.83	1.75
2	D	301	A1BUL	C62-C06	3.55	1.58	1.51
2	B	301	A1BUL	C62-C06	3.50	1.58	1.51
2	C	301	A1BUL	S58-N57	3.43	1.72	1.65
2	A	301	A1BUL	S58-N57	3.42	1.72	1.65
2	A	301	A1BUL	C60-S58	3.40	1.83	1.75
2	C	301	A1BUL	C62-C06	3.35	1.57	1.51
2	C	301	A1BUL	C60-S58	3.34	1.83	1.75
2	B	301	A1BUL	C60-S58	3.33	1.83	1.75
2	A	301	A1BUL	C62-C06	3.32	1.57	1.51
2	C	301	A1BUL	C33-C34	3.13	1.44	1.41
2	A	301	A1BUL	C33-C32	3.08	1.56	1.49
2	B	301	A1BUL	S58-N57	3.06	1.71	1.65
2	A	301	A1BUL	C33-C34	3.01	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	A1BUL	C33-C32	2.91	1.55	1.49
2	A	301	A1BUL	C13-C14	2.90	1.57	1.52
2	D	301	A1BUL	C13-N03	2.82	1.49	1.45
2	B	301	A1BUL	C33-C32	2.80	1.55	1.49
2	D	301	A1BUL	C33-C34	2.68	1.44	1.41
2	D	301	A1BUL	S58-N57	2.66	1.70	1.65
2	D	301	A1BUL	C13-C14	2.61	1.57	1.52
2	A	301	A1BUL	C13-N03	2.57	1.49	1.45
2	D	301	A1BUL	C33-C32	2.57	1.55	1.49
2	B	301	A1BUL	C33-C34	2.54	1.44	1.41
2	B	301	A1BUL	C13-N03	2.51	1.49	1.45
2	A	301	A1BUL	C40-C41	2.50	1.22	1.19
2	A	301	A1BUL	C21-C22	2.37	1.56	1.51
2	B	301	A1BUL	C13-C14	2.36	1.56	1.52
2	C	301	A1BUL	C36-CL39	2.31	1.79	1.73
2	A	301	A1BUL	C49-C50	2.31	1.54	1.50
2	C	301	A1BUL	C13-N03	2.29	1.49	1.45
2	C	301	A1BUL	C09-C05	2.29	1.54	1.49
2	A	301	A1BUL	O61-S58	2.28	1.47	1.43
2	C	301	A1BUL	O61-S58	2.28	1.47	1.43
2	A	301	A1BUL	C36-CL39	2.28	1.79	1.73
2	C	301	A1BUL	C21-C22	2.26	1.56	1.51
2	D	301	A1BUL	O15-C14	-2.23	1.18	1.23
2	B	301	A1BUL	O61-S58	2.21	1.47	1.43
2	B	301	A1BUL	O59-S58	2.20	1.47	1.43
2	D	301	A1BUL	O59-S58	2.20	1.47	1.43
2	D	301	A1BUL	C21-C22	2.18	1.56	1.51
2	B	301	A1BUL	C36-CL39	2.18	1.78	1.73
2	C	301	A1BUL	O59-S58	2.17	1.47	1.43
2	A	301	A1BUL	O59-S58	2.14	1.47	1.43
2	D	301	A1BUL	O61-S58	2.13	1.47	1.43
2	C	301	A1BUL	C13-C14	2.12	1.56	1.52
2	A	301	A1BUL	C06-C01	-2.11	1.49	1.51
2	B	301	A1BUL	C21-C22	2.07	1.56	1.51
2	D	301	A1BUL	C36-CL39	2.06	1.78	1.73
2	B	301	A1BUL	C40-C41	2.05	1.22	1.19
2	C	301	A1BUL	C49-C50	2.05	1.54	1.50
2	D	301	A1BUL	C49-C50	2.04	1.54	1.50
2	D	301	A1BUL	C40-C41	2.02	1.22	1.19
2	C	301	A1BUL	O15-C14	-2.01	1.19	1.23

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	A1BUL	C45-C42-C41	-35.90	75.72	109.99
2	C	301	A1BUL	C45-C42-C41	-35.39	76.21	109.99
2	A	301	A1BUL	C45-C42-C41	-34.78	76.79	109.99
2	B	301	A1BUL	C45-C42-C41	-34.39	77.16	109.99
2	C	301	A1BUL	C44-C42-C41	28.23	136.94	109.99
2	D	301	A1BUL	C44-C42-C41	27.15	135.91	109.99
2	B	301	A1BUL	C44-C42-C41	26.41	135.21	109.99
2	A	301	A1BUL	C44-C42-C41	25.36	134.20	109.99
2	C	301	A1BUL	O56-S43-O54	-22.91	99.18	118.01
2	D	301	A1BUL	O56-S43-O54	-22.42	99.58	118.01
2	B	301	A1BUL	O56-S43-O54	-21.94	99.98	118.01
2	A	301	A1BUL	O56-S43-O54	-21.41	100.41	118.01
2	B	301	A1BUL	C62-C06-C01	17.95	137.23	115.63
2	D	301	A1BUL	C62-C06-C01	16.96	136.04	115.63
2	C	301	A1BUL	C62-C06-C01	16.13	135.04	115.63
2	A	301	A1BUL	C62-C06-C01	15.88	134.74	115.63
2	A	301	A1BUL	O61-S58-O59	-13.11	101.30	118.87
2	C	301	A1BUL	O61-S58-O59	-12.68	101.88	118.87
2	B	301	A1BUL	O61-S58-O59	-12.44	102.19	118.87
2	D	301	A1BUL	O61-S58-O59	-11.97	102.83	118.87
2	A	301	A1BUL	C08-C07-C06	-8.95	101.64	108.40
2	D	301	A1BUL	C08-C07-C06	-8.74	101.81	108.40
2	C	301	A1BUL	C08-C07-C06	-8.40	102.06	108.40
2	B	301	A1BUL	C08-C07-C06	-8.35	102.10	108.40
2	C	301	A1BUL	C09-C05-N04	7.76	127.69	118.50
2	A	301	A1BUL	C09-C05-N04	7.64	127.55	118.50
2	B	301	A1BUL	C09-C05-N04	7.07	126.87	118.50
2	D	301	A1BUL	C09-C05-N04	7.07	126.87	118.50
2	C	301	A1BUL	C29-N28-C20	7.06	122.90	117.29
2	D	301	A1BUL	C29-N28-C20	6.96	122.83	117.29
2	B	301	A1BUL	C29-N28-C20	6.67	122.60	117.29
2	A	301	A1BUL	C29-N28-C20	6.47	122.44	117.29
2	C	301	A1BUL	C13-N03-N04	5.27	126.19	118.99
2	A	301	A1BUL	C01-C05-N04	-5.22	107.09	113.09
2	C	301	A1BUL	C01-C05-N04	-5.14	107.19	113.09
2	B	301	A1BUL	C09-C05-C01	-5.07	125.12	128.38
2	C	301	A1BUL	C09-C05-C01	-5.07	125.12	128.38
2	D	301	A1BUL	C09-C05-C01	-4.72	125.35	128.38
2	A	301	A1BUL	C09-C05-C01	-4.70	125.36	128.38
2	D	301	A1BUL	C01-C05-N04	-4.62	107.78	113.09
2	B	301	A1BUL	C01-C05-N04	-4.43	108.00	113.09
2	C	301	A1BUL	N57-C48-N47	4.30	127.74	119.03
2	B	301	A1BUL	C13-N03-N04	4.29	124.86	118.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	301	A1BUL	N57-C48-N47	4.14	127.42	119.03
2	D	301	A1BUL	C13-N03-N04	4.05	124.53	118.99
2	B	301	A1BUL	O56-S43-C55	3.88	113.31	108.42
2	B	301	A1BUL	F10-C09-C05	-3.81	106.96	112.39
2	B	301	A1BUL	N57-C48-N47	3.77	126.67	119.03
2	A	301	A1BUL	C14-C13-N03	3.63	118.68	111.89
2	B	301	A1BUL	C06-C01-C02	3.54	117.38	110.21
2	C	301	A1BUL	O56-S43-C55	3.41	112.72	108.42
2	D	301	A1BUL	C06-C01-C02	3.40	117.10	110.21
2	D	301	A1BUL	O61-S58-C60	3.21	113.34	108.26
2	D	301	A1BUL	O56-S43-C55	3.17	112.42	108.42
2	A	301	A1BUL	C13-N03-N04	3.15	123.29	118.99
2	A	301	A1BUL	C06-C01-C02	3.14	116.57	110.21
2	C	301	A1BUL	C06-C01-C02	3.05	116.39	110.21
2	D	301	A1BUL	C32-C33-C34	-2.99	120.26	124.44
2	C	301	A1BUL	C19-N16-C14	-2.90	119.11	123.44
2	A	301	A1BUL	O56-S43-C55	2.88	112.04	108.42
2	D	301	A1BUL	C31-C32-C20	2.82	120.79	117.94
2	B	301	A1BUL	O61-S58-C60	2.80	112.69	108.26
2	A	301	A1BUL	C02-N03-N04	-2.74	108.74	111.67
2	D	301	A1BUL	F18-C08-F17	2.72	118.12	105.19
2	D	301	A1BUL	C02-N03-N04	-2.68	108.81	111.67
2	A	301	A1BUL	O61-S58-C60	2.65	112.46	108.26
2	A	301	A1BUL	F18-C08-F17	2.61	117.63	105.19
2	B	301	A1BUL	F18-C08-F17	2.61	117.61	105.19
2	D	301	A1BUL	F12-C09-C05	-2.61	108.67	112.39
2	A	301	A1BUL	F11-C09-C05	-2.60	108.69	112.39
2	D	301	A1BUL	N57-C48-N47	2.56	124.21	119.03
2	C	301	A1BUL	C32-C33-C34	-2.54	120.89	124.44
2	D	301	A1BUL	O59-S58-C60	2.54	112.27	108.26
2	C	301	A1BUL	C14-C13-N03	-2.51	107.20	111.89
2	B	301	A1BUL	C34-C35-C36	2.51	121.52	118.10
2	A	301	A1BUL	O61-S58-N57	2.51	111.90	106.83
2	A	301	A1BUL	C30-C29-N28	-2.43	119.78	123.09
2	B	301	A1BUL	C02-N03-N04	-2.43	109.08	111.67
2	B	301	A1BUL	C06-C01-C05	-2.41	138.46	145.10
2	C	301	A1BUL	F12-C09-C05	-2.38	109.00	112.39
2	A	301	A1BUL	C38-C33-C32	-2.35	114.00	118.74
2	A	301	A1BUL	F51-C50-C49	-2.34	107.62	112.04
2	D	301	A1BUL	F10-C09-C05	-2.34	109.06	112.39
2	B	301	A1BUL	C50-C49-N46	-2.33	109.64	112.09
2	C	301	A1BUL	C34-C35-C36	2.33	121.27	118.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	A1BUL	F11-C09-C05	-2.32	109.09	112.39
2	D	301	A1BUL	C06-C01-C05	-2.32	138.72	145.10
2	A	301	A1BUL	C06-C01-C05	-2.32	138.73	145.10
2	C	301	A1BUL	O61-S58-C60	2.31	111.92	108.26
2	C	301	A1BUL	C06-C01-C05	-2.30	138.78	145.10
2	B	301	A1BUL	O61-S58-N57	2.27	111.42	106.83
2	A	301	A1BUL	C13-C14-N16	2.25	121.24	115.70
2	A	301	A1BUL	C40-C29-N28	2.24	121.07	116.62
2	A	301	A1BUL	O15-C14-N16	-2.22	119.19	122.95
2	D	301	A1BUL	C40-C29-N28	2.22	121.02	116.62
2	C	301	A1BUL	F18-C08-F17	2.21	115.73	105.19
2	C	301	A1BUL	F10-C09-C05	-2.19	109.27	112.39
2	A	301	A1BUL	C34-C35-C36	2.17	121.05	118.10
2	B	301	A1BUL	O59-S58-C60	2.16	111.68	108.26
2	D	301	A1BUL	O59-S58-N57	2.16	111.19	106.83
2	C	301	A1BUL	C30-C29-N28	-2.13	120.20	123.09
2	B	301	A1BUL	F11-C09-C05	-2.11	109.39	112.39
2	A	301	A1BUL	F12-C09-C05	-2.09	109.41	112.39
2	A	301	A1BUL	F10-C09-C05	-2.07	109.44	112.39
2	C	301	A1BUL	O59-S58-N57	2.04	110.96	106.83
2	D	301	A1BUL	F51-C50-C49	-2.04	108.19	112.04
2	A	301	A1BUL	C31-C32-C33	2.04	122.86	118.74
2	A	301	A1BUL	O59-S58-C60	2.04	111.48	108.26
2	C	301	A1BUL	C60-S58-N57	2.03	109.86	105.08
2	D	301	A1BUL	O61-S58-N57	2.03	110.92	106.83
2	C	301	A1BUL	C02-N03-N04	-2.02	109.51	111.67
2	B	301	A1BUL	F53-C50-C49	-2.01	108.25	112.04

There are no chirality outliers.

All (55) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	301	A1BUL	N03-C13-C14-N16
2	A	301	A1BUL	N03-C13-C14-O15
2	A	301	A1BUL	C14-C13-N03-C02
2	A	301	A1BUL	C14-C13-N03-N04
2	A	301	A1BUL	N16-C19-C20-C32
2	A	301	A1BUL	N16-C19-C20-N28
2	A	301	A1BUL	C29-C40-C41-C42
2	A	301	A1BUL	C41-C42-S43-O54
2	A	301	A1BUL	C41-C42-S43-O56
2	A	301	A1BUL	C35-C48-N57-S58

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Mol	Chain	Res	Type	Atoms
2	B	301	A1BUL	C41-C42-S43-O54
2	B	301	A1BUL	C41-C42-S43-O56
2	B	301	A1BUL	N46-C49-C50-F51
2	B	301	A1BUL	N46-C49-C50-F52
2	B	301	A1BUL	N46-C49-C50-F53
2	C	301	A1BUL	C41-C42-S43-O54
2	C	301	A1BUL	C41-C42-S43-O56
2	D	301	A1BUL	C20-C19-N16-C14
2	D	301	A1BUL	C29-C40-C41-C42
2	D	301	A1BUL	C41-C42-S43-O54
2	D	301	A1BUL	C41-C42-S43-O56
2	D	301	A1BUL	N46-C49-C50-F51
2	D	301	A1BUL	N46-C49-C50-F52
2	D	301	A1BUL	N46-C49-C50-F53
2	D	301	A1BUL	N03-C13-C14-O15
2	A	301	A1BUL	C21-C19-N16-C14
2	A	301	A1BUL	C01-C05-C09-F11
2	D	301	A1BUL	N03-C13-C14-N16
2	A	301	A1BUL	C01-C05-C09-F10
2	A	301	A1BUL	C01-C05-C09-F12
2	B	301	A1BUL	C01-C05-C09-F10
2	B	301	A1BUL	C01-C05-C09-F12
2	A	301	A1BUL	C20-C19-N16-C14
2	B	301	A1BUL	C01-C05-C09-F11
2	A	301	A1BUL	N04-C05-C09-F11
2	A	301	A1BUL	N04-C05-C09-F10
2	A	301	A1BUL	N04-C05-C09-F12
2	B	301	A1BUL	N04-C05-C09-F12
2	A	301	A1BUL	C19-C21-C22-C23
2	C	301	A1BUL	C29-C40-C41-C42
2	A	301	A1BUL	C48-N57-S58-O59
2	C	301	A1BUL	C48-N57-S58-O59
2	D	301	A1BUL	C48-N57-S58-O59
2	A	301	A1BUL	C45-C42-S43-O54
2	A	301	A1BUL	C45-C42-S43-O56
2	B	301	A1BUL	N04-C05-C09-F10
2	B	301	A1BUL	N04-C05-C09-F11
2	A	301	A1BUL	C19-C21-C22-C27
2	D	301	A1BUL	N47-C48-N57-S58
2	B	301	A1BUL	N28-C29-C40-C41
2	A	301	A1BUL	C48-N57-S58-C60
2	D	301	A1BUL	C35-C48-N57-S58

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Mol	Chain	Res	Type	Atoms
2	C	301	A1BUL	C21-C19-N16-C14
2	C	301	A1BUL	C48-N57-S58-C60
2	A	301	A1BUL	C21-C19-C20-C32

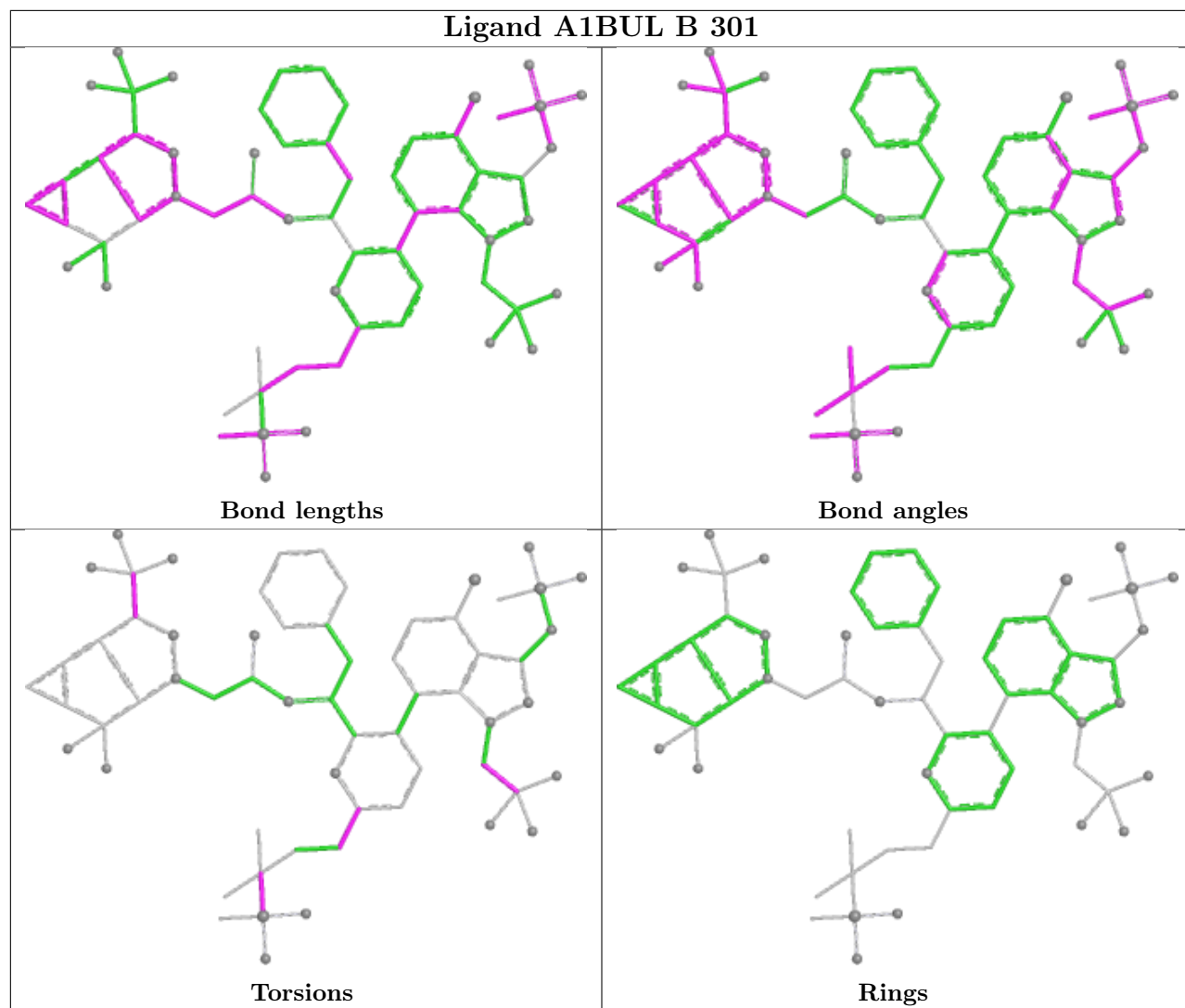
There are no ring outliers.

3 monomers are involved in 3 short contacts:

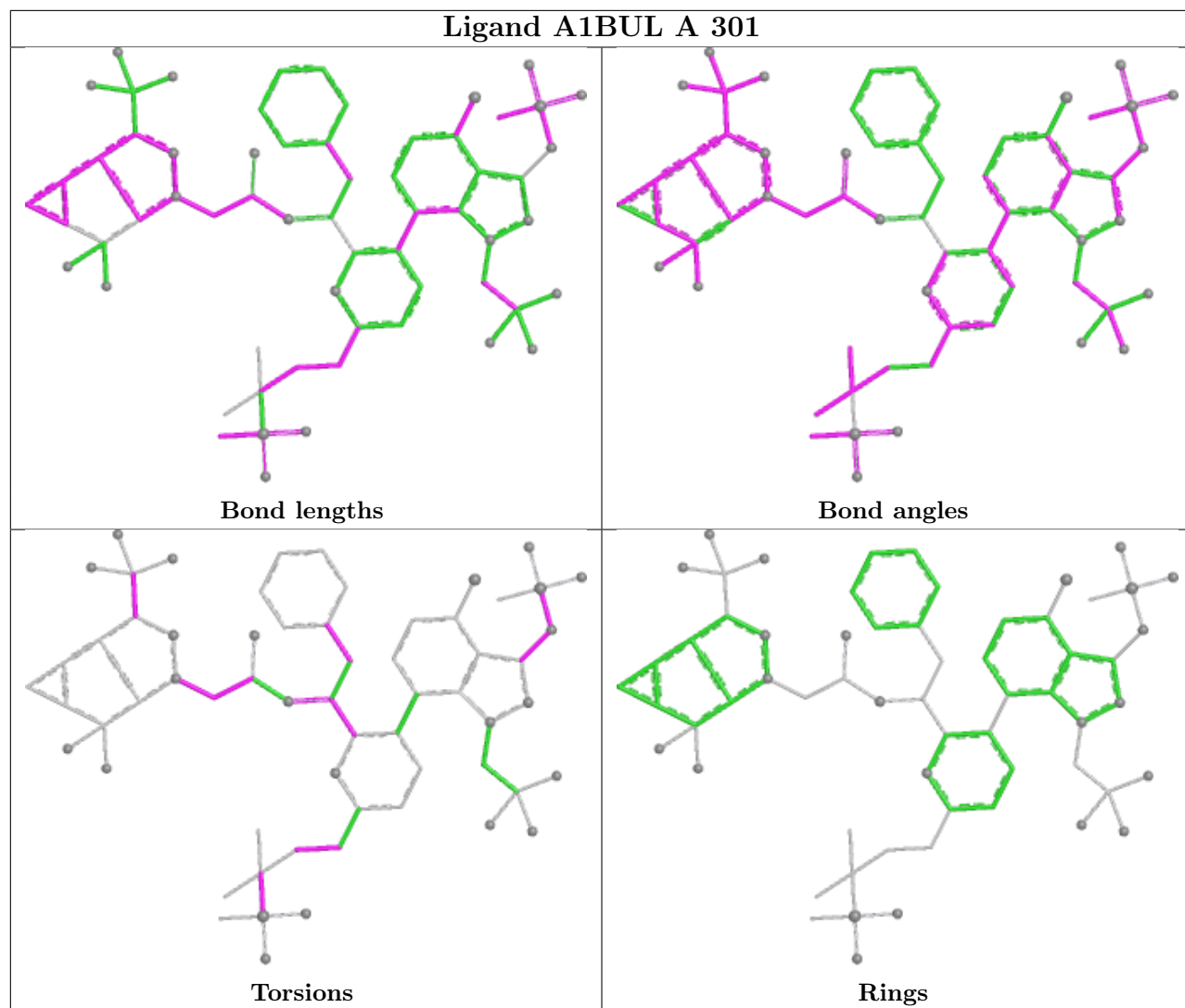
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	A1BUL	1	0
2	C	301	A1BUL	1	0
2	D	301	A1BUL	1	0

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

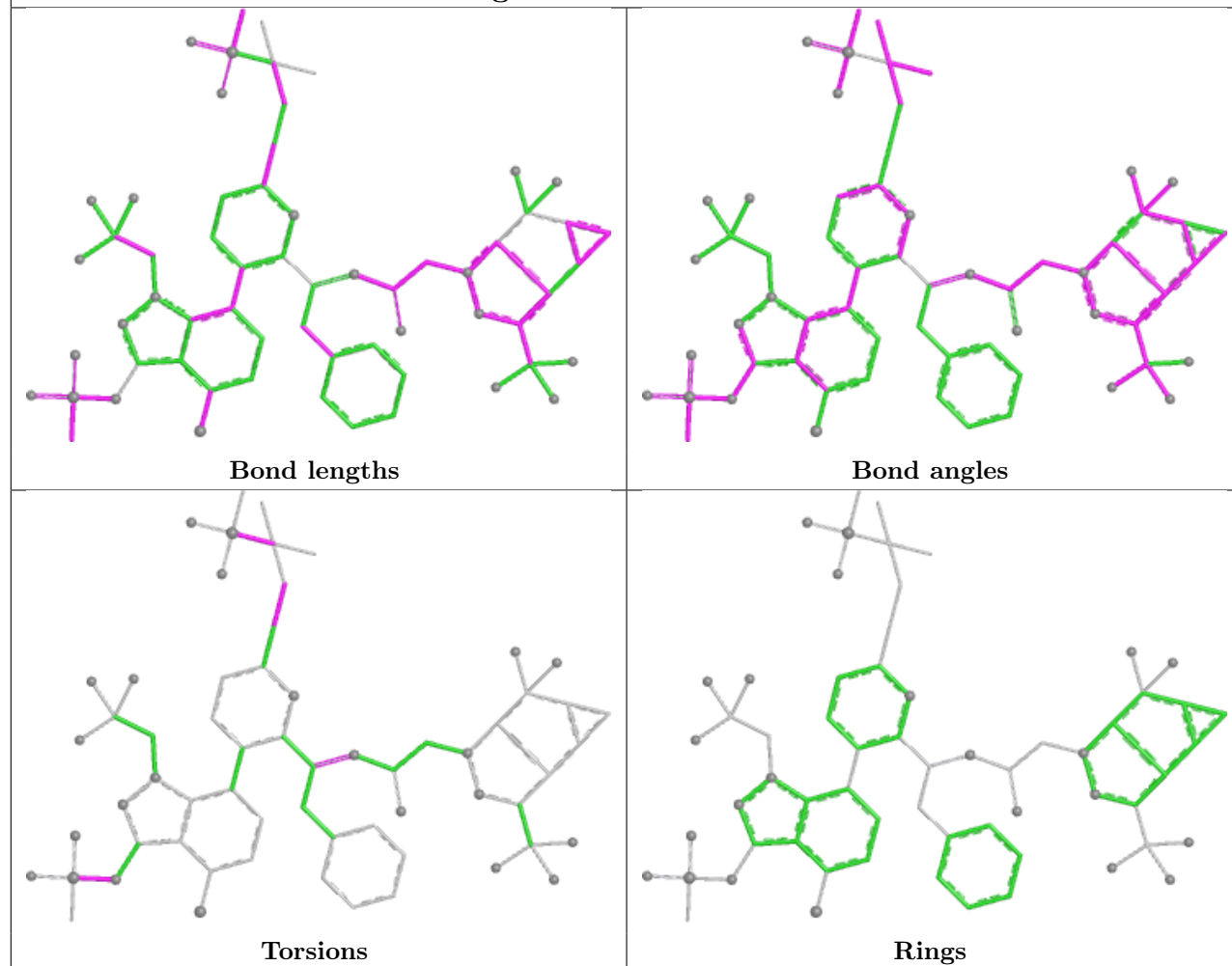
Ligand A1BUL B 301

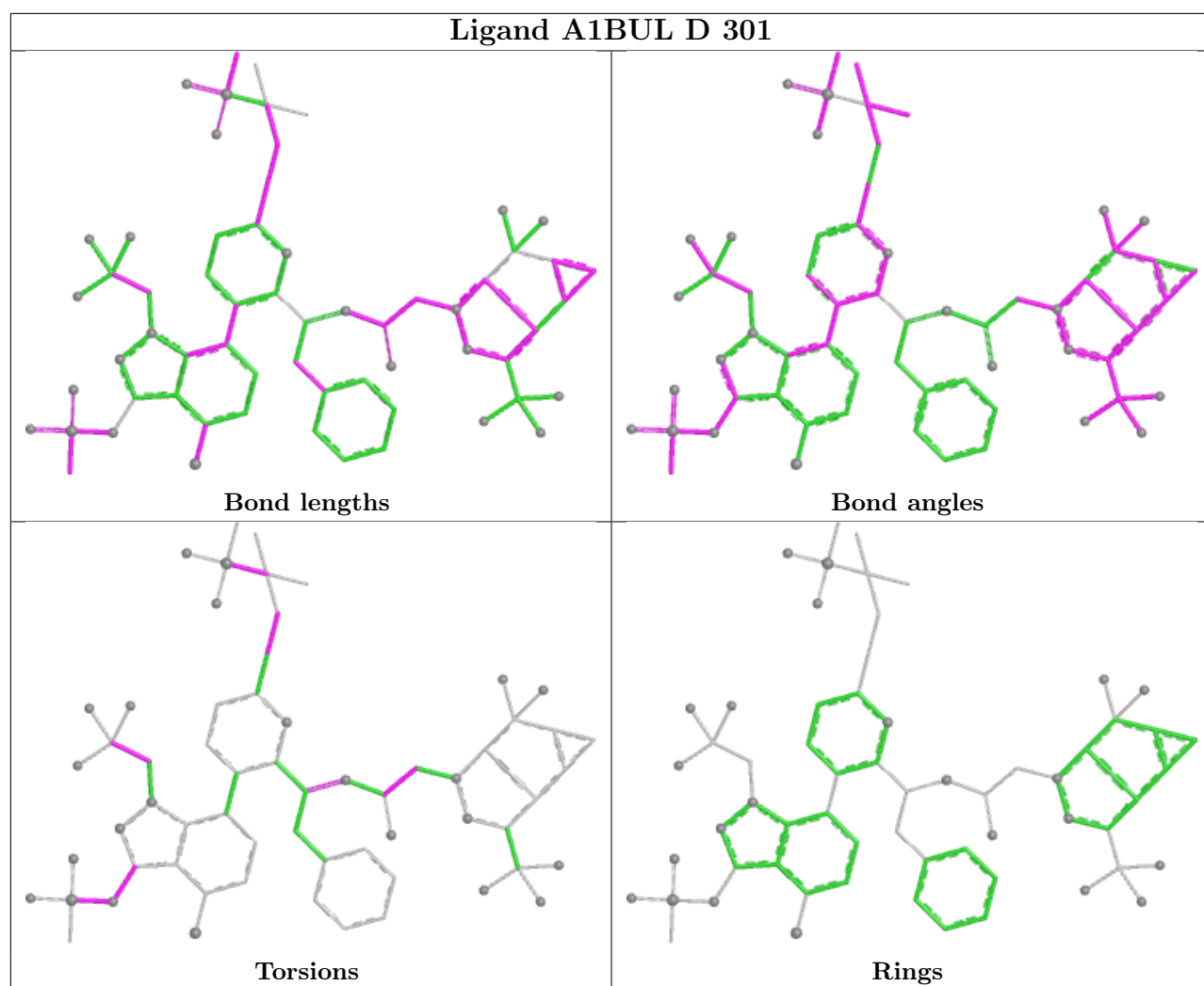


Ligand A1BUL A 301



Ligand A1BUL C 301





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	220/220 (100%)	0.57	11 (5%) 34 20	36, 64, 98, 134	0
1	B	220/220 (100%)	0.41	8 (3%) 46 29	44, 63, 107, 154	0
1	C	220/220 (100%)	0.67	17 (7%) 19 12	46, 69, 114, 171	0
1	D	220/220 (100%)	0.61	16 (7%) 21 13	45, 69, 111, 143	0
All	All	880/880 (100%)	0.57	52 (5%) 28 17	36, 66, 107, 171	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	86	VAL	5.0
1	A	153	ILE	4.3
1	A	198	CYS	4.0
1	C	92	ALA	3.8
1	B	152	ASP	3.7
1	D	92	ALA	3.6
1	C	107	THR	3.3
1	C	94	GLY	3.1
1	A	92	ALA	3.0
1	C	85	PRO	2.9
1	B	94	GLY	2.8
1	B	88	ALA	2.8
1	D	86	VAL	2.7
1	A	91	ILE	2.7
1	D	95	GLN	2.6
1	C	91	ILE	2.6
1	D	205	LEU	2.6
1	A	218	CYS	2.6
1	B	2	ILE	2.6
1	A	168	PHE	2.5
1	D	182	LYS	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	91	ILE	2.4
1	C	186	THR	2.4
1	A	104	ILE	2.4
1	A	211	LEU	2.4
1	A	157	PRO	2.4
1	D	87	HIS	2.3
1	D	152	ASP	2.3
1	C	106	GLY	2.2
1	A	154	ARG	2.2
1	D	85	PRO	2.2
1	D	157	PRO	2.2
1	A	150	ILE	2.2
1	C	118	MET	2.2
1	C	6	LEU	2.2
1	C	54	THR	2.1
1	D	101	GLY	2.1
1	B	113	GLU	2.1
1	C	7	GLN	2.1
1	C	62	HIS	2.1
1	B	57	ASN	2.1
1	D	124	ILE	2.1
1	B	95	GLN	2.1
1	C	99	PRO	2.1
1	C	127	GLY	2.1
1	C	100	ARG	2.1
1	C	198	CYS	2.1
1	D	161	PHE	2.1
1	D	181	VAL	2.0
1	D	211	LEU	2.0
1	D	107	THR	2.0
1	B	86	VAL	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](#)

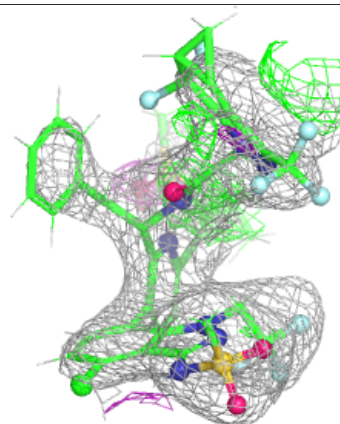
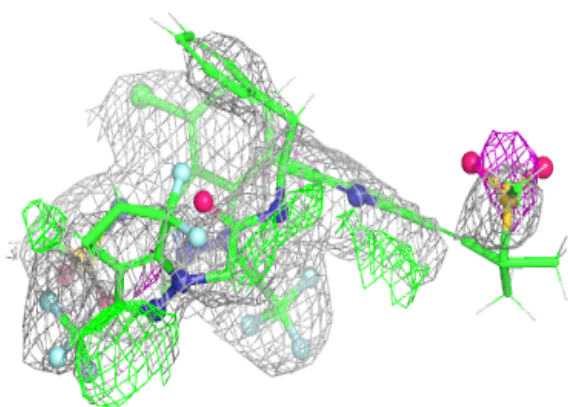
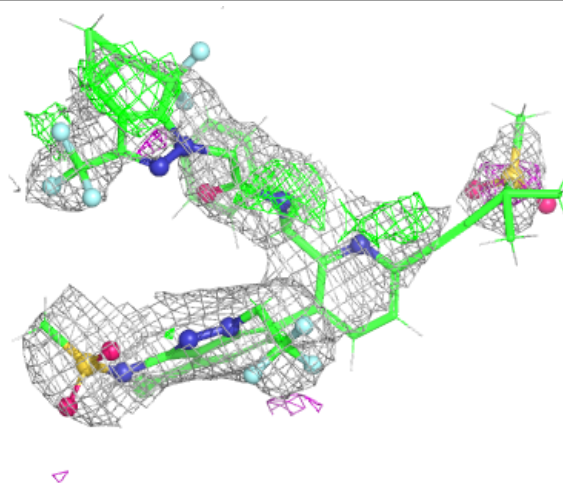
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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
2	A1BUL	C	301	62/62	0.75	0.25	57,64,80,83	96
2	A1BUL	B	301	62/62	0.79	0.17	51,60,73,84	0
2	A1BUL	A	301	62/62	0.82	0.16	42,52,69,76	0
2	A1BUL	D	301	62/62	0.83	0.17	43,57,74,76	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.

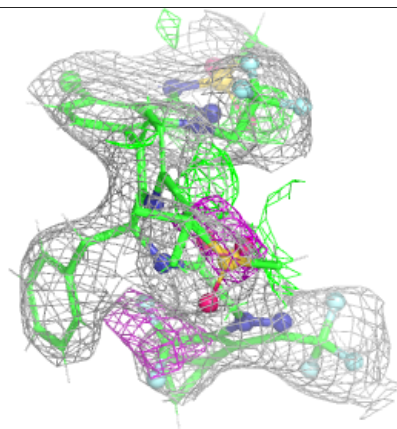
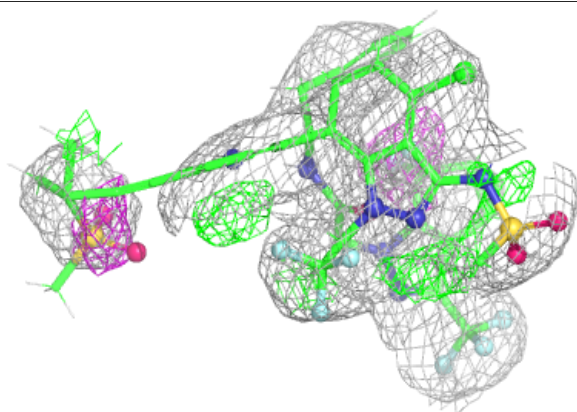
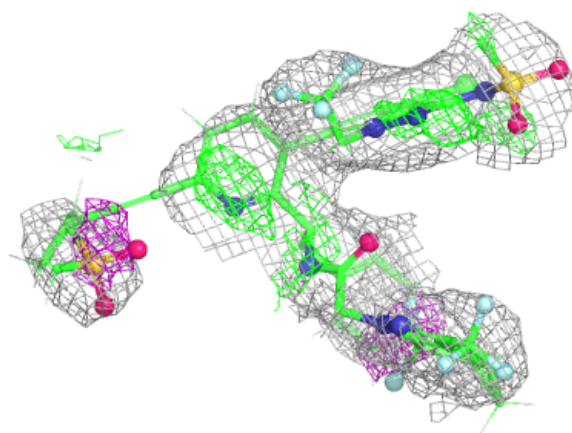
Electron density around A1BUL C 301:

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

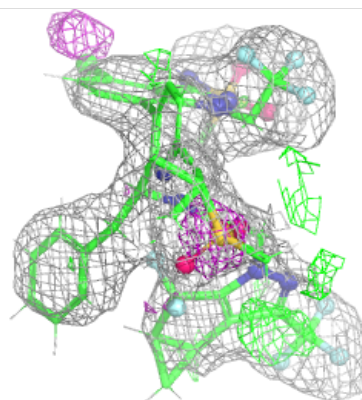
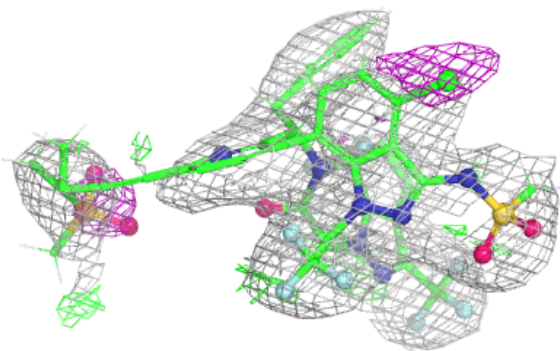
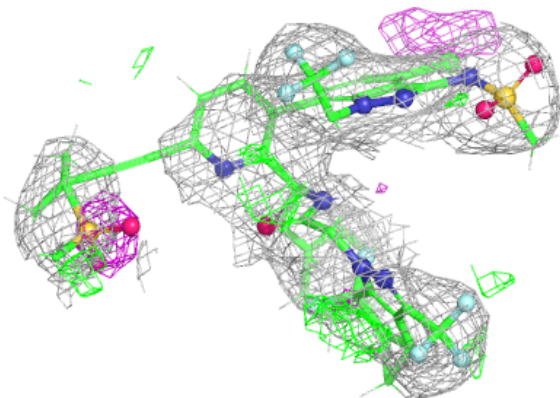


Electron density around A1BUL B 301:

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

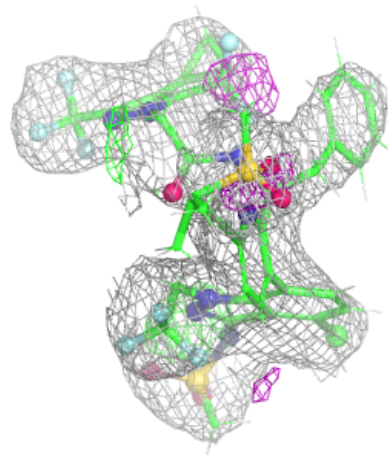
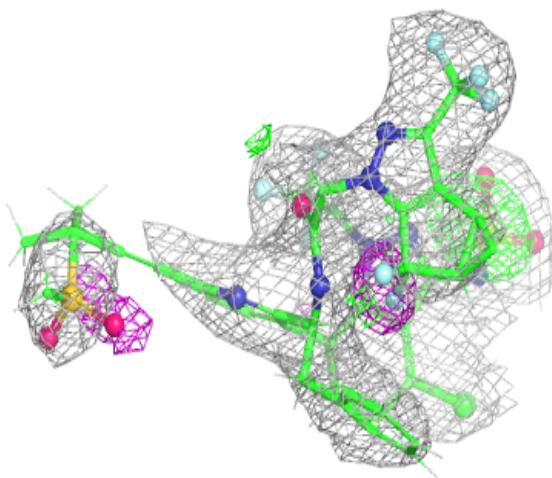
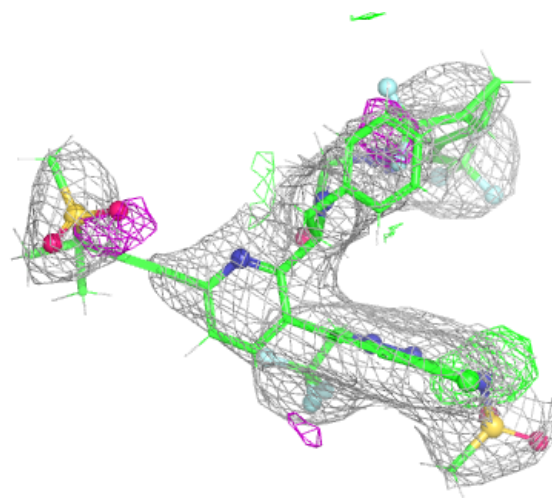
**Electron density around A1BUL A 301:**

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



Electron density around A1BUL 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 [i](#)

There are no such residues in this entry.