



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 09:19 AM UTC

PDB ID : 8QYQ / pdb_00008qyq
Title : Beta-cardiac myosin S1 fragment in the pre-powerstroke state complexed to Mavacamten
Authors : Robert-Paganin, J.; Kikuti, C.; Auguin, D.; Rety, S.; David, A.; Houdusse, A.
Deposited on : 2023-10-26
Resolution : 2.61 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

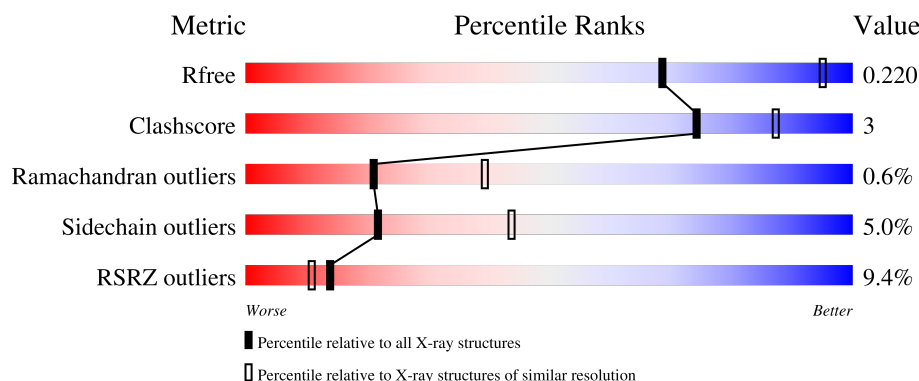
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.61 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	4951 (2.64-2.60)
Clashscore	190562	5303 (2.64-2.60)
Ramachandran outliers	187476	5217 (2.64-2.60)
Sidechain outliers	187428	5217 (2.64-2.60)
RSRZ outliers	180081	4950 (2.64-2.60)

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	807	8% 84% 11% ..
1	B	807	5% 82% 13% 5%
2	C	199	5% 63% 14% .. 21%
3	D	199	27% 36% 6% .. 57%

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 14993 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 Myosin-7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	781	Total	C	N	O	S	0	3	0
			6323	4043	1078	1168	34			
1	B	770	Total	C	N	O	S	0	2	0
			6219	3974	1062	1152	31			

- Molecule 2 is a protein called Myosin light chain 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	157	Total	C	N	O	S	0	0	0
			1240	781	205	244	10			

- Molecule 3 is a protein called Myosin light chain 3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	85	Total	C	N	O	S	0	0	0
			601	370	103	125	3			

There is a discrepancy between the modelled and reference sequences:

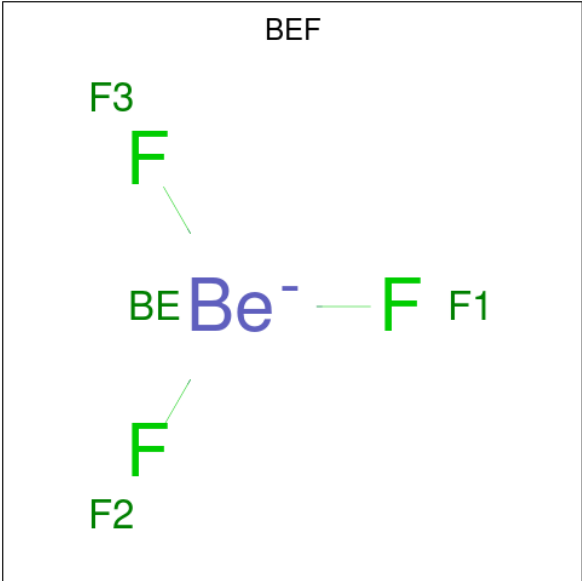
Chain	Residue	Modelled	Actual	Comment	Reference
D	151	VAL	THR	conflict	UNP P85100

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
4	B	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 5 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF₃) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	Be	F	0	0
			4	1	3		

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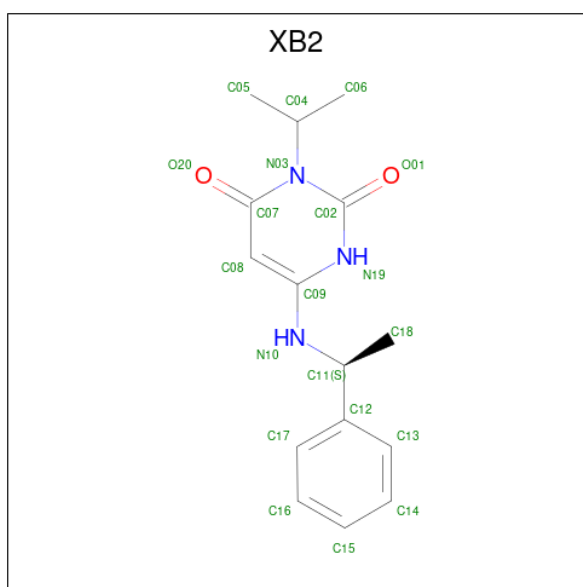
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	B	1	Total	Be	F	0	0
			4	1	3		

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total	Mg	0	0
			1	1		
6	B	1	Total	Mg	0	0
			1	1		

- Molecule 7 is Mavacamten (CCD ID: XB2) (formula: C₁₅H₁₉N₃O₂) (labeled as "Ligand of Interest" by depositor).



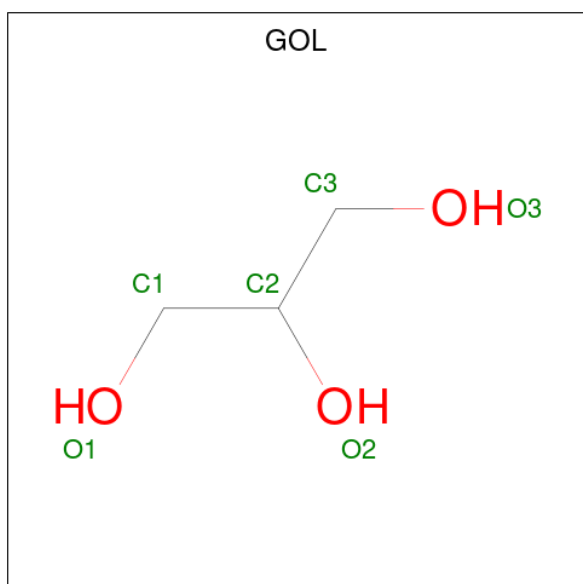
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	A	1	Total	C	N	O	0	0
			20	15	3	2		
7	B	1	Total	C	N	O	0	0
			20	15	3	2		

- Molecule 8 is FORMIC ACID (CCD ID: FMT) (formula: CH₂O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	A	1	Total	C	O	0	0
			3	1	2		
8	A	1	Total	C	O	0	0
			3	1	2		
8	A	1	Total	C	O	0	0
			3	1	2		
8	B	1	Total	C	O	0	0
			3	1	2		
8	B	1	Total	C	O	0	0
			3	1	2		

- Molecule 9 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	C	1	Total	C	O	0	0
			6	3	3		

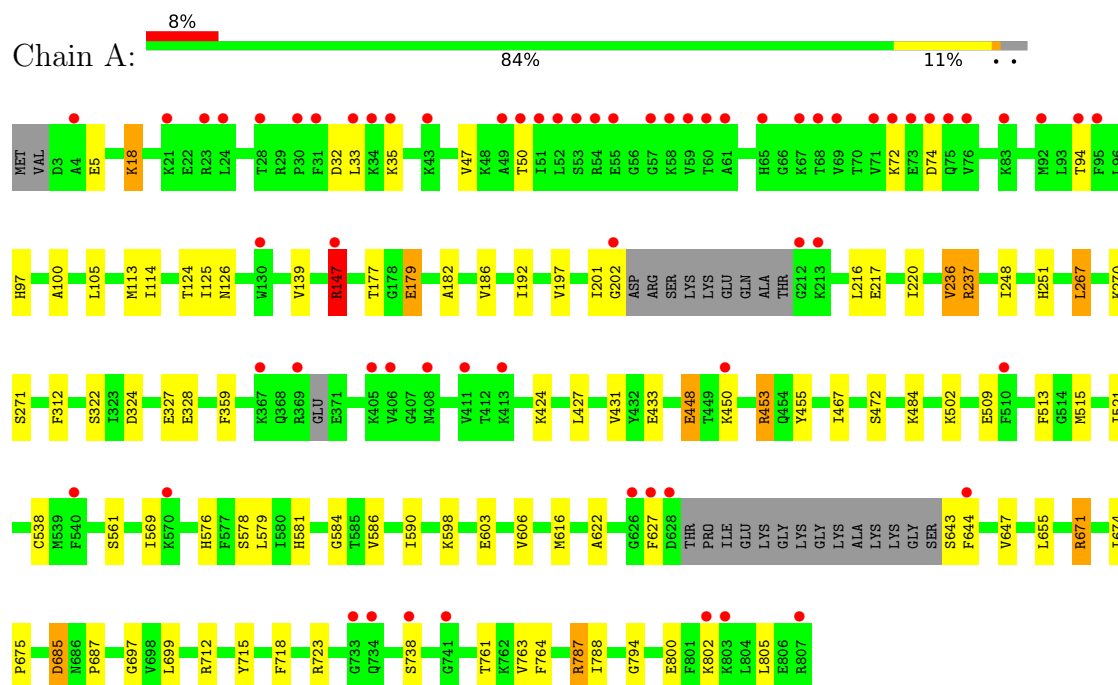
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	228	Total	O	0	0
			228	228		
10	B	242	Total	O	0	0
			242	242		
10	C	14	Total	O	0	0
			14	14		
10	D	1	Total	O	0	0
			1	1		

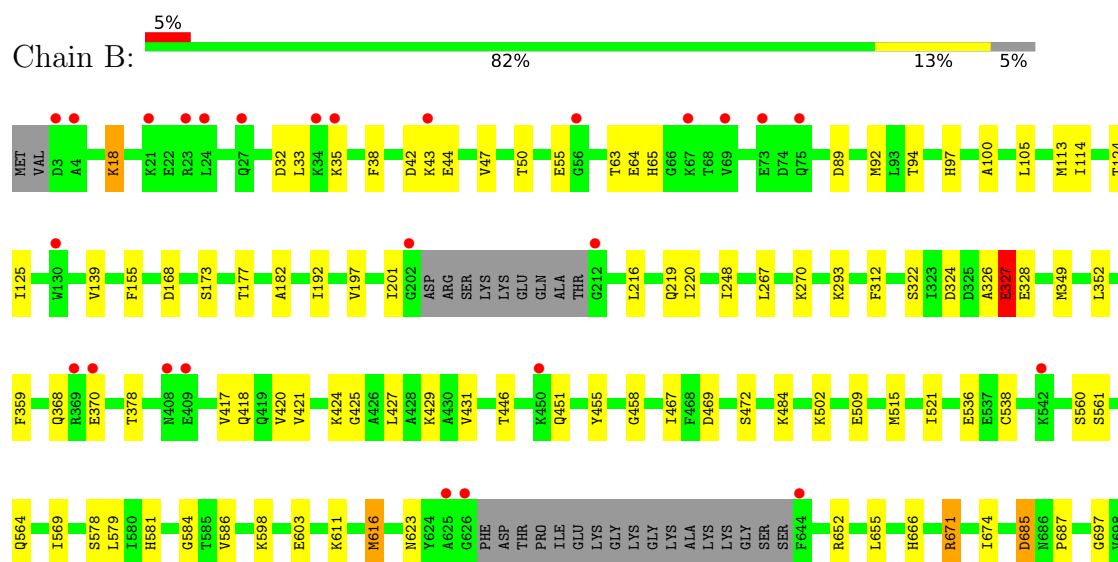
3 Residue-property plots [i](#)

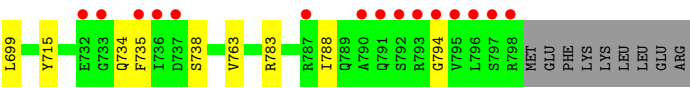
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Myosin-7

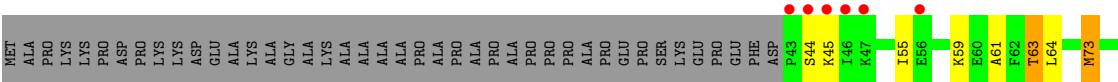


• Molecule 1: Myosin-7

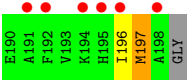
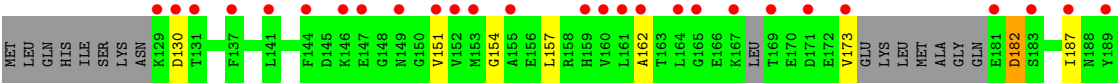
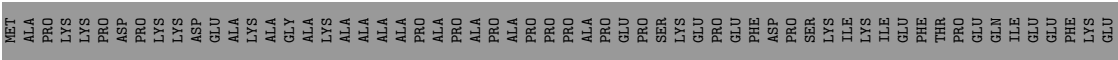
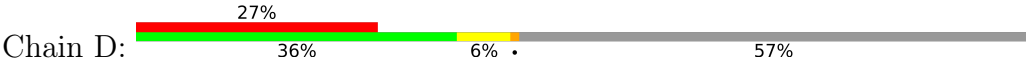




● Molecule 2: Myosin light chain 3



● Molecule 3: Myosin light chain 3



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	102.80Å 147.98Å 116.75Å 90.00° 91.62° 90.00°	Depositor
Resolution (Å)	91.64 – 2.61 91.64 – 2.61	Depositor EDS
% Data completeness (in resolution range)	66.0 (91.64-2.61) 66.0 (91.64-2.61)	Depositor EDS
R_{merge}	0.20	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.25 (at 2.62Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.178 , 0.217 0.185 , 0.220	Depositor DCC
R_{free} test set	3478 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	50.1	Xtriage
Anisotropy	0.106	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 79.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	14993	wwPDB-VP
Average B, all atoms (Å ²)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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: GOL, M3L, FMT, MG, ADP, BEF, XB2

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	0.86	1/6431 (0.0%)	1.36	24/8662 (0.3%)
1	B	0.86	1/6326 (0.0%)	1.36	25/8528 (0.3%)
2	C	0.86	0/1260	1.41	4/1690 (0.2%)
3	D	0.81	0/605	1.50	1/813 (0.1%)
All	All	0.86	2/14622 (0.0%)	1.37	54/19693 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	674	ILE	CA-C	6.75	1.58	1.53
1	A	674	ILE	CA-C	5.21	1.57	1.53

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	182	ASP	CA-CB-CG	8.37	120.97	112.60
1	B	424	LYS	N-CA-C	-7.41	98.49	110.20
2	C	107	GLU	N-CA-C	-7.12	105.12	113.88
1	A	179	GLU	CB-CG-CD	6.93	124.39	112.60
1	A	509	GLU	CB-CG-CD	6.86	124.25	112.60
1	B	155	PHE	CA-CB-CG	6.77	120.57	113.80
1	B	44	GLU	N-CA-C	-6.76	102.10	110.41
1	A	74	ASP	CA-C-N	6.63	129.49	120.54
1	A	74	ASP	C-N-CA	6.63	129.49	120.54
1	A	74	ASP	CA-CB-CG	6.32	118.92	112.60
1	A	472	SER	CA-C-N	6.22	128.90	120.38
1	A	472	SER	C-N-CA	6.22	128.90	120.38
1	A	685	ASP	CA-CB-CG	6.12	118.72	112.60
1	B	502	LYS	CA-C-N	6.02	128.63	120.38
1	B	502	LYS	C-N-CA	6.02	128.63	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	763	VAL	N-CA-CB	5.93	117.18	110.72
1	B	327	GLU	CB-CG-CD	5.73	122.34	112.60
1	A	718	PHE	CA-C-N	5.66	127.79	120.44
1	A	718	PHE	C-N-CA	5.66	127.79	120.44
1	A	622	ALA	CA-C-N	5.63	128.39	120.28
1	A	622	ALA	C-N-CA	5.63	128.39	120.28
1	B	685	ASP	CA-CB-CG	5.62	118.22	112.60
1	B	560	SER	CA-C-N	5.61	128.06	120.38
1	B	560	SER	C-N-CA	5.61	128.06	120.38
1	A	502	LYS	CA-C-N	5.55	127.99	120.38
1	A	502	LYS	C-N-CA	5.55	127.99	120.38
1	A	236	VAL	N-CA-CB	5.50	116.98	110.55
1	B	312	PHE	CA-CB-CG	5.45	119.25	113.80
1	B	469	ASP	N-CA-C	-5.45	106.13	112.89
1	B	370	GLU	N-CA-C	5.43	117.77	109.95
1	A	271	SER	CA-C-N	5.31	127.39	120.28
1	A	271	SER	C-N-CA	5.31	127.39	120.28
1	A	794	GLY	CA-C-N	5.31	127.19	120.72
1	A	794	GLY	C-N-CA	5.31	127.19	120.72
1	A	450	LYS	CA-C-N	5.31	127.77	120.39
1	A	450	LYS	C-N-CA	5.31	127.77	120.39
1	B	794	GLY	CA-C-N	5.24	127.11	120.72
1	B	794	GLY	C-N-CA	5.24	127.11	120.72
1	B	38	PHE	CA-CB-CG	5.22	119.03	113.80
1	A	788	ILE	N-CA-C	-5.22	105.62	110.53
2	C	174	GLU	CA-C-N	5.20	127.25	120.28
2	C	174	GLU	C-N-CA	5.20	127.25	120.28
1	B	44	GLU	CA-C-N	-5.18	111.98	121.52
1	B	44	GLU	C-N-CA	-5.18	111.98	121.52
1	A	182	ALA	N-CA-C	5.18	116.73	111.14
1	A	312	PHE	CA-CB-CG	5.17	118.97	113.80
1	B	788	ILE	N-CA-C	-5.16	105.82	110.82
1	B	420	VAL	CA-C-N	5.10	127.45	120.46
1	B	420	VAL	C-N-CA	5.10	127.45	120.46
2	C	188	ASN	N-CA-C	-5.08	100.79	108.67
1	B	182	ALA	N-CA-C	5.06	116.61	111.14
1	B	168	ASP	CA-CB-CG	5.06	117.66	112.60
1	B	472	SER	CA-C-N	5.02	127.26	120.38
1	B	472	SER	C-N-CA	5.02	127.26	120.38

There are no chirality outliers.

There are no planarity outliers.

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	6323	0	6298	38	0
1	B	6219	0	6190	34	0
2	C	1240	0	1226	16	0
3	D	601	0	522	5	0
4	A	27	0	12	1	0
4	B	27	0	12	0	0
5	A	4	0	0	0	0
5	B	4	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
7	A	20	0	0	0	0
7	B	20	0	0	0	0
8	A	9	0	6	1	0
8	B	6	0	4	0	0
9	C	6	0	8	0	0
10	A	228	0	0	2	0
10	B	242	0	0	0	0
10	C	14	0	0	0	0
10	D	1	0	0	0	0
All	All	14993	0	14278	88	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 3.

All (88) 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:B:89:ASP:HB3	1:B:92:MET:HE2	1.66	0.78
2:C:154:GLY:HA2	2:C:187:ILE:HD12	1.71	0.72
1:A:513:PHE:H	8:A:1005:FMT:H	1.55	0.72
3:D:154:GLY:HA2	3:D:187:ILE:HD12	1.73	0.70
1:A:251:HIS:HB3	1:A:453:ARG:HG2	1.73	0.69
2:C:61:ALA:HA	2:C:64:LEU:HD12	1.79	0.62
1:B:417:VAL:O	1:B:421:VAL:HG23	2.01	0.61
1:B:349:MET:HG2	1:B:616:MET:HE1	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:GLU:HB3	1:A:237:ARG:NH2	2.18	0.58
1:A:147:ARG:HD3	10:A:1105:HOH:O	2.04	0.58
1:A:179:GLU:HB3	1:A:237:ARG:HH21	1.68	0.58
1:B:538:CYS:HA	1:B:598:LYS:HE2	1.88	0.56
1:B:192:ILE:HD11	1:B:248:ILE:HD13	1.87	0.56
1:A:685:ASP:OD1	1:A:687:PRO:HD2	2.08	0.54
1:A:627:PHE:HB2	1:A:644:PHE:H	1.71	0.54
1:A:538:CYS:HA	1:A:598:LYS:HE2	1.90	0.54
2:C:142:ARG:HG3	2:C:189:TYR:OH	2.07	0.54
1:A:192:ILE:HD11	1:A:248:ILE:HD13	1.91	0.53
1:B:685:ASP:OD1	1:B:687:PRO:HD2	2.07	0.53
1:A:202:GLY:HA3	10:A:1319:HOH:O	2.08	0.53
1:A:715:TYR:CE1	1:A:763:VAL:HG22	2.44	0.52
1:A:324:ASP:O	1:A:328:GLU:HG2	2.08	0.52
1:B:324:ASP:O	1:B:328:GLU:HG2	2.09	0.51
1:A:715:TYR:HB3	1:A:738:SER:HB3	1.92	0.51
1:A:761:THR:HG22	1:B:378:THR:HG23	1.92	0.51
3:D:157:LEU:HD23	3:D:187:ILE:HD13	1.93	0.51
2:C:157:LEU:HD23	2:C:187:ILE:HD13	1.93	0.50
1:B:734:GLN:HG2	1:B:735:PHE:N	2.26	0.49
1:B:35:LYS:HB3	1:B:50:THR:HG23	1.93	0.49
1:A:35:LYS:HB3	1:A:50:THR:HG23	1.95	0.49
2:C:158:ARG:HH12	2:C:174:GLU:HA	1.78	0.48
1:A:216:LEU:O	1:A:220:ILE:HG13	2.13	0.47
3:D:162:ALA:HB2	3:D:173:VAL:HG21	1.97	0.47
1:A:427:LEU:O	1:A:431:VAL:HG23	2.14	0.47
1:B:216:LEU:O	1:B:220:ILE:HG13	2.15	0.47
1:A:105:LEU:HB3	1:A:125:ILE:HD11	1.97	0.46
1:B:715:TYR:HB3	1:B:738:SER:HB3	1.96	0.46
2:C:100:LEU:HD23	2:C:121:MET:HE1	1.98	0.46
1:A:177:THR:OG1	1:A:671:ARG:HD2	2.15	0.46
1:B:425:GLY:O	1:B:429:LYS:HG3	2.15	0.46
1:B:611:LYS:HB3	2:C:147:GLU:HB2	1.96	0.46
1:B:32:ASP:HB3	1:B:35:LYS:HB2	1.97	0.46
1:B:427:LEU:O	1:B:431:VAL:HG23	2.16	0.46
2:C:63:THR:HG23	2:C:73:MET:SD	2.56	0.45
1:A:32:ASP:HB3	1:A:35:LYS:HB2	1.98	0.45
1:B:63:THR:C	1:B:65:HIS:H	2.24	0.45
1:A:186:VAL:HG11	4:A:1001:ADP:C5	2.52	0.45
1:B:219:GLN:NE2	1:B:446:THR:HG22	2.32	0.44
1:B:97:HIS:CE1	1:B:100:ALA:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:515:MET:HE2	1:B:697:GLY:HA3	2.00	0.43
1:A:267:LEU:HD11	1:A:647:VAL:HG13	2.00	0.43
1:B:89:ASP:HB3	1:B:92:MET:CE	2.44	0.43
1:B:293:LYS:HD3	1:B:326:ALA:HB1	2.00	0.43
1:A:627:PHE:HD2	1:A:643:SER:N	2.16	0.43
1:A:712:ARG:HD3	1:A:764:PHE:CE2	2.53	0.43
1:B:352:LEU:HD12	1:B:616:MET:HE2	2.01	0.43
3:D:197:MET:HE3	3:D:197:MET:HB3	1.95	0.43
1:A:787:ARG:HD3	2:C:131:THR:HA	2.00	0.43
1:A:448:GLU:O	1:A:448:GLU:HG2	2.19	0.43
1:A:18:LYS:HD3	1:A:113:MET:HE1	2.01	0.43
1:B:173:SER:HA	1:B:458:GLY:O	2.19	0.42
1:A:114:ILE:O	1:A:124:THR:HA	2.19	0.42
1:B:105:LEU:HB3	1:B:125:ILE:HD11	2.00	0.42
2:C:90:ASN:ND2	2:C:90:ASN:N	2.67	0.42
3:D:85:ARG:HA	3:D:89:GLN:O	2.19	0.42
1:B:581:HIS:HB2	1:B:584:GLY:O	2.19	0.42
1:B:564:GLN:HB2	1:B:578:SER:OG	2.20	0.42
1:A:97:HIS:CE1	1:A:100:ALA:HB2	2.55	0.42
1:A:467:ILE:HG12	1:A:586:VAL:HG22	2.02	0.42
1:B:324:ASP:OD2	1:B:327:GLU:HG2	2.19	0.42
1:A:581:HIS:HB2	1:A:584:GLY:O	2.20	0.41
2:C:85:ARG:HA	2:C:89:GLN:O	2.19	0.41
2:C:134:TYR:CE1	2:C:194:LYS:HG3	2.55	0.41
1:B:114:ILE:O	1:B:124:THR:HA	2.19	0.41
1:A:139:VAL:HG11	1:A:197:VAL:HB	2.02	0.41
1:A:515:MET:HE2	1:A:697:GLY:HA3	2.03	0.41
1:B:467:ILE:HG12	1:B:586:VAL:HG22	2.03	0.41
1:B:18:LYS:HD3	1:B:113:MET:HE1	2.01	0.41
1:B:177:THR:OG1	1:B:671:ARG:HD2	2.21	0.41
2:C:99:VAL:HB	2:C:121:MET:HG2	2.02	0.41
1:A:723:ARG:HH22	2:C:135:GLU:CG	2.34	0.41
1:A:802:LYS:HA	1:A:805:LEU:HD12	2.03	0.41
1:A:576:HIS:ND1	1:A:590:ILE:HG13	2.36	0.41
1:A:723:ARG:HH22	2:C:135:GLU:HG2	1.86	0.41
1:A:126:ASN:HB3	1:A:675:PRO:HD3	2.03	0.41
1:B:139:VAL:HG11	1:B:197:VAL:HB	2.02	0.40
1:B:734:GLN:HG2	1:B:735:PHE:H	1.85	0.40
2:C:55:ILE:HG12	2:C:119:LEU:HD21	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	774/807 (96%)	742 (96%)	28 (4%)	4 (0%)	24	44
1	B	764/807 (95%)	736 (96%)	23 (3%)	5 (1%)	18	35
2	C	155/199 (78%)	148 (96%)	6 (4%)	1 (1%)	21	39
3	D	77/199 (39%)	76 (99%)	1 (1%)	0	100	100
All	All	1770/2012 (88%)	1702 (96%)	58 (3%)	10 (1%)	21	39

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	201	ILE
1	A	267	LEU
1	B	55	GLU
1	B	267	LEU
1	A	72	LYS
1	B	201	ILE
1	B	43	LYS
2	C	44	SER
1	B	64	GLU
1	A	147	ARG

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	677/695 (97%)	645 (95%)	32 (5%)	23	46

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	665/695 (96%)	636 (96%)	29 (4%)	25	48
2	C	136/165 (82%)	127 (93%)	9 (7%)	15	32
3	D	54/165 (33%)	48 (89%)	6 (11%)	6	11
All	All	1532/1720 (89%)	1456 (95%)	76 (5%)	22	44

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	GLU
1	A	18	LYS
1	A	33	LEU
1	A	47	VAL
1	A	94	THR
1	A	147	ARG
1	A	217	GLU
1	A	236	VAL
1	A	237	ARG
1	A	270	LYS
1	A	322	SER
1	A	327	GLU
1	A	359	PHE
1	A	424	LYS
1	A	433	GLU
1	A	448	GLU
1	A	453	ARG
1	A	455	TYR
1	A	484	LYS
1	A	521	ILE
1	A	561	SER
1	A	569	ILE
1	A	578	SER
1	A	579	LEU
1	A	603	GLU
1	A	606	VAL
1	A	616	MET
1	A	655	LEU
1	A	671	ARG
1	A	699	LEU
1	A	787	ARG
1	A	800	GLU
1	B	18	LYS

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Mol	Chain	Res	Type
1	B	33	LEU
1	B	42	ASP
1	B	47	VAL
1	B	94	THR
1	B	270	LYS
1	B	322	SER
1	B	327	GLU
1	B	359	PHE
1	B	368	GLN
1	B	418	GLN
1	B	451	GLN
1	B	455	TYR
1	B	484	LYS
1	B	509	GLU
1	B	521	ILE
1	B	536	GLU
1	B	561	SER
1	B	569	ILE
1	B	579	LEU
1	B	603	GLU
1	B	616	MET
1	B	623	ASN
1	B	652	ARG
1	B	655	LEU
1	B	666	HIS
1	B	671	ARG
1	B	699	LEU
1	B	783	ARG
2	C	45	LYS
2	C	59	LYS
2	C	63	THR
2	C	73	MET
2	C	82	ASP
2	C	90	ASN
2	C	130	ASP
2	C	151	THR
2	C	174	GLU
3	D	92	THR
3	D	130	ASP
3	D	151	VAL
3	D	182	ASP
3	D	196	ILE

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Mol	Chain	Res	Type
3	D	197	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	187	ASN
1	A	193	GLN
1	A	418	GLN
1	A	595	GLN
1	A	666	HIS
1	A	696	ASN
1	A	726	ASN
1	B	75	GLN
1	B	160	ASN
1	B	187	ASN
1	B	193	GLN
1	B	562	ASN
1	B	595	GLN
1	B	666	HIS
1	B	696	ASN
2	C	105	GLN
2	C	149	ASN
3	D	93	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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
1	M3L	B	129	1	10,11,12	0.78	0	9,14,16	0.79	0
1	M3L	A	129	1	10,11,12	0.63	0	9,14,16	0.81	0
1	M3L	A	549	1	10,11,12	0.45	0	9,14,16	0.47	0
1	M3L	B	549	1	10,11,12	0.43	0	9,14,16	0.50	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
1	M3L	B	129	1	-	0/9/10/12	-
1	M3L	A	129	1	-	0/9/10/12	-
1	M3L	A	549	1	-	1/9/10/12	-
1	M3L	B	549	1	-	1/9/10/12	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	549	M3L	CA-CB-CG-CD
1	B	549	M3L	CA-CB-CG-CD

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates

There are no oligosaccharides in this entry.

5.6 Ligand geometry

Of 14 ligands modelled in this entry, 2 are monoatomic - leaving 12 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	FMT	A	1005	-	2,2,2	1.30	0	1,1,1	1.06	0
5	BEF	B	1002	4	0,3,3	-	-	-	-	-
8	FMT	B	1004	-	2,2,2	1.21	0	1,1,1	1.04	0
8	FMT	A	1006	-	2,2,2	1.41	0	1,1,1	1.09	0
9	GOL	C	201	-	5,5,5	0.14	0	5,5,5	0.34	0
4	ADP	B	1001	6,5	28,29,29	0.63	1 (3%)	43,45,45	0.43	0
8	FMT	A	1007	-	2,2,2	1.45	0	1,1,1	0.79	0
8	FMT	B	1005	-	2,2,2	1.41	0	1,1,1	1.02	0
4	ADP	A	1001	6,5	28,29,29	0.38	0	43,45,45	0.59	1 (2%)
7	XB2	B	1003	-	19,21,21	4.13	6 (31%)	26,29,29	1.85	8 (30%)
5	BEF	A	1002	4	0,3,3	-	-	-	-	-
7	XB2	A	1004	-	19,21,21	4.10	6 (31%)	26,29,29	1.68	5 (19%)

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
7	XB2	A	1004	-	-	0/10/12/12	0/2/2/2
4	ADP	B	1001	6,5	-	2/16/32/32	0/3/3/3
4	ADP	A	1001	6,5	-	2/16/32/32	0/3/3/3
7	XB2	B	1003	-	-	0/10/12/12	0/2/2/2
9	GOL	C	201	-	-	0/4/4/4	-

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	B	1003	XB2	O01-C02	14.45	1.48	1.23
7	A	1004	XB2	O01-C02	14.02	1.47	1.23
7	A	1004	XB2	O20-C07	7.76	1.40	1.23
7	B	1003	XB2	O20-C07	7.39	1.39	1.23
7	A	1004	XB2	C13-C12	4.66	1.46	1.39
7	B	1003	XB2	C13-C12	4.23	1.45	1.39
7	A	1004	XB2	C16-C15	3.68	1.46	1.38
7	B	1003	XB2	C16-C15	3.54	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	1004	XB2	C02-N03	-3.20	1.32	1.38
7	B	1003	XB2	C02-N03	-2.63	1.33	1.38
7	B	1003	XB2	C07-N03	-2.41	1.36	1.40
4	B	1001	ADP	PB-O2B	-2.30	1.46	1.54
7	A	1004	XB2	C07-N03	-2.30	1.36	1.40

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	B	1003	XB2	N19-C02-N03	4.39	121.22	115.66
7	A	1004	XB2	N19-C02-N03	4.21	120.99	115.66
7	B	1003	XB2	C08-C07-N03	3.65	120.92	115.28
7	A	1004	XB2	C08-C07-N03	3.46	120.62	115.28
7	A	1004	XB2	C07-C08-C09	-3.36	116.62	121.02
7	B	1003	XB2	O20-C07-C08	-3.07	118.04	125.61
7	B	1003	XB2	C07-C08-C09	-3.01	117.07	121.02
7	A	1004	XB2	C06-C04-N03	-2.70	107.91	111.69
7	A	1004	XB2	C05-C04-N03	2.66	115.41	111.69
7	B	1003	XB2	O01-C02-N19	-2.58	116.73	121.49
7	B	1003	XB2	C17-C12-C13	2.43	121.31	118.30
7	B	1003	XB2	C18-C11-C12	-2.41	106.55	112.22
7	B	1003	XB2	C04-N03-C02	2.33	122.49	117.43
4	A	1001	ADP	O3B-PB-O2B	2.19	116.01	107.80

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	1001	ADP	PA-O3A-PB-O3B
4	B	1001	ADP	PA-O3A-PB-O3B
4	A	1001	ADP	PA-O3A-PB-O1B
4	B	1001	ADP	PA-O3A-PB-O1B

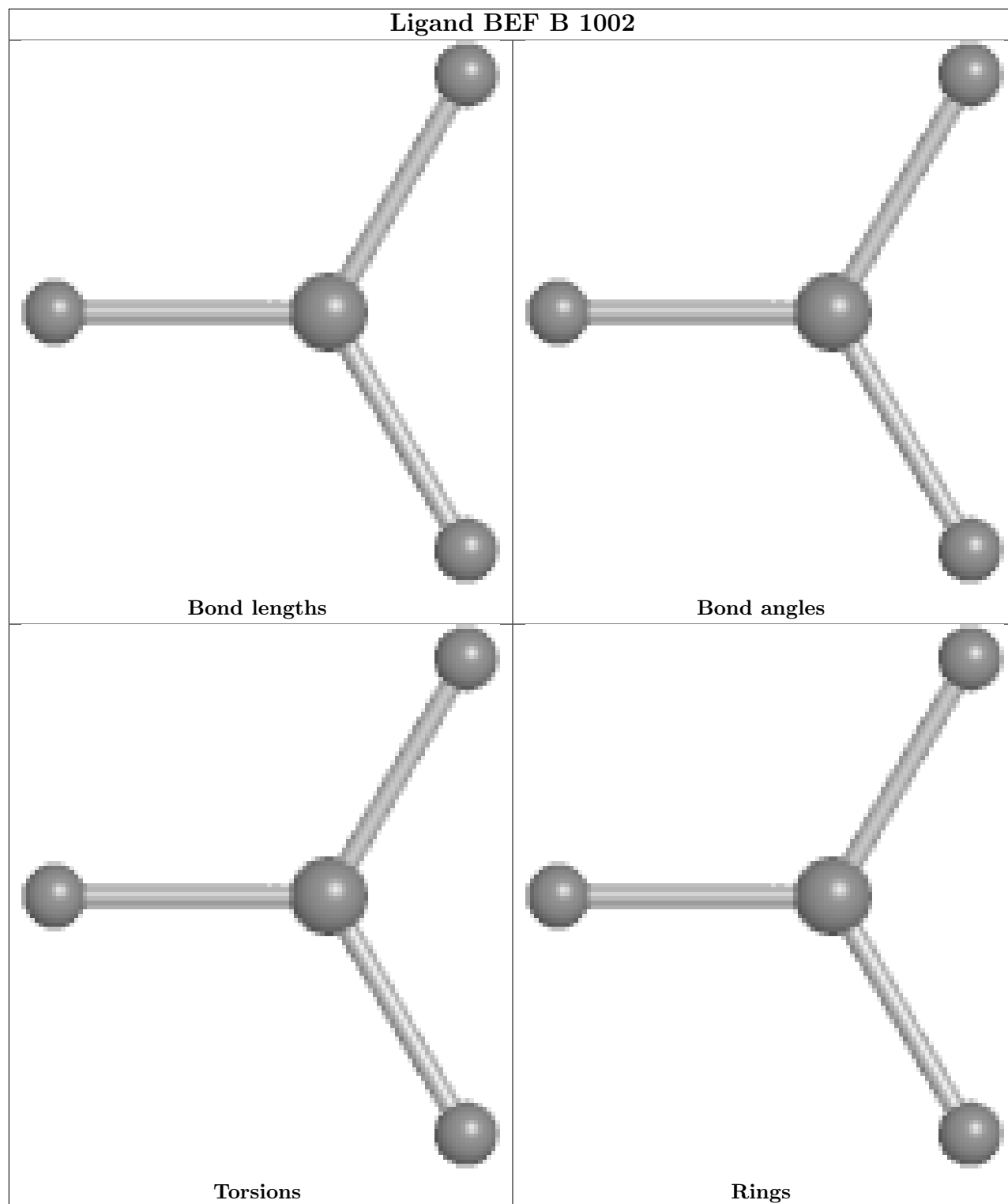
There are no ring outliers.

2 monomers are involved in 2 short contacts:

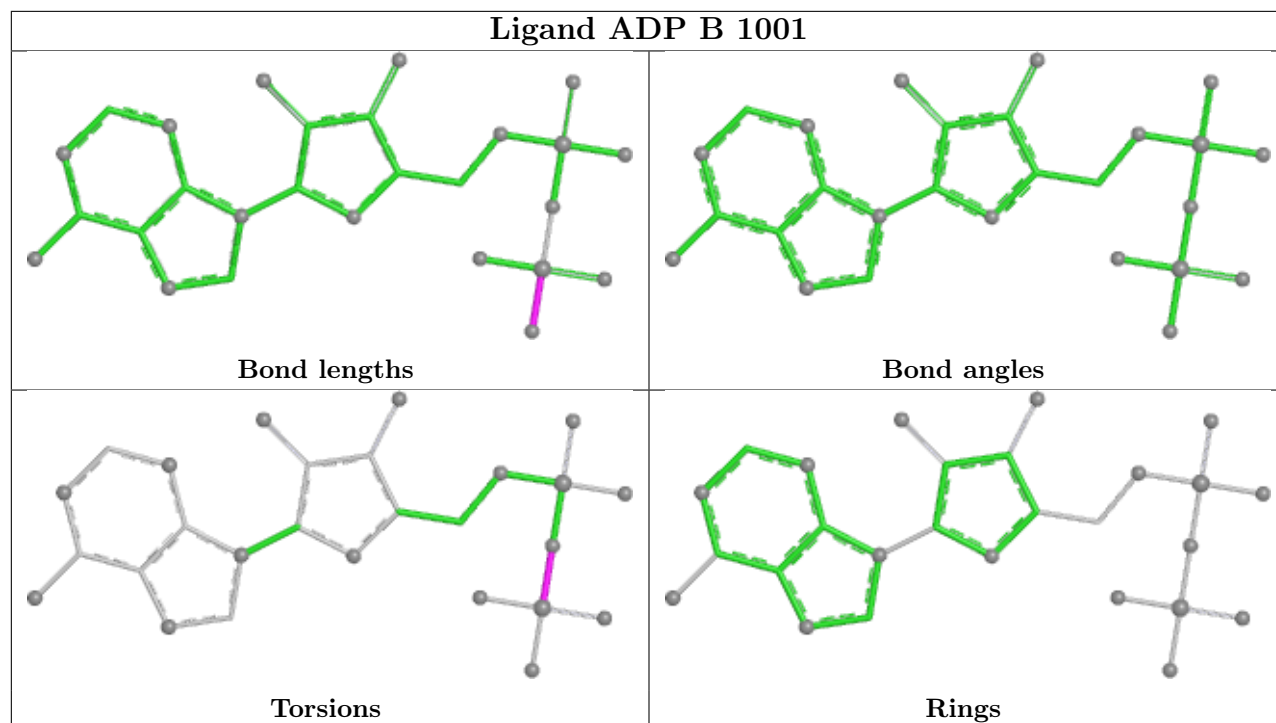
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	1005	FMT	1	0
4	A	1001	ADP	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths,

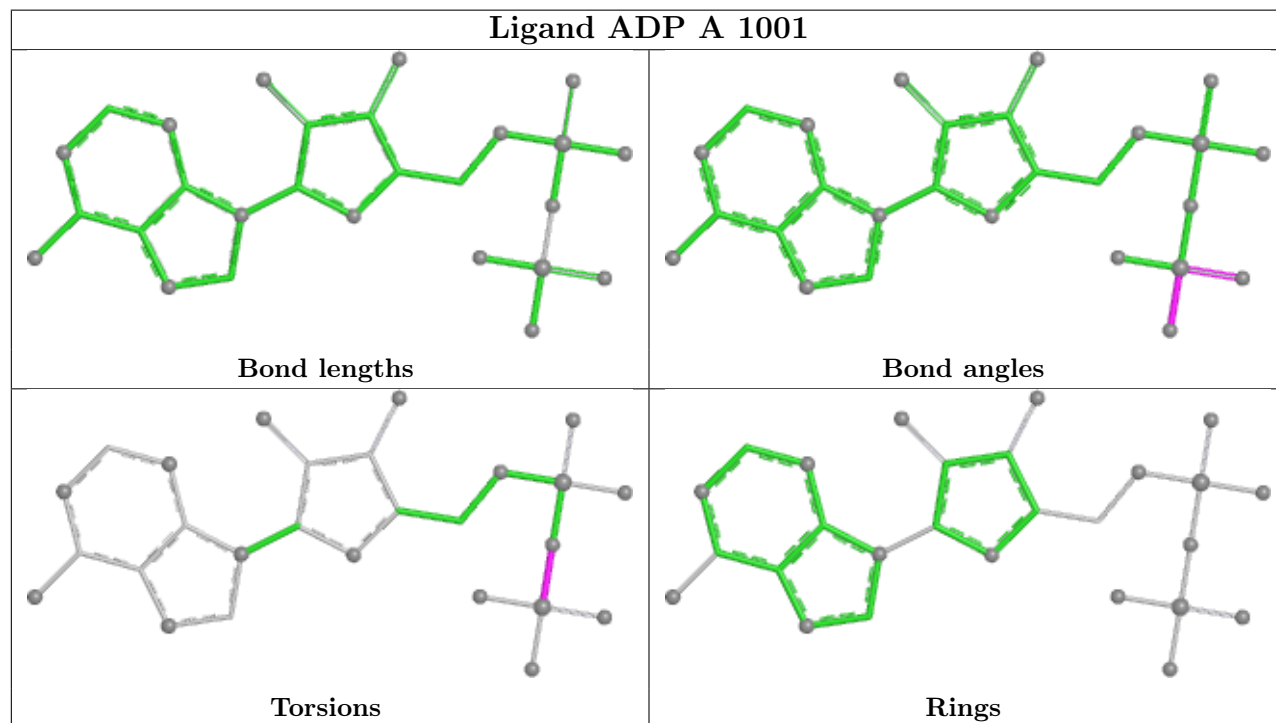
bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 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.

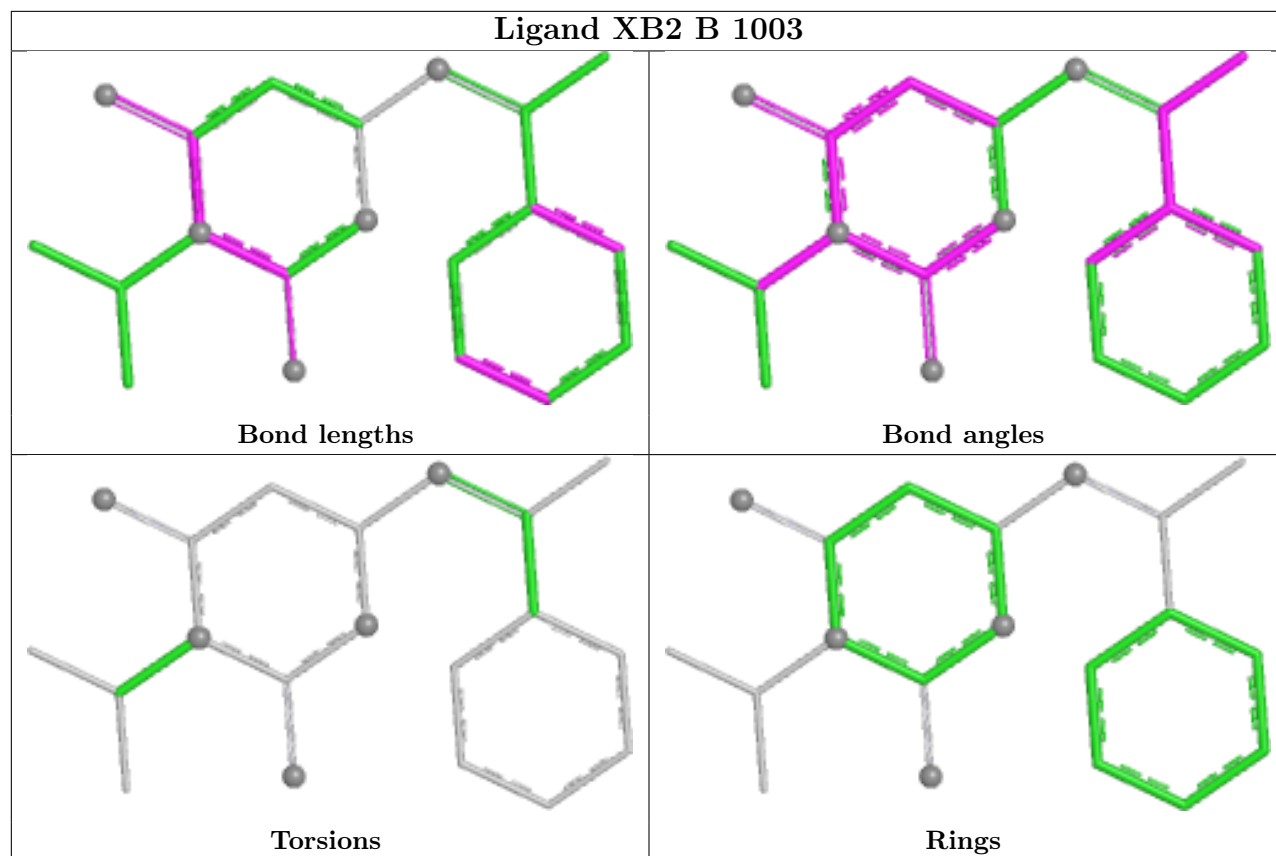


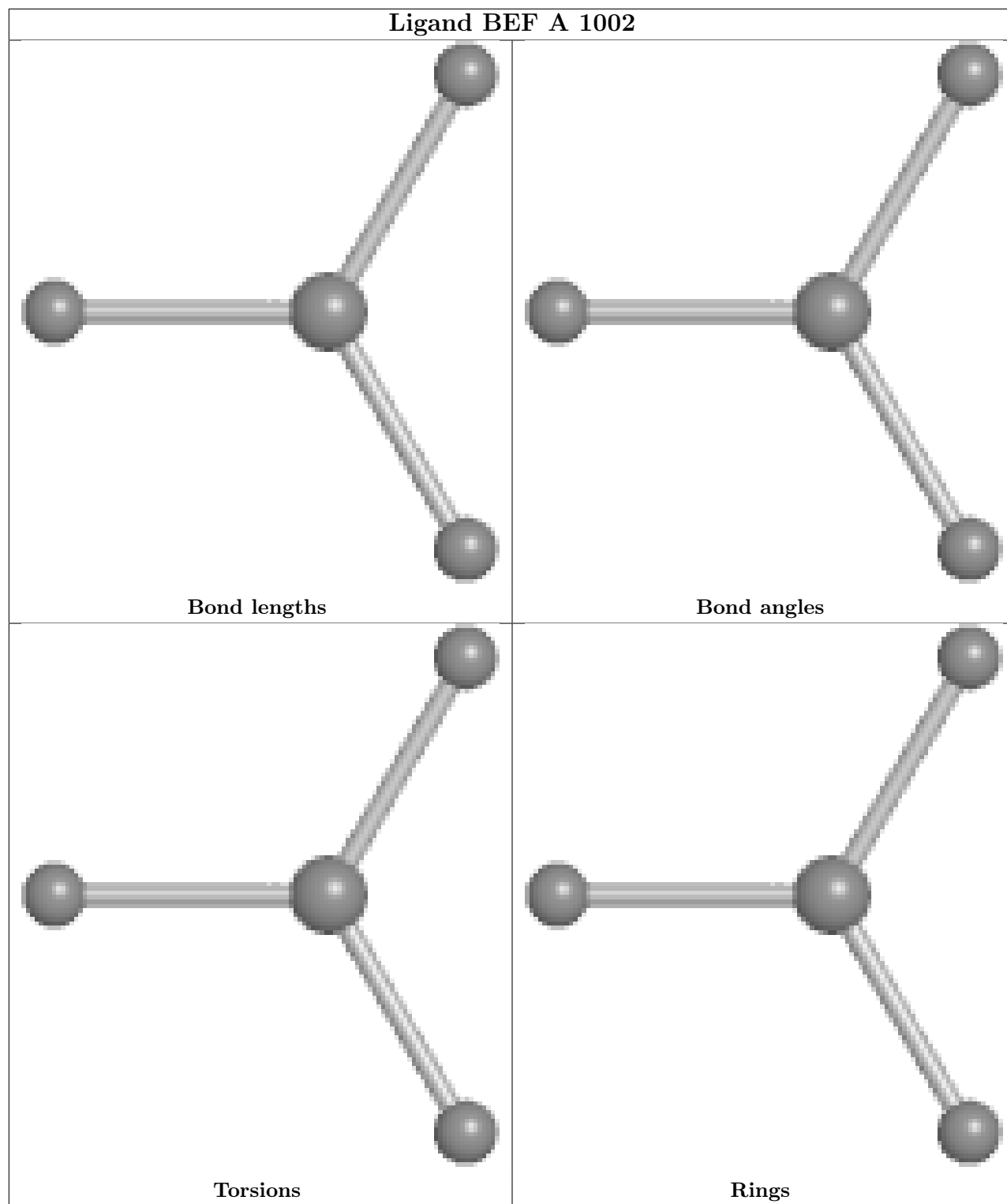
Ligand ADP B 1001

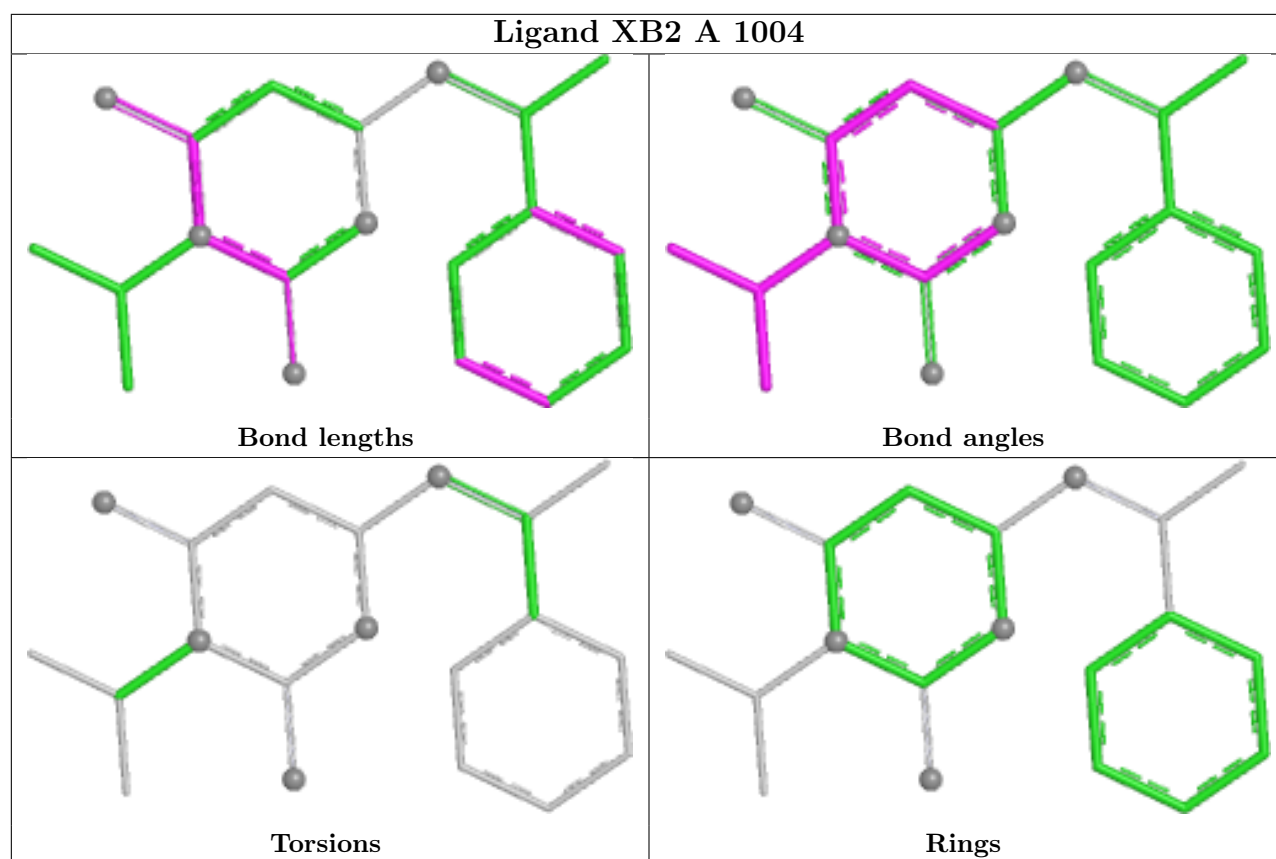


Ligand ADP A 1001









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	779/807 (96%)	0.15	64 (8%)	17 14	21, 51, 117, 163	3 (0%)
1	B	768/807 (95%)	0.01	41 (5%)	32 27	20, 49, 108, 200	2 (0%)
2	C	157/199 (78%)	0.56	10 (6%)	25 21	42, 79, 127, 163	0
3	D	85/199 (42%)	2.71	54 (63%)	0 0	101, 149, 178, 196	0
All	All	1789/2012 (88%)	0.24	169 (9%)	14 11	20, 54, 138, 200	5 (0%)

All (169) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	D	83	VAL	6.3
1	B	796	LEU	6.0
3	D	80	CYS	6.0
3	D	96	VAL	5.8
1	A	147	ARG	5.7
1	A	628	ASP	5.5
3	D	198	ALA	5.2
1	B	735	PHE	5.2
1	B	202	GLY	5.2
1	B	798	ARG	5.1
1	A	130[A]	TRP	5.0
2	C	43	PRO	5.0
3	D	94	ALA	4.7
2	C	47	LYS	4.7
1	A	60	THR	4.6
3	D	89	GLN	4.6
1	A	202	GLY	4.6
1	A	57	GLY	4.5
1	A	34	LYS	4.5
1	B	736	ILE	4.4
3	D	84	LEU	4.4

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Mol	Chain	Res	Type	RSRZ
3	D	82	ASP	4.4
3	D	167	LYS	4.3
1	A	67	LYS	4.3
1	B	790	ALA	4.3
3	D	129	LYS	4.2
1	A	52	LEU	4.2
1	A	733	GLY	4.2
3	D	102	LYS	4.2
3	D	86	ALA	4.2
1	B	794	GLY	4.2
1	B	626	GLY	4.1
1	A	59	VAL	4.0
3	D	160	VAL	4.0
3	D	173	VAL	3.9
3	D	164	LEU	3.9
3	D	144	PHE	3.9
1	A	212	GLY	3.9
1	A	627	PHE	3.8
3	D	95	GLU	3.8
3	D	100	LEU	3.8
3	D	161	LEU	3.8
2	C	45	LYS	3.8
3	D	141	LEU	3.8
3	D	131	THR	3.8
3	D	97	LEU	3.8
1	A	61	ALA	3.7
3	D	162	ALA	3.7
1	A	35	LYS	3.7
1	A	58	LYS	3.7
3	D	87	LEU	3.6
3	D	92	THR	3.6
3	D	90	ASN	3.6
3	D	171	ASP	3.6
3	D	146	LYS	3.6
3	D	151	VAL	3.6
1	B	369	ARG	3.5
1	B	130[A]	TRP	3.5
1	A	411	VAL	3.5
1	A	570	LYS	3.5
1	B	795	VAL	3.5
1	A	54	ARG	3.5
1	A	369	ARG	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	644	PHE	3.5
1	A	71	VAL	3.4
1	B	67	LYS	3.4
1	A	807	ARG	3.4
1	A	72	LYS	3.3
1	A	51	ILE	3.3
1	A	74	ASP	3.3
1	B	733	GLY	3.3
1	B	791	GLN	3.2
3	D	169	THR	3.2
1	B	792	SER	3.2
3	D	155	ALA	3.2
1	B	3	ASP	3.1
1	A	92[A]	MET	3.1
1	B	797	SER	3.1
3	D	130	ASP	3.1
1	A	24	LEU	3.0
1	A	626	GLY	3.0
2	C	104	LYS	3.0
1	B	732	GLU	3.0
1	A	21	LYS	3.0
3	D	85	ARG	3.0
1	A	50	THR	3.0
1	A	75	GLN	2.9
3	D	91	PRO	2.9
1	A	69	VAL	2.9
1	A	95	PHE	2.9
3	D	99	VAL	2.9
1	B	212	GLY	2.8
3	D	81	GLY	2.8
1	A	30	PRO	2.8
2	C	46	ILE	2.8
1	A	408	ASN	2.8
1	A	31	PHE	2.8
1	B	409	GLU	2.8
1	A	741	GLY	2.8
1	A	43	LYS	2.8
2	C	44	SER	2.8
3	D	101	GLY	2.7
2	C	156	GLU	2.7
1	A	213	LYS	2.7
1	A	73	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	408	ASN	2.7
1	B	35	LYS	2.7
1	B	450	LYS	2.7
1	B	644	PHE	2.7
1	A	49	ALA	2.6
1	B	43	LYS	2.6
3	D	153	MET	2.6
1	A	53	SER	2.6
1	B	793	ARG	2.6
3	D	189	TYR	2.6
3	D	194	LYS	2.6
1	A	76	VAL	2.6
1	B	625	ALA	2.6
3	D	165	GLY	2.5
1	A	33	LEU	2.5
2	C	56	GLU	2.5
1	A	367	LYS	2.5
1	A	450	LYS	2.5
3	D	149	ASN	2.5
3	D	187	ILE	2.5
2	C	132	GLY	2.4
1	A	405	LYS	2.4
1	A	68	THR	2.4
2	C	169	THR	2.4
3	D	196	ILE	2.4
1	B	737	ASP	2.4
3	D	88	GLY	2.4
1	A	413	LYS	2.4
3	D	183	SER	2.4
1	B	34	LYS	2.4
1	A	83	LYS	2.3
1	A	802	LYS	2.3
1	B	542	LYS	2.3
1	A	510	PHE	2.3
1	B	370	GLU	2.3
3	D	195	HIS	2.2
1	B	21	LYS	2.2
1	B	27	GLN	2.2
1	B	69	VAL	2.2
3	D	152	VAL	2.2
1	A	55	GLU	2.2
1	A	738	SER	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	406	VAL	2.2
1	A	540	PHE	2.2
1	B	4	ALA	2.2
1	A	28	THR	2.2
1	A	94	THR	2.2
1	A	23	ARG	2.2
3	D	192	PHE	2.2
1	A	4	ALA	2.1
3	D	191	ALA	2.1
3	D	181	GLU	2.1
1	B	787	ARG	2.1
1	A	734	GLN	2.1
1	A	65	HIS	2.1
3	D	137	PHE	2.1
1	B	23	ARG	2.0
1	B	75	GLN	2.0
3	D	159	HIS	2.0
1	B	56	GLY	2.0
1	B	73	GLU	2.0
3	D	147	GLU	2.0
1	A	803	LYS	2.0
1	B	24	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($\text{\AA}^2$)	Q<0.9
1	M3L	B	129	12/13	0.95	0.10	47,50,54,58	0
1	M3L	B	549	12/13	0.95	0.10	50,56,61,63	0
1	M3L	A	129	12/13	0.96	0.09	47,50,53,54	0
1	M3L	A	549	12/13	0.96	0.09	53,58,65,65	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

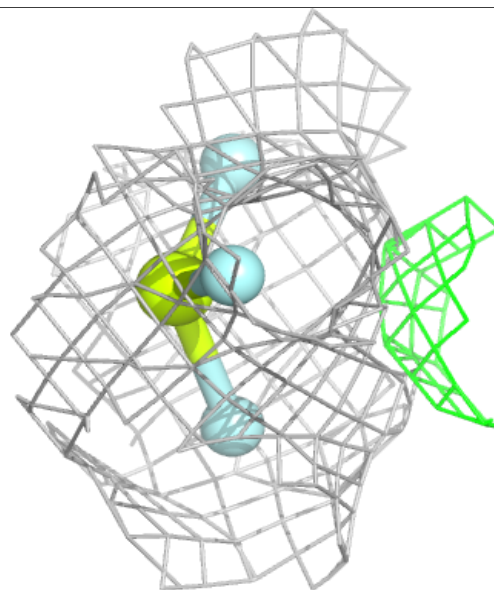
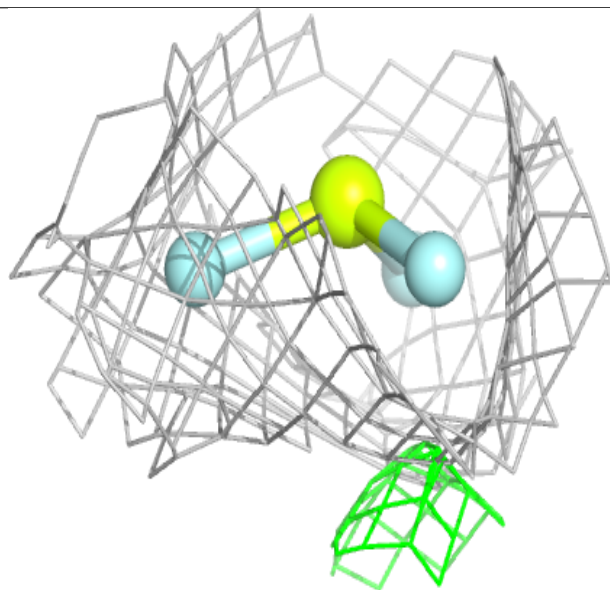
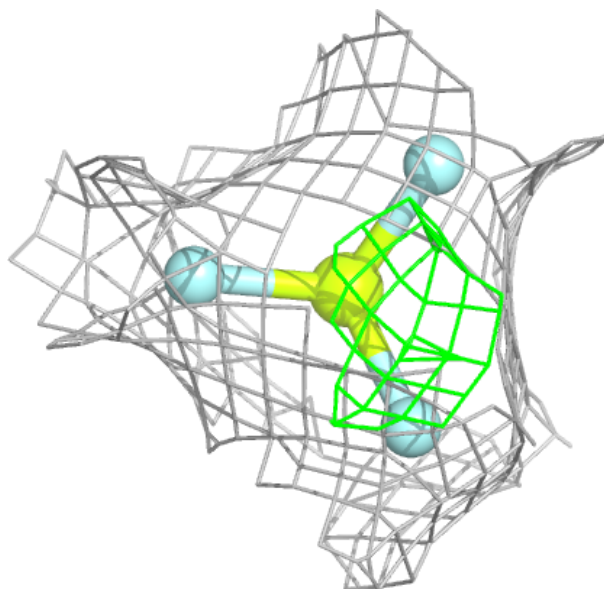
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
8	FMT	A	1007	3/3	0.89	0.22	69,69,72,75	0
9	GOL	C	201	6/6	0.89	0.12	70,78,80,82	0
8	FMT	A	1006	3/3	0.91	0.22	50,50,52,54	0
8	FMT	B	1005	3/3	0.92	0.24	60,60,60,61	0
8	FMT	A	1005	3/3	0.93	0.14	42,42,43,43	0
8	FMT	B	1004	3/3	0.96	0.09	51,51,53,55	0
5	BEF	B	1002	4/4	0.97	0.07	34,37,38,41	0
7	XB2	A	1004	20/20	0.98	0.05	20,29,44,45	0
7	XB2	B	1003	20/20	0.98	0.06	33,42,49,51	0
4	ADP	B	1001	27/27	0.98	0.05	35,40,45,48	0
4	ADP	A	1001	27/27	0.98	0.05	35,41,45,52	0
5	BEF	A	1002	4/4	0.99	0.07	31,32,34,38	0
6	MG	A	1003	1/1	1.00	0.04	27,27,27,27	0
6	MG	B	1006	1/1	1.00	0.03	35,35,35,35	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.

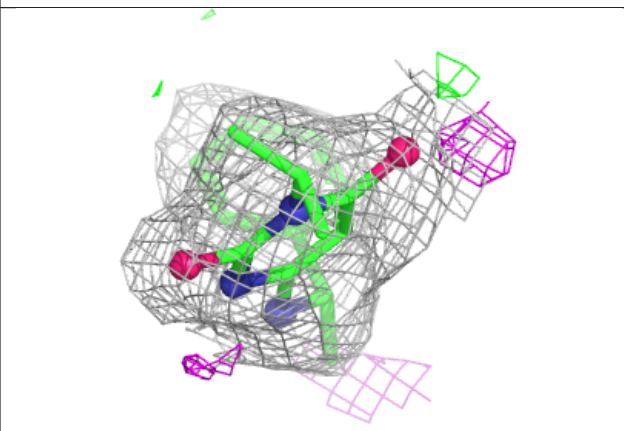
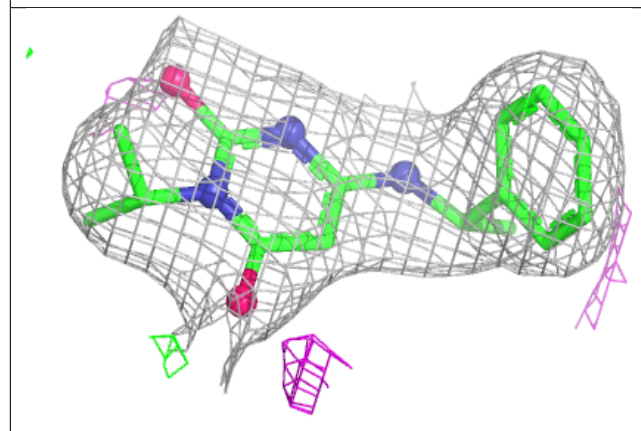
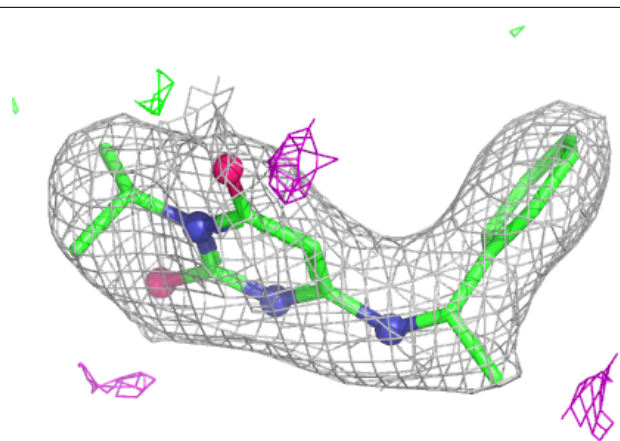
Electron density around BEF B 1002:

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

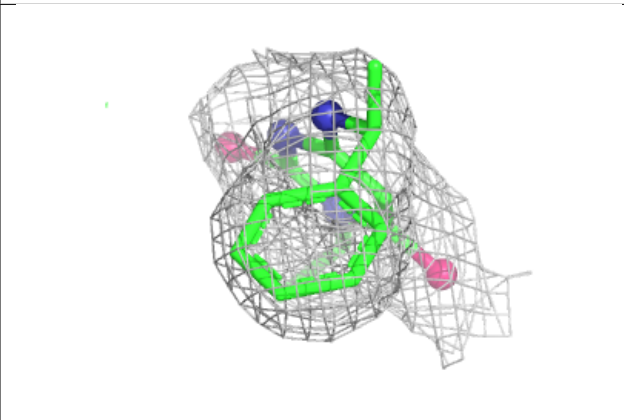
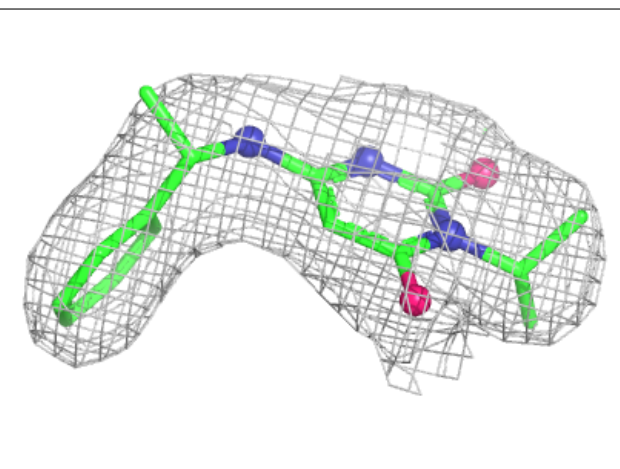


Electron density around XB2 A 1004:

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

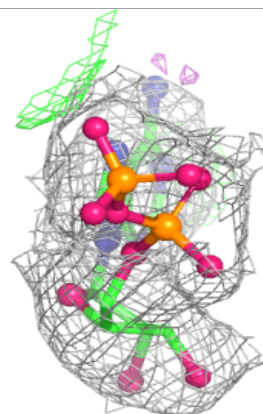
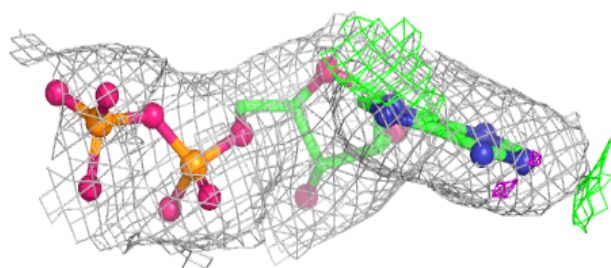
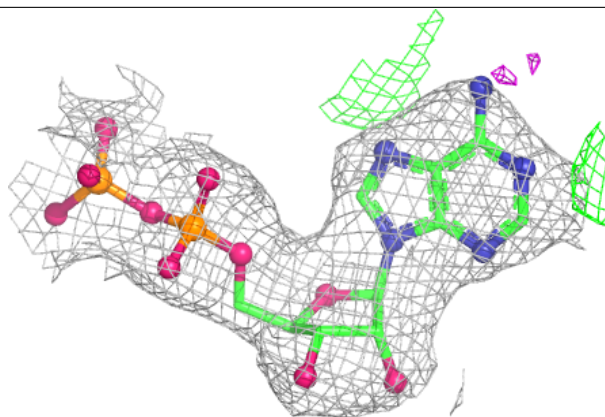
**Electron density around XB2 B 1003:**

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

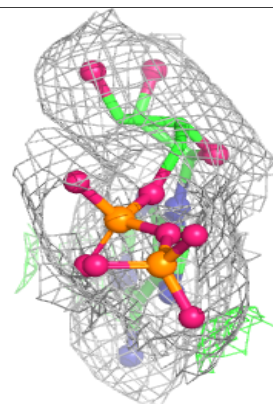
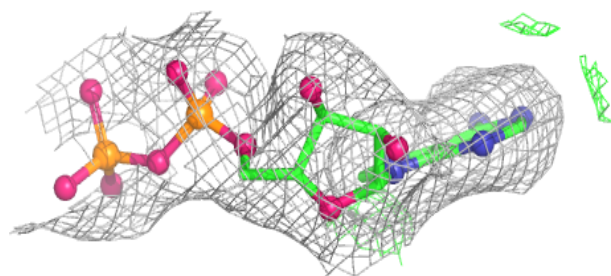
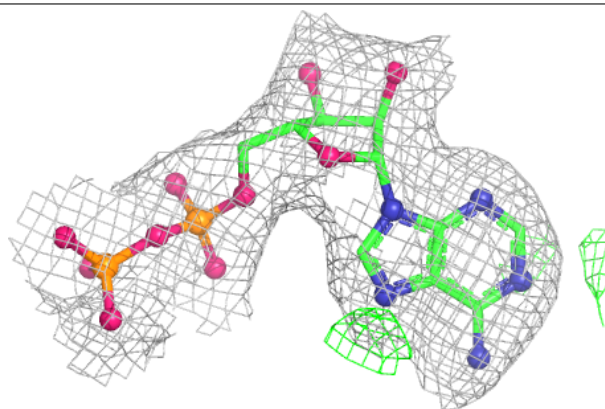


Electron density around ADP B 1001:

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

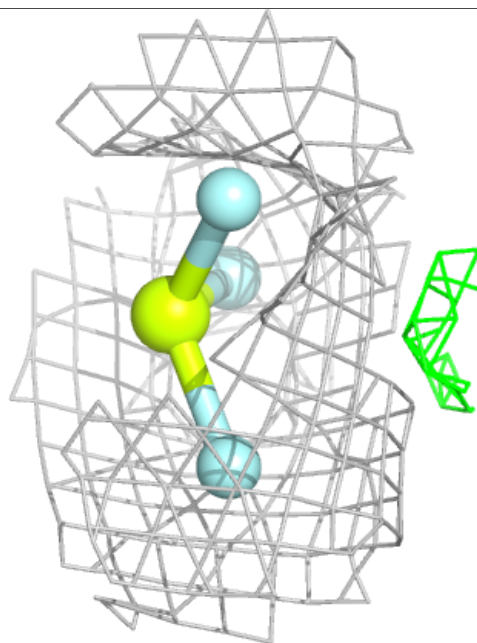
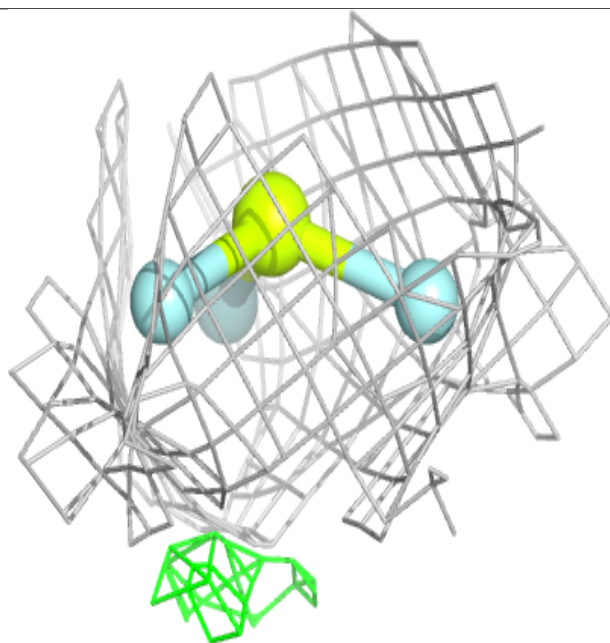
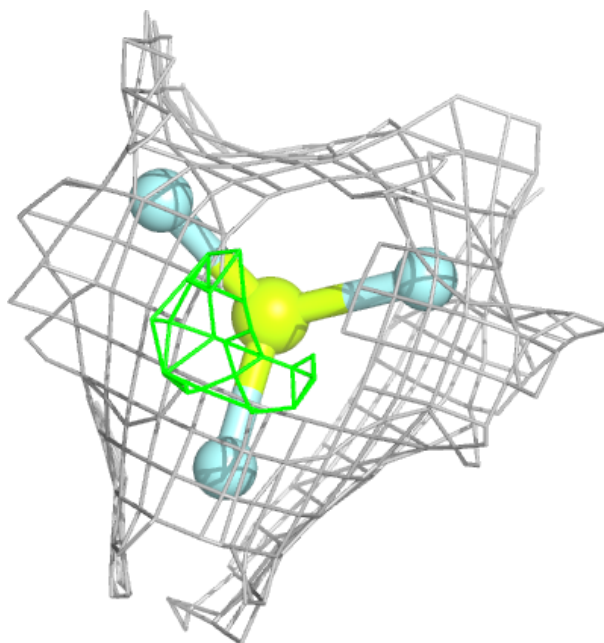
**Electron density around ADP A 1001:**

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



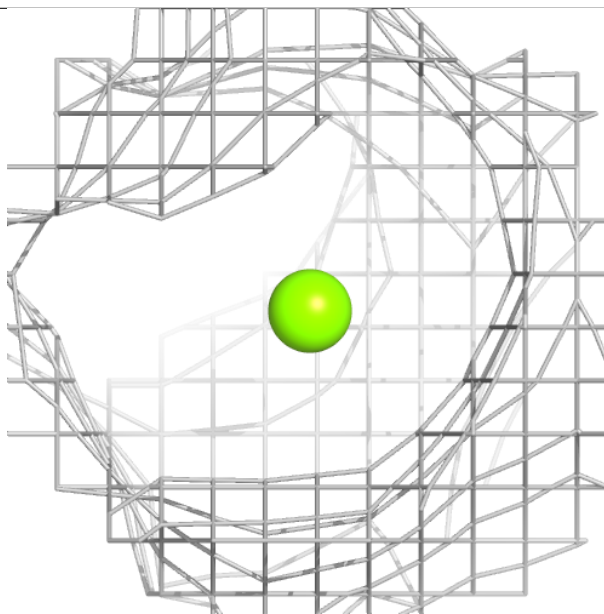
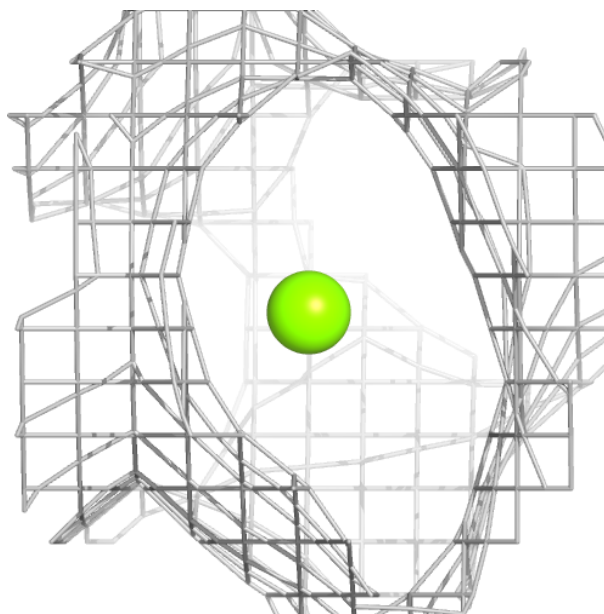
Electron density around BEF A 1002:

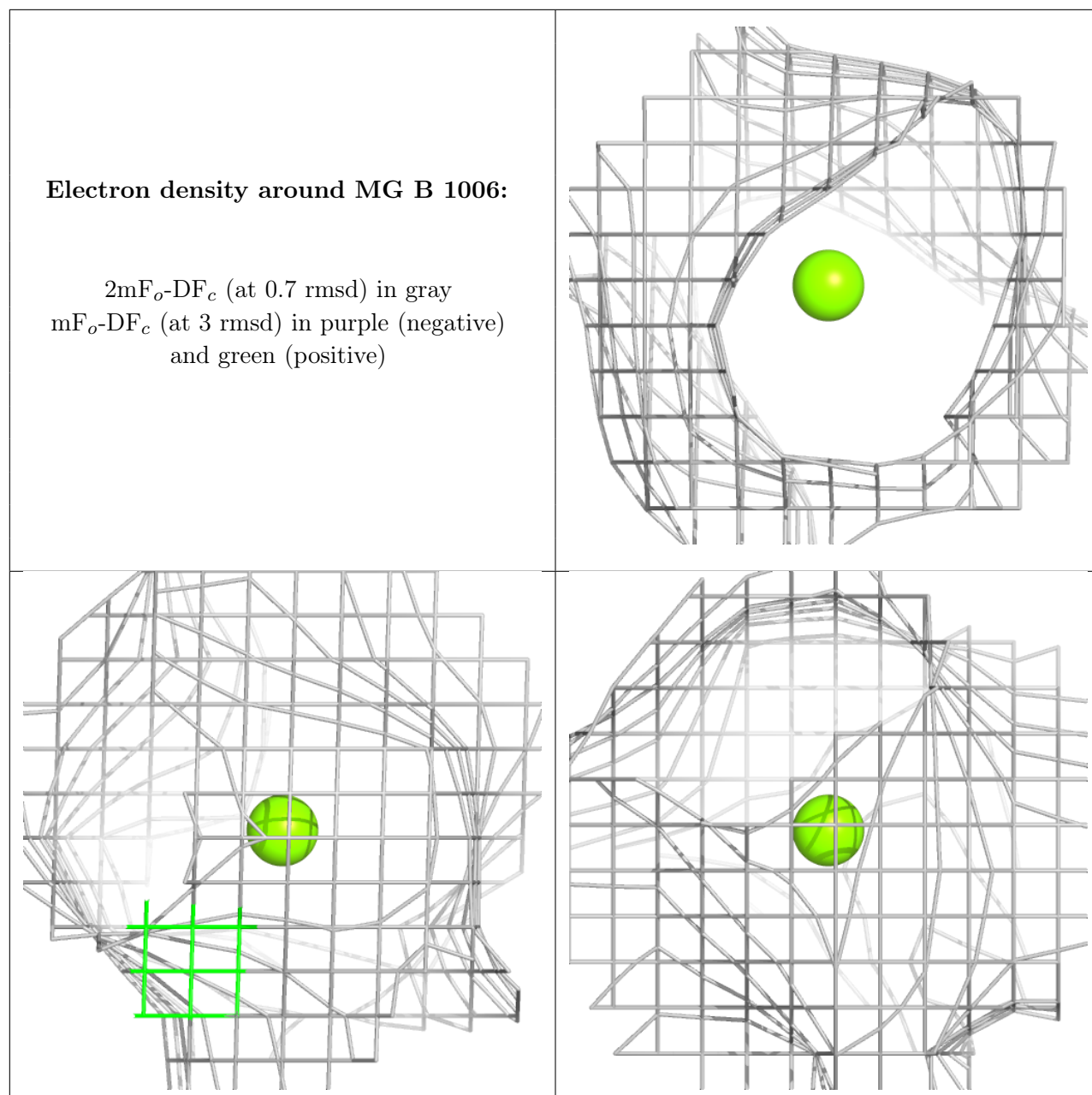
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around MG A 1003:

$2mF_o-DF_c$ (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.