



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 25, 2026 – 05:48 PM EDT

PDB ID : 6FWS / pdb_00006fws
Title : Structure of DinG in complex with ssDNA and ADPBeF
Authors : Cheng, K.; Wigley, D.
Deposited on : 2018-03-07
Resolution : 2.50 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

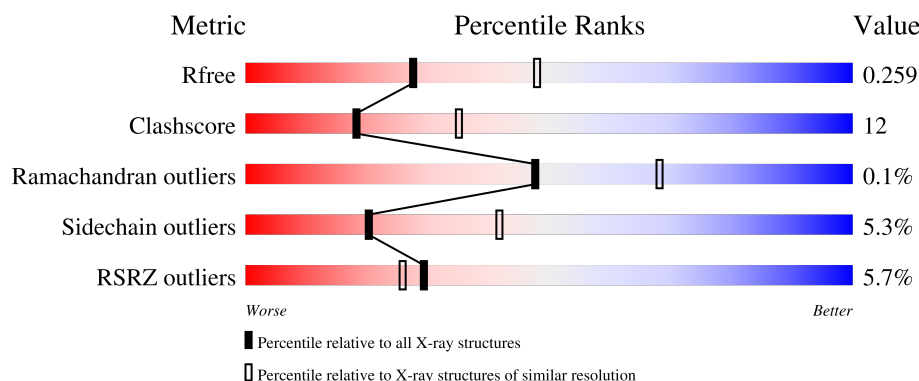
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	716	4% 73% 21% • •
1	B	716	6% 70% 24% • 5%
2	C	11	18% 36% 64%
3	D	10	10% 20% 80%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SF4	A	801	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 11747 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 ATP-dependent DNA helicase DinG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	686	Total	C	N	O	S	0	0	0
			5456	3475	960	995	26			
1	B	683	Total	C	N	O	S	0	0	0
			5438	3464	960	989	25			

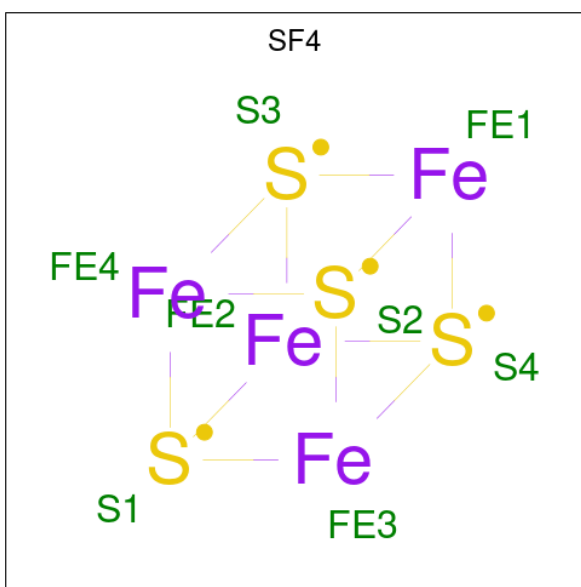
- Molecule 2 is a DNA chain called DNA (5'-D(*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*T)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	11	Total	C	N	O	P	0	0	0
			216	110	22	74	10			

- Molecule 3 is a DNA chain called DNA (5'-D(*TP*TP*TP*TP*TP*TP*TP*TP*TP*T)-3').

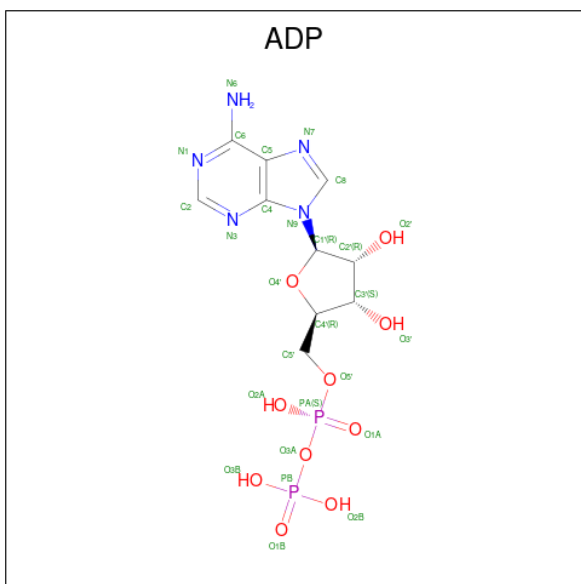
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	10	Total	C	N	O	P	0	0	0
			196	100	20	67	9			

- Molecule 4 is IRON/SULFUR CLUSTER (CCD ID: SF4) (formula: Fe₄S₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total 8	Fe 4	S 4	0	0
4	B	1	Total 8	Fe 4	S 4	0	0

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{10}\text{P}_2$) (labeled as "Ligand of Interest" by depositor).



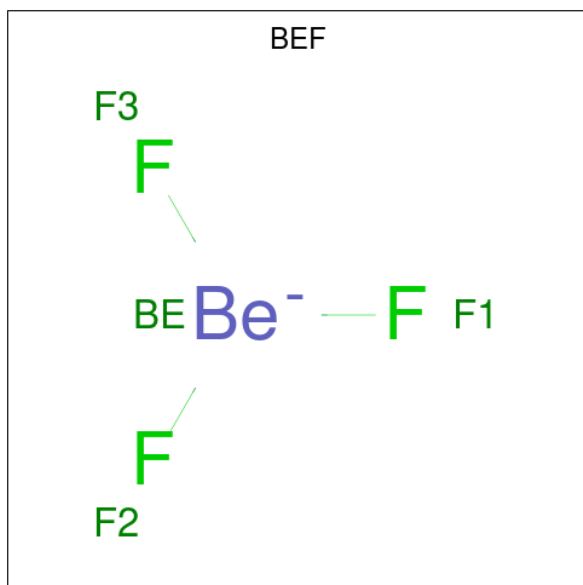
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

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

- Molecule 6 is BERYLLIUM TRIFLUORIDE ION (CCD ID: BEF) (formula: BeF₃) (labeled as "Ligand of Interest" by depositor).



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

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

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

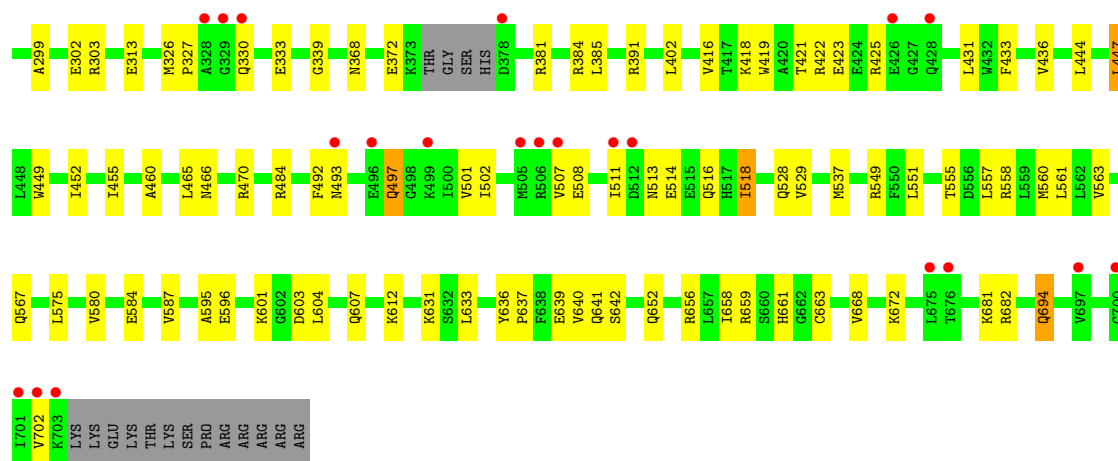
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	186	Total	O	0	0
			186	186		

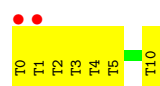
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	9	Total 9	O 9	0	0
8	B	159	Total 159	O 159	0	0
8	D	7	Total 7	O 7	0	0



- Molecule 2: DNA (5'-D(*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*T)-3')



- Molecule 3: DNA (5'-D(*TP*TP*TP*TP*TP*TP*TP*TP*TP*T)-3')



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	109.77Å 119.75Å 126.74Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	63.37 – 2.50 63.37 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.0 (63.37-2.50) 99.0 (63.37-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.93 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.219 , 0.256 0.223 , 0.259	Depositor DCC
R_{free} test set	2821 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å ²)	32.7	Xtriage
Anisotropy	0.520	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 41.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	11747	wwPDB-VP
Average B, all atoms (Å ²)	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.99% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SF4, BEF, MG, ADP

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	0.37	0/5564	0.62	2/7537 (0.0%)
1	B	0.41	1/5546 (0.0%)	0.64	5/7512 (0.1%)
2	C	0.58	0/237	0.83	0/365
3	D	0.51	0/215	0.84	0/331
All	All	0.40	1/11562 (0.0%)	0.64	7/15745 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	47	GLY	C-O	-9.64	1.11	1.23

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	676	THR	N-CA-C	10.69	123.01	111.36
1	B	93	TYR	N-CA-C	6.33	118.18	111.28
1	B	99	LEU	CA-C-N	-5.78	113.00	122.54
1	B	99	LEU	C-N-CA	-5.78	113.00	122.54
1	A	527	GLU	CB-CG-CD	-5.35	103.50	112.60
1	B	694	GLN	CA-C-N	5.16	125.06	119.85
1	B	694	GLN	C-N-CA	5.16	125.06	119.85

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen

atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5456	0	5540	118	0
1	B	5438	0	5527	144	0
2	C	216	0	131	9	0
3	D	196	0	119	8	0
4	A	8	0	0	2	0
4	B	8	0	0	0	0
5	A	27	0	12	0	0
5	B	27	0	12	0	0
6	A	4	0	0	0	0
6	B	4	0	0	1	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
8	A	186	0	0	25	0
8	B	159	0	0	36	0
8	C	9	0	0	2	0
8	D	7	0	0	1	0
All	All	11747	0	11341	274	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 12.

All (274) 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:507:VAL:CG2	8:B:930:HOH:O	1.95	1.11
1:B:507:VAL:HG22	8:B:930:HOH:O	1.57	1.02
1:B:243:LEU:O	8:B:901:HOH:O	1.81	0.97
1:A:596:GLU:OE1	8:A:901:HOH:O	1.83	0.95
1:A:378:ASP:OD2	8:A:903:HOH:O	1.85	0.95
1:A:689:VAL:O	8:A:902:HOH:O	1.84	0.93
2:C:10:DT:O3'	8:C:101:HOH:O	1.87	0.92
1:B:529:VAL:HG11	1:B:560:MET:HE1	1.53	0.90
1:A:381:ARG:NH1	8:A:903:HOH:O	2.07	0.88
1:B:46:GLU:OE1	8:B:902:HOH:O	1.93	0.86
1:A:514:GLU:OE2	1:A:545:ARG:NH2	2.09	0.85
1:B:391:ARG:NH1	8:B:908:HOH:O	2.09	0.85
1:A:182:ASP:OD2	8:A:904:HOH:O	1.95	0.84
1:A:152:GLU:HA	1:A:155:ARG:HG3	1.58	0.84
1:A:162:ASP:HA	1:A:165:THR:HG22	1.60	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:596:GLU:O	8:B:903:HOH:O	1.95	0.84
1:A:578:LYS:HD2	1:A:578:LYS:N	1.92	0.83
1:A:577:ARG:NH2	8:A:908:HOH:O	2.12	0.81
1:B:205:CYS:N	8:B:909:HOH:O	2.13	0.80
1:B:603:ASP:OD1	8:B:904:HOH:O	1.99	0.80
1:B:508:GLU:HG2	1:B:672:LYS:HE3	1.64	0.79
1:B:507:VAL:HG23	8:B:930:HOH:O	1.64	0.79
1:B:176:ASP:OD2	8:B:906:HOH:O	2.02	0.77
1:B:144:GLU:OE1	8:B:905:HOH:O	2.03	0.76
1:B:125:THR:OG1	1:B:160:LYS:NZ	2.19	0.76
1:A:185:ARG:O	8:A:906:HOH:O	2.03	0.76
4:A:801:SF4:S4	8:A:919:HOH:O	2.44	0.75
1:A:560:MET:HE3	1:A:585:ARG:HB3	1.68	0.74
1:B:497:GLN:HE22	1:B:661:HIS:HA	1.52	0.74
1:A:145:LEU:HD22	1:A:186:ARG:HD2	1.68	0.74
1:A:450:ARG:NH2	8:A:912:HOH:O	2.21	0.73
2:C:4:DT:H2"	2:C:5:DT:H72	1.69	0.72
1:B:596:GLU:HG2	1:B:652:GLN:HG2	1.71	0.72
1:B:287:MET:HE1	1:B:295:ILE:HG23	1.71	0.72
3:D:6:DT:OP1	8:D:101:HOH:O	2.08	0.71
1:B:73:ARG:HH12	1:B:104:ILE:HG21	1.55	0.70
1:A:578:LYS:HD2	1:A:578:LYS:H	1.55	0.70
1:A:24:ASP:OD1	8:A:907:HOH:O	2.09	0.70
1:A:145:LEU:HD13	1:A:186:ARG:HB3	1.73	0.70
1:B:73:ARG:NH1	1:B:104:ILE:HG21	2.07	0.69
1:A:574:GLU:O	1:A:578:LYS:HD3	1.92	0.69
1:B:470:ARG:NH2	1:B:640:VAL:O	2.26	0.69
1:A:673:ARG:HA	1:A:676:THR:HB	1.75	0.69
1:B:73:ARG:HH12	1:B:104:ILE:CG2	2.05	0.68
1:A:505:MET:HE3	1:A:520:GLU:HB3	1.75	0.68
1:A:404:ARG:NH1	8:A:918:HOH:O	2.26	0.67
1:B:273:ARG:NH2	8:B:917:HOH:O	2.19	0.67
1:B:232:GLU:HG2	1:B:447:LEU:HD21	1.76	0.67
3:D:2:DT:H5"	3:D:2:DT:H6	1.59	0.67
1:A:520:GLU:HG2	1:A:697:VAL:HG11	1.77	0.66
1:B:205:CYS:SG	8:B:1054:HOH:O	2.54	0.66
1:B:682:ARG:HD3	8:B:907:HOH:O	1.96	0.65
1:A:162:ASP:HA	1:A:165:THR:CG2	2.26	0.65
1:B:188:SER:O	8:B:910:HOH:O	2.15	0.65
1:A:506:ARG:HG2	1:A:520:GLU:OE2	1.97	0.64
2:C:10:DT:OP2	8:C:102:HOH:O	2.15	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:612:LYS:O	8:A:909:HOH:O	2.16	0.63
1:B:612:LYS:O	8:B:911:HOH:O	2.15	0.63
1:B:333:GLU:HG3	1:B:421:THR:HG22	1.80	0.63
1:A:537:MET:HG3	1:A:587:VAL:HG22	1.82	0.62
1:B:236:VAL:HG22	1:B:237:LEU:HG	1.80	0.61
1:B:497:GLN:NE2	1:B:661:HIS:HA	2.16	0.61
1:B:242:ASN:ND2	8:B:925:HOH:O	2.34	0.61
1:A:574:GLU:O	1:A:578:LYS:CD	2.49	0.60
1:B:529:VAL:CG1	1:B:560:MET:HE1	2.30	0.60
1:A:102:LYS:HD3	8:A:1059:HOH:O	2.01	0.59
1:B:402:LEU:HD21	1:B:433:PHE:HB3	1.83	0.59
1:B:41:THR:OG1	1:B:484:ARG:NH2	2.26	0.59
1:B:507:VAL:CG2	1:B:513:ASN:ND2	2.66	0.59
1:B:497:GLN:HG2	1:B:663:CYS:O	2.03	0.59
1:A:152:GLU:OE1	1:A:186:ARG:NH2	2.35	0.58
1:A:514:GLU:HG2	1:A:518:ILE:HD13	1.86	0.58
1:A:575:LEU:O	1:A:579:ARG:HG3	2.04	0.58
1:B:507:VAL:HG21	1:B:513:ASN:CG	2.29	0.58
1:B:652:GLN:NE2	8:B:903:HOH:O	2.34	0.58
1:A:131:GLU:OE2	1:A:131:GLU:N	2.25	0.58
1:B:636:TYR:CE2	3:D:1:DT:H2'	2.39	0.57
1:A:120:CYS:SG	1:A:122:ARG:HG2	2.44	0.57
1:A:381:ARG:HD3	8:A:903:HOH:O	2.03	0.57
1:B:551:LEU:HD11	1:B:563:VAL:HG11	1.85	0.57
1:A:637:PRO:O	1:A:641:GLN:HG2	2.05	0.57
1:B:106:ASP:OD1	1:B:106:ASP:N	2.37	0.56
1:A:17:ALA:HB1	1:A:103:ILE:HD12	1.86	0.56
1:A:247:LEU:HD13	1:A:253:LEU:HD22	1.87	0.56
1:B:22:ILE:HD11	1:B:99:LEU:HD21	1.87	0.56
1:B:133:THR:H	1:B:146:THR:HG21	1.70	0.56
1:B:137:LEU:HD12	1:B:137:LEU:H	1.70	0.56
1:A:384:ARG:HB2	8:A:925:HOH:O	2.06	0.56
1:B:217:ALA:O	8:B:912:HOH:O	2.17	0.56
1:A:205:CYS:HG	1:A:208:PHE:HD2	1.52	0.56
1:B:73:ARG:HH22	1:B:106:ASP:CG	2.15	0.55
1:B:155:ARG:HG3	1:B:158:LYS:HE3	1.88	0.55
1:A:677:LYS:HE2	2:C:3:DT:OP1	2.07	0.55
1:B:652:GLN:O	1:B:656:ARG:NH2	2.38	0.55
1:A:424:GLU:HG2	1:A:429:LEU:HD23	1.87	0.55
1:B:90:ASP:CG	1:B:174:HIS:HE2	2.14	0.55
1:B:537:MET:HG2	1:B:607:GLN:HB3	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4:THR:HG23	8:A:942:HOH:O	2.06	0.54
3:D:4:DT:H2"	3:D:5:DT:H71	1.90	0.54
1:B:114:GLY:HA3	3:D:9:DT:H5"	1.90	0.54
1:B:449:TRP:O	8:B:914:HOH:O	2.19	0.54
1:A:119:VAL:HG23	1:A:187:LEU:HB3	1.90	0.54
1:A:529:VAL:HG13	1:A:560:MET:HE1	1.90	0.54
1:B:73:ARG:NH2	1:B:106:ASP:OD2	2.41	0.53
1:B:513:ASN:ND2	8:B:930:HOH:O	2.38	0.53
1:B:142:ASP:HB2	8:B:987:HOH:O	2.08	0.53
1:A:636:TYR:HB2	2:C:1:DT:O4	2.08	0.53
1:B:4:THR:O	1:B:8:LYS:HG3	2.09	0.53
3:D:9:DT:H2'	3:D:10:DT:C5	2.44	0.53
1:B:514:GLU:HG2	1:B:518:ILE:HD12	1.90	0.53
1:B:601:LYS:HG2	8:B:953:HOH:O	2.08	0.53
1:B:555:THR:O	1:B:558:ARG:HB2	2.08	0.53
1:A:531:SER:HB3	1:A:533:LYS:HG3	1.90	0.52
1:B:528:GLN:O	8:B:915:HOH:O	2.19	0.52
1:B:21:GLN:OE1	1:B:102:LYS:HG2	2.08	0.52
1:B:205:CYS:HB2	1:B:208:PHE:HD2	1.74	0.52
1:A:638:PHE:N	8:A:929:HOH:O	2.38	0.52
1:B:119:VAL:HG23	1:B:187:LEU:HB3	1.91	0.52
1:B:145:LEU:N	8:B:905:HOH:O	2.02	0.52
1:A:262:GLU:HG3	1:A:436:VAL:HG22	1.91	0.52
1:A:54:ALA:HB3	1:A:60:LYS:HD3	1.91	0.52
1:A:75:GLU:OE2	8:A:910:HOH:O	2.19	0.52
1:A:124:LEU:HD21	1:A:160:LYS:HA	1.92	0.52
1:A:205:CYS:SG	1:A:208:PHE:HD2	2.31	0.52
1:A:130:THR:O	1:A:132:PRO:HD3	2.09	0.52
1:B:313:GLU:OE1	8:B:913:HOH:O	2.18	0.51
1:A:101:LYS:NZ	1:A:107:LEU:O	2.43	0.51
1:A:344:GLU:H	1:A:344:GLU:CD	2.18	0.51
1:B:637:PRO:O	1:B:641:GLN:HG2	2.11	0.51
1:B:240:PRO:HB3	1:B:452:ILE:HD13	1.93	0.51
1:A:1:MET:HG3	8:B:969:HOH:O	2.09	0.51
1:A:122:ARG:NH1	4:A:801:SF4:S4	2.84	0.51
1:A:287:MET:HE1	1:A:295:ILE:HG23	1.91	0.51
1:B:34:MET:HG2	1:B:63:SER:HB3	1.93	0.51
1:B:302:GLU:O	8:B:916:HOH:O	2.19	0.51
1:B:132:PRO:HA	1:B:146:THR:HG23	1.94	0.50
1:B:287:MET:HE2	1:B:299:ALA:HB1	1.93	0.50
1:A:424:GLU:HG2	1:A:429:LEU:CD2	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:ILE:O	1:B:75:GLU:HG3	2.12	0.50
1:B:452:ILE:HB	1:B:455:ILE:HD11	1.92	0.50
1:A:638:PHE:CD1	2:C:2:DT:H2"	2.47	0.50
1:B:60:LYS:NZ	6:B:803:BEF:F1	2.35	0.50
1:B:381:ARG:NH2	8:B:933:HOH:O	2.42	0.50
1:A:569:ARG:HA	1:A:572:LEU:HD12	1.94	0.50
1:A:130:THR:N	8:A:905:HOH:O	2.00	0.50
1:A:625:THR:O	1:A:628:GLU:HG2	2.12	0.50
1:B:291:ARG:HH11	1:B:295:ILE:HD11	1.76	0.50
1:A:338:MET:SD	1:A:628:GLU:HG3	2.52	0.50
1:B:3:LEU:O	1:B:8:LYS:HE3	2.11	0.50
1:A:561:LEU:HD23	1:A:587:VAL:HB	1.94	0.49
1:B:465:LEU:N	8:B:920:HOH:O	2.45	0.49
1:B:507:VAL:HG11	1:B:516:GLN:CG	2.43	0.49
1:B:268:THR:HG22	1:B:270:PRO:HD2	1.93	0.49
1:B:595:ALA:C	1:B:656:ARG:HD2	2.37	0.49
1:B:580:VAL:HG11	1:B:604:LEU:HA	1.94	0.49
1:A:452:ILE:HB	1:A:455:ILE:HD11	1.95	0.49
1:B:567:GLN:NE2	8:B:906:HOH:O	2.32	0.49
1:B:327:PRO:O	1:B:422:ARG:NH2	2.45	0.48
1:A:55:PRO:HD2	1:A:58:VAL:HG21	1.94	0.48
1:A:508:GLU:OE1	1:A:676:THR:HG21	2.14	0.48
1:B:278:LEU:HD23	1:B:391:ARG:HH12	1.79	0.48
1:A:295:ILE:HD12	1:A:295:ILE:H	1.79	0.48
1:A:463:ARG:HD2	1:A:468:PHE:CE2	2.49	0.48
1:A:508:GLU:CD	1:A:676:THR:HG21	2.38	0.48
1:A:247:LEU:HD12	1:A:457:VAL:HG22	1.96	0.47
1:B:557:LEU:HB3	1:B:560:MET:HE2	1.95	0.47
1:A:265:ALA:HB3	1:A:402:LEU:HD22	1.96	0.47
1:A:161:GLY:O	1:A:165:THR:N	2.33	0.47
1:A:578:LYS:H	1:A:578:LYS:CD	2.27	0.47
1:B:137:LEU:HA	1:B:140:PHE:HB2	1.96	0.47
1:B:416:VAL:HB	1:B:418:LYS:HE2	1.96	0.47
1:A:607:GLN:HG3	1:A:666:GLU:HG3	1.96	0.47
1:B:95:LYS:C	1:B:98:PRO:HD2	2.40	0.47
1:B:339:GLY:O	1:B:418:LYS:HE3	2.14	0.47
1:B:35:ILE:HG23	1:B:67:PRO:HG3	1.97	0.47
1:B:507:VAL:HG11	1:B:516:GLN:HG3	1.96	0.47
1:B:26:ILE:HD13	1:B:661:HIS:HB2	1.97	0.46
1:A:168:TRP:CD1	1:A:175:THR:HB	2.50	0.46
1:B:326:MET:HE1	1:B:431:LEU:HD11	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:103:ILE:HG22	1:B:104:ILE:HG13	1.96	0.46
1:B:639:GLU:OE2	1:B:682:ARG:NH1	2.46	0.46
1:B:278:LEU:CD2	1:B:391:ARG:NH1	2.78	0.46
1:B:66:ILE:HB	1:B:67:PRO:HD3	1.97	0.46
1:A:331:GLU:OE2	1:A:424:GLU:N	2.43	0.46
1:A:694:GLN:OE1	8:A:913:HOH:O	2.21	0.46
1:B:73:ARG:NH1	1:B:104:ILE:CG2	2.72	0.46
1:A:34:MET:HG2	1:A:63:SER:HB3	1.98	0.45
1:A:264:SER:OG	1:A:434:HIS:ND1	2.39	0.45
1:A:661:HIS:O	8:A:911:HOH:O	2.21	0.45
1:B:549:ARG:HA	1:B:549:ARG:HD2	1.69	0.45
1:A:273:ARG:NH1	8:A:937:HOH:O	2.49	0.45
1:A:89:GLN:HG2	1:A:221:VAL:HG12	1.98	0.45
1:A:145:LEU:HA	1:A:145:LEU:HD23	1.62	0.45
1:B:54:ALA:HB3	1:B:60:LYS:HE3	1.98	0.45
1:A:331:GLU:HA	1:A:422:ARG:O	2.17	0.45
1:A:75:GLU:HB3	1:A:77:LYS:HG3	1.99	0.44
1:A:445:GLU:HA	1:A:449:TRP:HB2	2.00	0.44
1:B:168:TRP:CD1	1:B:175:THR:HB	2.52	0.44
1:B:82:SER:OG	1:B:224:HIS:ND1	2.42	0.44
1:B:90:ASP:OD1	1:B:174:HIS:NE2	2.38	0.44
1:B:211:ARG:O	1:B:214:ILE:HB	2.17	0.44
1:A:371:SER:O	1:A:374:THR:OG1	2.29	0.44
2:C:0:DT:C5	2:C:1:DT:C5	3.06	0.44
1:B:54:ALA:O	1:B:60:LYS:HE3	2.17	0.44
2:C:0:DT:H73	2:C:1:DT:H73	2.00	0.44
1:B:501:VAL:O	1:B:668:VAL:HA	2.18	0.44
8:A:918:HOH:O	1:B:303:ARG:NH2	2.31	0.44
1:A:326:MET:HB2	1:A:422:ARG:NH2	2.33	0.43
1:B:384:ARG:NH2	8:B:932:HOH:O	2.39	0.43
1:A:228:MET:HE2	1:A:253:LEU:HD11	2.00	0.43
1:B:327:PRO:HB2	1:B:330:GLN:CD	2.43	0.43
1:B:419:TRP:HZ3	1:B:436:VAL:HG12	1.84	0.43
1:A:19:GLN:HG2	1:A:25:PHE:CD1	2.53	0.43
1:A:127:LEU:HB3	1:A:156:CYS:SG	2.59	0.43
1:B:265:ALA:HB3	1:B:402:LEU:HD22	2.00	0.43
1:B:656:ARG:O	1:B:659:ARG:HD3	2.18	0.43
1:A:615:PHE:CG	2:C:3:DT:H4'	2.53	0.43
1:A:575:LEU:HD23	1:A:575:LEU:HA	1.91	0.43
1:B:73:ARG:NH2	1:B:106:ASP:CG	2.77	0.43
1:A:339:GLY:O	1:A:418:LYS:HE3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:137:LEU:O	1:B:141:LEU:HG	2.19	0.42
3:D:8:DT:H2''	3:D:9:DT:O5'	2.19	0.42
1:A:239:ASP:O	1:A:243:LEU:HG	2.18	0.42
1:A:574:GLU:C	1:A:578:LYS:HD3	2.44	0.42
1:A:500:ILE:O	1:A:692:ILE:HA	2.20	0.42
1:B:508:GLU:N	8:B:930:HOH:O	2.51	0.42
1:A:642:SER:OG	8:A:914:HOH:O	2.21	0.42
1:A:651:ILE:HD11	1:A:686:ALA:HB1	2.01	0.42
3:D:2:DT:H6	3:D:2:DT:C5'	2.30	0.42
1:A:505:MET:HA	1:A:520:GLU:OE2	2.19	0.42
1:B:561:LEU:HD23	1:B:587:VAL:HB	2.00	0.42
1:B:13:ALA:O	1:B:16:LYS:HB3	2.20	0.42
1:B:28:ARG:NH2	1:B:492:PHE:HZ	2.18	0.42
1:A:119:VAL:HG11	1:A:168:TRP:CZ3	2.54	0.41
1:B:26:ILE:CD1	1:B:661:HIS:HB2	2.49	0.41
1:A:135:GLN:H	1:A:135:GLN:HG2	1.70	0.41
1:B:69:ILE:CD1	1:B:100:LEU:HD11	2.50	0.41
1:A:296:PRO:HA	1:A:297:PRO:HD2	1.94	0.41
1:A:674:LEU:O	1:A:680:GLY:HA3	2.21	0.41
1:A:261:LEU:HD12	1:A:440:VAL:HG22	2.02	0.41
1:B:493:ASN:O	1:B:497:GLN:HB2	2.19	0.41
1:B:682:ARG:NH1	8:B:907:HOH:O	2.06	0.41
1:A:158:LYS:HD2	1:A:158:LYS:HA	1.89	0.41
1:B:54:ALA:O	1:B:460:ALA:HA	2.21	0.41
1:B:161:GLY:O	1:B:165:THR:HB	2.20	0.41
1:B:230:ALA:HA	1:B:236:VAL:HG13	2.02	0.41
1:B:507:VAL:CG2	1:B:513:ASN:CG	2.93	0.41
1:A:205:CYS:SG	1:A:208:PHE:CD2	3.13	0.41
1:B:257:ALA:HB2	1:B:444:LEU:HD21	2.02	0.41
1:B:3:LEU:HD12	1:B:40:LYS:HG3	2.02	0.41
1:B:22:ILE:O	1:B:25:PHE:HB2	2.21	0.41
1:B:658:ILE:O	8:B:919:HOH:O	2.22	0.41
1:A:127:LEU:O	1:A:147:PRO:HG3	2.20	0.41
1:B:9:ALA:O	1:B:12:ALA:HB3	2.21	0.41
1:A:19:GLN:HG2	1:A:25:PHE:CE1	2.56	0.41
1:A:406:ALA:O	1:A:418:LYS:NZ	2.44	0.41
1:A:438:ILE:HD11	1:A:625:THR:HG22	2.03	0.41
1:B:21:GLN:CD	1:B:102:LYS:HG2	2.46	0.41
1:B:511:ILE:HD12	1:B:511:ILE:HA	1.86	0.40
1:B:580:VAL:HB	1:B:604:LEU:HD23	2.03	0.40
1:A:82:SER:HA	1:A:222:ALA:O	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:VAL:HG13	1:A:668:VAL:HG13	2.03	0.40
1:B:211:ARG:NH1	1:B:236:VAL:HB	2.36	0.40
1:B:384:ARG:HA	1:B:384:ARG:HD2	1.84	0.40
1:A:273:ARG:HB2	1:A:312:TYR:CE1	2.57	0.40
1:B:502:ILE:O	1:B:694:GLN:HA	2.21	0.40
1:A:676:THR:HG22	1:A:677:LYS:HG2	2.02	0.40
1:B:55:PRO:HD2	1:B:58:VAL:HG21	2.03	0.40
1:B:682:ARG:HG2	8:B:999:HOH:O	2.21	0.40
1:A:281:LYS:O	8:A:915:HOH:O	2.22	0.40
1:B:132:PRO:HA	1:B:146:THR:CG2	2.52	0.40
1:B:271:TRP:O	1:B:275:GLN:HG2	2.21	0.40
1:B:595:ALA:O	1:B:656:ARG:HD2	2.21	0.40
1:B:596:GLU:O	1:B:656:ARG:CZ	2.69	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	680/716 (95%)	655 (96%)	25 (4%)	0	100	100
1	B	677/716 (95%)	650 (96%)	26 (4%)	1 (0%)	48	68
All	All	1357/1432 (95%)	1305 (96%)	51 (4%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	135	GLN

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	588/618 (95%)	556 (95%)	32 (5%)	20	41
1	B	586/618 (95%)	556 (95%)	30 (5%)	21	43
All	All	1174/1236 (95%)	1112 (95%)	62 (5%)	20	42

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	75	GLU
1	A	76	GLN
1	A	100	LEU
1	A	120	CYS
1	A	131	GLU
1	A	133	THR
1	A	141	LEU
1	A	150	GLN
1	A	151	GLU
1	A	163	LEU
1	A	167	LYS
1	A	176	ASP
1	A	189	THR
1	A	205	CYS
1	A	209	VAL
1	A	236	VAL
1	A	287	MET
1	A	333	GLU
1	A	440	VAL
1	A	443	GLN
1	A	450	ARG
1	A	452	ILE
1	A	518	ILE
1	A	532	LYS
1	A	555	THR
1	A	560	MET
1	A	618	ILE

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Mol	Chain	Res	Type
1	A	642	SER
1	A	676	THR
1	A	678	ASN
1	A	696	GLU
1	A	702	VAL
1	B	100	LEU
1	B	102	LYS
1	B	138	LEU
1	B	143	ASP
1	B	163	LEU
1	B	165	THR
1	B	176	ASP
1	B	189	THR
1	B	205	CYS
1	B	216	GLU
1	B	232	GLU
1	B	236	VAL
1	B	274	LEU
1	B	291	ARG
1	B	368	ASN
1	B	372	GLU
1	B	385	LEU
1	B	423	GLU
1	B	425	ARG
1	B	447	LEU
1	B	466	ASN
1	B	497	GLN
1	B	518	ILE
1	B	575	LEU
1	B	584	GLU
1	B	631	LYS
1	B	633	LEU
1	B	642	SER
1	B	681	LYS
1	B	702	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	428	GLN
1	A	516	GLN

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Mol	Chain	Res	Type
1	A	592	GLN
1	B	21	GLN
1	B	215	GLN
1	B	307	HIS
1	B	319	ASN
1	B	388	GLN
1	B	443	GLN
1	B	466	ASN
1	B	494	HIS
1	B	497	GLN
1	B	592	GLN
1	B	649	ASN
1	B	653	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](#)

Of 8 ligands modelled in this entry, 2 are monoatomic - leaving 6 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	$\# Z > 2$
6	BEF	B	803	5	0,3,3	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	SF4	A	801	-	0,12,12	-	-	-		
4	SF4	B	801	1	0,12,12	-	-	-		
5	ADP	B	802	6,7	28,29,29	1.42	6 (21%)	43,45,45	1.90	11 (25%)
5	ADP	A	802	6,7	28,29,29	1.40	5 (17%)	43,45,45	1.95	12 (27%)
6	BEF	A	803	5	0,3,3	-	-	-		

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	SF4	A	801	-	-	-	0/6/5/5
5	ADP	A	802	6,7	-	8/16/32/32	0/3/3/3
4	SF4	B	801	1	-	-	0/6/5/5
5	ADP	B	802	6,7	-	6/16/32/32	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	802	ADP	C5-C4	4.54	1.47	1.39
5	A	802	ADP	C5-C4	4.29	1.46	1.39
5	A	802	ADP	C5-C6	2.67	1.48	1.41
5	B	802	ADP	C5-C6	2.53	1.48	1.41
5	A	802	ADP	C4-N9	-2.43	1.32	1.37
5	A	802	ADP	C5-N7	-2.41	1.34	1.39
5	B	802	ADP	PA-O3A	2.36	1.62	1.59
5	B	802	ADP	C5-N7	-2.26	1.35	1.39
5	A	802	ADP	C8-N7	2.26	1.36	1.31
5	B	802	ADP	C4-N9	-2.13	1.33	1.37
5	B	802	ADP	C8-N7	2.11	1.35	1.31

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	802	ADP	C5-C4-N3	-5.27	119.46	126.72
5	B	802	ADP	C5-C4-N3	-5.26	119.47	126.72
5	B	802	ADP	N3-C4-N9	4.49	134.80	127.17
5	A	802	ADP	C4-C5-N7	-4.03	105.98	110.58
5	A	802	ADP	N3-C4-N9	4.01	133.99	127.17
5	B	802	ADP	N3-C2-N1	-3.75	122.91	128.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	802	ADP	C2-N3-C4	3.66	120.77	111.83
5	B	802	ADP	C4-N9-C8	3.54	109.45	105.74
5	A	802	ADP	C2-N3-C4	3.39	120.12	111.83
5	B	802	ADP	C4-C5-N7	-3.35	106.76	110.58
5	A	802	ADP	C4-N9-C8	3.32	109.22	105.74
5	A	802	ADP	N3-C2-N1	-2.95	124.12	128.58
5	A	802	ADP	C5-N7-C8	2.91	108.03	103.45
5	A	802	ADP	O4'-C1'-N9	-2.84	102.64	108.09
5	B	802	ADP	C5-N7-C8	2.68	107.67	103.45
5	A	802	ADP	N9-C8-N7	-2.62	110.22	113.94
5	B	802	ADP	N9-C8-N7	-2.49	110.40	113.94
5	A	802	ADP	C5'-C4'-C3'	-2.45	106.39	115.21
5	A	802	ADP	C6-C5-N7	2.36	136.65	132.09
5	B	802	ADP	C6-C5-N7	2.31	136.54	132.09
5	B	802	ADP	C2-N1-C6	2.25	122.43	118.73
5	B	802	ADP	O3'-C3'-C2'	-2.14	104.96	111.82
5	A	802	ADP	O3A-PB-O1B	-2.13	99.85	111.04

There are no chirality outliers.

All (14) torsion outliers are listed below:

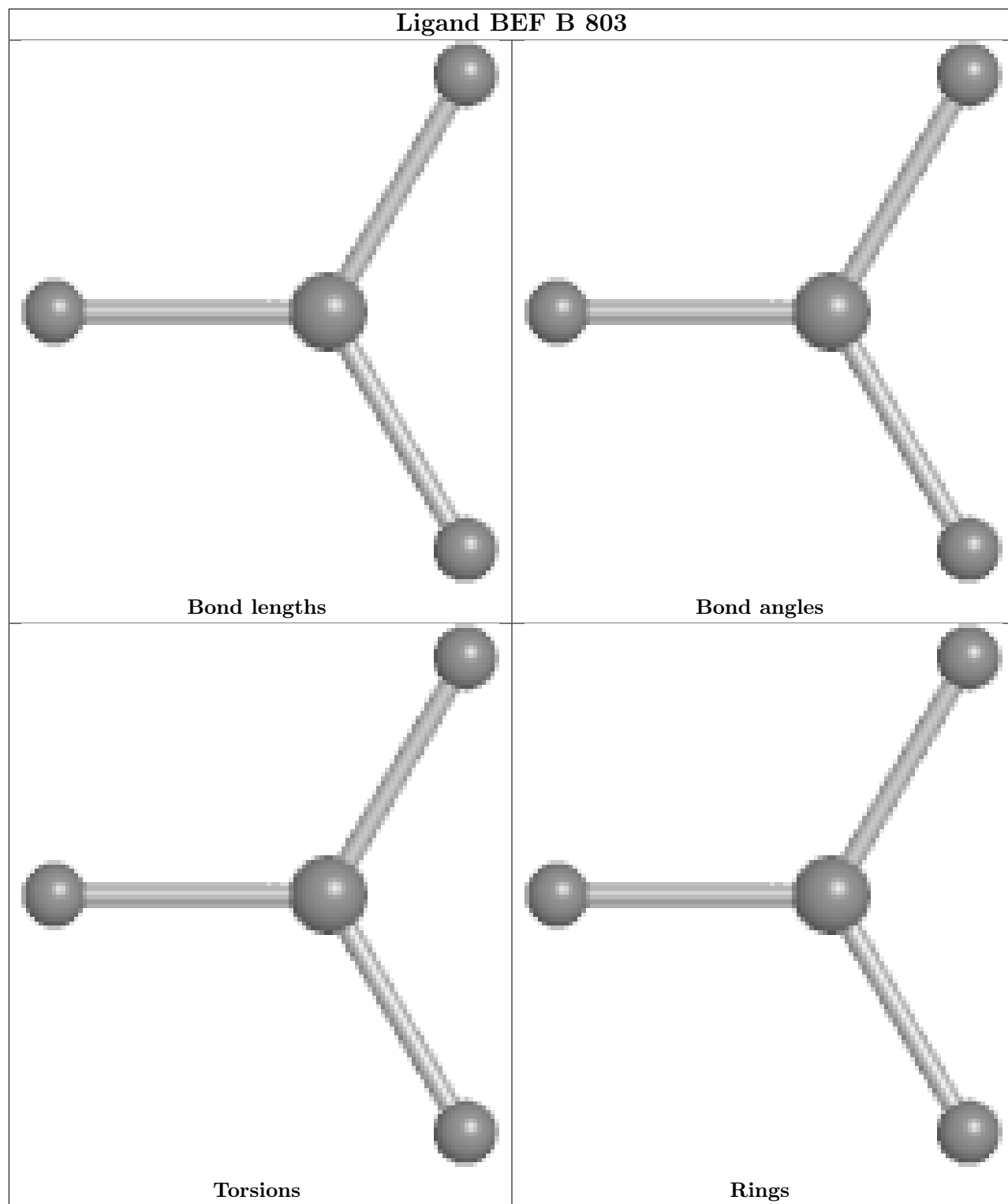
Mol	Chain	Res	Type	Atoms
5	A	802	ADP	PA-O3A-PB-O3B
5	A	802	ADP	C5'-O5'-PA-O1A
5	B	802	ADP	PA-O3A-PB-O2B
5	B	802	ADP	C2'-C1'-N9-C8
5	B	802	ADP	C2'-C1'-N9-C4
5	A	802	ADP	C2'-C1'-N9-C8
5	A	802	ADP	C5'-O5'-PA-O3A
5	A	802	ADP	C2'-C1'-N9-C4
5	A	802	ADP	O4'-C1'-N9-C8
5	A	802	ADP	PA-O3A-PB-O2B
5	B	802	ADP	PA-O3A-PB-O3B
5	B	802	ADP	O4'-C1'-N9-C8
5	B	802	ADP	PA-O3A-PB-O1B
5	A	802	ADP	O4'-C4'-C5'-O5'

There are no ring outliers.

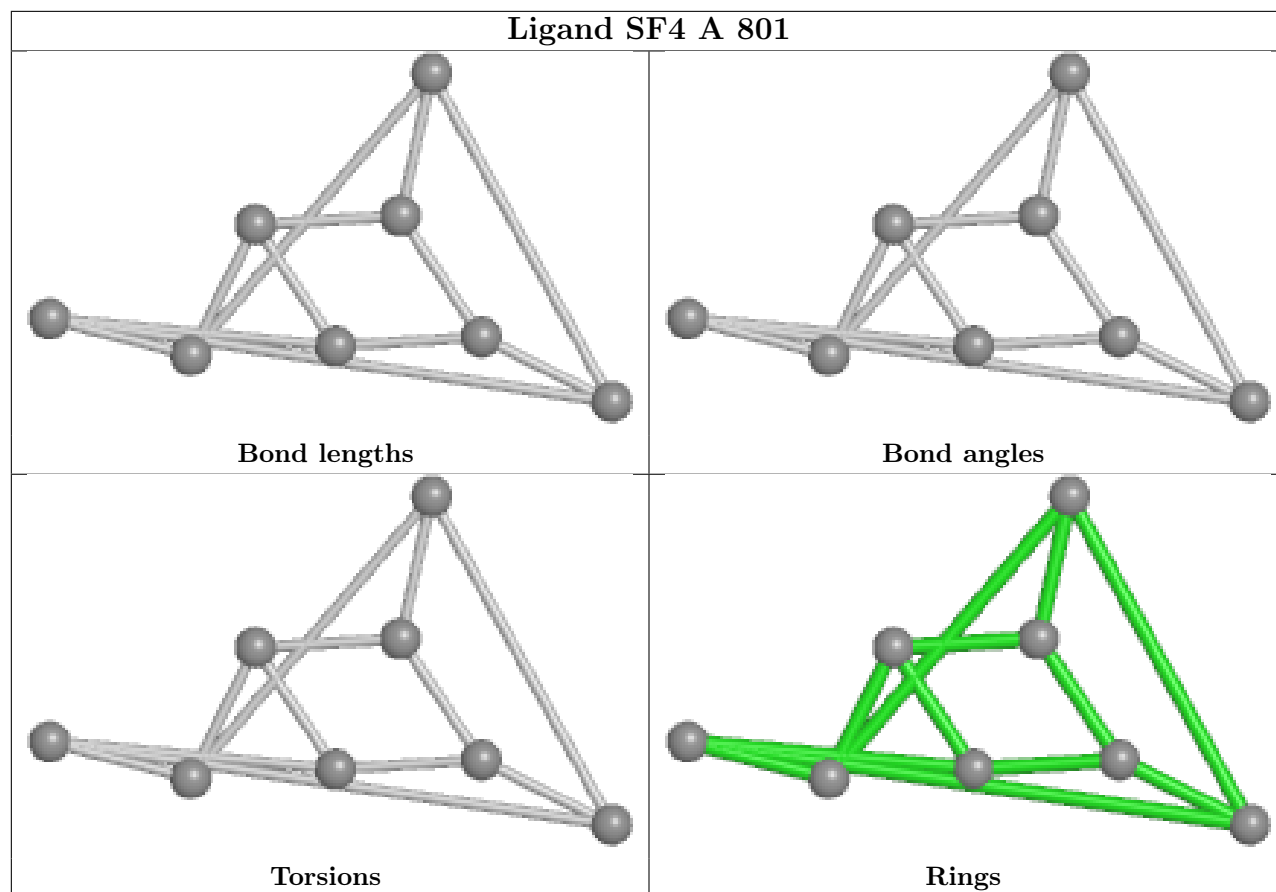
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	803	BEF	1	0
4	A	801	SF4	2	0

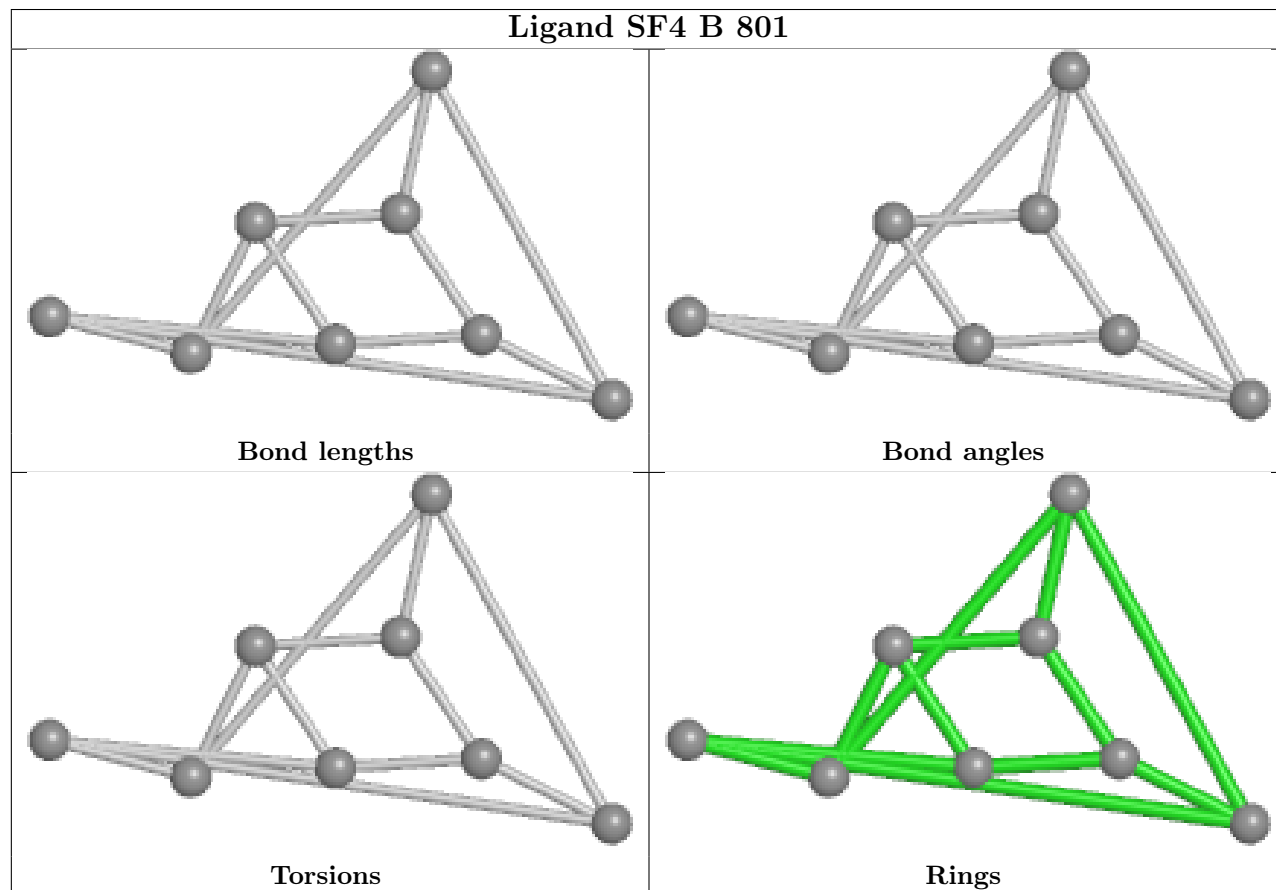
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

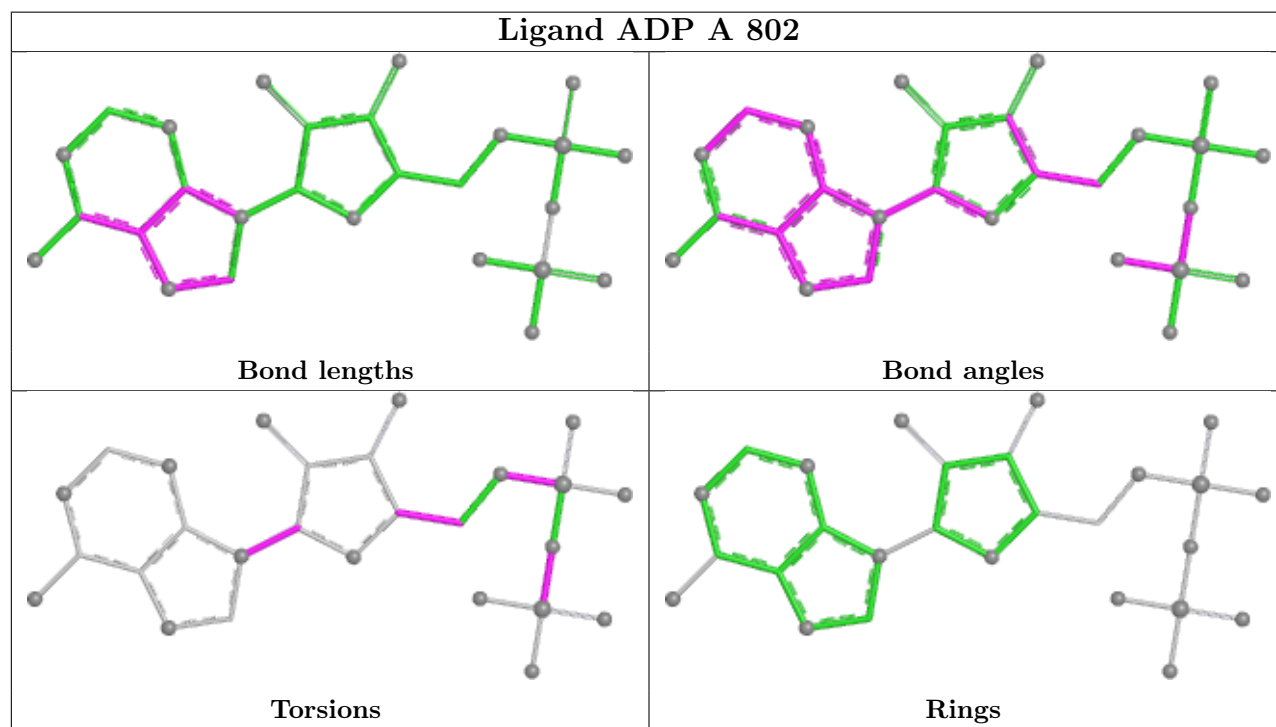
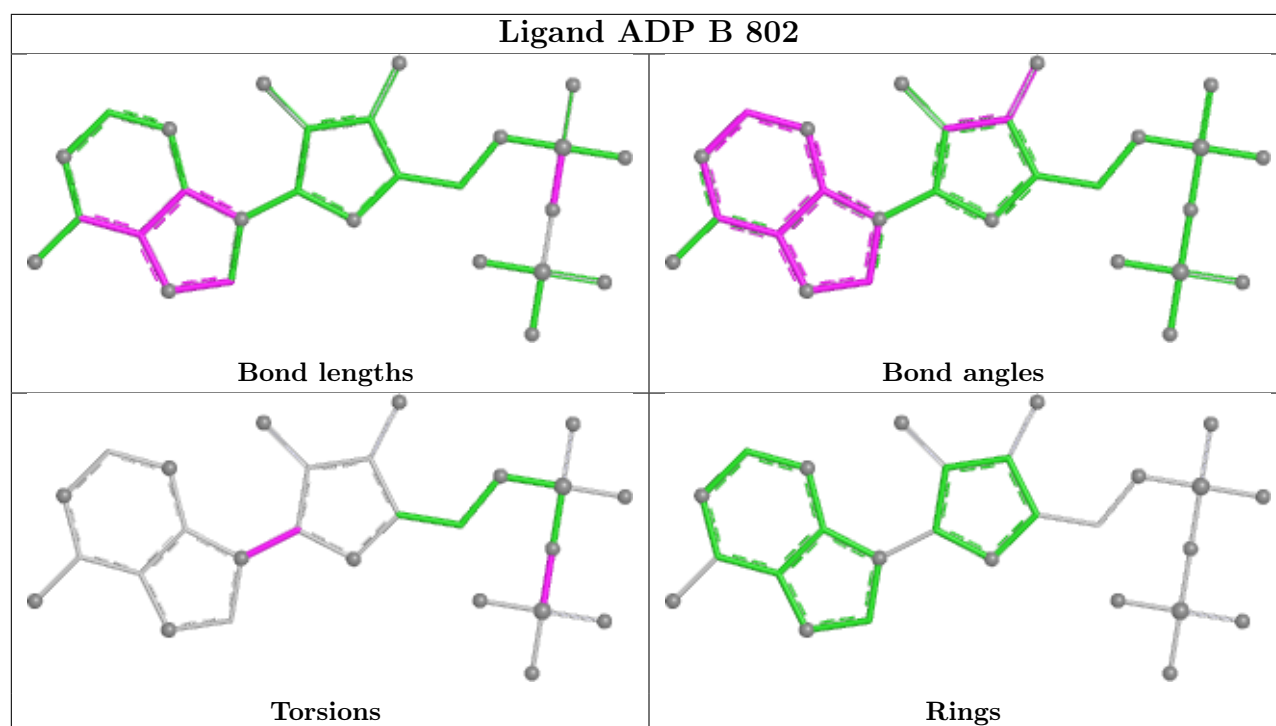


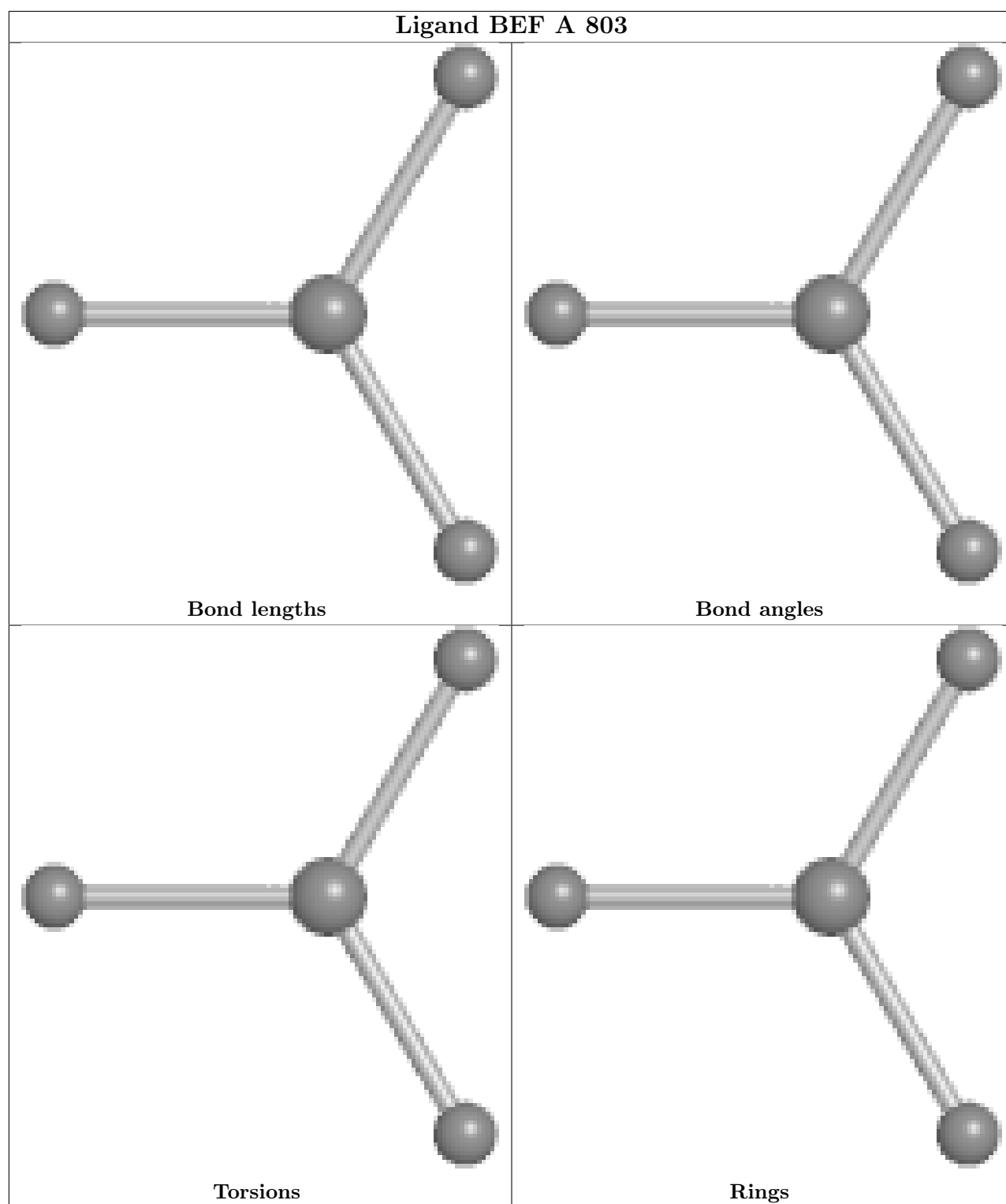
Ligand SF4 A 801



Ligand SF4 B 801







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

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	686/716 (95%)	0.17	32 (4%) 36 32	19, 33, 64, 80	0
1	B	683/716 (95%)	0.48	44 (6%) 25 22	20, 39, 65, 77	0
2	C	11/11 (100%)	0.71	2 (18%) 3 2	36, 50, 72, 73	0
3	D	10/10 (100%)	0.54	1 (10%) 12 10	33, 48, 74, 76	0
All	All	1390/1453 (95%)	0.33	79 (5%) 29 26	19, 36, 64, 80	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	378	ASP	4.7
1	B	328	ALA	4.6
1	B	702	VAL	4.3
1	B	2	ALA	4.1
1	A	133	THR	4.1
1	A	511	ILE	3.9
1	B	507	VAL	3.7
1	B	511	ILE	3.6
1	A	132	PRO	3.6
1	B	233	SER	3.6
1	A	166	TYR	3.4
1	A	165	THR	3.4
1	B	329	GLY	3.4
1	B	23	PRO	3.3
1	B	24	ASP	3.3
1	A	142	ASP	3.3
1	B	137	LEU	3.2
1	A	130	THR	3.2
1	A	129	SER	3.2
1	B	701	ILE	3.2
3	D	1	DT	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	512	ASP	3.1
1	A	146	THR	3.0
1	A	209	VAL	3.0
2	C	0	DT	2.9
1	A	624	ILE	2.9
1	A	163	LEU	2.9
1	A	134	GLN	2.9
1	B	506	ARG	2.8
1	B	428	GLN	2.8
1	B	21	GLN	2.8
1	B	22	ILE	2.7
1	A	233	SER	2.7
1	A	128	ALA	2.7
1	A	527	GLU	2.7
1	B	20	GLU	2.7
1	B	102	LYS	2.6
1	A	145	LEU	2.6
1	B	496	GLU	2.6
1	A	162	ASP	2.6
1	B	138	LEU	2.6
1	B	426	GLU	2.6
1	A	189	THR	2.5
1	B	189	THR	2.5
1	A	144	GLU	2.5
1	B	19	GLN	2.5
1	B	210	ALA	2.4
1	B	676	THR	2.4
1	B	703	LYS	2.4
1	A	164	ASP	2.4
1	B	103	ILE	2.4
1	B	165	THR	2.4
1	A	150	GLN	2.4
1	B	675	LEU	2.4
1	B	133	THR	2.3
1	A	167	LYS	2.3
1	B	493	ASN	2.3
1	A	168	TRP	2.3
1	B	505	MET	2.3
1	B	16	LYS	2.3
1	A	510	SER	2.3
1	B	26	ILE	2.3
1	B	293	LYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	131	GLU	2.2
1	B	212(A)	ARG	2.2
1	B	140	PHE	2.2
1	B	700	GLY	2.2
1	A	618	ILE	2.2
1	A	127	LEU	2.1
1	A	379	ILE	2.1
1	B	330	GLN	2.1
2	C	1	DT	2.1
1	B	6	ALA	2.1
1	B	142	ASP	2.1
1	B	697	VAL	2.0
1	B	499	LYS	2.0
1	A	619	ASP	2.0
1	B	378	ASP	2.0
1	A	170	GLY	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(Å ²)	Q<0.9
4	SF4	A	801	8/8	0.78	0.12	83,113,150,165	0
4	SF4	B	801	8/8	0.84	0.13	84,100,150,173	0
5	ADP	B	802	27/27	0.95	0.09	29,39,52,54	0
6	BEF	A	803	4/4	0.95	0.07	26,26,28,31	0
6	BEF	B	803	4/4	0.95	0.07	26,26,29,31	0
5	ADP	A	802	27/27	0.97	0.07	23,29,35,38	0
7	MG	B	804	1/1	0.98	0.03	31,31,31,31	0

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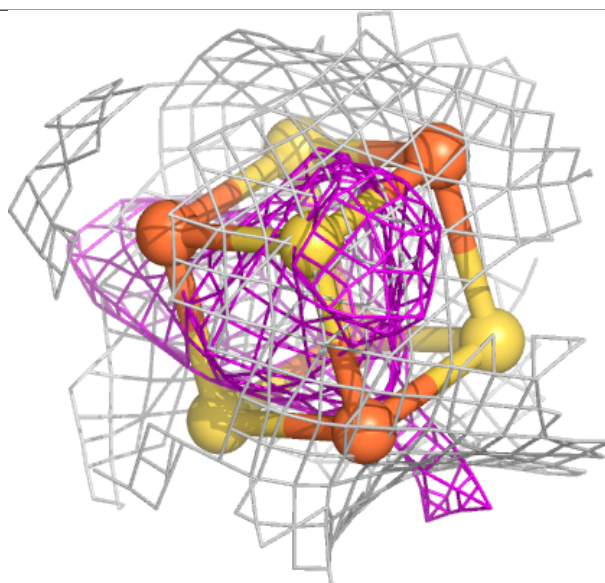
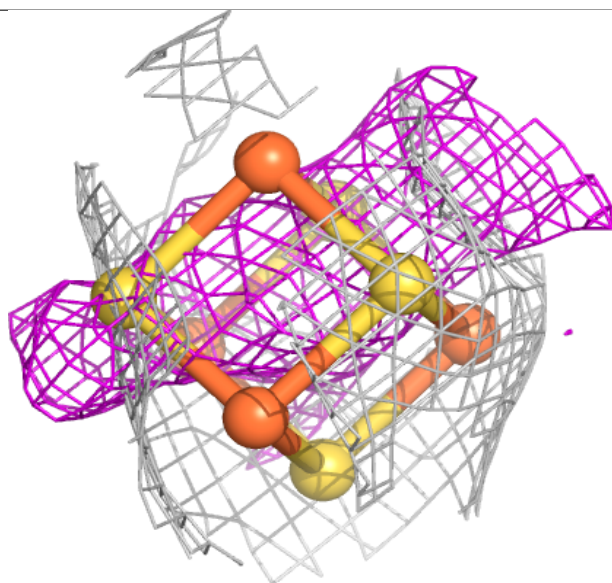
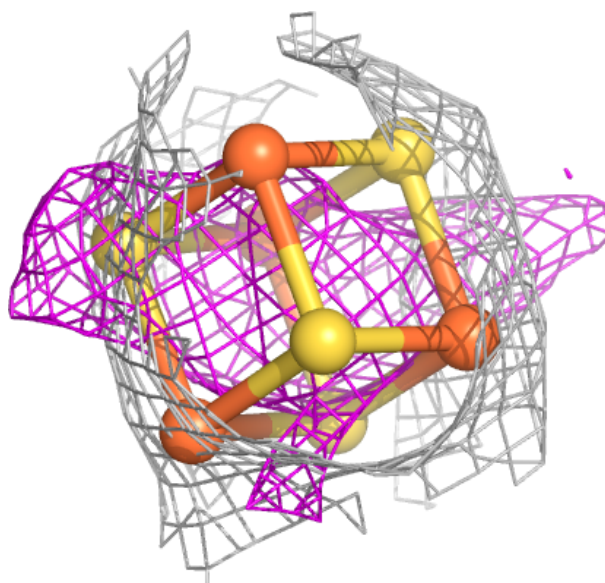
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
7	MG	A	804	1/1	0.99	0.04	25,25,25,25	0

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.

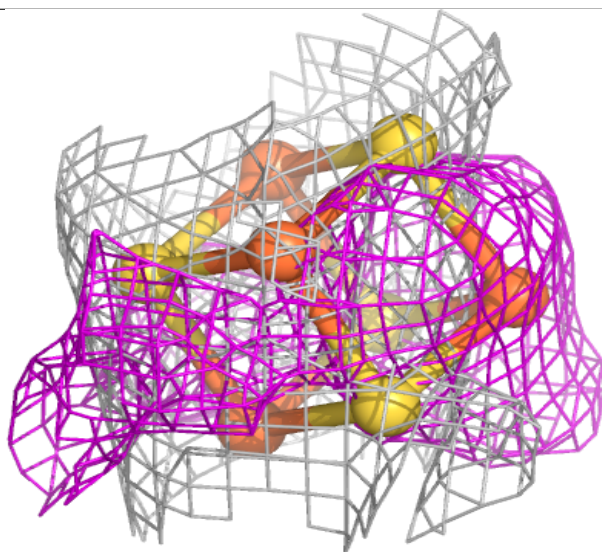
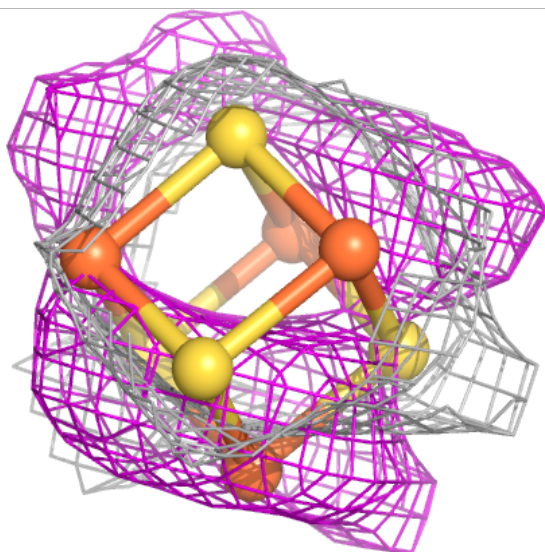
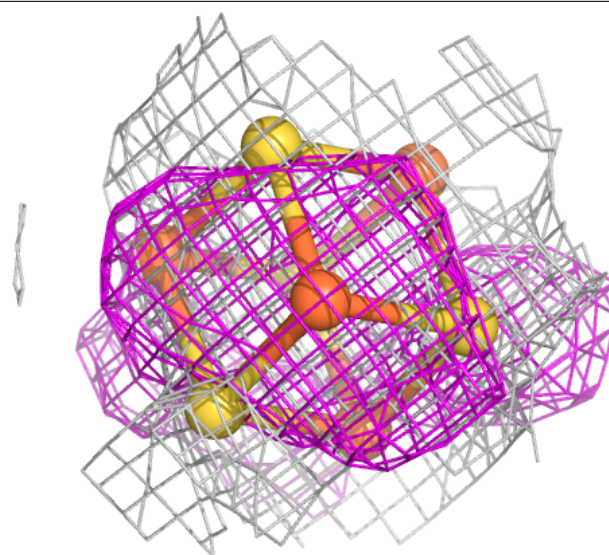
Electron density around SF4 A 801:

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



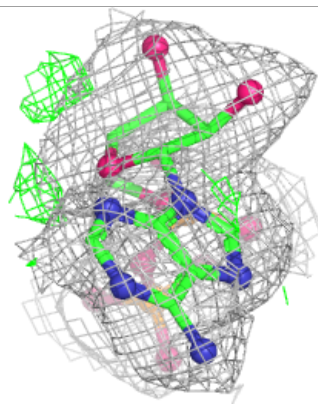
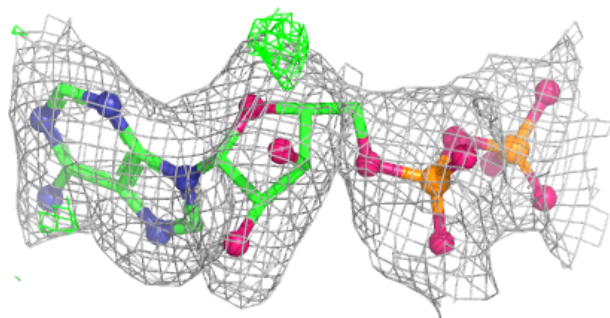
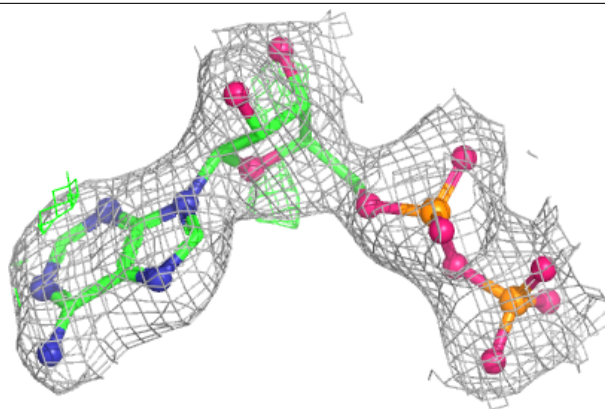
Electron density around SF4 B 801:

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



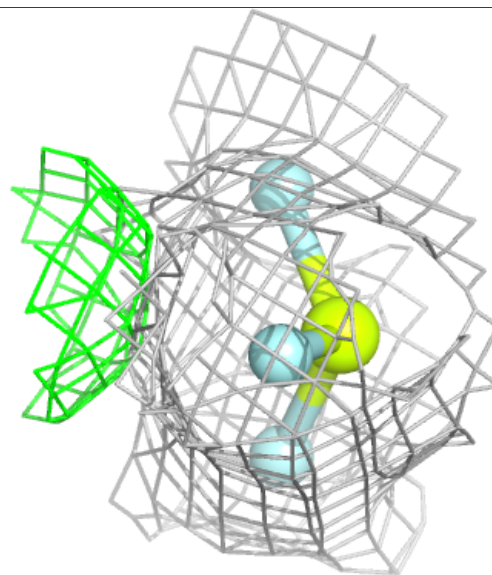
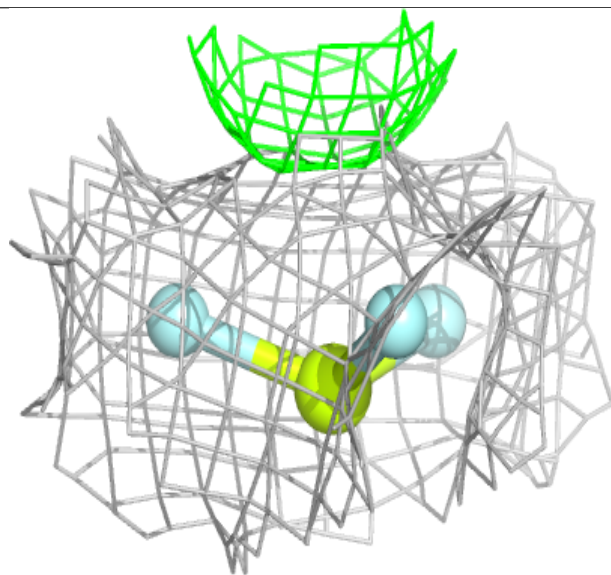
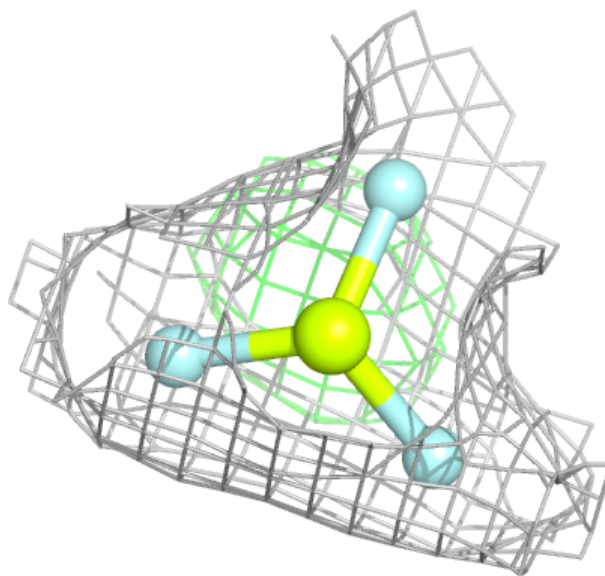
Electron density around ADP B 802:

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



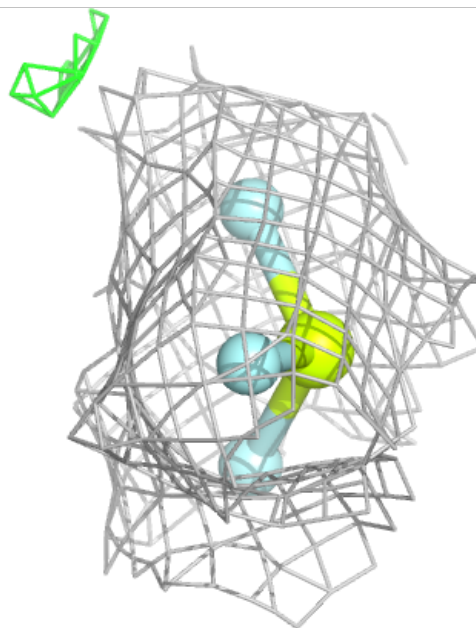
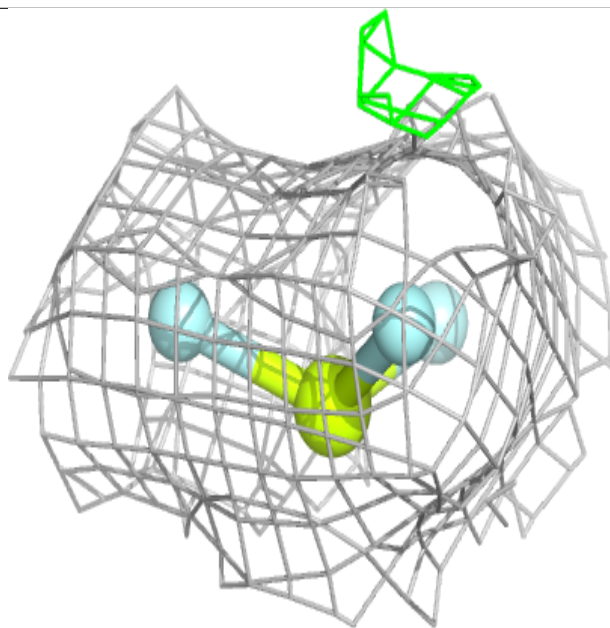
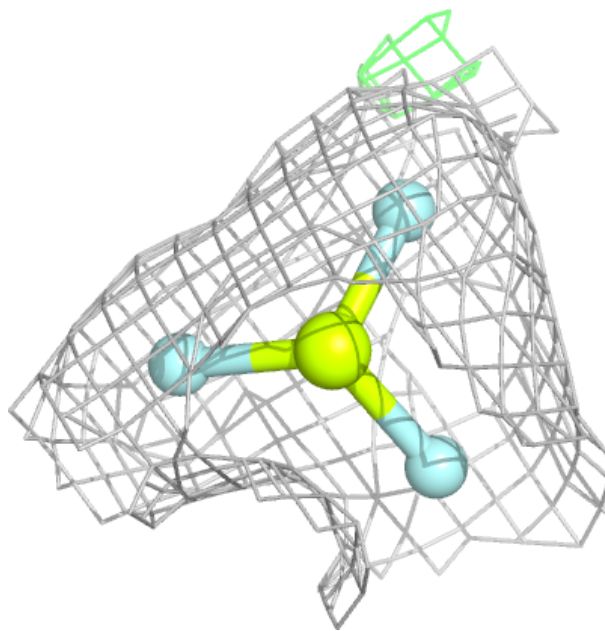
Electron density around BEF A 803:

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



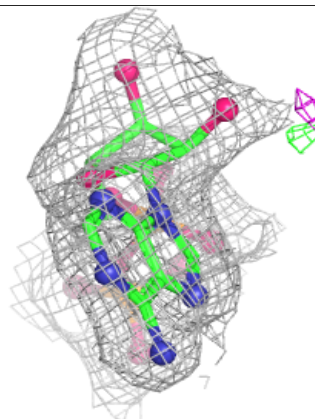
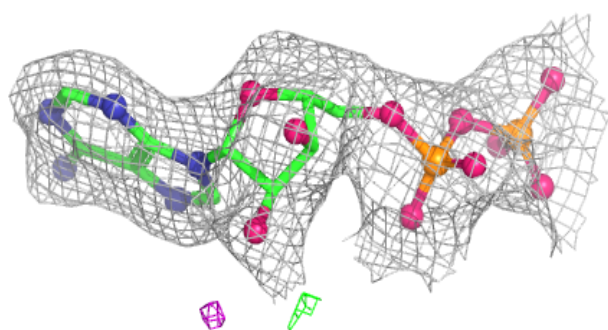
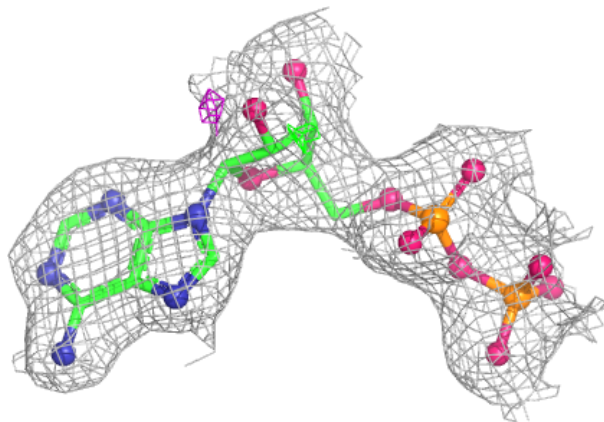
Electron density around BEF B 803:

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



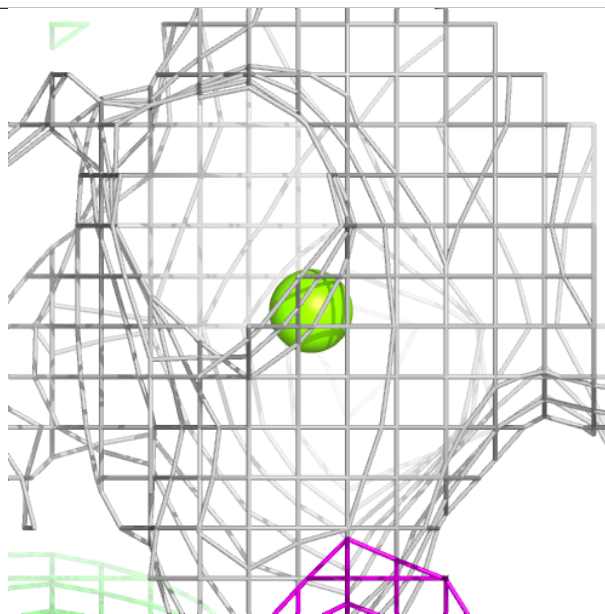
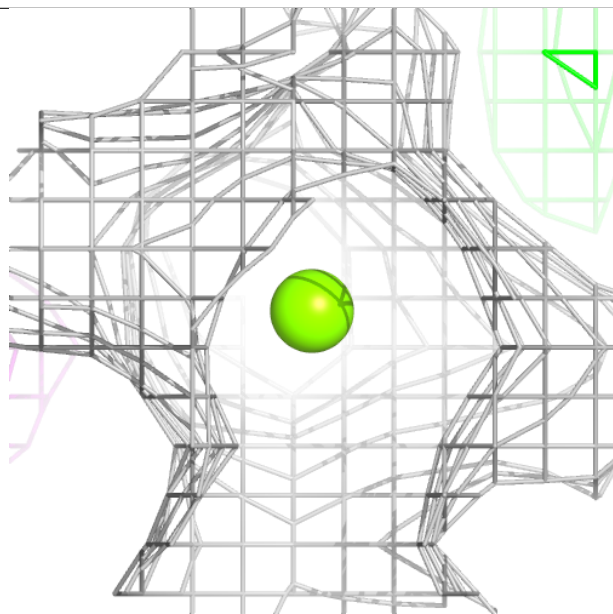
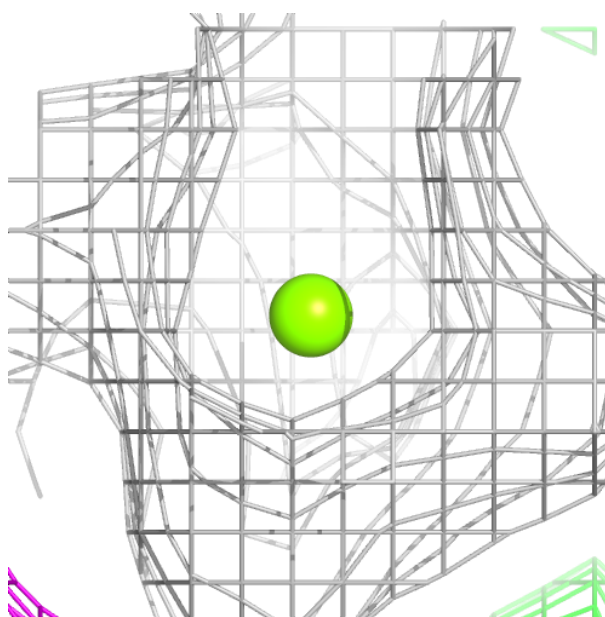
Electron density around ADP A 802:

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



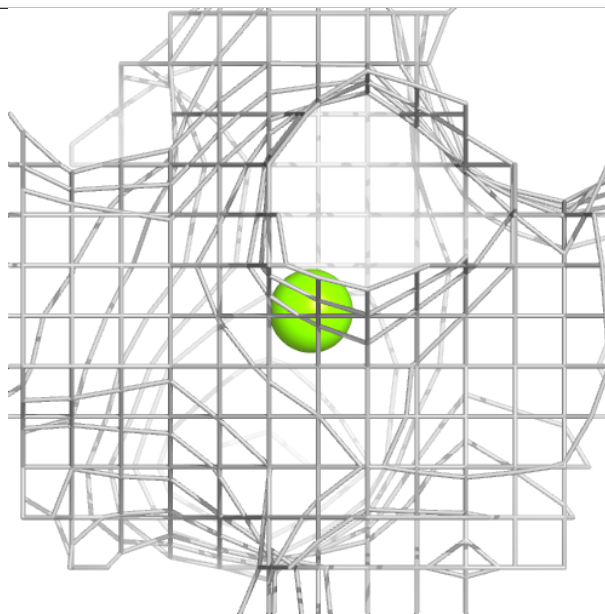
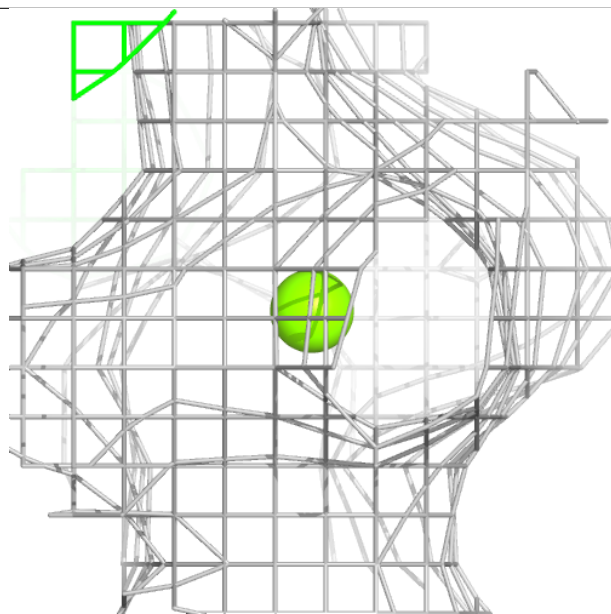
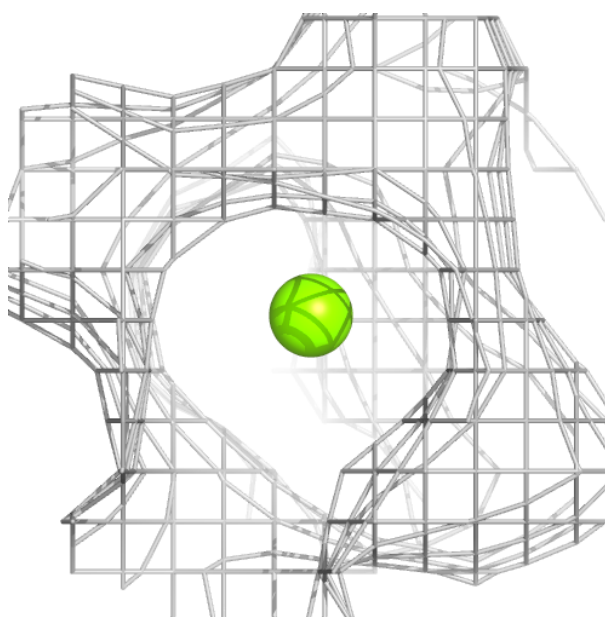
Electron density around MG B 804:

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



Electron density around MG A 804:

$2mF_o-DF_c$ (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.