Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 01:40 pm BST

PDB ID	:	6FWS
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 following versions of software and data (see references ⓘ) were used in the production of this report:

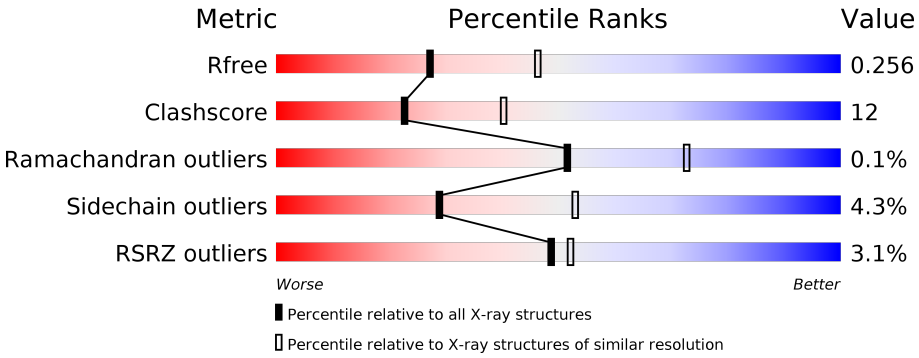
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (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 on 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 <=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	3% 74% 20%
1	B	716	3% 71% 24% 5%
2	C	11	9% 36% 55% 9%
3	D	10	10% 20% 70% 10%

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 crite-

ria:

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			

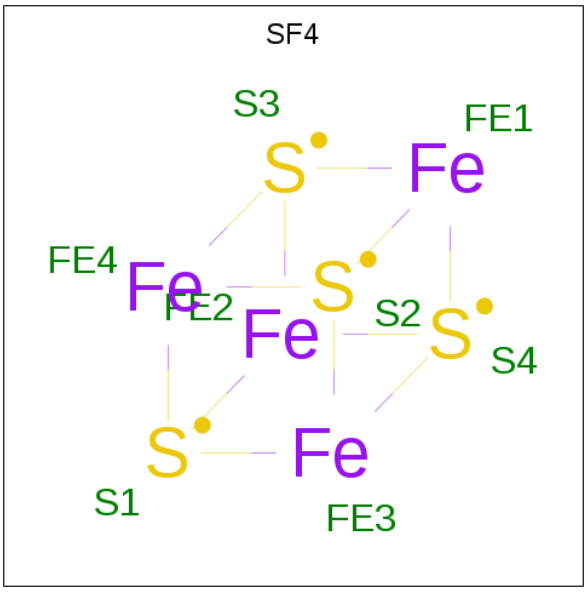
- Molecule 2 is a DNA chain called DNA (5'-D(*TP*TP*TP*TP*TP*TP*TP*TP*TP*TP*T)-3').

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').

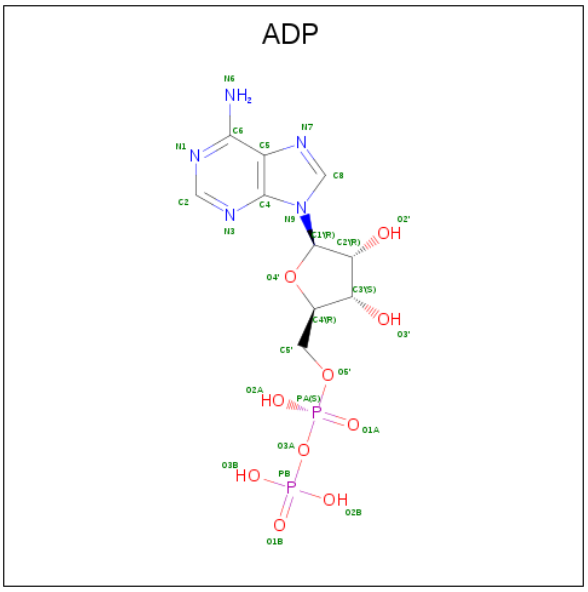
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	10	Total	C	N	O	P	0	0	0
			196	100	20	67	9			

- Molecule 4 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4) (labeled as "Ligand of Interest" by author).



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

- Molecule 5 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$) (labeled as "Ligand of Interest" by author).



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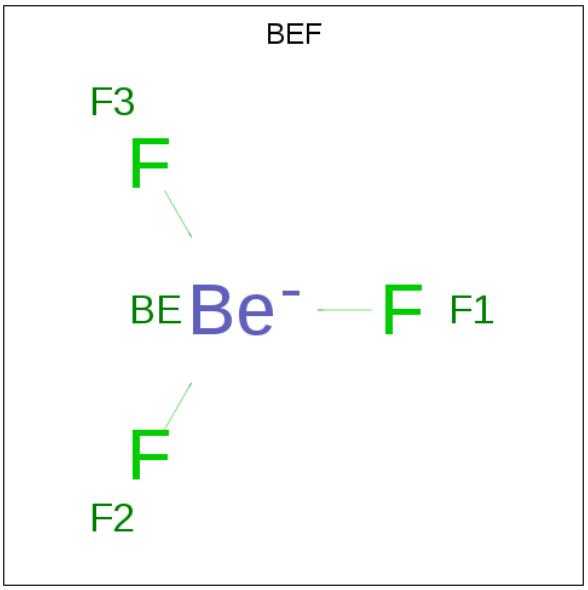
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 6 is BERYLLIUM TRIFLUORIDE ION (three-letter code: BEF) (formula: BeF_3) (labeled as "Ligand of Interest" by author).



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 (three-letter code: MG) (formula: Mg) (labeled as "Ligand of Interest" by author).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	B	1	Total	Mg		0	0
			1	1			
7	A	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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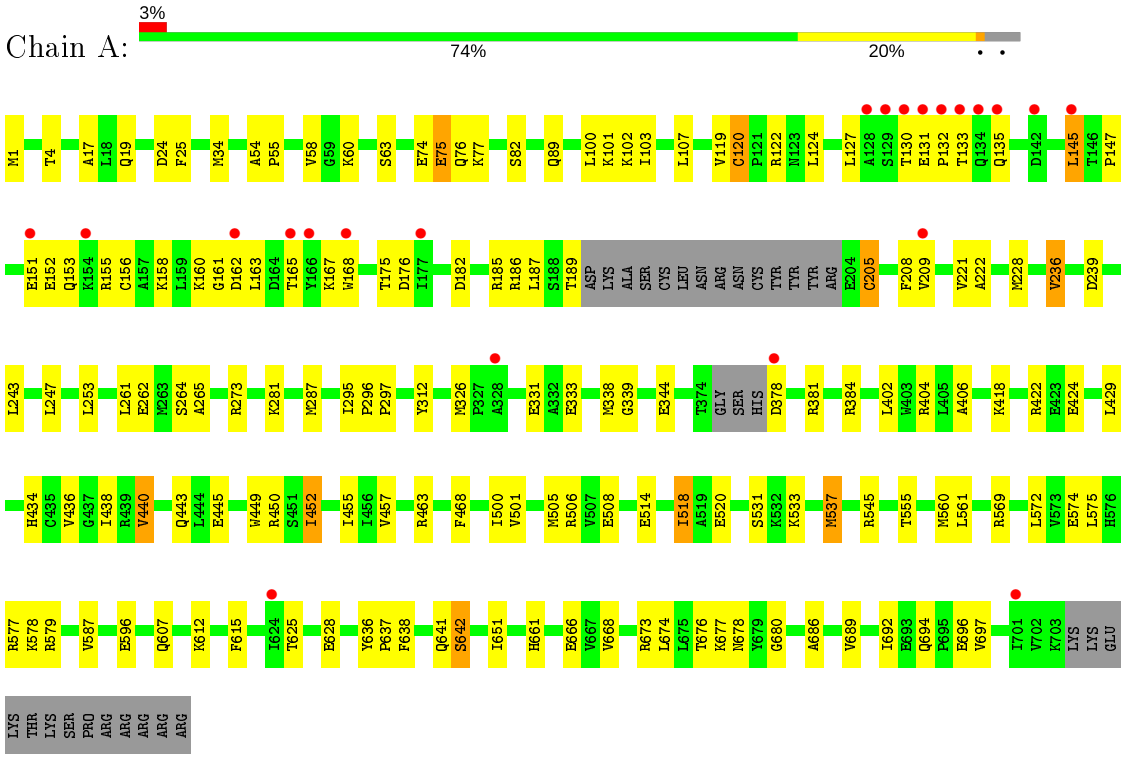
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	C	9	Total O 9 9	0	0
8	B	159	Total O 159 159	0	0
8	D	7	Total O 7 7	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

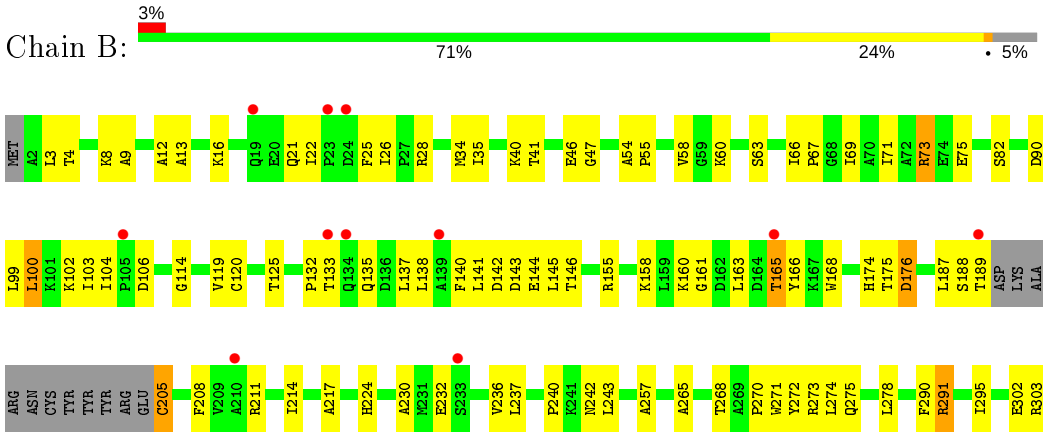
- Molecule 1: ATP-dependent DNA helicase DinG

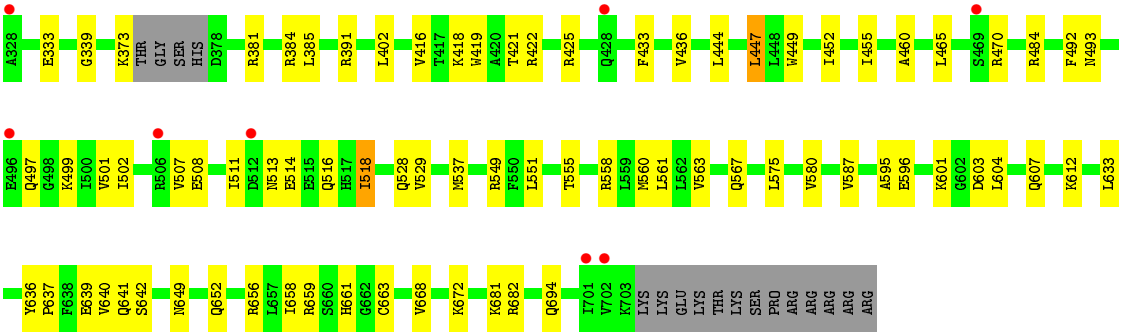
Chain A:



- Molecule 1: ATP-dependent DNA helicase DinG

Chain B:





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

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [1]	2.93 (at 2.51Å)	Xtriage
Refinement program	PHENIX (1.11.1_2575: ???)	Depositor
R, R_{free}	0.219 , 0.256 0.219 , 0.256	Depositor DCC
R_{free} test set	2806 reflections (4.85%)	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)	0.34 , 46.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: 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	0.41	0/5564	0.60	2/7537 (0.0%)
1	B	0.42	1/5546 (0.0%)	0.60	1/7512 (0.0%)
2	C	1.25	1/237 (0.4%)	1.55	0/365
3	D	1.09	0/215	1.47	1/331 (0.3%)
All	All	0.47	2/11562 (0.0%)	0.67	4/15745 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	47	GLY	C-O	-7.89	1.11	1.23
2	C	1	DT	C3'-O3'	-5.36	1.36	1.44

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	145	LEU	CA-CB-CG	-6.07	101.34	115.30
1	B	166	TYR	CB-CG-CD2	-5.29	117.83	121.00
1	A	236	VAL	CG1-CB-CG2	5.08	119.04	110.90
3	D	9	DT	N3-C4-O4	5.03	122.92	119.90

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	5456	0	5540	113	0
1	B	5438	0	5527	136	0
2	C	216	0	131	10	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	262	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 (262) 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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
1:B:596:GLU:HG2	1:B:652:GLN:HG2	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: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:H6	3:D:2:DT:H5"	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:90:ASP:OD1	1:B:174:HIS:NE2	2.38	0.57
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:B:22:ILE:HD11	1:B:99:LEU:HD21	1.87	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: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:B:155:ARG:HG3	1:B:158:LYS:HE3	1.88	0.55
1:B:652:GLN:O	1:B:656:ARG:NH2	2.38	0.55
1:A:677:LYS:HE2	2:C:3:DT:OP1	2.07	0.55
1:A:424:GLU:HG2	1:A:429:LEU:HD23	1.87	0.55
1:A:505:MET:HE3	1:A:520:GLU:HB3	1.88	0.55
1:B:537:MET:HG2	1:B:607:GLN:HB3	1.88	0.54
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:449:TRP:O	8:B:914:HOH:O	2.19	0.54
1:B:114:GLY:HA3	3:D:9:DT:H5"	1.90	0.54
1:A:119:VAL:HG23	1:A:187:LEU:HB3	1.90	0.54
1:B:507:VAL:HG21	1:B:513:ASN:CG	2.29	0.53
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:B:4:THR:O	1:B:8:LYS:HG3	2.09	0.53
1:A:636:TYR:HB2	2:C:1:DT:O4	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:145:LEU:N	8:B:905:HOH:O	2.02	0.52
1:B:119:VAL:HG23	1:B:187:LEU:HB3	1.91	0.52
1:A:262:GLU:HG3	1:A:436:VAL:HG22	1.91	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: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:130:THR:O	1:A:132:PRO:HD3	2.09	0.52
2:C:5:DT:H71	2:C:5:DT:OP2	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: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:B:73:ARG:HH22	1:B:106:ASP:CG	2.15	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:B:302:GLU:O	8:B:916:HOH:O	2.19	0.51
1:B:34:MET:HG2	1:B:63:SER:HB3	1.93	0.51
1:B:132:PRO:HA	1:B:146:THR:HG23	1.94	0.50
1:A:424:GLU:HG2	1:A:429:LEU:CD2	2.41	0.50
1:B:452:ILE:HB	1:B:455:ILE:HD11	1.92	0.50
1:B:71:ILE:O	1:B:75:GLU:HG3	2.12	0.50
1:A:638:PHE:CD1	2:C:2:DT:H2"	2.47	0.50
1:B:381:ARG:NH2	8:B:933:HOH:O	2.42	0.50
1:B:60:LYS:NZ	6:B:803:BEF:F1	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:508:GLU:OE1	1:A:676:THR:HG21	2.14	0.48
1:A:55:PRO:HD2	1:A:58:VAL:HG21	1.94	0.48
1:B:278:LEU:HD23	1:B:391:ARG:HH12	1.79	0.48
1:A:295:ILE:H	1:A:295:ILE:HD12	1.79	0.48
1:A:463:ARG:HD2	1:A:468:PHE:CE2	2.49	0.48
1:A:247:LEU:HD12	1:A:457:VAL:HG22	1.96	0.47
1:A:265:ALA:HB3	1:A:402:LEU:HD22	1.96	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:161:GLY:O	1:A:165:THR:N	2.33	0.47
1:A:578:LYS:CD	1:A:578:LYS:H	2.27	0.47
1:A:607:GLN:HG3	1:A:666:GLU:HG3	1.96	0.47
1:B:339:GLY:O	1:B:418:LYS:HE3	2.14	0.47
1:B:507:VAL:HG11	1:B:516:GLN:HG3	1.96	0.47
1:B:35:ILE:HG23	1:B:67:PRO:HG3	1.97	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:A:344:GLU:H	1:A:344:GLU:CD	2.18	0.46
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:A:228:MET:HE2	1:A:253:LEU:HD11	1.98	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:HD2	1:B:549:ARG:HA	1.69	0.45
1:A:273:ARG:NH1	8:A:937:HOH:O	2.49	0.45
1:A:145:LEU:HD23	1:A:145:LEU:HA	1.62	0.45
1:A:89:GLN:HG2	1:A:221:VAL:HG12	1.98	0.45
2:C:4:DT:H2"	2:C:5:DT:H71	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:595:ALA:C	1:B:656:ARG:HD2	2.37	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:211:ARG:O	1:B:214:ILE:HB	2.17	0.44
1:B:82:SER:OG	1:B:224:HIS:ND1	2.42	0.44
1:B:54:ALA:O	1:B:60:LYS:HE3	2.17	0.44
2:C:0:DT:C5	2:C:1:DT:C5	3.06	0.44
1:B:501:VAL:O	1:B:668:VAL:HA	2.18	0.44
2:C:0:DT:H73	2:C:1:DT:H73	2.00	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:B:529:VAL:HG11	1:B:560:MET:HE3	2.00	0.43
1:A:508:GLU:CD	1:A:676:THR:HG21	2.38	0.43
1:B:529:VAL:HG11	1:B:560:MET:CE	2.47	0.43
1:B:419:TRP:HZ3	1:B:436:VAL:HG12	1.84	0.43
1:A:127:LEU:HB3	1:A:156:CYS:SG	2.59	0.43
1:A:19:GLN:HG2	1:A:25:PHE:CD1	2.53	0.43
1:A:505:MET:CE	1:A:520:GLU:HB3	2.49	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:HA	1:A:575:LEU:HD23	1.91	0.43
1:B:290:PHE:O	1:B:373:LYS:NZ	2.39	0.43
1:A:339:GLY:O	1:A:418:LYS:HE3	2.19	0.42
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: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:C5'	3:D:2:DT:H6	2.30	0.42
1:A:505:MET:HA	1:A:520:GLU:OE2	2.19	0.42
1:B:95:LYS:C	1:B:98:PRO:HD2	2.40	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:54:ALA:O	1:B:460:ALA:HA	2.21	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:22:ILE:O	1:B:25:PHE:HB2	2.21	0.41
1:B:3:LEU:HD12	1:B:40:LYS:HG3	2.02	0.41
1:B:658:ILE:O	8:B:919:HOH:O	2.22	0.41
1:B:9:ALA:O	1:B:12:ALA:HB3	2.21	0.41
1:A:127:LEU:O	1:A:147:PRO:HG3	2.20	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: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:501:VAL:HG13	1:A:668:VAL:HG13	2.03	0.40
1:A:82:SER:HA	1:A:222:ALA:O	2.20	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%)	51 73
All	All	1357/1432 (95%)	1305 (96%)	51 (4%)	1 (0%)	51 73

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	135	GLN

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	588/618 (95%)	561 (95%)	27 (5%)	27 50
1	B	586/618 (95%)	563 (96%)	23 (4%)	32 57
All	All	1174/1236 (95%)	1124 (96%)	50 (4%)	29 53

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	74	GLU
1	A	75	GLU
1	A	76	GLN
1	A	100	LEU
1	A	120	CYS

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Mol	Chain	Res	Type
1	A	133	THR
1	A	151	GLU
1	A	153	GLN
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	452	ILE
1	A	518	ILE
1	A	537	MET
1	A	555	THR
1	A	560	MET
1	A	642	SER
1	A	678	ASN
1	A	696	GLU
1	B	73	ARG
1	B	100	LEU
1	B	120	CYS
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	272	TYR
1	B	274	LEU
1	B	291	ARG
1	B	385	LEU
1	B	425	ARG
1	B	447	LEU
1	B	499	LYS
1	B	518	ILE
1	B	575	LEU
1	B	633	LEU

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Mol	Chain	Res	Type
1	B	642	SER
1	B	649	ASN
1	B	681	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	33	GLN
1	B	307	HIS
1	B	497	GLN
1	B	649	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	$\#\|Z\| > 2$
4	SF4	A	801	-	0,12,12	0.00	-	-		

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	ADP	B	802	7,6	24,29,29	1.00	1 (4%)	29,45,45	1.46	5 (17%)
6	BEF	B	803	5	0,3,3	0.00	-	-		
4	SF4	B	801	1	0,12,12	0.00	-	-		
6	BEF	A	803	5	0,3,3	0.00	-	-		
5	ADP	A	802	7,6	24,29,29	0.97	1 (4%)	29,45,45	1.52	6 (20%)

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
4	SF4	B	801	1	-	-	0/6/5/5
5	ADP	B	802	7,6	-	3/12/32/32	0/3/3/3
5	ADP	A	802	7,6	-	6/12/32/32	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	802	ADP	C5-C4	2.36	1.47	1.40
5	A	802	ADP	C5-C4	2.20	1.46	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	802	ADP	N3-C2-N1	-3.69	122.91	128.68
5	A	802	ADP	C4-C5-N7	-3.28	105.98	109.40
5	A	802	ADP	N3-C2-N1	-2.92	124.12	128.68
5	B	802	ADP	PA-O3A-PB	-2.86	123.03	132.83
5	A	802	ADP	PA-O3A-PB	-2.70	123.56	132.83
5	B	802	ADP	C4-C5-N7	-2.54	106.76	109.40
5	A	802	ADP	C1'-N9-C4	-2.48	122.28	126.64
5	A	802	ADP	C5'-C4'-C3'	-2.35	106.39	115.18
5	B	802	ADP	C2-N1-C6	2.15	122.43	118.75
5	B	802	ADP	O3'-C3'-C2'	-2.12	104.96	111.82
5	A	802	ADP	O3A-PB-O1B	-2.04	99.85	111.19

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	B	802	ADP	PA-O3A-PB-O2B
5	A	802	ADP	PA-O3A-PB-O3B
5	A	802	ADP	C5'-O5'-PA-O1A
5	A	802	ADP	C5'-O5'-PA-O3A
5	A	802	ADP	O4'-C4'-C5'-O5'
5	B	802	ADP	PA-O3A-PB-O3B
5	A	802	ADP	PA-O3A-PB-O2B
5	A	802	ADP	C5'-O5'-PA-O2A
5	B	802	ADP	PA-O3A-PB-O1B

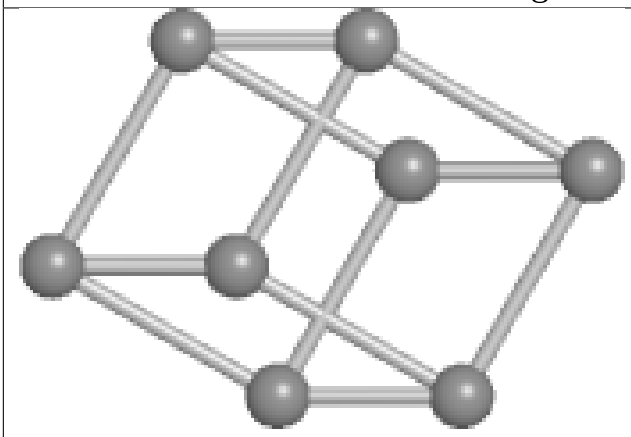
There are no ring outliers.

2 monomers are involved in 3 short contacts:

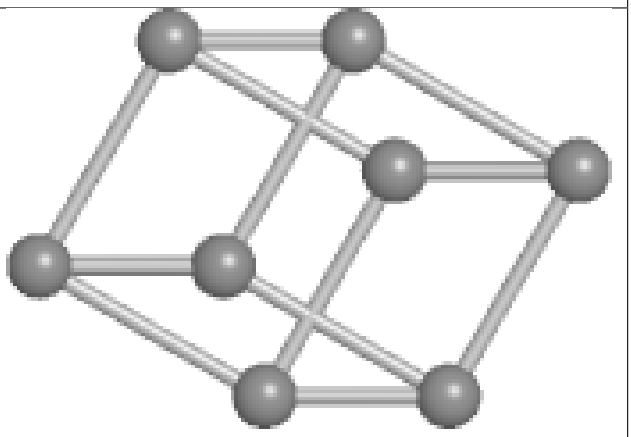
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	801	SF4	2	0
6	B	803	BEF	1	0

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 then 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.

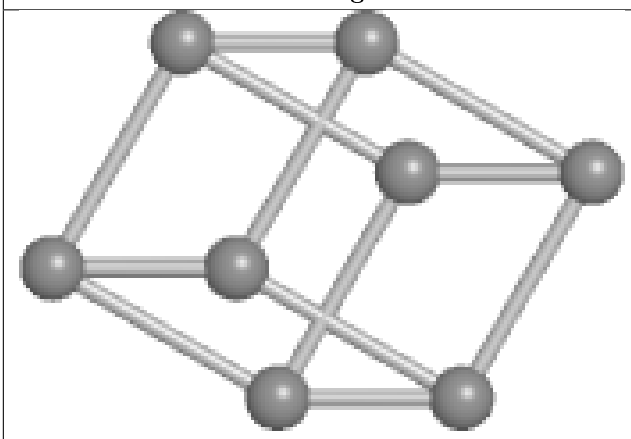
Ligand SF4 A 801



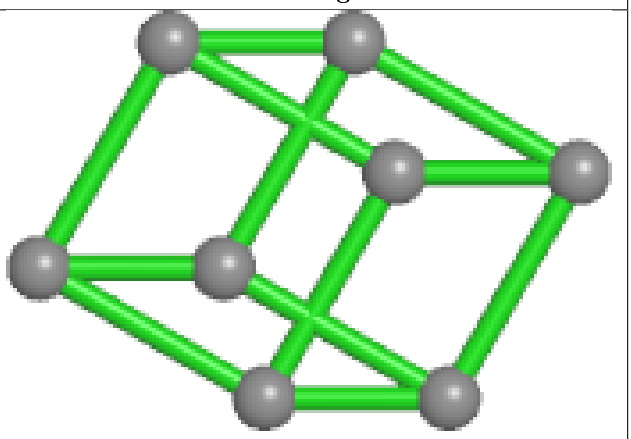
Bond lengths



Bond angles

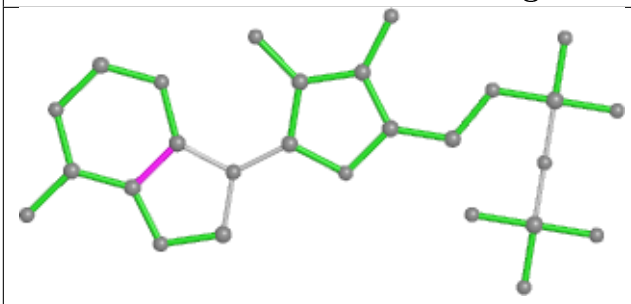


Torsions

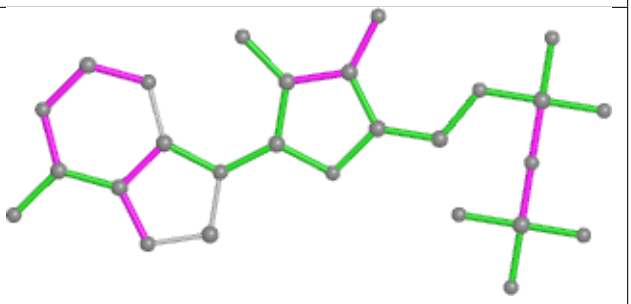


Rings

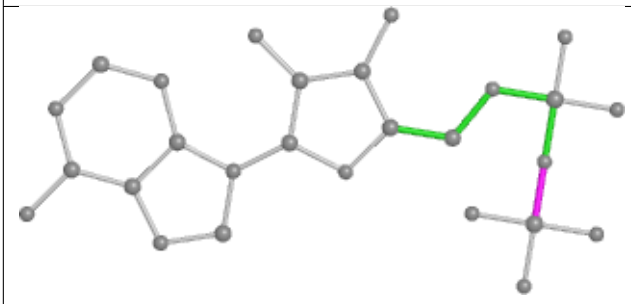
Ligand ADP B 802



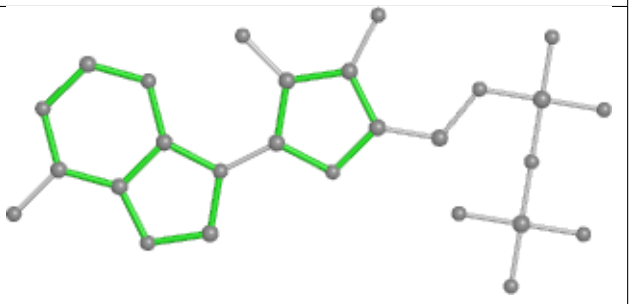
Bond lengths



Bond angles

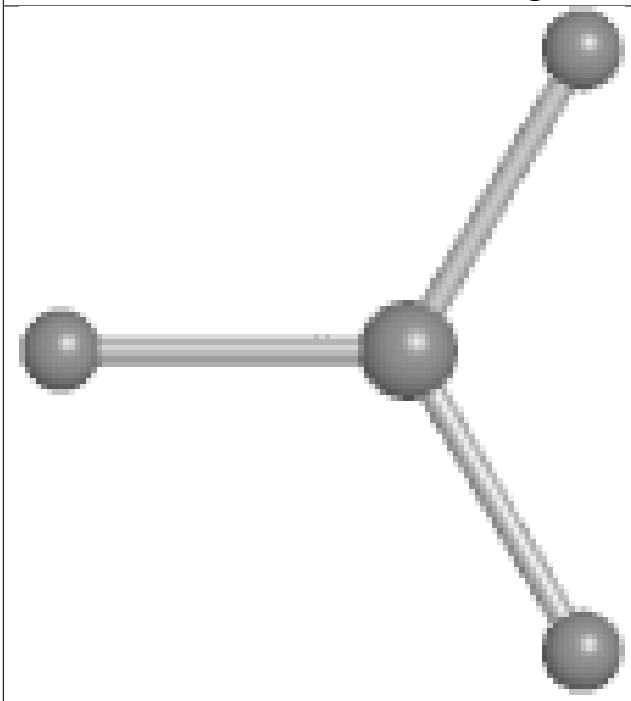


Torsions

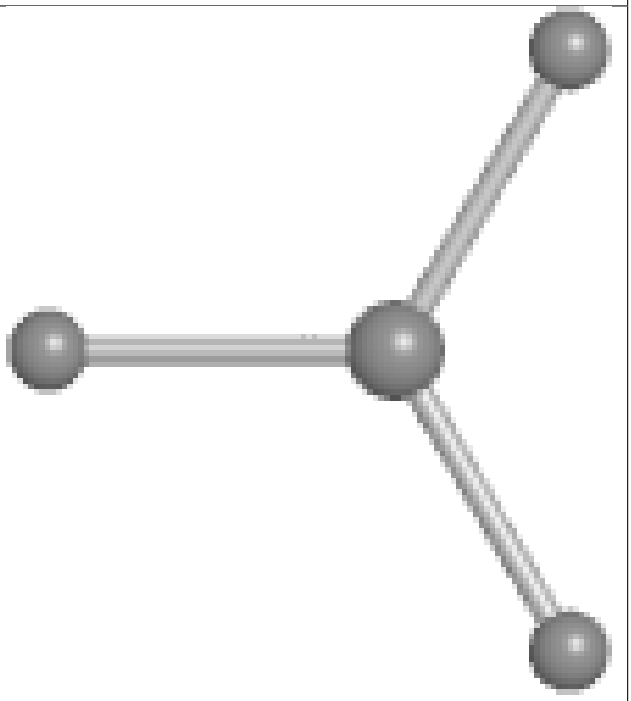


Rings

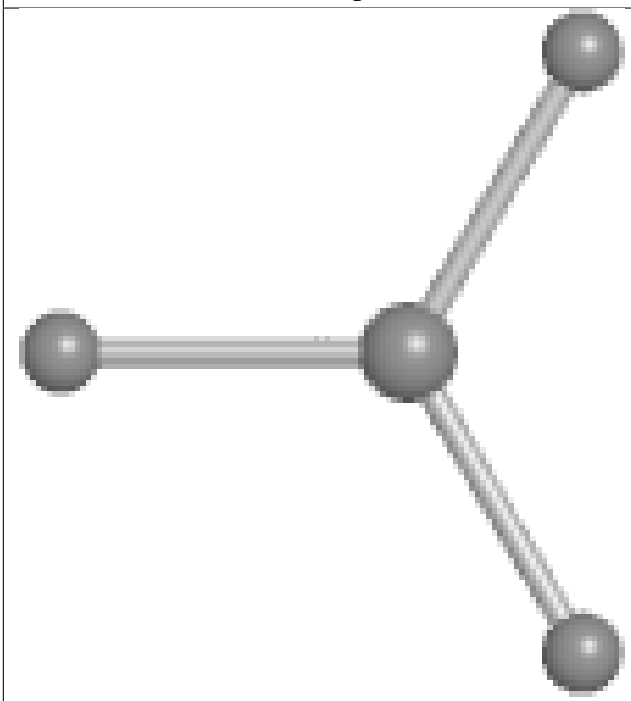
Ligand BEF B 803



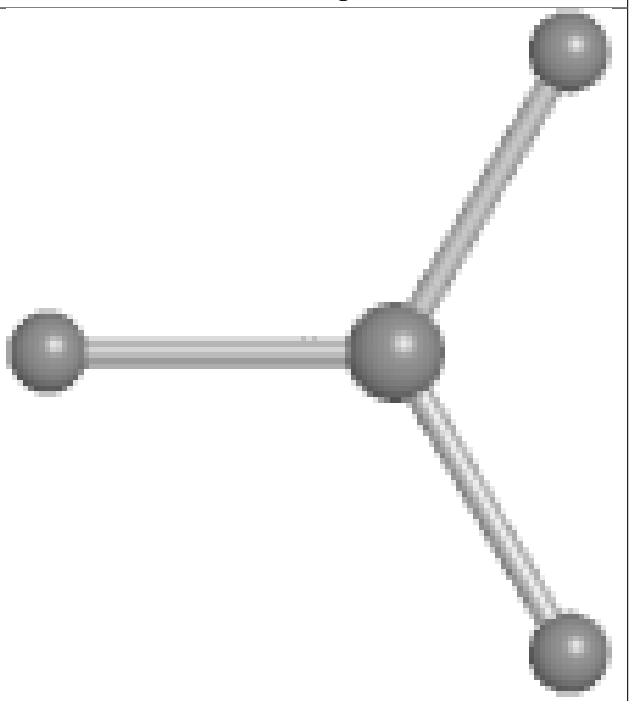
Bond lengths



Bond angles

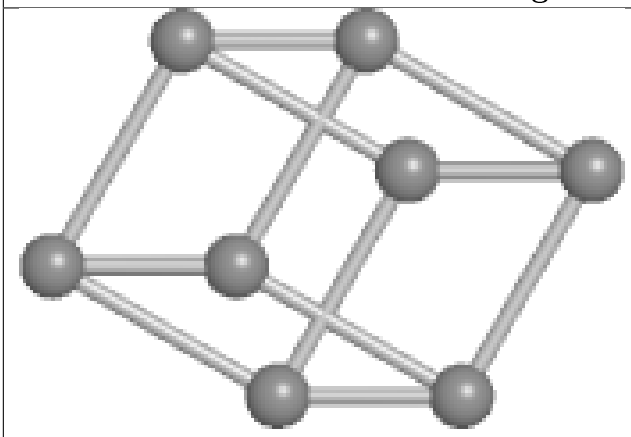


Torsions

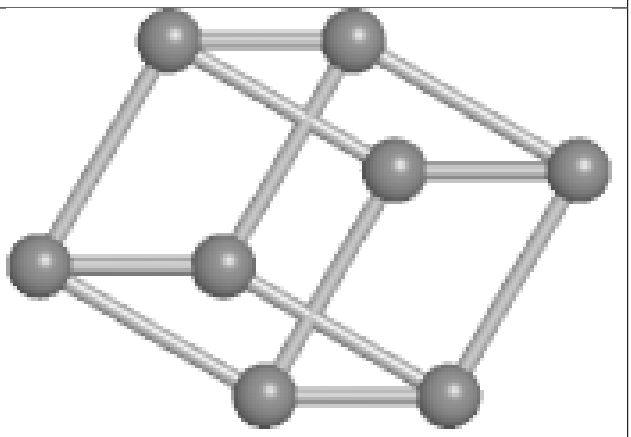


Rings

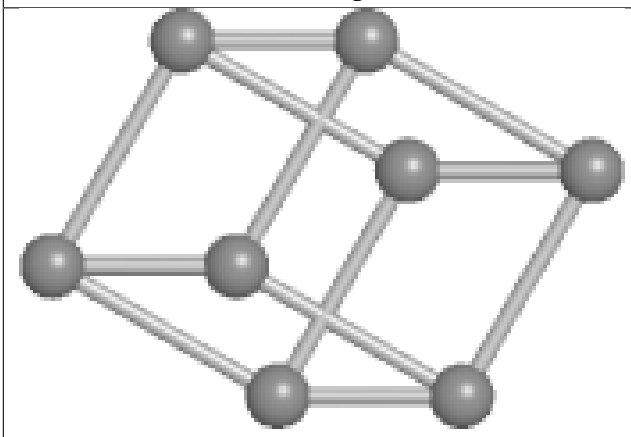
Ligand SF4 B 801



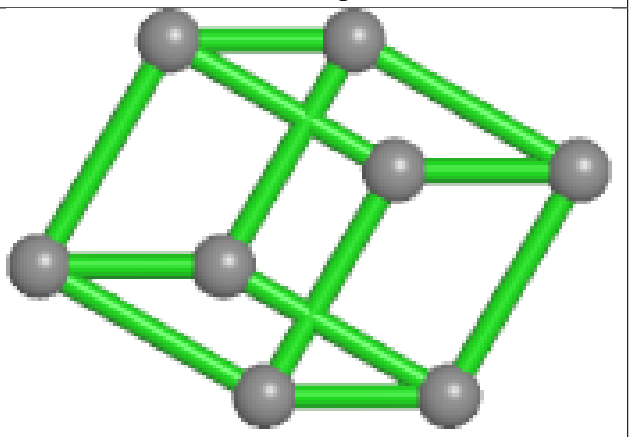
Bond lengths



Bond angles

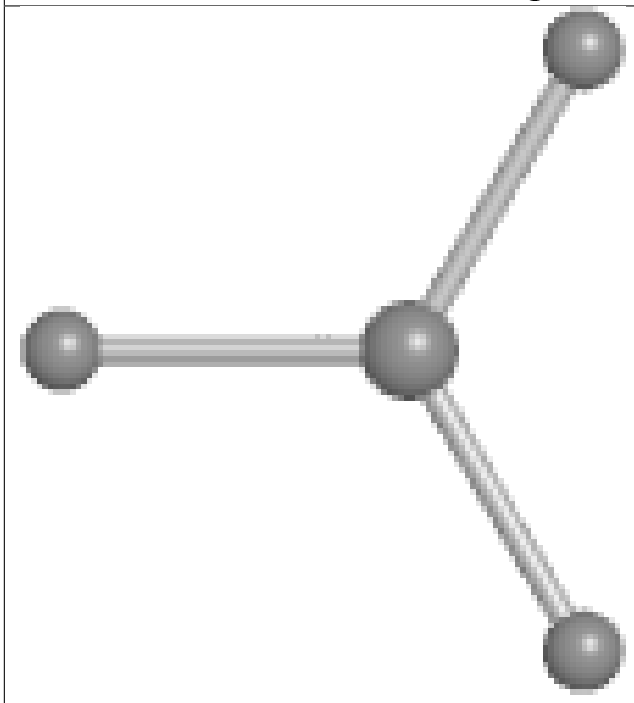


Torsions

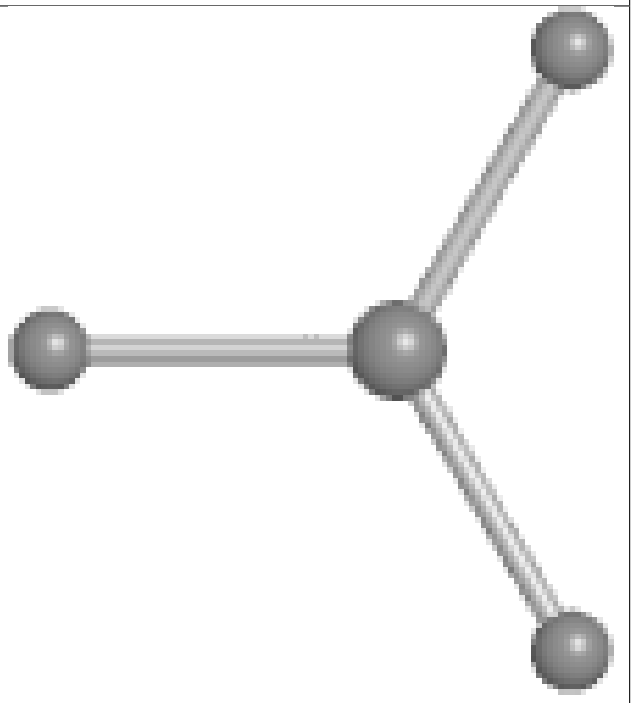


Rings

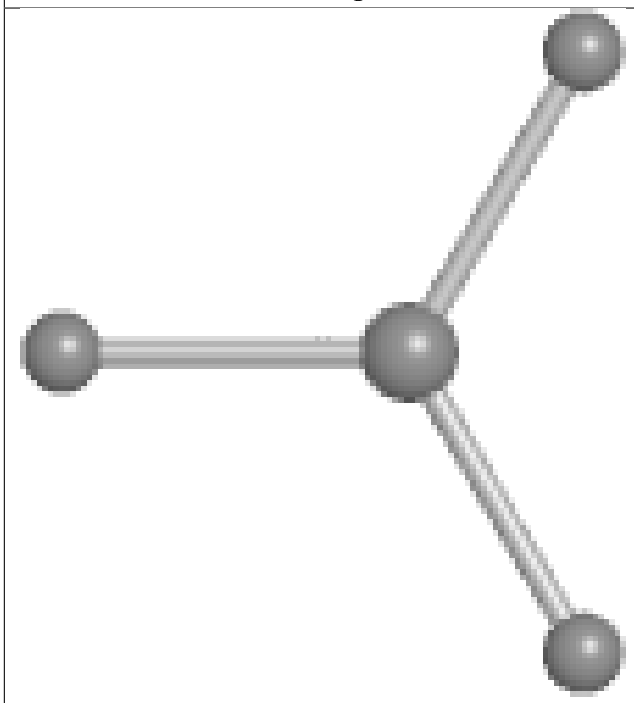
Ligand BEF A 803



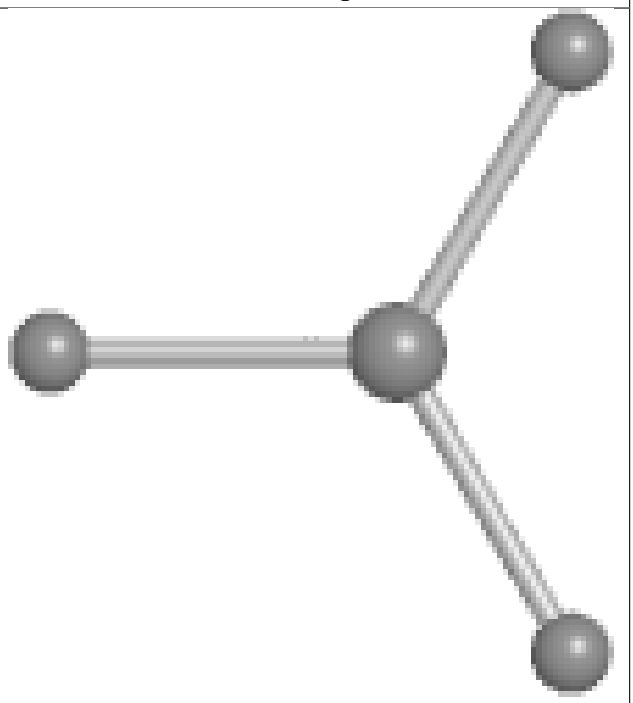
Bond lengths



Bond angles

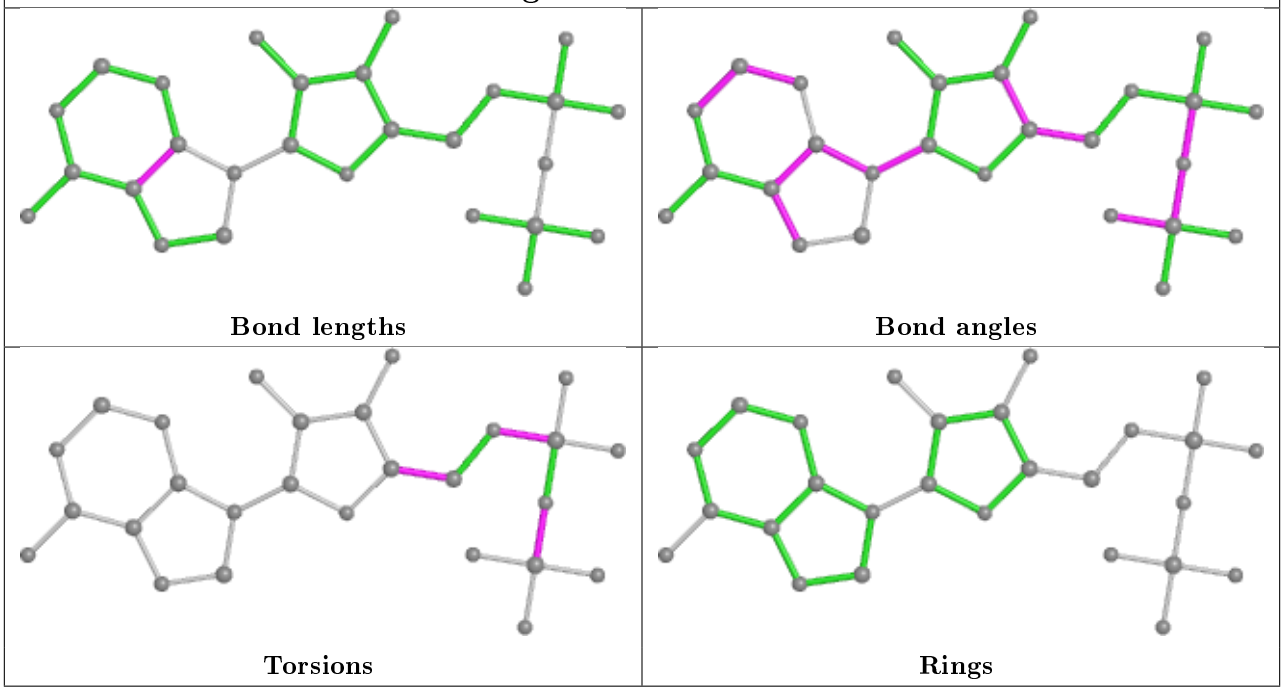


Torsions



Rings

Ligand ADP A 802



5.7 Other polymers

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, 95^{th} 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%)	0.04	22 (3%) 47 51	19, 33, 64, 80	0
1	B	683/716 (95%)	0.15	19 (2%) 53 56	20, 39, 65, 77	0
2	C	11/11 (100%)	0.08	1 (9%) 9 9	36, 50, 72, 73	0
3	D	10/10 (100%)	0.22	1 (10%) 7 6	33, 48, 74, 76	0
All	All	1390/1453 (95%)	0.10	43 (3%) 49 52	19, 36, 64, 80	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	133	THR	5.4
1	A	378	ASP	4.4
1	B	328	ALA	4.4
1	A	165	THR	4.1
1	B	233	SER	3.8
1	A	134	GLN	3.8
1	A	132	PRO	3.7
1	A	328	ALA	3.3
1	A	131	GLU	3.2
1	A	142	ASP	3.2
1	B	133	THR	3.2
1	A	130	THR	3.2
1	A	151	GLU	3.0
1	B	19	GLN	2.9
1	A	154	LYS	2.9
1	A	129	SER	2.8
1	B	210	ALA	2.8
1	A	145	LEU	2.7
1	A	209	VAL	2.6
1	B	24	ASP	2.6
1	B	512	ASP	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	166	TYR	2.5
1	B	701	ILE	2.5
1	B	134	GLN	2.5
1	B	139	ALA	2.5
1	B	23	PRO	2.4
1	B	428	GLN	2.4
1	A	135	GLN	2.4
1	B	702	VAL	2.3
1	B	105	PRO	2.3
1	B	506	ARG	2.3
1	A	168	TRP	2.3
2	C	0	DT	2.3
1	A	177	ILE	2.3
1	B	189	THR	2.2
1	B	165	THR	2.2
3	D	1	DT	2.2
1	A	162	ASP	2.1
1	A	128	ALA	2.1
1	A	624	ILE	2.1
1	B	496	GLU	2.1
1	A	701	ILE	2.0
1	B	469	SER	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 carbohydrates 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, 95^{th} 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	0.83	0.21	83,113,150,165	0

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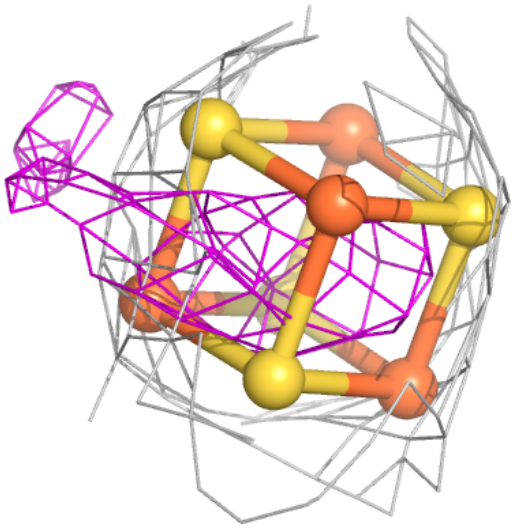
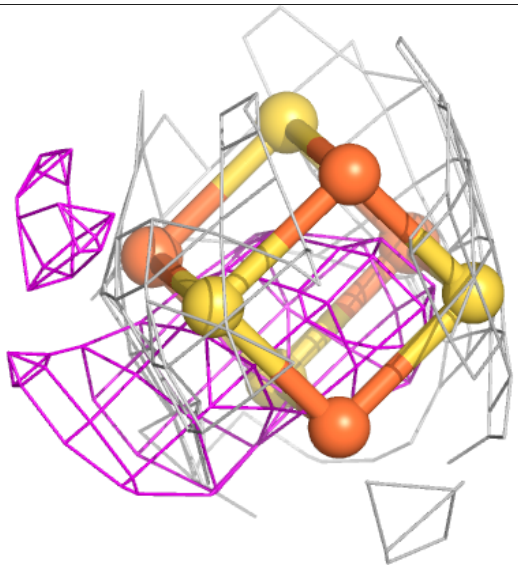
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	SF4	B	801	8/8	0.89	0.22	84,100,150,173	0
7	MG	B	804	1/1	0.94	0.09	31,31,31,31	0
6	BEF	A	803	4/4	0.94	0.11	26,26,28,31	0
5	ADP	B	802	27/27	0.96	0.13	29,39,52,54	0
6	BEF	B	803	4/4	0.96	0.10	26,26,29,31	0
5	ADP	A	802	27/27	0.97	0.15	23,29,35,38	0
7	MG	A	804	1/1	0.99	0.11	25,25,25,25	0

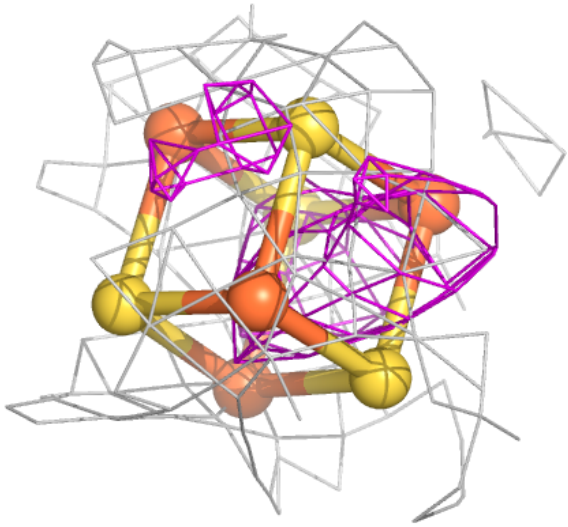
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation 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)

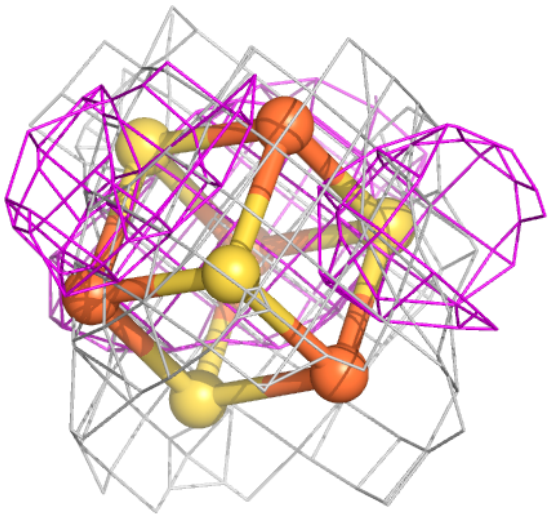


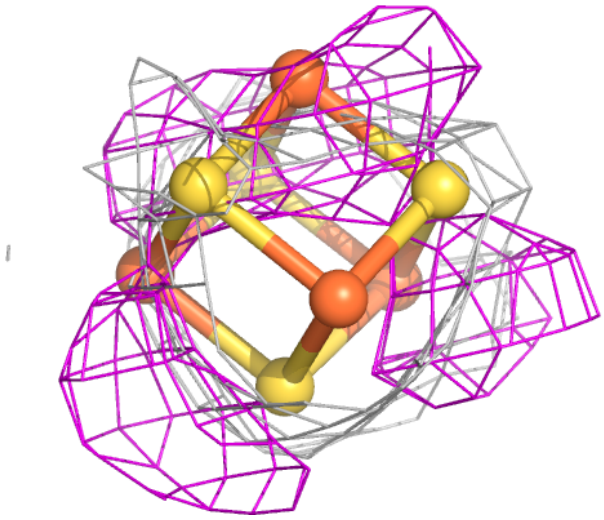


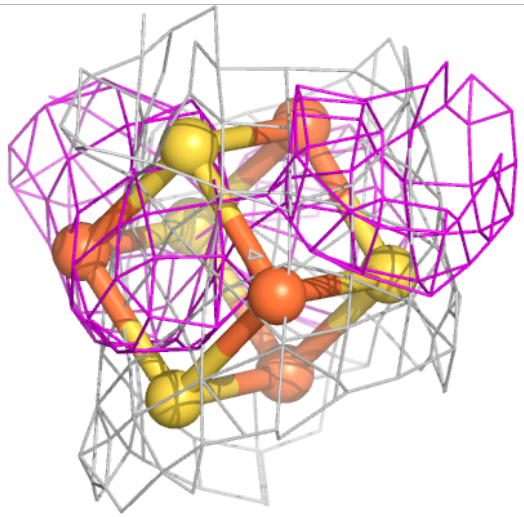


Electron density around SF4 B 801:

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

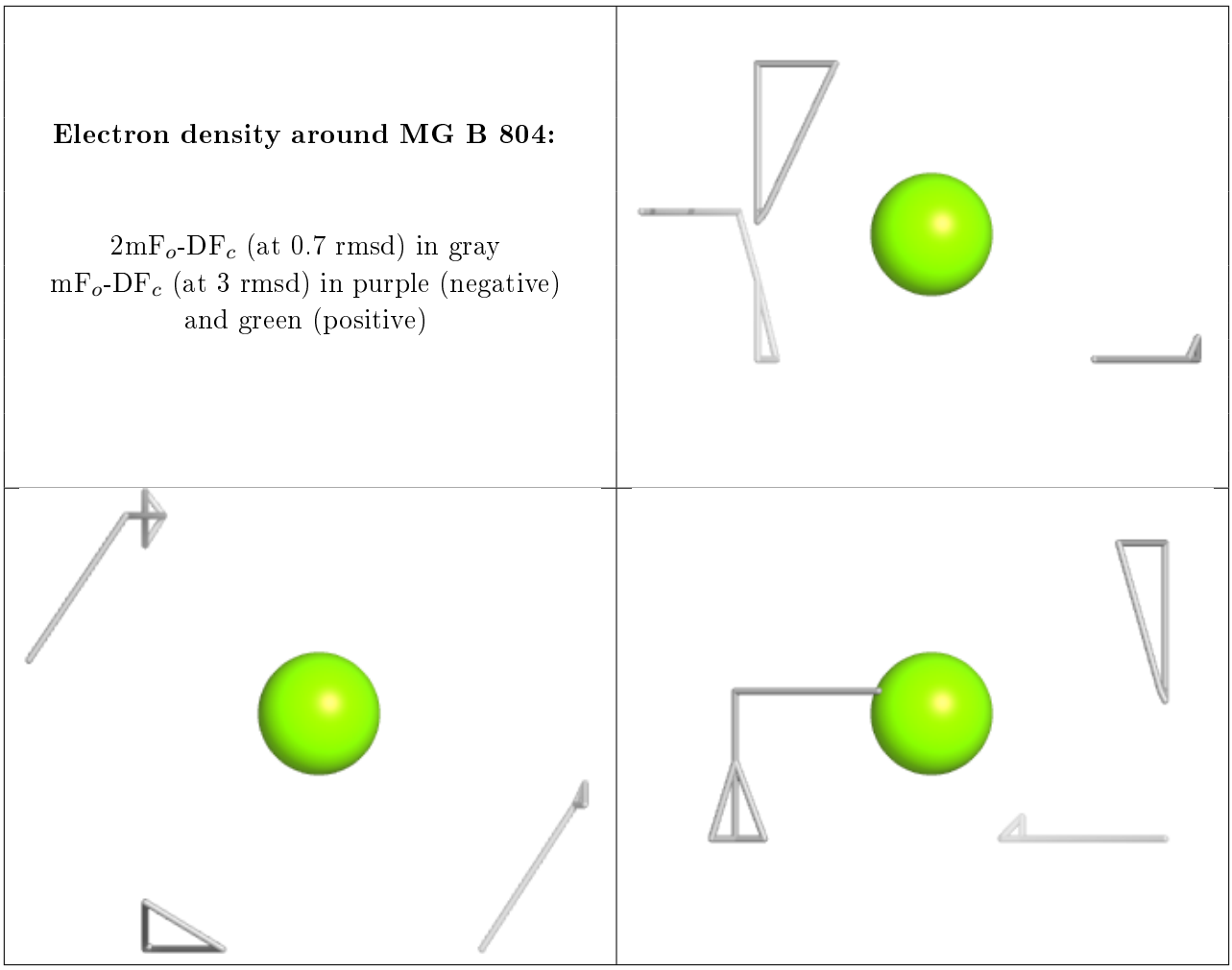






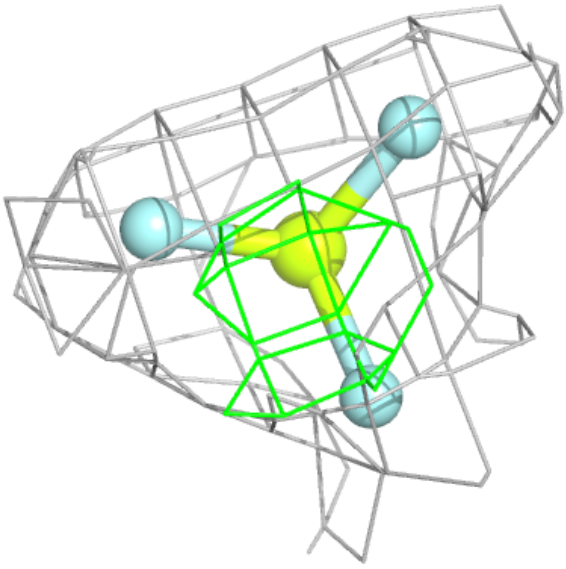
Electron density around MG B 804:

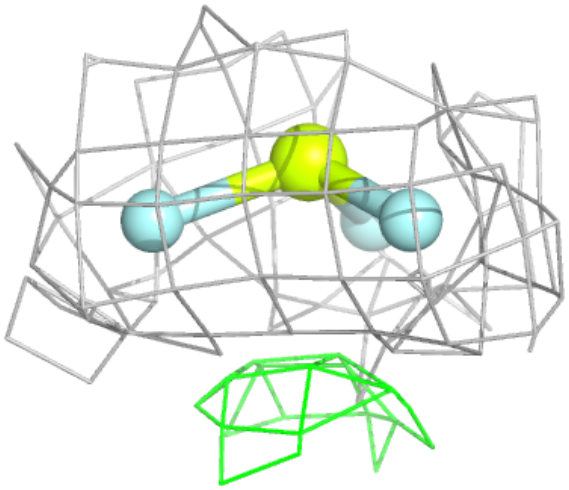
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

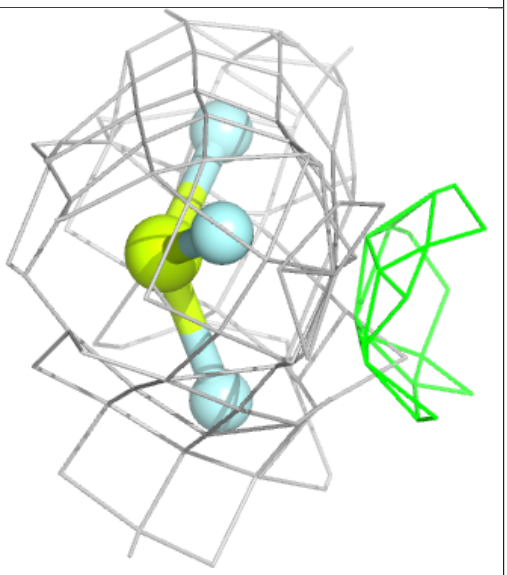


Electron density around BEF A 803:

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

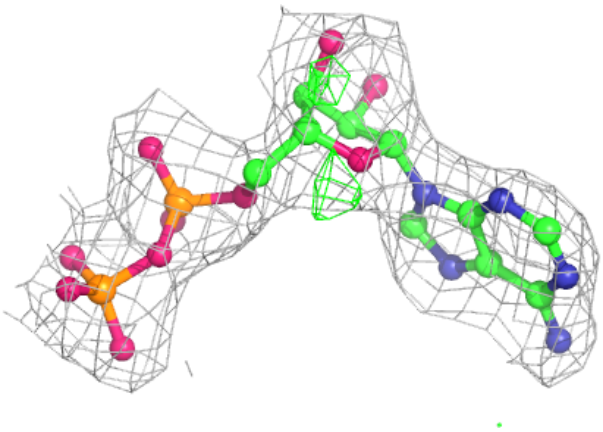


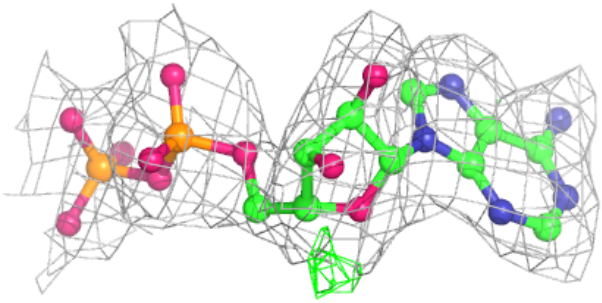


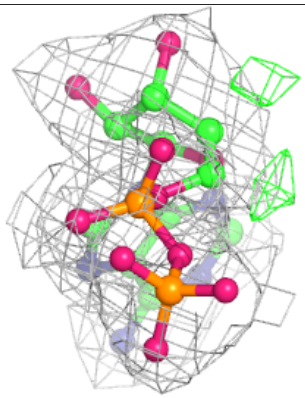


Electron density around ADP B 802:

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

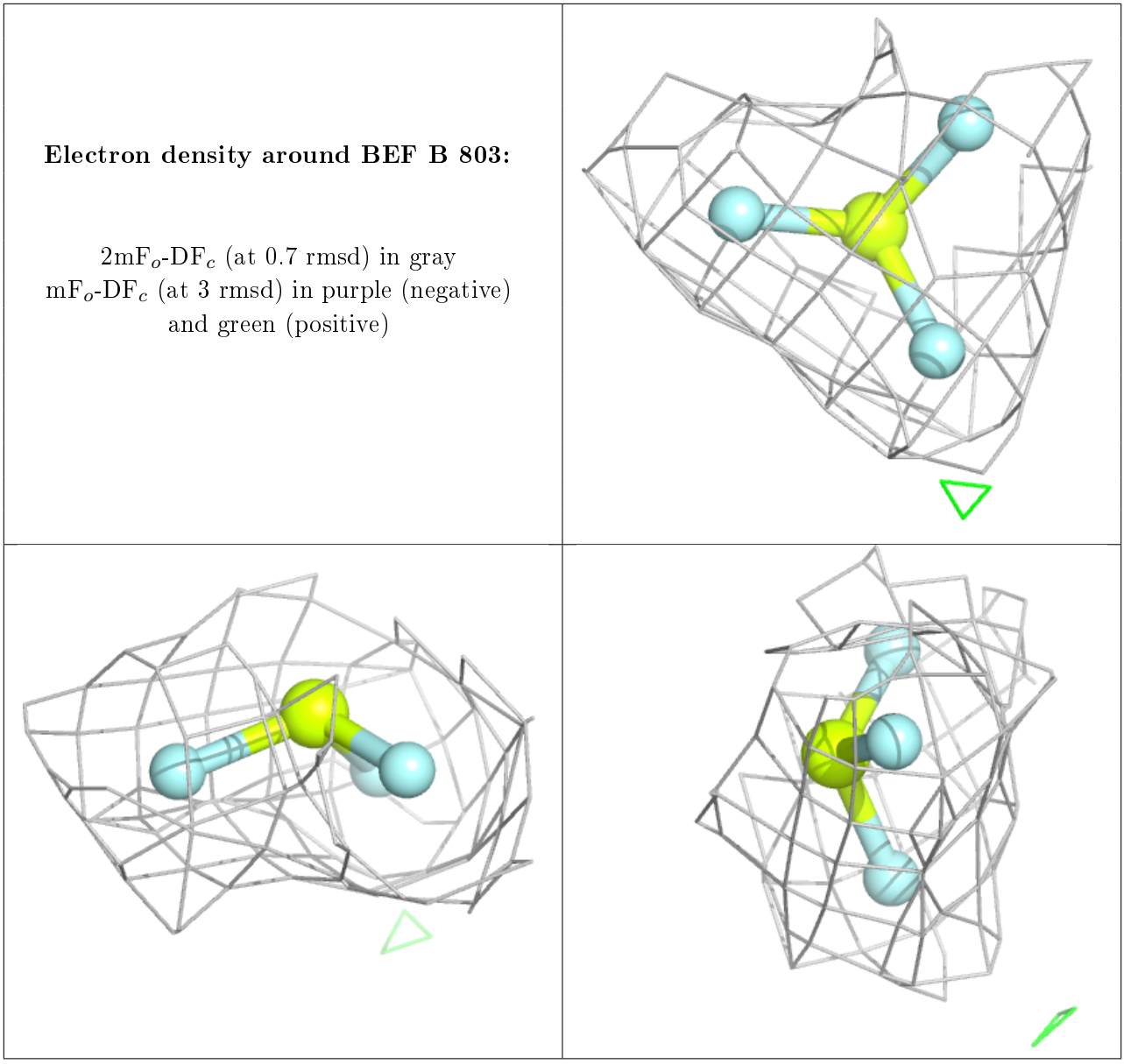






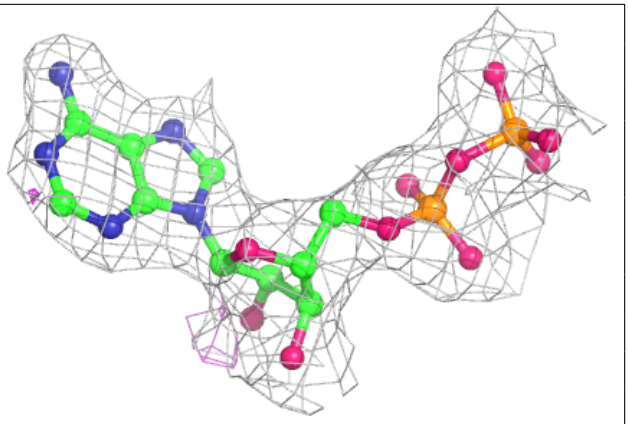
Electron density around BEF B 803:

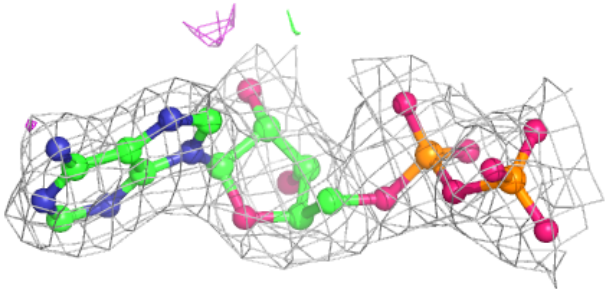
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

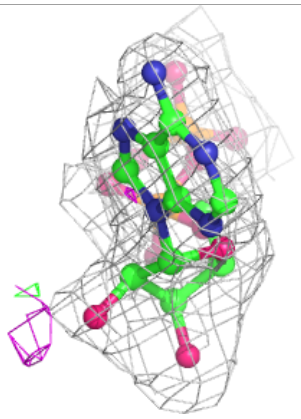


Electron density around ADP A 802:

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

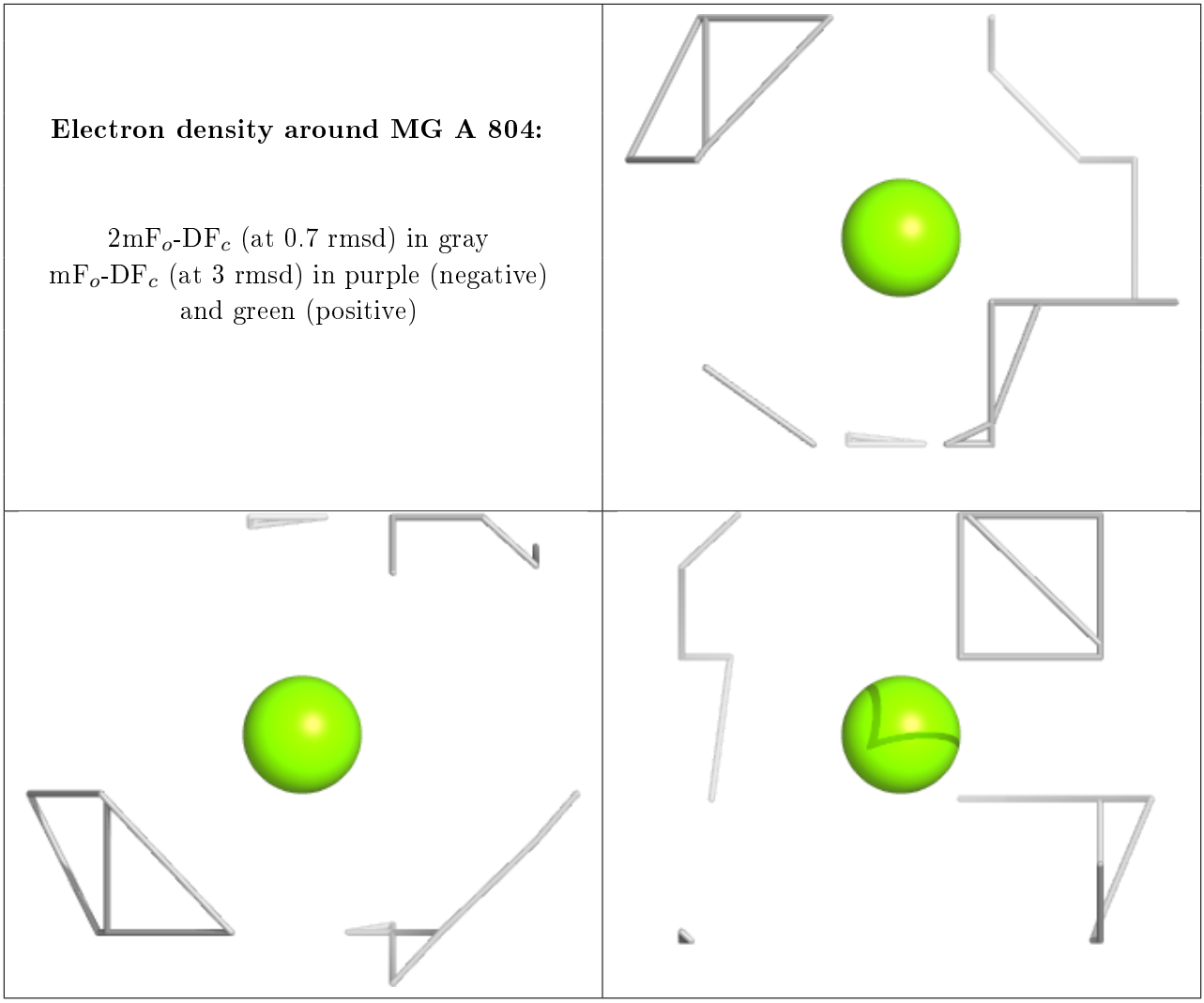






Electron density around MG A 804:

$2mF_o$-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

There are no such residues in this entry.