



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:12 AM UTC

PDB ID : 5DAC / pdb_00005dac
Title : ATP-gamma-S bound Rad50 from Chaetomium thermophilum in complex with DNA
Authors : Seifert, F.U.; Lammens, K.; Stoeck, G.; Kessler, B.; Hopfner, K.-P.
Deposited on : 2015-08-19
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

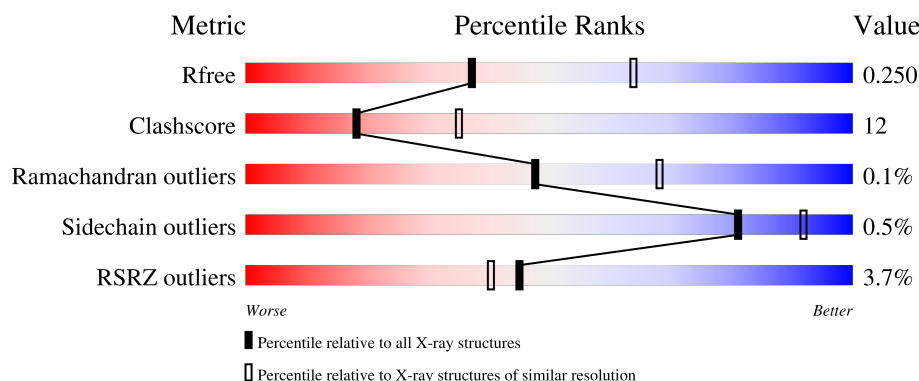
1 Overall quality at a glance

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	449	4% 73% 22% • •
1	B	449	3% 71% 24% • •
2	C	15	47% 53%
3	D	15	53% 47%

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	15	Total	C	N	O	P	0	0	0
			285	135	45	90	15			

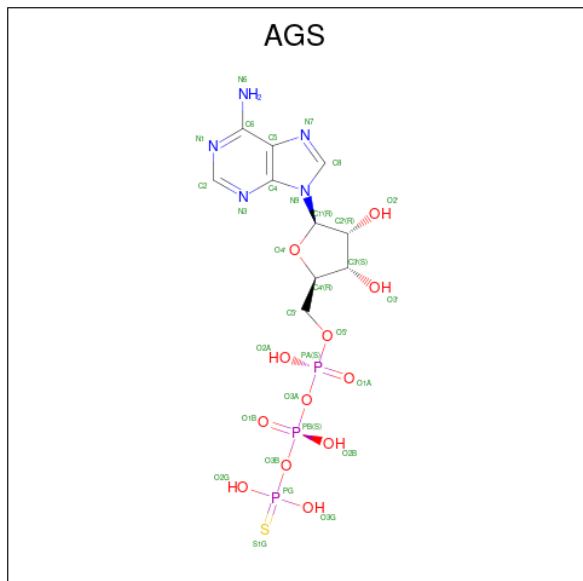
- Molecule 3 is a DNA chain called DNA (5'-D(P*GP*GP*GP*GP*GP*GP*GP*GP*GP*G P*GP*GP*GP*GP*G)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	15	Total	C	N	O	P	0	0	0
			330	150	75	90	15			

- Molecule 4 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

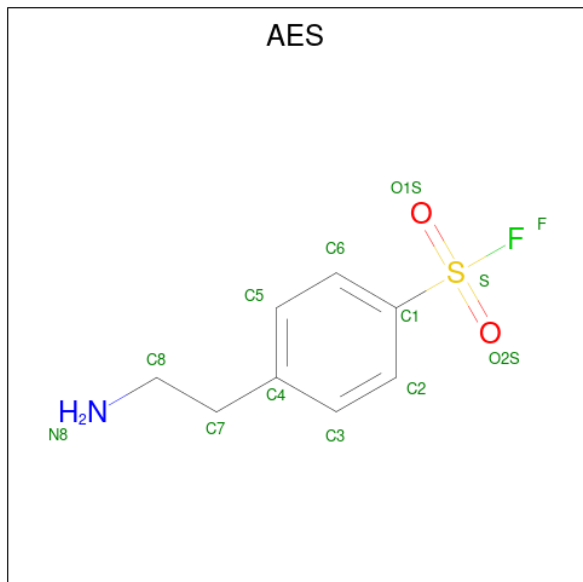
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	Mg	0	0
			1	1		
4	B	1	Total	Mg	0	0
			1	1		

- Molecule 5 is PHOSPHOTHIOPHOSPHORIC ACID-ADENYLATE ESTER (CCD ID: AGS) (formula: C₁₀H₁₆N₅O₁₂P₃S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		
5	B	1	Total	C	N	O	P	S	0	0
			31	10	5	12	3	1		

- Molecule 6 is 4-(2-AMINOETHYL)BENZENESULFONYL FLUORIDE (CCD ID: AES) (formula: $C_8H_{10}FNO_2S$).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
6	A	1	Total	C	F	H	N	O	S	0	0
			23	8	1	10	1	2	1		
6	B	1	Total	C	F	H	N	O	S	0	0
			23	8	1	10	1	2	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	51	Total	O	0	0
			51	51		
7	B	53	Total	O	0	0
			53	53		

Chain C:  47% 53%



- Molecule 3: DNA (5'-D(P*GP*GP*GP*GP*GP*GP*GP*GP*GP*GP*GP*GP*GP*GP*GP*GP*G)-3')

Chain D:  53% 47%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	92.31Å 97.08Å 115.01Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.48 – 2.50 49.48 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (49.48-2.50) 99.5 (49.48-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.20	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.9_1692	Depositor
R, R_{free}	0.210 , 0.246 0.218 , 0.250	Depositor DCC
R_{free} test set	1806 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	56.0	Xtriage
Anisotropy	0.187	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 62.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7660	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.68% 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: AGS, AES, MG

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	0.51	0/3461	0.95	14/4658 (0.3%)
1	B	0.53	0/3458	0.92	9/4655 (0.2%)
2	C	0.35	0/314	0.60	0/476
3	D	0.38	0/374	0.62	0/581
All	All	0.51	0/7607	0.91	23/10370 (0.2%)

There are no bond length outliers.

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	122	ASN	N-CA-C	-7.81	95.99	108.73
1	A	19	HIS	CA-C-N	7.33	127.31	119.76
1	A	19	HIS	C-N-CA	7.33	127.31	119.76
1	B	68	ASP	CA-C-N	6.38	126.59	119.32
1	B	68	ASP	C-N-CA	6.38	126.59	119.32
1	A	109	ARG	N-CA-C	6.32	119.16	110.24
1	B	91	GLU	N-CA-C	6.27	118.87	110.35
1	B	168	GLU	CA-C-N	6.22	127.61	119.84
1	B	168	GLU	C-N-CA	6.22	127.61	119.84
1	B	1268	LEU	N-CA-C	5.95	119.22	109.76
1	B	126	ARG	N-CA-C	5.82	119.74	109.96
1	A	107	ASN	N-CA-C	5.79	118.54	111.82
1	A	106	ASN	N-CA-C	-5.68	101.22	110.20
1	A	104	GLN	N-CA-C	5.62	117.32	110.41
1	A	168	GLU	CA-C-N	5.48	126.69	119.84
1	A	168	GLU	C-N-CA	5.48	126.69	119.84
1	B	16	GLY	CA-C-N	5.29	125.75	120.04
1	B	16	GLY	C-N-CA	5.29	125.75	120.04
1	A	68	ASP	CA-C-N	5.28	125.34	119.32
1	A	68	ASP	C-N-CA	5.28	125.34	119.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	13	ARG	CB-CA-C	-5.20	110.56	116.54
1	A	146	VAL	CA-C-N	5.14	125.67	120.38
1	A	146	VAL	C-N-CA	5.14	125.67	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	3417	0	3475	81	0
1	B	3414	0	3473	73	0
2	C	285	0	166	6	0
3	D	330	0	166	6	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
5	A	31	0	12	2	0
5	B	31	0	12	3	0
6	A	13	10	10	1	0
6	B	13	10	10	1	0
7	A	51	0	0	3	0
7	B	53	0	0	3	0
All	All	7640	20	7324	162	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 (162) 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)
2:C:9:DC:H2''	2:C:10:DC:C6	2.09	0.88
1:B:1194:MET:HE2	1:B:1203:MET:HA	1.57	0.85
1:A:1206:ARG:O	5:B:1402:AGS:H2'	1.78	0.83
1:A:193:ARG:HA	1:A:1130:MET:HE1	1.61	0.83
1:B:193:ARG:CZ	1:B:1183:GLY:HA3	2.11	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1159:THR:HG22	1:B:1254:SER:OG	1.81	0.80
5:A:1402:AGS:H2'	1:B:1206:ARG:O	1.82	0.80
1:A:211:VAL:HG13	7:A:1529:HOH:O	1.82	0.79
1:B:1140:TYR:CE1	1:B:1144:MET:HE3	2.19	0.77
1:A:70:ASP:OD2	1:A:109:ARG:NH2	2.23	0.71
1:B:76:GLU:OE2	1:B:78:ARG:NH1	2.24	0.70
1:B:1307:ARG:NH1	7:B:1502:HOH:O	2.24	0.69
1:B:1207:CYS:SG	1:B:1212:LYS:HG3	2.33	0.68
1:A:89:ILE:HG13	1:A:91:GLU:HG3	1.78	0.66
1:B:193:ARG:HA	1:B:1130:MET:HE1	1.78	0.66
1:B:1228:CYS:HB2	1:B:1231:CYS:SG	2.36	0.65
1:A:160:ASP:OD1	7:A:1501:HOH:O	2.14	0.65
1:A:1146:GLU:HG2	1:A:1150:ARG:NH1	2.12	0.65
1:B:164:TRP:CG	1:B:165:PRO:HD3	2.32	0.64
1:B:40:LYS:HE2	5:B:1402:AGS:O2B	1.98	0.64
1:A:72:VAL:HG13	1:A:74:GLU:H	1.62	0.63
1:B:1102:LEU:O	1:B:1106:LYS:HG3	1.98	0.63
1:B:1138:MET:HE2	1:B:1186:ARG:NE	2.14	0.63
1:B:99:ILE:HD12	1:B:113:THR:HA	1.80	0.62
1:A:2:SER:OG	1:A:88:THR:HA	2.00	0.62
1:A:1138:MET:HE3	1:A:1186:ARG:NH1	2.15	0.61
1:B:1179:SER:OG	1:B:1182:SER:OG	2.18	0.60
1:B:141:SER:HB2	1:B:146:VAL:O	2.01	0.60
1:B:68:ASP:OD2	1:B:109:ARG:NH1	2.33	0.60
1:A:1240:THR:HA	1:A:1243:LEU:HD12	1.83	0.59
1:A:1194:MET:HE2	1:A:1203:MET:HA	1.84	0.58
1:A:217:LYS:HD3	1:A:1109:TYR:HD2	1.69	0.58
1:B:1161:GLN:HG3	1:B:1246:ASP:HB3	1.85	0.58
1:B:1201:MET:HE2	1:B:1206:ARG:HD3	1.85	0.57
1:B:1201:MET:CE	1:B:1206:ARG:HD3	2.34	0.57
1:B:173:LYS:NZ	1:B:177:ASP:OD2	2.36	0.57
1:A:189:ILE:HG23	1:A:1130:MET:HG3	1.86	0.57
1:B:100:GLN:HB2	1:B:114:LEU:HD11	1.86	0.57
1:A:180:PHE:CZ	1:A:1145:MET:HE3	2.41	0.56
1:B:138:LYS:O	1:B:142:GLU:HB2	2.06	0.55
1:B:104:GLN:HB2	1:B:106:ASN:OD1	2.07	0.55
1:A:1145:MET:HE2	1:A:1148:ILE:HD12	1.90	0.54
1:A:5:GLU:OE2	1:A:86:ARG:NH1	2.40	0.54
1:A:68:ASP:OD2	1:A:70:ASP:HB2	2.07	0.54
3:D:2:DG:H4'	3:D:3:DG:OP1	2.06	0.54
1:A:76:GLU:OE2	1:A:100:GLN:NE2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:LEU:HD12	1:A:121:ARG:N	2.22	0.54
1:A:193:ARG:CA	1:A:1130:MET:HE1	2.36	0.54
1:B:1278:GLU:HG3	7:B:1540:HOH:O	2.08	0.54
1:B:164:TRP:CD2	1:B:165:PRO:HD3	2.43	0.53
1:B:97:ARG:NH2	1:B:137:ASP:OD1	2.38	0.53
1:B:1256:HIS:ND1	1:B:1283:MET:O	2.38	0.53
1:A:1144:MET:CE	1:A:1226:SER:HB3	2.39	0.53
1:B:61:ARG:O	1:B:62:ASN:HB2	2.09	0.52
1:B:2:SER:OG	1:B:144:LEU:O	2.14	0.52
2:C:6:DC:H2''	2:C:7:DC:C6	2.45	0.52
1:B:1178:THR:OG1	1:B:1184:THR:HG22	2.10	0.51
1:A:1138:MET:HE2	1:A:1186:ARG:HD3	1.90	0.51
1:A:5:GLU:OE2	1:A:86:ARG:HD2	2.10	0.51
1:B:139:LEU:O	1:B:143:LYS:HG2	2.10	0.51
1:B:48:LYS:HE2	1:B:152:ASP:HA	1.92	0.51
3:D:10:DG:C2	3:D:11:DG:C2	3.00	0.51
1:A:1144:MET:HE1	1:A:1226:SER:HB3	1.93	0.50
1:B:203:LEU:HG	1:B:207:LYS:HE3	1.94	0.50
3:D:5:DG:H2''	3:D:6:DG:C8	2.47	0.50
1:B:204:LYS:O	1:B:208:GLU:HG2	2.11	0.50
1:A:1207:CYS:SG	1:A:1212:LYS:HG3	2.51	0.50
1:A:32:ILE:HB	1:A:1273:ILE:HG13	1.94	0.49
1:B:1179:SER:HG	1:B:1182:SER:HG	1.50	0.49
1:B:79:ALA:HB3	1:B:99:ILE:HG23	1.93	0.49
2:C:9:DC:H2''	2:C:10:DC:H6	1.74	0.49
1:A:1135:HIS:O	1:A:1139:GLN:HG2	2.13	0.49
1:A:180:PHE:HZ	1:A:1145:MET:HE3	1.76	0.49
1:A:1201:MET:HE1	1:B:71:LEU:HD11	1.95	0.48
1:A:5:GLU:CD	1:A:86:ARG:HH11	2.21	0.48
1:A:94:VAL:HG13	1:A:119:LEU:HB3	1.94	0.48
1:A:1163:THR:HB	1:B:1301:GLN:HE22	1.78	0.48
1:A:136:LEU:O	1:A:140:VAL:HG23	2.14	0.48
1:A:217:LYS:HD3	1:A:1109:TYR:CD2	2.48	0.48
1:A:60:THR:O	1:A:111:GLN:NE2	2.46	0.48
1:A:40:LYS:HE2	5:A:1402:AGS:O1B	2.14	0.47
1:A:118:LEU:HB2	1:A:136:LEU:HD22	1.96	0.47
1:B:72:VAL:HG13	1:B:74:GLU:H	1.79	0.47
1:B:206:LEU:HB3	1:B:1116:VAL:HG22	1.96	0.47
1:A:1294:ARG:HB3	1:A:1306:VAL:CG2	2.45	0.47
1:A:120:LEU:HD12	1:A:121:ARG:H	1.79	0.47
1:A:164:TRP:CG	1:A:165:PRO:HD3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1252:ALA:HB2	1:B:1279:PHE:CD1	2.50	0.47
1:A:44:ILE:HD11	1:A:1273:ILE:HD11	1.96	0.47
1:A:166:MET:HE2	1:A:1207:CYS:SG	2.55	0.46
1:A:172:LEU:HD11	1:A:176:PHE:HE2	1.80	0.46
1:A:1145:MET:HE2	1:A:1145:MET:HA	1.96	0.46
1:A:1225:GLU:HB2	6:A:1403:AES:H81	1.98	0.46
1:B:146:VAL:HG11	1:B:155:ILE:HD12	1.98	0.46
1:B:27:THR:HG23	1:B:1268:LEU:O	2.16	0.46
1:A:35:TYR:O	1:A:38:SER:OG	2.27	0.46
1:B:1260:LYS:HE3	1:B:1288:PHE:CE1	2.51	0.46
1:A:57:PRO:O	1:A:58:ASN:HB2	2.17	0.45
1:B:17:PRO:HD3	1:B:67:HIS:CD2	2.51	0.45
1:A:192:ILE:HG22	1:A:1130:MET:HE3	1.98	0.45
1:B:1155:LEU:O	1:B:1159:THR:HG23	2.16	0.45
1:B:8:SER:HB3	1:B:82:LYS:HB2	1.99	0.45
1:B:168:GLU:H	1:B:168:GLU:CD	2.24	0.45
1:A:4:ILE:O	1:A:4:ILE:HG13	2.17	0.45
1:A:164:TRP:N	1:A:165:PRO:CD	2.80	0.45
2:C:13:DC:H2"	2:C:14:DC:C6	2.52	0.45
1:B:1179:SER:O	1:B:1183:GLY:N	2.51	0.44
1:A:193:ARG:N	1:A:1130:MET:HE2	2.32	0.44
1:B:1249:ARG:HG3	1:B:1282:TYR:CD1	2.52	0.44
2:C:11:DC:H2"	2:C:12:DC:C6	2.52	0.44
1:A:8:SER:HB3	1:A:82:LYS:HB2	2.00	0.44
1:B:192:ILE:HG22	1:B:1130:MET:HE3	2.00	0.44
1:B:1207:CYS:SG	1:B:1212:LYS:CG	3.05	0.44
1:B:1291:ASP:OD2	1:B:1307:ARG:HD2	2.18	0.44
1:A:174:LYS:O	1:A:178:GLU:HG3	2.18	0.44
1:A:13:ARG:O	1:A:67:HIS:ND1	2.44	0.44
1:A:1278:GLU:HG3	1:A:1282:TYR:HE2	1.81	0.44
1:A:110:THR:HG23	3:D:6:DG:OP1	2.19	0.43
1:A:31:LEU:HD11	1:A:1280:LEU:HD21	2.00	0.43
1:B:1160:TYR:CE2	1:B:1162:GLY:HA3	2.53	0.43
1:A:1146:GLU:HG2	1:A:1150:ARG:CZ	2.47	0.43
1:B:34:GLY:O	1:B:40:LYS:NZ	2.45	0.43
1:A:48:LYS:HE3	1:A:152:ASP:HA	1.99	0.43
1:B:119:LEU:HD12	1:B:119:LEU:C	2.43	0.43
1:B:1178:THR:HA	1:B:1183:GLY:O	2.19	0.43
1:A:38:SER:HB3	1:A:1295:VAL:O	2.19	0.43
1:B:1163:THR:O	1:B:1196:LYS:HE2	2.19	0.43
1:B:102:LEU:O	1:B:109:ARG:HA	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:11:DC:H2''	2:C:12:DC:C5	2.54	0.43
1:B:79:ALA:HB3	1:B:99:ILE:CG2	2.49	0.43
3:D:11:DG:C2	3:D:12:DG:C2	3.06	0.42
1:A:173:LYS:HE2	1:A:1188:TYR:O	2.19	0.42
1:A:1147:GLN:HG2	1:A:1150:ARG:HH21	1.84	0.42
1:B:1129:GLY:O	1:B:1133:VAL:HG23	2.20	0.42
1:A:166:MET:HE1	1:A:1203:MET:HB3	2.01	0.42
1:B:161:ASP:OD2	1:B:175:ARG:NH2	2.53	0.42
1:B:1279:PHE:CZ	1:B:1283:MET:CE	3.02	0.42
1:A:1163:THR:HB	1:B:1301:GLN:NE2	2.35	0.42
1:A:1144:MET:HE2	1:A:1227:PHE:CE1	2.55	0.42
1:A:1147:GLN:CG	1:A:1150:ARG:HH21	2.33	0.42
1:A:69:PRO:O	1:A:72:VAL:HG12	2.19	0.42
1:A:203:LEU:HD22	1:A:1123:ILE:HD12	2.02	0.42
1:A:214:LYS:HE2	7:A:1529:HOH:O	2.18	0.42
1:A:1146:GLU:CD	1:A:1150:ARG:HH12	2.27	0.42
1:B:66:ILE:HD12	1:B:66:ILE:N	2.35	0.41
1:B:173:LYS:HE2	1:B:1188:TYR:O	2.20	0.41
1:A:70:ASP:CG	1:A:109:ARG:NH2	2.77	0.41
1:B:133:VAL:HG12	7:B:1505:HOH:O	2.19	0.41
1:A:1208:SER:HB2	5:B:1402:AGS:PG	2.60	0.41
1:B:150:ILE:HD11	1:B:179:ILE:HG23	2.02	0.41
1:B:1225:GLU:HB2	6:B:1403:AES:H72	2.02	0.41
3:D:2:DG:H2''	3:D:3:DG:O5'	2.21	0.41
1:A:174:LYS:HG2	1:A:178:GLU:OE2	2.21	0.41
1:A:1299:GLU:OE1	1:A:1299:GLU:N	2.41	0.41
1:A:1254:SER:O	1:A:1258:ILE:HG13	2.21	0.41
1:A:1296:LYS:O	1:A:1303:SER:HA	2.21	0.41
1:A:144:LEU:HD23	1:A:144:LEU:HA	1.94	0.40
1:B:92:SER:OG	1:B:121:ARG:NH2	2.54	0.40
1:A:89:ILE:H	1:A:89:ILE:HG12	1.73	0.40
1:A:66:ILE:HD12	1:A:66:ILE:N	2.36	0.40
1:B:209:ARG:HG2	1:B:1112:THR:HG21	2.03	0.40
1:A:193:ARG:CA	1:A:1130:MET:CE	2.99	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	428/449 (95%)	420 (98%)	7 (2%)	1 (0%)	43	63
1	B	428/449 (95%)	421 (98%)	7 (2%)	0	100	100
All	All	856/898 (95%)	841 (98%)	14 (2%)	1 (0%)	48	68

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	181	GLU

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	380/389 (98%)	379 (100%)	1 (0%)	86	94
1	B	380/389 (98%)	377 (99%)	3 (1%)	73	88
All	All	760/778 (98%)	756 (100%)	4 (0%)	81	92

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	94	VAL
1	B	206	LEU
1	B	1150	ARG
1	B	1191	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	58	ASN
1	A	111	GLN
1	A	1135	HIS
1	A	1238	GLN
1	A	1267	ASN
1	B	58	ASN
1	B	1238	GLN
1	B	1301	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 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	$\# Z > 2$
5	AGS	B	1402	4	32,33,33	0.62	1 (3%)	45,52,52	0.81	1 (2%)
6	AES	B	1403	-	12,13,13	1.19	0	17,18,18	2.53	4 (23%)
6	AES	A	1403	-	12,13,13	1.10	1 (8%)	17,18,18	2.46	8 (47%)
5	AGS	A	1402	4	32,33,33	0.76	2 (6%)	45,52,52	0.62	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
5	AGS	B	1402	4	-	3/21/38/38	0/3/3/3
6	AES	B	1403	-	-	2/9/9/9	0/1/1/1
6	AES	A	1403	-	-	4/9/9/9	0/1/1/1
5	AGS	A	1402	4	-	6/21/38/38	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1402	AGS	PB-O3A	-2.85	1.56	1.59
5	B	1402	AGS	PG-S1G	2.59	1.96	1.90
5	A	1402	AGS	PG-S1G	2.48	1.96	1.90
6	A	1403	AES	C7-C4	2.01	1.57	1.51

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	1403	AES	O2S-S-O1S	-6.60	99.33	119.18
6	B	1403	AES	C6-C1-S	6.47	123.84	119.25
6	B	1403	AES	O2S-S-O1S	-6.13	100.73	119.18
6	A	1403	AES	C6-C1-S	4.24	122.26	119.25
6	B	1403	AES	F-S-O1S	2.93	112.89	106.35
6	A	1403	AES	C6-C1-C2	-2.88	116.72	120.47
6	A	1403	AES	F-S-O2S	2.77	112.53	106.35
6	B	1403	AES	C6-C1-C2	-2.56	117.12	120.47
5	B	1402	AGS	PB-O3B-PG	-2.51	123.97	133.17
6	A	1403	AES	C2-C1-S	2.51	121.03	119.25
6	A	1403	AES	F-S-O1S	2.38	111.65	106.35
6	A	1403	AES	C3-C2-C1	2.35	121.73	119.44
6	A	1403	AES	C5-C6-C1	2.14	121.52	119.44

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	1402	AGS	C5'-O5'-PA-O1A
5	A	1402	AGS	C5'-O5'-PA-O2A
5	A	1402	AGS	C5'-O5'-PA-O3A

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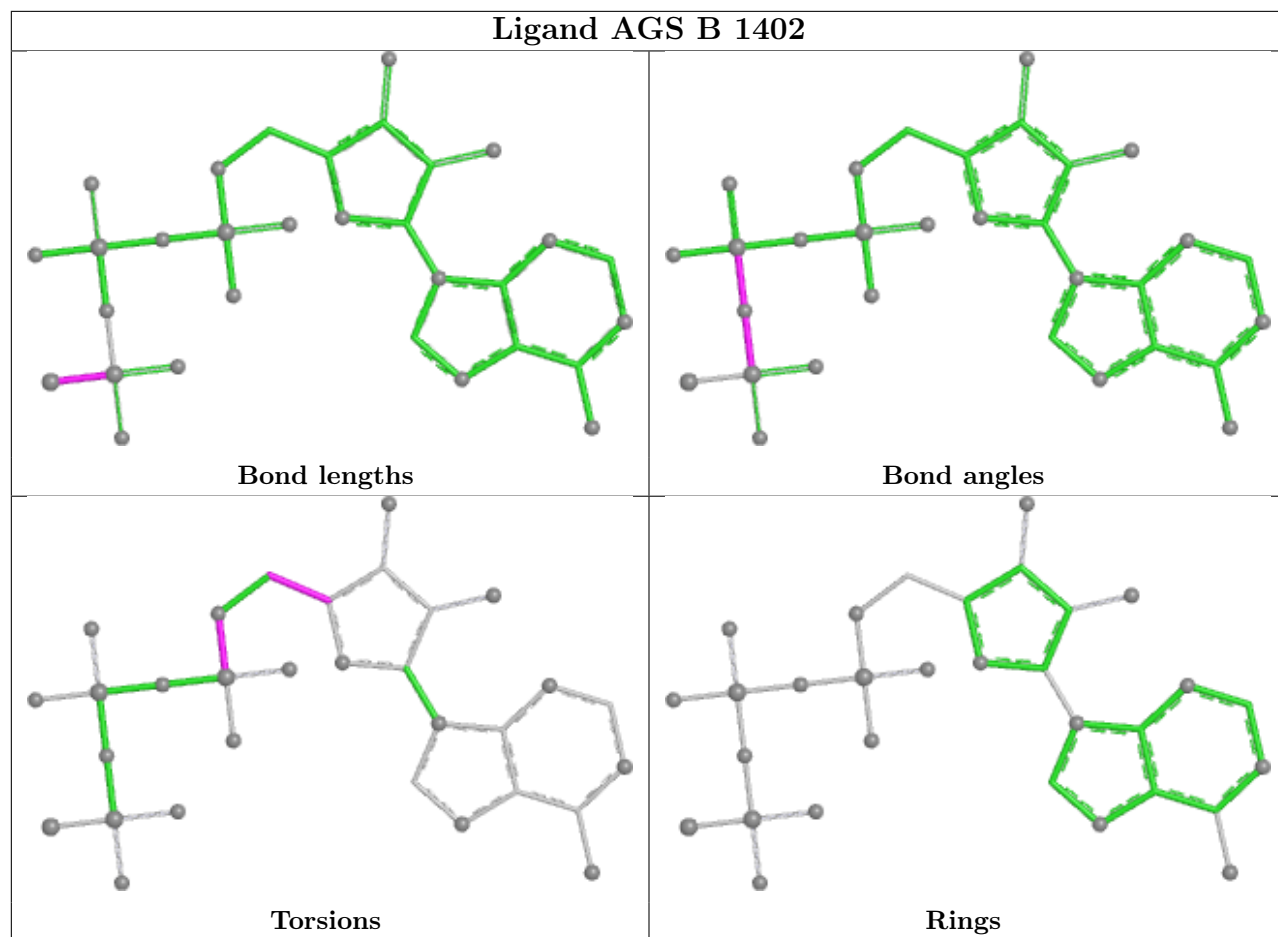
Mol	Chain	Res	Type	Atoms
5	A	1402	AGS	O4'-C4'-C5'-O5'
5	B	1402	AGS	C5'-O5'-PA-O1A
6	A	1403	AES	C2-C1-S-O2S
6	A	1403	AES	C6-C1-S-O2S
5	A	1402	AGS	C3'-C4'-C5'-O5'
5	B	1402	AGS	O4'-C4'-C5'-O5'
6	A	1403	AES	C2-C1-S-F
6	A	1403	AES	C6-C1-S-F
5	A	1402	AGS	PG-O3B-PB-O2B
6	B	1403	AES	C2-C1-S-O2S
6	B	1403	AES	C6-C1-S-O2S
5	B	1402	AGS	C3'-C4'-C5'-O5'

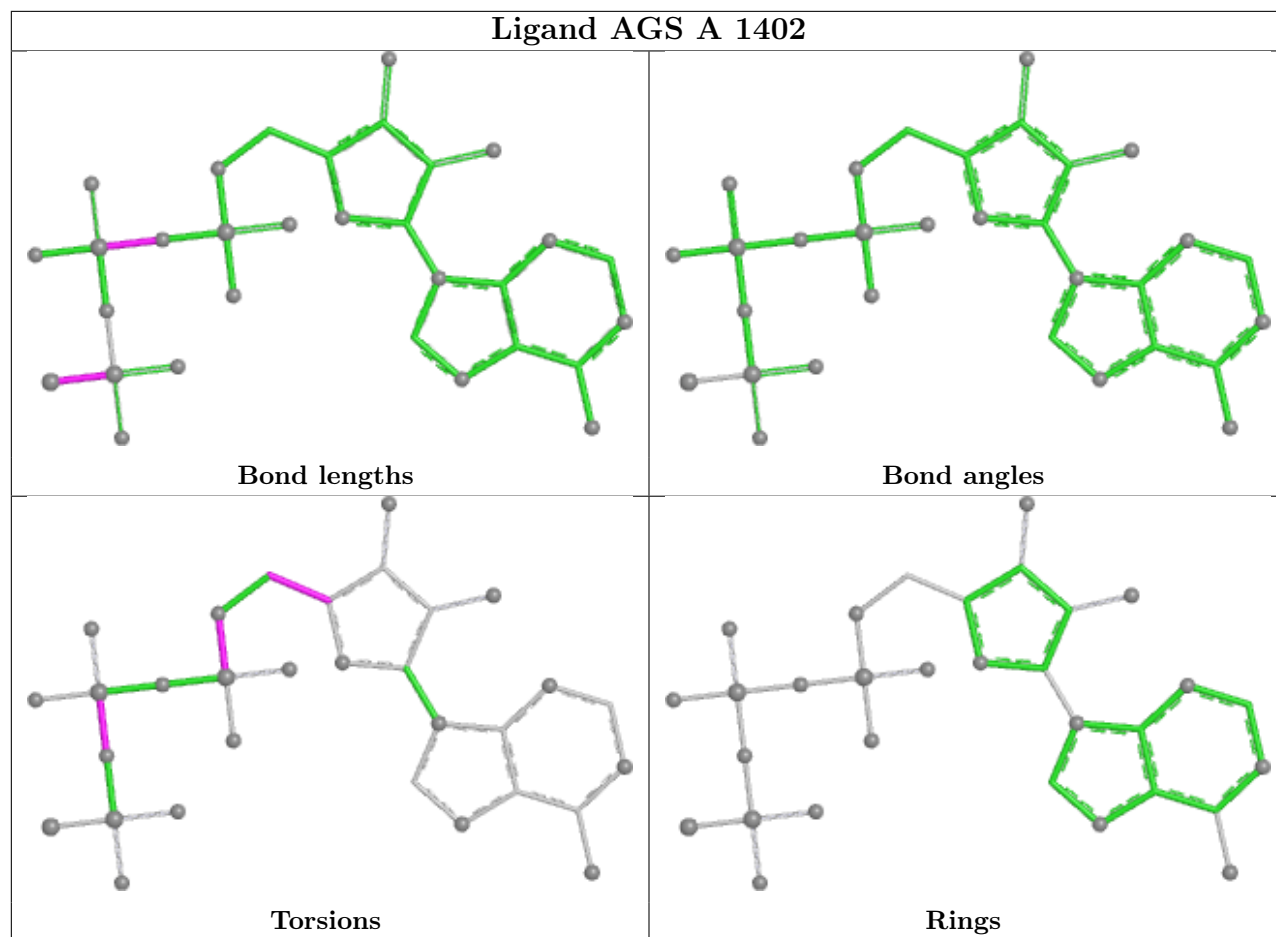
There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1402	AGS	3	0
6	B	1403	AES	1	0
6	A	1403	AES	1	0
5	A	1402	AGS	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.





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	431/449 (95%)	0.23	19 (4%) 39 34	29, 55, 90, 121	84 (19%)
1	B	432/449 (96%)	0.17	14 (3%) 50 46	23, 53, 90, 160	49 (11%)
2	C	15/15 (100%)	0.71	0 100 100	96, 147, 186, 188	0
3	D	15/15 (100%)	1.20	0 100 100	118, 161, 193, 205	0
All	All	893/928 (96%)	0.23	33 (3%) 45 40	23, 54, 102, 205	133 (14%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1176	SER	4.1
1	B	1100	LEU	3.8
1	A	103	VAL	3.6
1	B	1267	ASN	3.4
1	A	1182	SER	3.2
1	A	1179	SER	3.2
1	B	1182	SER	3.1
1	B	107	ASN	2.9
1	A	1183	GLY	2.9
1	A	182	ALA	2.8
1	A	1311	THR	2.8
1	B	135	GLU	2.8
1	B	1227	PHE	2.7
1	A	1184	THR	2.6
1	B	1183	GLY	2.6
1	A	2	SER	2.6
1	A	1178	THR	2.5
1	A	106	ASN	2.5
1	B	1231	CYS	2.5
1	B	124	GLY	2.5
1	A	1173	ASP	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	1284	GLN	2.4
1	B	1184	THR	2.3
1	B	125	GLU	2.3
1	A	122	ASN	2.3
1	A	1175	GLU	2.2
1	A	59	SER	2.2
1	A	102	LEU	2.2
1	A	123	ASN	2.1
1	B	1265	GLN	2.1
1	A	1180	SER	2.1
1	B	1310	ILE	2.0
1	A	104	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

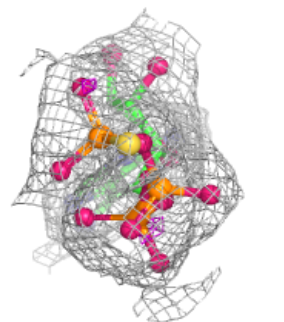
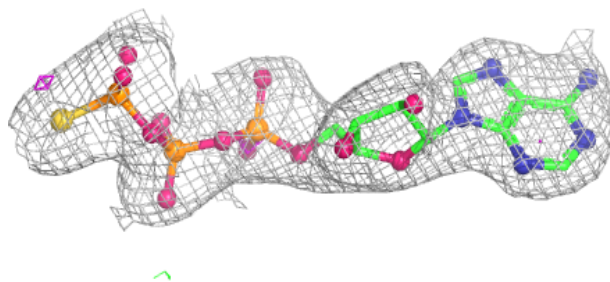
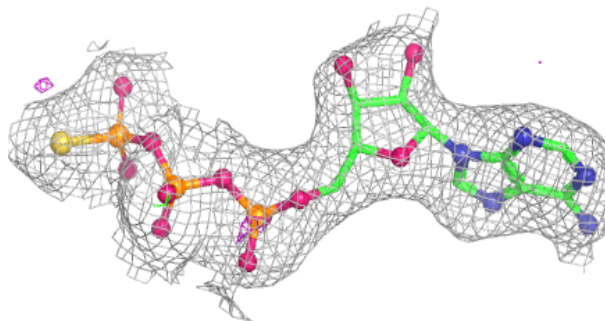
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	AES	A	1403	13/13	0.84	0.17	23,91,92,92	0
6	AES	B	1403	13/13	0.84	0.18	23,97,100,100	0
5	AGS	A	1402	31/31	0.97	0.07	41,47,50,52	0
4	MG	B	1401	1/1	0.98	0.04	42,42,42,42	0
5	AGS	B	1402	31/31	0.98	0.06	33,43,51,52	0
4	MG	A	1401	1/1	1.00	0.03	49,49,49,49	0

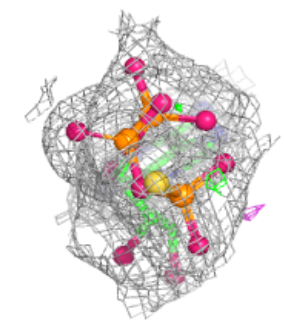
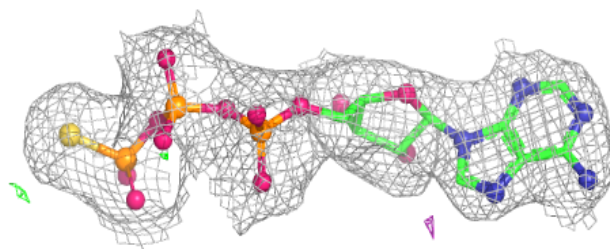
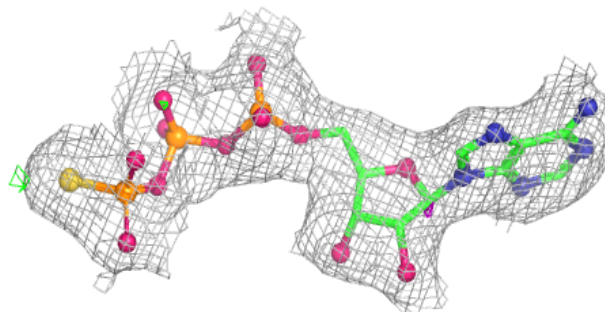
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around AGS A 1402:

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

**Electron density around AGS B 1402:**

$2mF_o-DF_c$ (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.