



wwPDB X-ray Structure Validation Summary Report ⓘ

May 25, 2020 – 10:36 am BST

PDB ID : 1XFV
Title : Crystal structure of anthrax edema factor (EF) in complex with calmodulin and 3' deoxy-ATP
Authors : Shen, Q.; Zhukovskaya, N.L.; Guo, Q.; Florian, J.; Tang, W.J.
Deposited on : 2004-09-15
Resolution : 3.35 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

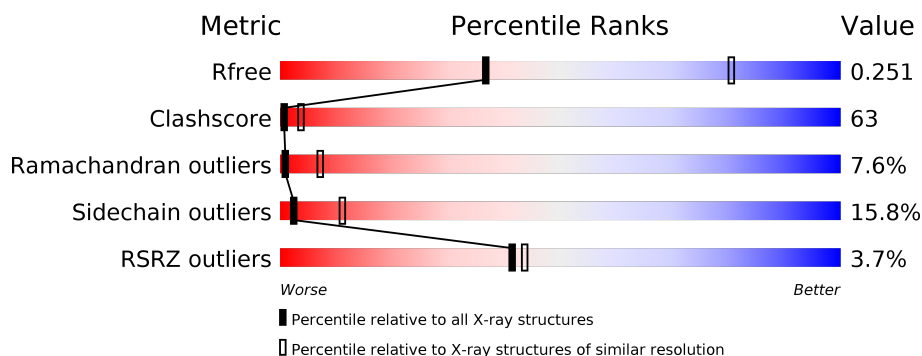
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.35 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	1558 (3.42-3.30)
Clashscore	141614	1627 (3.42-3.30)
Ramachandran outliers	138981	1599 (3.42-3.30)
Sidechain outliers	138945	1598 (3.42-3.30)
RSRZ outliers	127900	1507 (3.42-3.30)

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 $\leq 5\%$. 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	777	
1	B	777	
1	C	777	
1	D	777	
1	E	777	
1	F	777	

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Mol	Chain	Length	Quality of chain
2	O	149	<div><div><div>%</div><div><div></div><div>24%</div><div>61%</div><div>13%</div></div><div></div></div></div>
2	P	149	<div><div><div>%</div><div><div></div><div>22%</div><div>64%</div><div>12%</div></div><div></div></div></div>
2	Q	149	<div><div><div>%</div><div><div></div><div>23%</div><div>62%</div><div>13%</div></div><div></div></div></div>
2	R	149	<div><div><div>%</div><div><div></div><div>21%</div><div>63%</div><div>13%</div></div><div></div></div></div>
2	S	149	<div><div><div>3%</div><div><div></div><div>22%</div><div>63%</div><div>13%</div></div><div></div></div></div>
2	T	149	<div><div><div>%</div><div><div></div><div>23%</div><div>62%</div><div>13%</div></div><div></div></div></div>

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 43044 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 Calmodulin-sensitive adenylate cyclase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	735	Total	C	N	O	S	0	0	0
			5992	3828	995	1163	6			
1	B	735	Total	C	N	O	S	0	0	0
			5992	3828	995	1163	6			
1	C	735	Total	C	N	O	S	0	0	0
			5992	3828	995	1163	6			
1	D	735	Total	C	N	O	S	0	0	0
			5992	3828	995	1163	6			
1	E	735	Total	C	N	O	S	0	0	0
			5992	3828	995	1163	6			
1	F	735	Total	C	N	O	S	0	0	0
			5992	3828	995	1163	6			

There are 54 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	24	MET	-	INITIATING METHIONINE	UNP P40136
A	25	HIS	-	EXPRESSION TAG	UNP P40136
A	26	HIS	-	EXPRESSION TAG	UNP P40136
A	27	HIS	-	EXPRESSION TAG	UNP P40136
A	28	HIS	-	EXPRESSION TAG	UNP P40136
A	29	HIS	-	EXPRESSION TAG	UNP P40136
A	30	HIS	-	EXPRESSION TAG	UNP P40136
A	31	ALA	-	CLONING ARTIFACT	UNP P40136
A	32	ALA	-	CLONING ARTIFACT	UNP P40136
B	24	MET	-	INITIATING METHIONINE	UNP P40136
B	25	HIS	-	EXPRESSION TAG	UNP P40136
B	26	HIS	-	EXPRESSION TAG	UNP P40136
B	27	HIS	-	EXPRESSION TAG	UNP P40136
B	28	HIS	-	EXPRESSION TAG	UNP P40136
B	29	HIS	-	EXPRESSION TAG	UNP P40136
B	30	HIS	-	EXPRESSION TAG	UNP P40136
B	31	ALA	-	CLONING ARTIFACT	UNP P40136

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Chain	Residue	Modelled	Actual	Comment	Reference
B	32	ALA	-	CLONING ARTIFACT	UNP P40136
C	24	MET	-	INITIATING METHIONINE	UNP P40136
C	25	HIS	-	EXPRESSION TAG	UNP P40136
C	26	HIS	-	EXPRESSION TAG	UNP P40136
C	27	HIS	-	EXPRESSION TAG	UNP P40136
C	28	HIS	-	EXPRESSION TAG	UNP P40136
C	29	HIS	-	EXPRESSION TAG	UNP P40136
C	30	HIS	-	EXPRESSION TAG	UNP P40136
C	31	ALA	-	CLONING ARTIFACT	UNP P40136
C	32	ALA	-	CLONING ARTIFACT	UNP P40136
D	24	MET	-	INITIATING METHIONINE	UNP P40136
D	25	HIS	-	EXPRESSION TAG	UNP P40136
D	26	HIS	-	EXPRESSION TAG	UNP P40136
D	27	HIS	-	EXPRESSION TAG	UNP P40136
D	28	HIS	-	EXPRESSION TAG	UNP P40136
D	29	HIS	-	EXPRESSION TAG	UNP P40136
D	30	HIS	-	EXPRESSION TAG	UNP P40136
D	31	ALA	-	CLONING ARTIFACT	UNP P40136
D	32	ALA	-	CLONING ARTIFACT	UNP P40136
E	24	MET	-	INITIATING METHIONINE	UNP P40136
E	25	HIS	-	EXPRESSION TAG	UNP P40136
E	26	HIS	-	EXPRESSION TAG	UNP P40136
E	27	HIS	-	EXPRESSION TAG	UNP P40136
E	28	HIS	-	EXPRESSION TAG	UNP P40136
E	29	HIS	-	EXPRESSION TAG	UNP P40136
E	30	HIS	-	EXPRESSION TAG	UNP P40136
E	31	ALA	-	CLONING ARTIFACT	UNP P40136
E	32	ALA	-	CLONING ARTIFACT	UNP P40136
F	24	MET	-	INITIATING METHIONINE	UNP P40136
F	25	HIS	-	EXPRESSION TAG	UNP P40136
F	26	HIS	-	EXPRESSION TAG	UNP P40136
F	27	HIS	-	EXPRESSION TAG	UNP P40136
F	28	HIS	-	EXPRESSION TAG	UNP P40136
F	29	HIS	-	EXPRESSION TAG	UNP P40136
F	30	HIS	-	EXPRESSION TAG	UNP P40136
F	31	ALA	-	CLONING ARTIFACT	UNP P40136
F	32	ALA	-	CLONING ARTIFACT	UNP P40136

- Molecule 2 is a protein called Calmodulin 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	146	Total	C	N	O	S	0	0	0
			1146	702	186	249	9			

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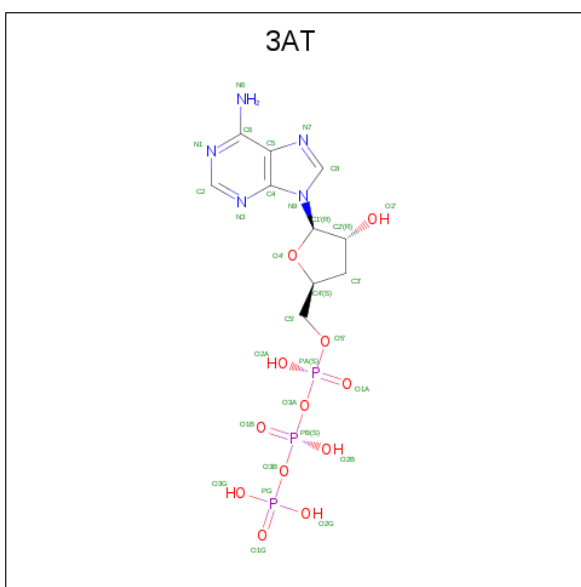
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	P	146	Total 1146	C 702	N 186	O 249	S 9	0	0	0
2	Q	146	Total 1146	C 702	N 186	O 249	S 9	0	0	0
2	R	146	Total 1146	C 702	N 186	O 249	S 9	0	0	0
2	S	146	Total 1146	C 702	N 186	O 249	S 9	0	0	0
2	T	146	Total 1146	C 702	N 186	O 249	S 9	0	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	2	Total 2	Mg 2	0	0
3	E	2	Total 2	Mg 2	0	0
3	B	2	Total 2	Mg 2	0	0
3	C	2	Total 2	Mg 2	0	0
3	A	2	Total 2	Mg 2	0	0
3	F	2	Total 2	Mg 2	0	0

- Molecule 4 is 3'-DEOXYADENOSINE-5'-TRIPHOSPHATE (three-letter code: 3AT) (formula: C₁₀H₁₆N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 30	C 10	N 5	O 12	P 3	0	0
4	B	1	Total 30	C 10	N 5	O 12	P 3	0	0
4	C	1	Total 30	C 10	N 5	O 12	P 3	0	0
4	D	1	Total 30	C 10	N 5	O 12	P 3	0	0
4	E	1	Total 30	C 10	N 5	O 12	P 3	0	0
4	F	1	Total 30	C 10	N 5	O 12	P 3	0	0

- Molecule 5 is CALCIUM ION (three-letter code: CA) (formula: Ca).

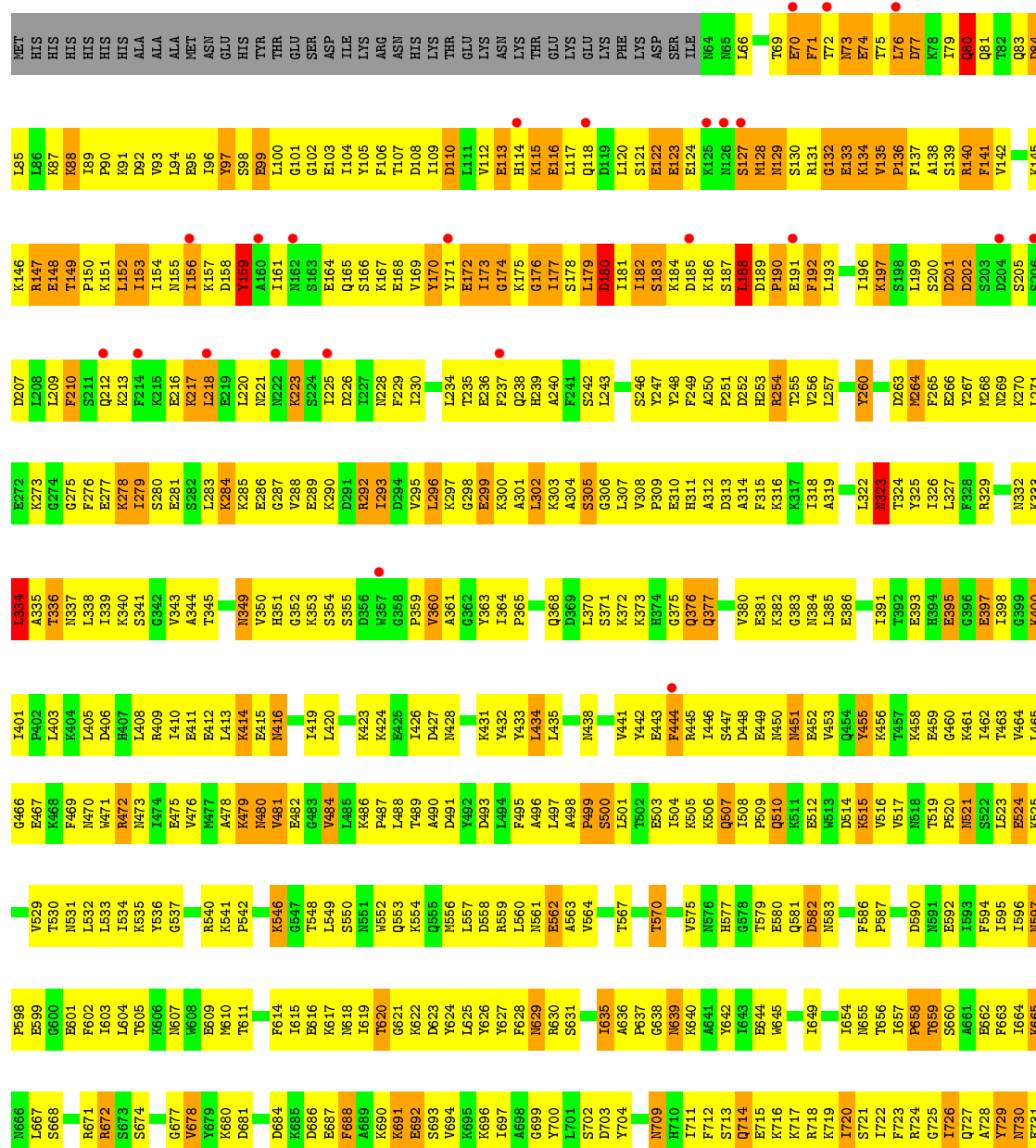
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	P	3	Total Ca 3 3	0	0
5	Q	3	Total Ca 3 3	0	0
5	T	3	Total Ca 3 3	0	0
5	O	3	Total Ca 3 3	0	0
5	R	3	Total Ca 3 3	0	0
5	S	3	Total Ca 3 3	0	0

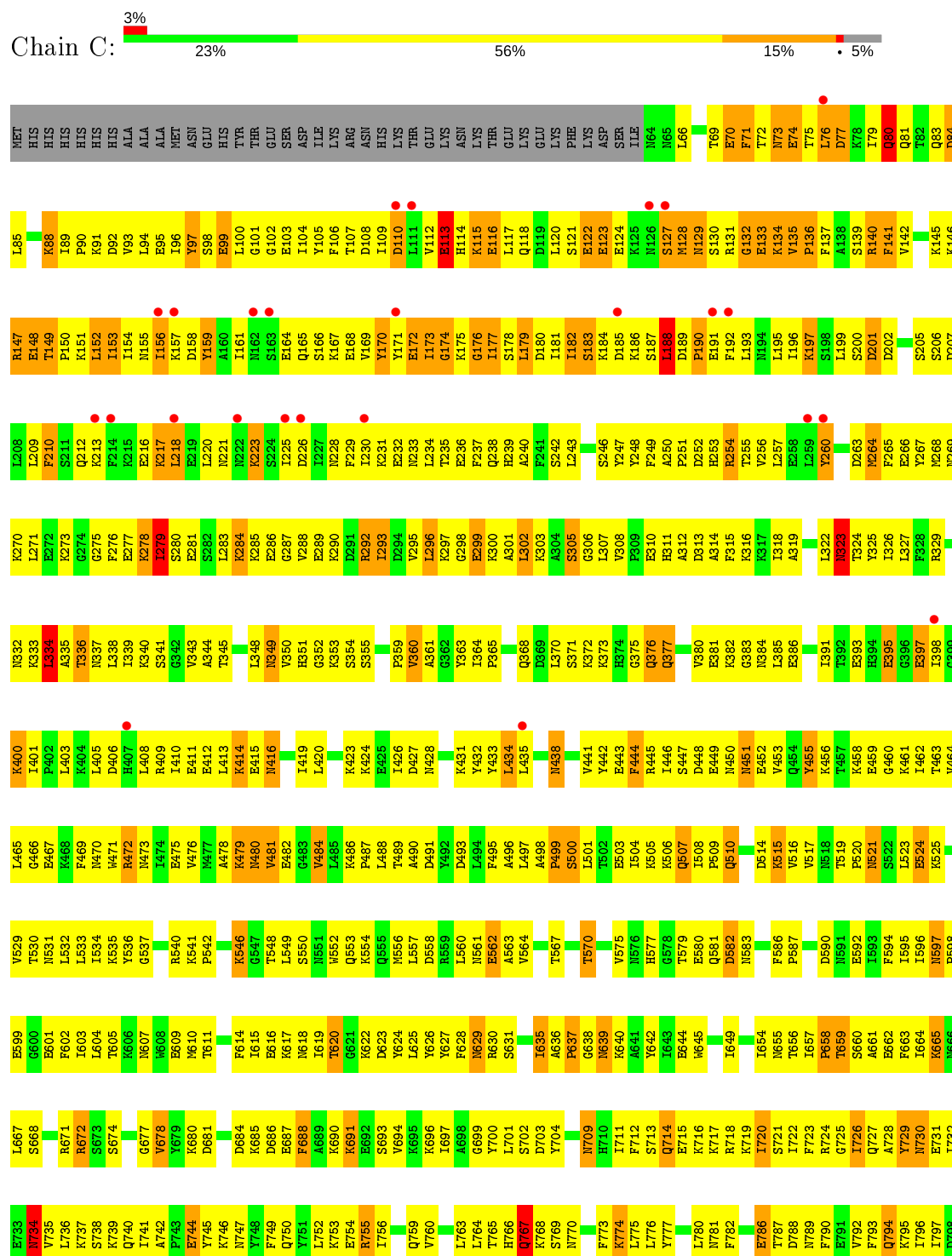
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	1	Total 1	O 1	0	0
6	B	1	Total 1	O 1	0	0
6	C	1	Total 1	O 1	0	0
6	D	1	Total 1	O 1	0	0
6	E	1	Total 1	O 1	0	0
6	F	1	Total 1	O 1	0	0



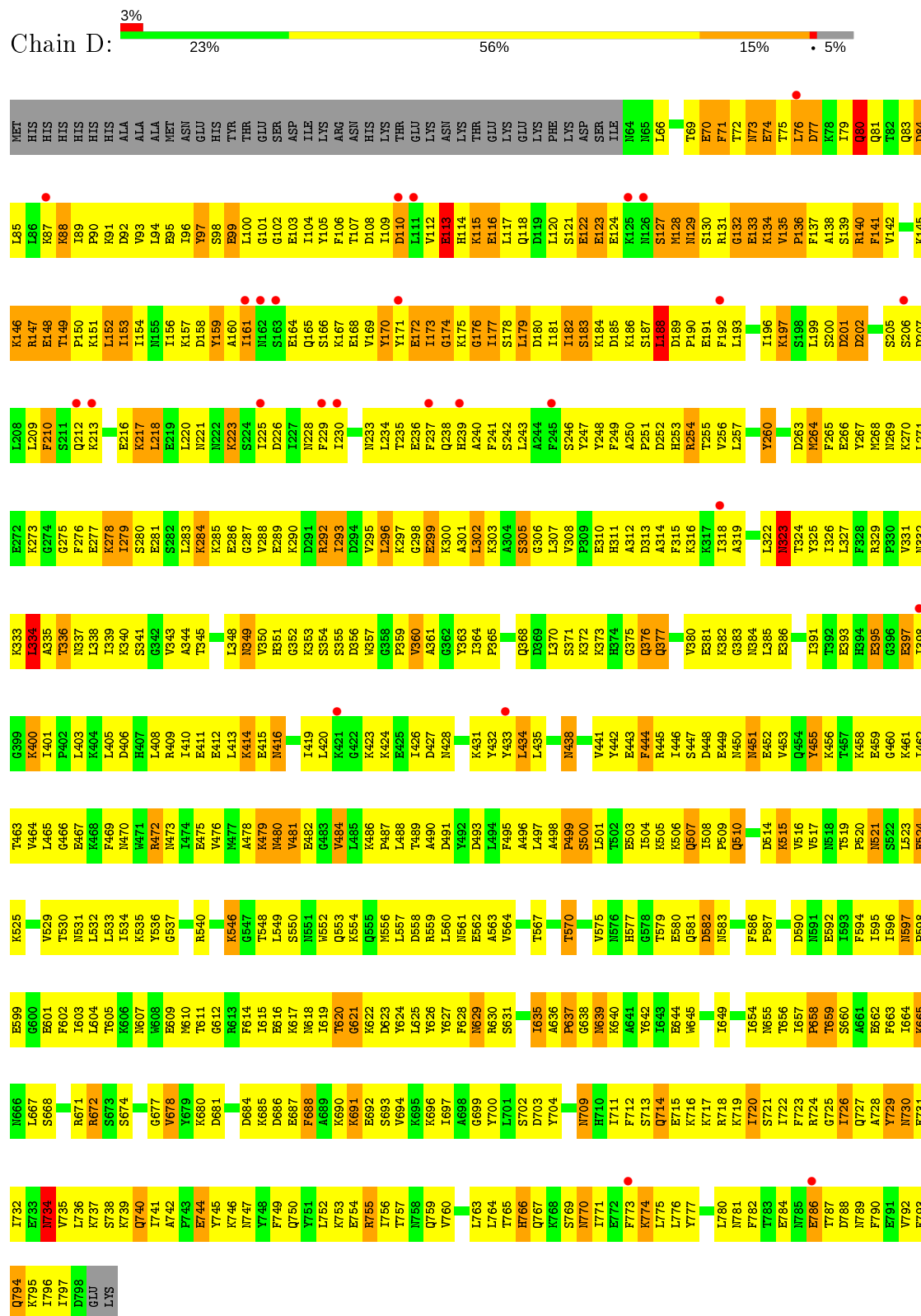
● Molecule 1: Calmodulin-sensitive adenylate cyclase





GLU
LYS

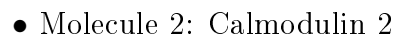
• Molecule 1: Calmodulin-sensitive adenylate cyclase

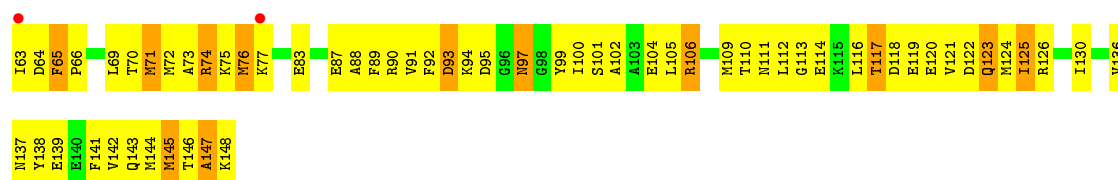


Chain E: 4% 23% 55% 15% 5%

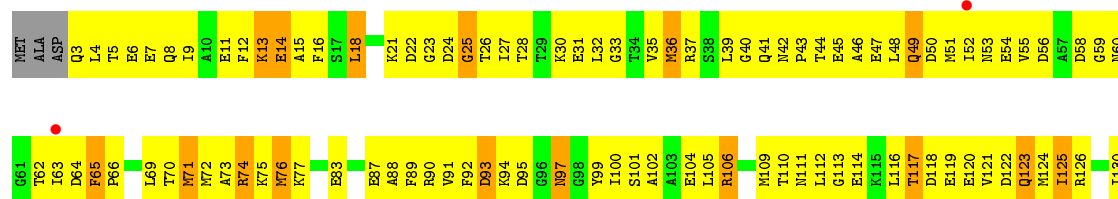
Item	Value 1	Value 2	Value 3	Value 4	Value 5	Value 6	Value 7	Value 8	Value 9	Value 10	Category
MET	147	148	149	150	151	152	153	154	155	156	157
HIS	157	158	159	160	161	162	163	164	165	166	167
HIS	167	168	169	170	171	172	173	174	175	176	177
HIS	177	178	179	180	181	182	183	184	185	186	187
HIS	187	188	189	190	191	192	193	194	195	196	197
HIS	197	198	199	200	201	202	203	204	205	206	207
HIS	207	208	209	210	211	212	213	214	215	216	217
HIS	217	218	219	220	221	222	223	224	225	226	227
HIS	227	228	229	230	231	232	233	234	235	236	237
HIS	237	238	239	240	241	242	243	244	245	246	247
ALA	247	248	249	250	251	252	253	254	255	256	257
ALA	257	258	259	260	261	262	263	264	265	266	267
ALA	267	268	269	270	271	272	273	274	275	276	277
ALA	277	278	279	280	281	282	283	284	285	286	287
ALA	287	288	289	290	291	292	293	294	295	296	297
ALA	297	298	299	300	301	302	303	304	305	306	307
ALA	307	308	309	310	311	312	313	314	315	316	317
ALA	317	318	319	320	321	322	323	324	325	326	327
ALA	327	328	329	330	331	332	333	334	335	336	337
ALA	337	338	339	340	341	342	343	344	345	346	347
ALA	347	348	349	350	351	352	353	354	355	356	357
ALA	357	358	359	360	361	362	363	364	365	366	367
ALA	367	368	369	370	371	372	373	374	375	376	377
ALA	377	378	379	380	381	382	383	384	385	386	387
ALA	387	388	389	390	391	392	393	394	395	396	397
ALA	397	398	399	400	401	402	403	404	405	406	407
ALA	407	408	409	410	411	412	413	414	415	416	417
ALA	417	418	419	420	421	422	423	424	425	426	427
ALA	427	428	429	430	431	432	433	434	435	436	437
ALA	437	438	439	440	441	442	443	444	445	446	447
ALA	447	448	449	450	451	452	453	454	455	456	457
ALA	457	458	459	460	461	462	463	464	465	466	467
ALA	467	468	469	470	471	472	473	474	475	476	477
ALA	477	478	479	480	481	482	483	484	485	486	487
ALA	487	488	489	490	491	492	493	494	495	496	497
ALA	497	498	499	500	501	502	503	504	505	506	507
ALA	507	508	509	510	511	512	513	514	515	516	517

Chain F: 5% 24% 55% 15% 5%

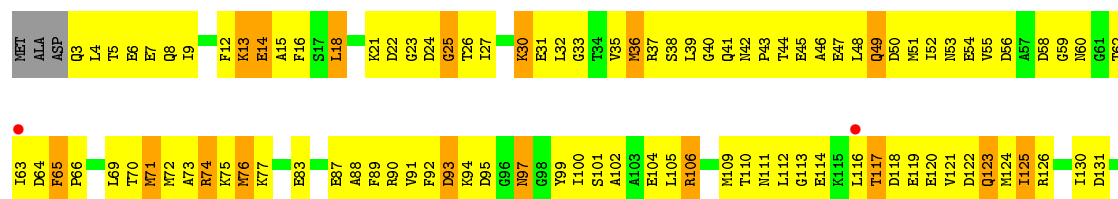




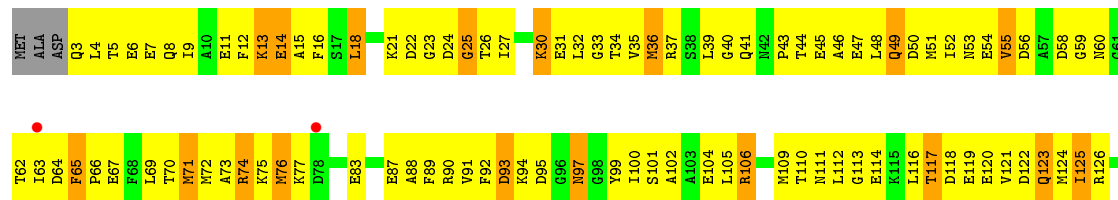
● Molecule 2: Calmodulin 2



● Molecule 2: Calmodulin 2



● Molecule 2: Calmodulin 2

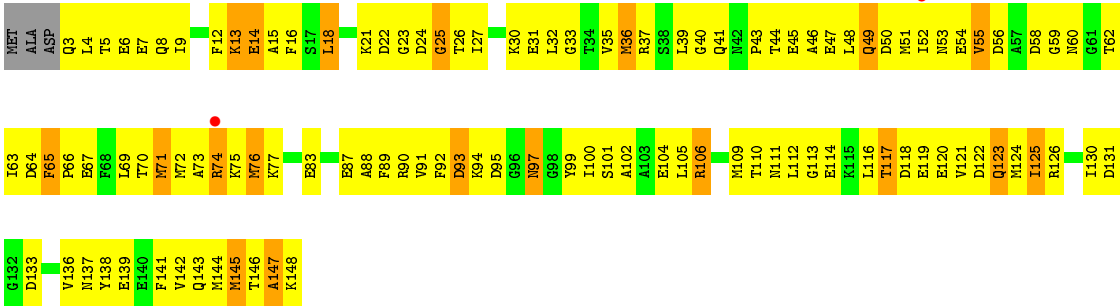


● Molecule 2: Calmodulin 2





• Molecule 2: Calmodulin 2



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	184.60Å 319.29Å 142.05Å 90.00° 90.22° 90.00°	Depositor
Resolution (Å)	29.57 – 3.35 35.51 – 3.35	Depositor EDS
% Data completeness (in resolution range)	92.6 (29.57-3.35) 91.6 (35.51-3.35)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 3.32Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.263 , 0.282 0.234 , 0.251	Depositor DCC
R_{free} test set	5790 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	97.5	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 56.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.458 for -1/2*h+1/2*k,3/2*h+1/2*k,-l 0.458 for -1/2*h-1/2*k,-3/2*h+1/2*k,-l 0.440 for 1/2*h+1/2*k,3/2*h-1/2*k,-l 0.447 for 1/2*h-1/2*k,-3/2*h-1/2*k,-l 0.439 for -h,-k,l	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	43044	wwPDB-VP
Average B, all atoms (Å ²)	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% 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: CA, MG, 3AT

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	0.53	0/6104	0.82	13/8208 (0.2%)
1	B	0.54	0/6104	0.83	13/8208 (0.2%)
1	C	0.56	1/6104 (0.0%)	0.89	22/8208 (0.3%)
1	D	0.56	3/6104 (0.0%)	0.85	15/8208 (0.2%)
1	E	0.56	2/6104 (0.0%)	0.85	16/8208 (0.2%)
1	F	0.54	0/6104	0.84	12/8208 (0.1%)
2	O	0.53	0/1158	0.76	0/1553
2	P	0.54	0/1158	0.76	0/1553
2	Q	0.55	0/1158	0.75	0/1553
2	R	0.55	0/1158	0.76	0/1553
2	S	0.56	0/1158	0.76	0/1553
2	T	0.56	0/1158	0.76	0/1553
All	All	0.55	6/43572 (0.0%)	0.83	91/58566 (0.2%)

The worst 5 of 6 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	740	GLN	C-N	-5.88	1.20	1.34
1	C	766	HIS	C-N	-5.74	1.20	1.34
1	D	784	GLU	C-N	5.50	1.46	1.34
1	D	621	GLY	C-N	5.27	1.46	1.34
1	E	784	GLU	C-N	5.14	1.45	1.34

The worst 5 of 91 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	766	HIS	O-C-N	-15.18	98.42	122.70
1	C	767	GLN	CA-C-N	12.73	145.20	117.20
1	C	766	HIS	CG-ND1-CE1	9.42	121.39	108.20
1	C	766	HIS	ND1-CG-CD2	-8.71	93.81	106.00
1	C	767	GLN	O-C-N	-7.95	109.99	122.70

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	5992	0	6010	771	2
1	B	5992	0	6010	765	2
1	C	5992	0	6010	770	2
1	D	5992	0	6009	771	3
1	E	5992	0	6009	772	3
1	F	5992	0	6010	755	1
2	O	1146	0	1071	150	0
2	P	1146	0	1071	157	0
2	Q	1146	0	1071	155	0
2	R	1146	0	1071	157	0
2	S	1146	0	1071	162	0
2	T	1146	0	1071	157	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	2	0	0	0	0
3	F	2	0	0	0	0
4	A	30	0	12	1	0
4	B	30	0	12	1	0
4	C	30	0	12	1	0
4	D	30	0	12	1	0
4	E	30	0	12	1	0
4	F	30	0	12	1	0
5	O	3	0	0	0	0
5	P	3	0	0	0	0
5	Q	3	0	0	0	0
5	R	3	0	0	0	0
5	S	3	0	0	0	0
5	T	3	0	0	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	D	1	0	0	0	0
6	E	1	0	0	0	0
6	F	1	0	0	0	0
All	All	43044	0	42556	5389	8

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 63.

The worst 5 of 5389 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:E:179:LEU:O	1:E:183:SER:CB	1.74	1.36
1:D:179:LEU:O	1:D:183:SER:CB	1.77	1.30
1:F:179:LEU:O	1:F:183:SER:CB	1.80	1.30
1:C:179:LEU:O	1:C:183:SER:CB	1.77	1.30
1:F:188:LEU:H	1:F:188:LEU:CD2	1.46	1.27

The worst 5 of 8 symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:685:LYS:NZ	1:D:685:LYS:NZ[2_657]	2.03	0.17
1:A:75:THR:CG2	1:E:786:GLU:O[4_556]	2.09	0.11
1:B:786:GLU:O	1:D:75:THR:CG2[4_656]	2.12	0.08
1:F:75:THR:CG2	1:F:786:GLU:O[2_557]	2.13	0.07
1:B:75:THR:CG2	1:D:786:GLU:O[4_656]	2.14	0.06

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	733/777 (94%)	497 (68%)	179 (24%)	57 (8%)	1	6
1	B	733/777 (94%)	494 (67%)	183 (25%)	56 (8%)	1	7
1	C	733/777 (94%)	491 (67%)	187 (26%)	55 (8%)	1	7
1	D	733/777 (94%)	492 (67%)	187 (26%)	54 (7%)	1	7
1	E	733/777 (94%)	490 (67%)	186 (25%)	57 (8%)	1	6
1	F	733/777 (94%)	492 (67%)	186 (25%)	55 (8%)	1	7
2	O	144/149 (97%)	103 (72%)	30 (21%)	11 (8%)	1	7
2	P	144/149 (97%)	103 (72%)	30 (21%)	11 (8%)	1	7
2	Q	144/149 (97%)	103 (72%)	30 (21%)	11 (8%)	1	7
2	R	144/149 (97%)	103 (72%)	29 (20%)	12 (8%)	1	6
2	S	144/149 (97%)	103 (72%)	30 (21%)	11 (8%)	1	7
2	T	144/149 (97%)	103 (72%)	30 (21%)	11 (8%)	1	7
All	All	5262/5556 (95%)	3574 (68%)	1287 (24%)	401 (8%)	1	7

5 of 401 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	176	GLY
1	A	183	SER
1	A	302	LEU
1	A	787	THR
1	B	137	PHE

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	664/705 (94%)	562 (85%)	102 (15%)	2	12
1	B	664/705 (94%)	558 (84%)	106 (16%)	2	10
1	C	664/705 (94%)	560 (84%)	104 (16%)	2	11
1	D	664/705 (94%)	558 (84%)	106 (16%)	2	10

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	664/705 (94%)	558 (84%)	106 (16%)	2	10
1	F	664/705 (94%)	558 (84%)	106 (16%)	2	10
2	O	123/127 (97%)	103 (84%)	20 (16%)	2	10
2	P	123/127 (97%)	105 (85%)	18 (15%)	3	13
2	Q	123/127 (97%)	104 (85%)	19 (15%)	2	12
2	R	123/127 (97%)	103 (84%)	20 (16%)	2	10
2	S	123/127 (97%)	105 (85%)	18 (15%)	3	13
2	T	123/127 (97%)	104 (85%)	19 (15%)	2	12
All	All	4722/4992 (95%)	3978 (84%)	744 (16%)	2	11

5 of 744 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	156	ILE
1	D	786	GLU
2	R	13	LYS
1	D	201	ASP
1	D	444	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 225 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	770	ASN
1	D	581	GLN
2	O	49	GLN
1	D	64	ASN
1	D	376	GLN

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 [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 36 ligands modelled in this entry, 30 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	3AT	E	907	3	25,32,32	1.37	4 (16%)	28,50,50	1.29	3 (10%)
4	3AT	A	903	3	25,32,32	1.42	4 (16%)	28,50,50	1.32	3 (10%)
4	3AT	D	906	3	25,32,32	1.44	4 (16%)	28,50,50	1.30	3 (10%)
4	3AT	C	905	3	25,32,32	1.46	4 (16%)	28,50,50	1.33	3 (10%)
4	3AT	B	904	3	25,32,32	1.40	4 (16%)	28,50,50	1.34	3 (10%)
4	3AT	F	908	3	25,32,32	1.37	4 (16%)	28,50,50	1.33	3 (10%)

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	3AT	E	907	3	-	7/18/34/34	0/3/3/3
4	3AT	A	903	3	-	7/18/34/34	0/3/3/3
4	3AT	D	906	3	-	7/18/34/34	0/3/3/3
4	3AT	C	905	3	-	7/18/34/34	0/3/3/3
4	3AT	B	904	3	-	7/18/34/34	0/3/3/3
4	3AT	F	908	3	-	7/18/34/34	0/3/3/3

The worst 5 of 24 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	906	3AT	C4-N3	3.60	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	903	3AT	C4-N3	3.40	1.40	1.35
4	C	905	3AT	C4-N3	3.33	1.40	1.35
4	B	904	3AT	C4-N3	3.07	1.39	1.35
4	C	905	3AT	PG-O2G	-2.99	1.43	1.54

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	908	3AT	O4'-C1'-C2'	-4.13	100.89	106.93
4	B	904	3AT	O4'-C1'-C2'	-4.05	101.01	106.93
4	C	905	3AT	O4'-C1'-C2'	-3.96	101.14	106.93
4	A	903	3AT	O4'-C1'-C2'	-3.87	101.27	106.93
4	E	907	3AT	O4'-C1'-C2'	-3.80	101.38	106.93

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	E	907	3AT	PB-O3B-PG-O2G
4	E	907	3AT	O4'-C4'-C5'-O5'
4	E	907	3AT	C3'-C4'-C5'-O5'
4	A	903	3AT	PB-O3B-PG-O2G
4	A	903	3AT	O4'-C4'-C5'-O5'

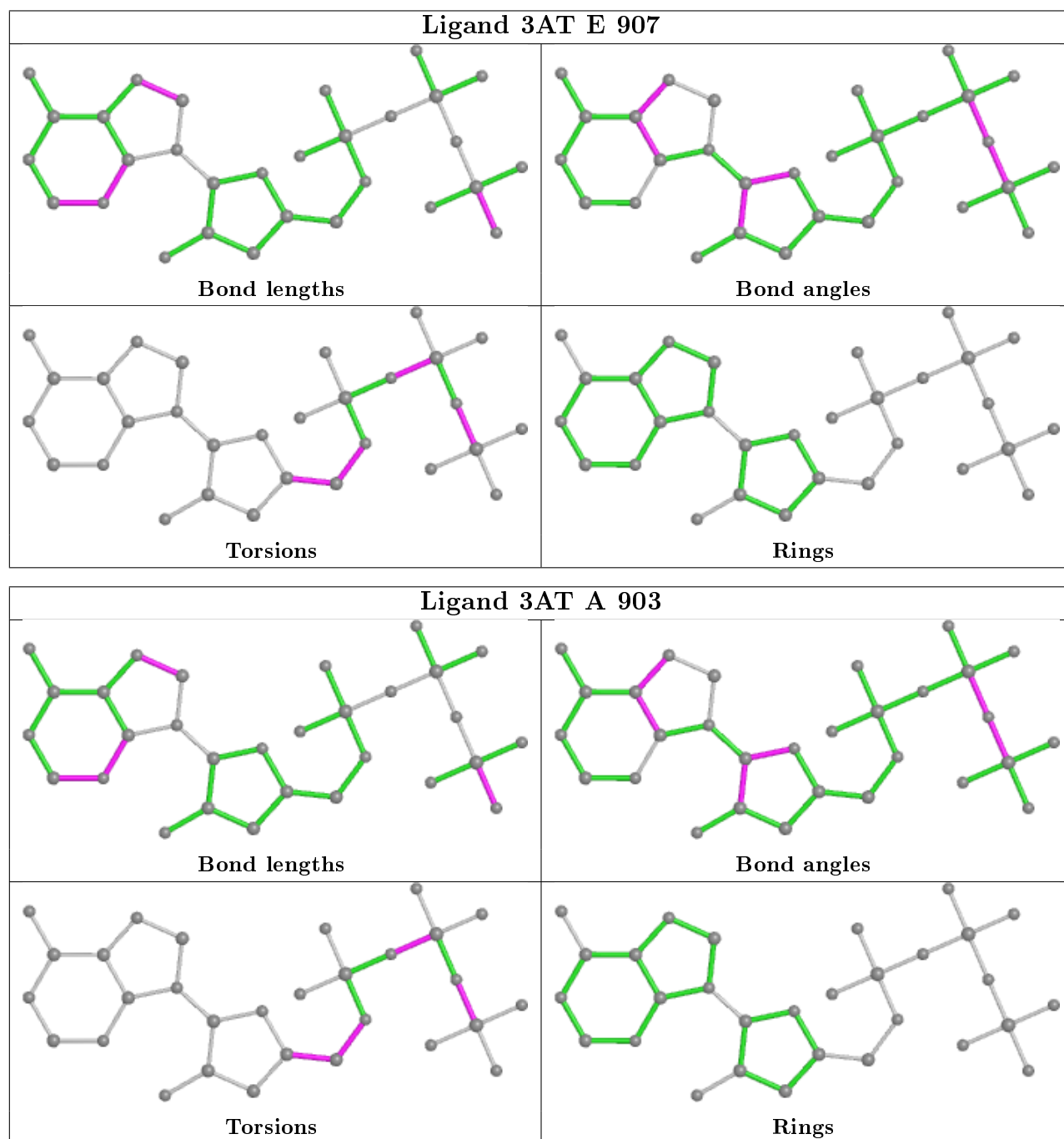
There are no ring outliers.

6 monomers are involved in 6 short contacts:

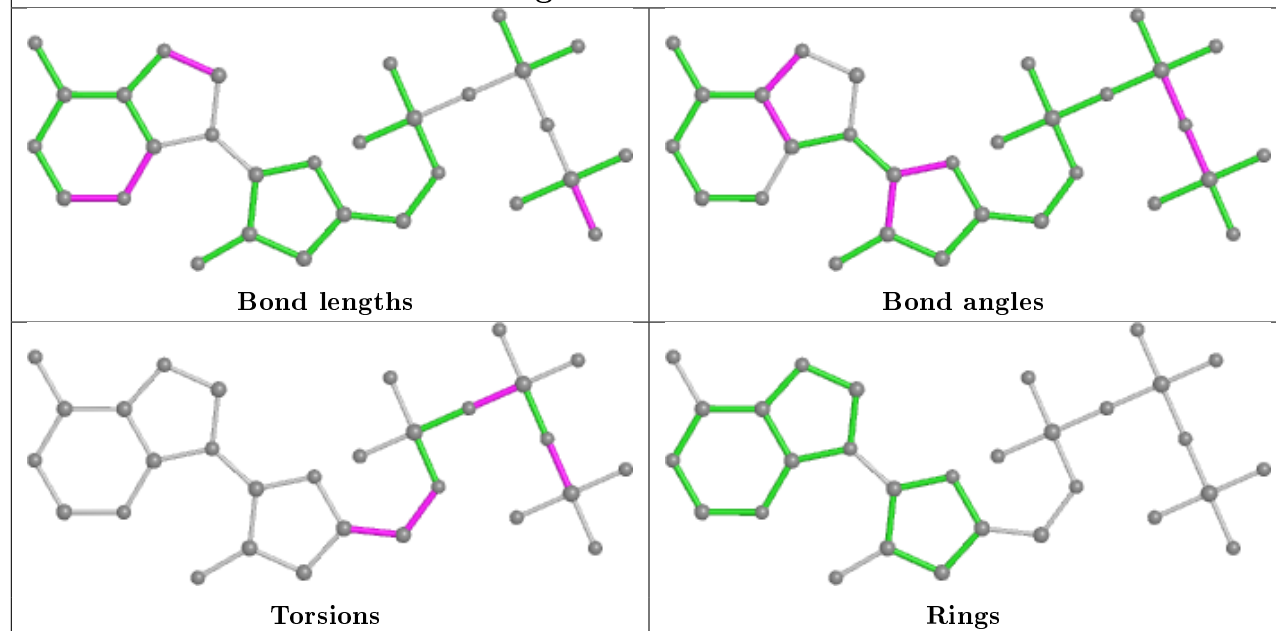
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	E	907	3AT	1	0
4	A	903	3AT	1	0
4	D	906	3AT	1	0
4	C	905	3AT	1	0
4	B	904	3AT	1	0
4	F	908	3AT	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be

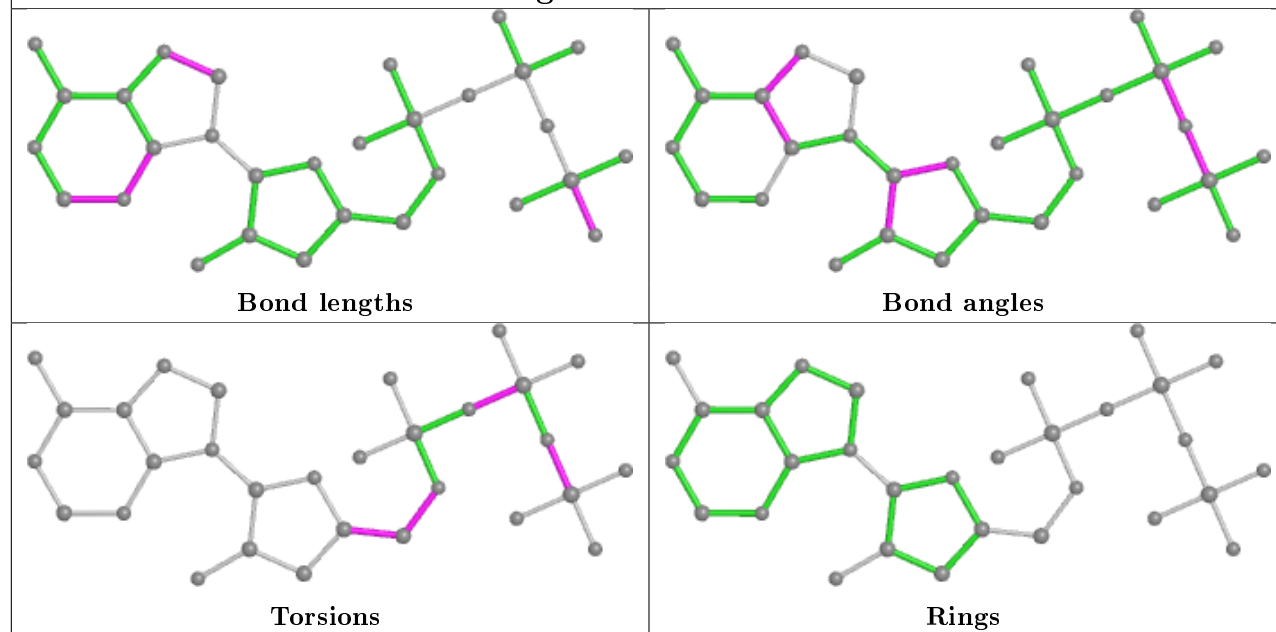
highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

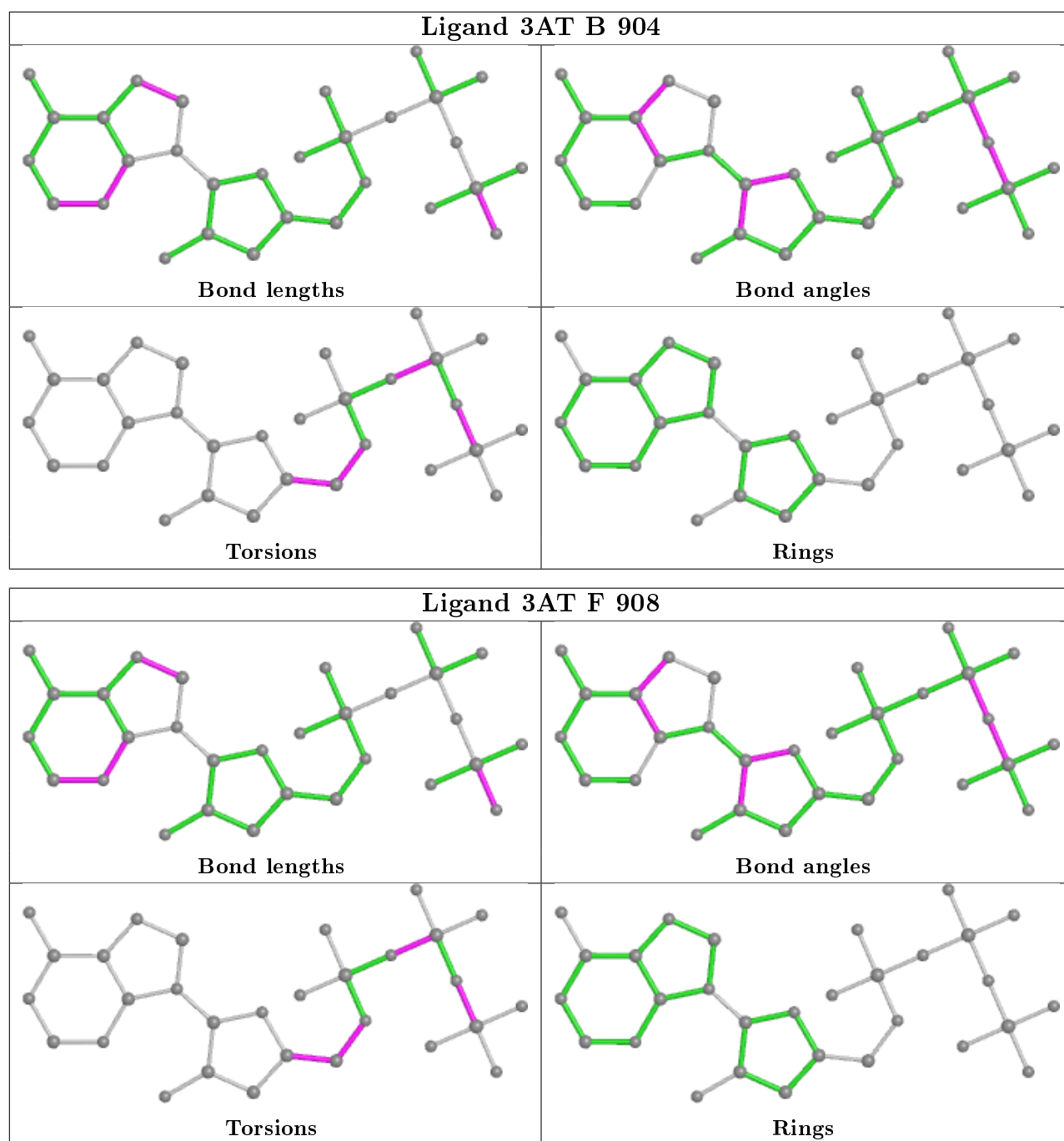


Ligand 3AT D 906



Ligand 3AT C 905





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	735/777 (94%)	0.32	35 (4%) 30 33	26, 80, 136, 148	0
1	B	735/777 (94%)	0.25	26 (3%) 44 46	27, 80, 136, 148	0
1	C	735/777 (94%)	0.27	25 (3%) 45 47	27, 80, 136, 148	0
1	D	735/777 (94%)	0.28	26 (3%) 44 46	27, 80, 136, 150	0
1	E	735/777 (94%)	0.29	31 (4%) 36 38	26, 80, 136, 148	0
1	F	735/777 (94%)	0.31	37 (5%) 28 31	27, 80, 136, 148	0
2	O	146/149 (97%)	0.09	2 (1%) 75 78	33, 63, 124, 131	0
2	P	146/149 (97%)	0.09	2 (1%) 75 78	33, 63, 124, 131	0
2	Q	146/149 (97%)	0.08	2 (1%) 75 78	33, 62, 124, 131	0
2	R	146/149 (97%)	0.12	2 (1%) 75 78	33, 63, 124, 131	0
2	S	146/149 (97%)	0.11	4 (2%) 54 57	32, 62, 124, 131	0
2	T	146/149 (97%)	0.09	2 (1%) 75 78	33, 62, 124, 131	0
All	All	5286/5556 (95%)	0.26	194 (3%) 41 43	26, 76, 134, 150	0

The worst 5 of 194 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	126	ASN	8.6
1	D	162	ASN	7.5
1	D	171	TYR	7.3
1	A	222	ASN	7.2
1	B	126	ASN	7.1

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

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	3AT	A	903	30/30	0.92	0.24	60,74,93,94	0
4	3AT	C	905	30/30	0.92	0.22	62,73,94,95	0
4	3AT	F	908	30/30	0.92	0.21	61,75,94,95	0
4	3AT	E	907	30/30	0.93	0.22	60,74,96,97	0
4	3AT	B	904	30/30	0.93	0.23	58,73,93,94	0
3	MG	C	903	1/1	0.93	0.15	9,9,9,9	0
4	3AT	D	906	30/30	0.93	0.21	58,74,94,95	0
5	CA	Q	705	1/1	0.93	0.11	55,55,55,55	0
5	CA	O	701	1/1	0.94	0.07	51,51,51,51	0
3	MG	B	902	1/1	0.94	0.21	17,17,17,17	0
5	CA	T	811	1/1	0.95	0.16	33,33,33,33	0
3	MG	D	904	1/1	0.95	0.17	8,8,8,8	0
5	CA	Q	805	1/1	0.95	0.17	27,27,27,27	0
5	CA	S	809	1/1	0.95	0.16	26,26,26,26	0
5	CA	S	709	1/1	0.96	0.11	57,57,57,57	0
5	CA	R	707	1/1	0.96	0.10	62,62,62,62	0
5	CA	T	711	1/1	0.96	0.10	55,55,55,55	0
3	MG	A	901	1/1	0.97	0.19	5,5,5,5	0
3	MG	D	905	1/1	0.97	0.10	43,43,43,43	0
5	CA	P	703	1/1	0.97	0.15	62,62,62,62	0
3	MG	A	902	1/1	0.97	0.16	28,28,28,28	0
3	MG	E	906	1/1	0.97	0.14	26,26,26,26	0
3	MG	F	906	1/1	0.97	0.15	11,11,11,11	0
5	CA	R	807	1/1	0.97	0.14	33,33,33,33	0
5	CA	Q	806	1/1	0.97	0.16	57,57,57,57	0
5	CA	R	808	1/1	0.98	0.11	54,54,54,54	0
3	MG	F	907	1/1	0.98	0.11	34,34,34,34	0
5	CA	O	802	1/1	0.98	0.14	52,52,52,52	0
3	MG	E	905	1/1	0.98	0.14	20,20,20,20	0
5	CA	O	801	1/1	0.98	0.16	30,30,30,30	0
5	CA	P	804	1/1	0.98	0.10	52,52,52,52	0
3	MG	B	903	1/1	0.98	0.13	25,25,25,25	0

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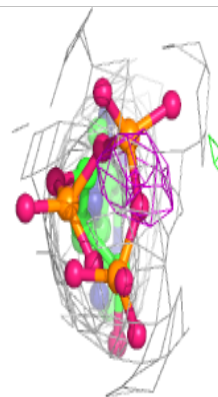
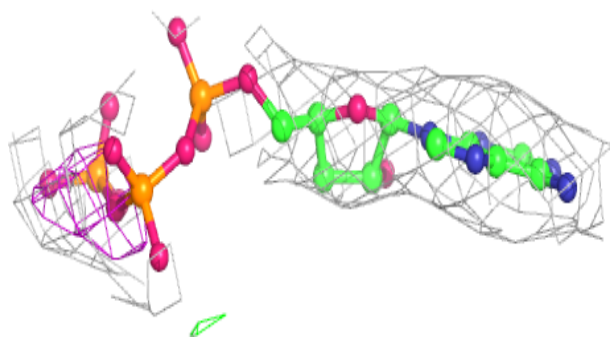
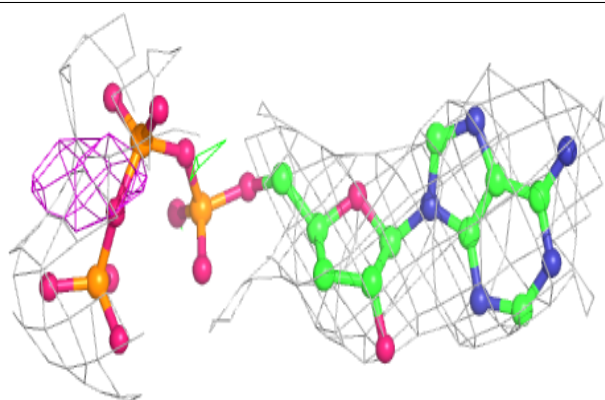
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	MG	C	904	1/1	0.98	0.15	26,26,26,26	0
5	CA	T	812	1/1	0.98	0.16	49,49,49,49	0
5	CA	P	803	1/1	0.98	0.14	31,31,31,31	0
5	CA	S	810	1/1	0.99	0.12	56,56,56,56	0

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.

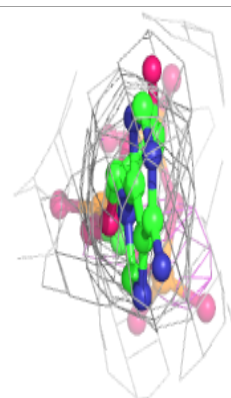
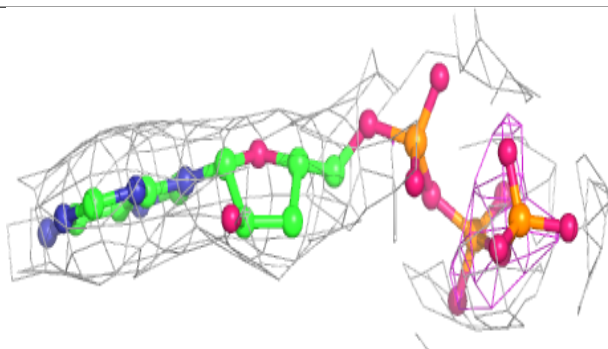
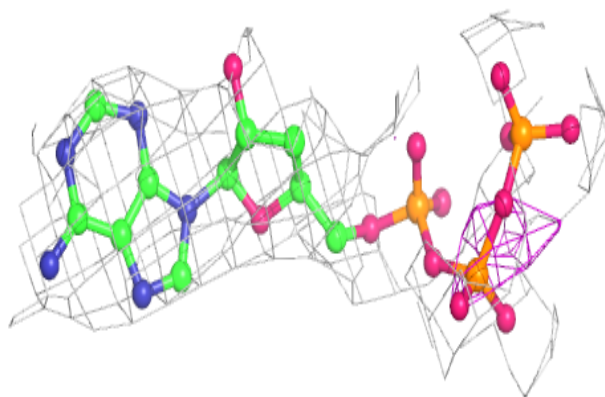
Electron density around 3AT A 903:

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

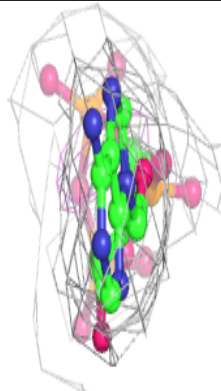
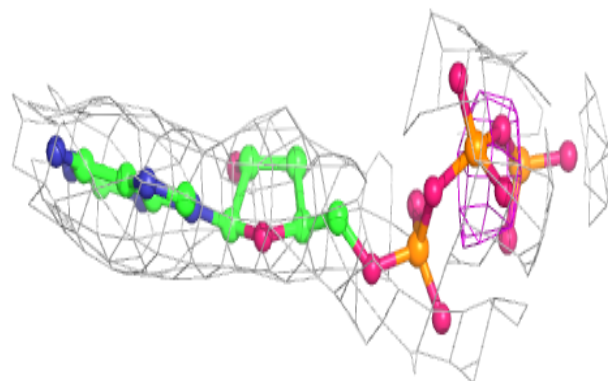
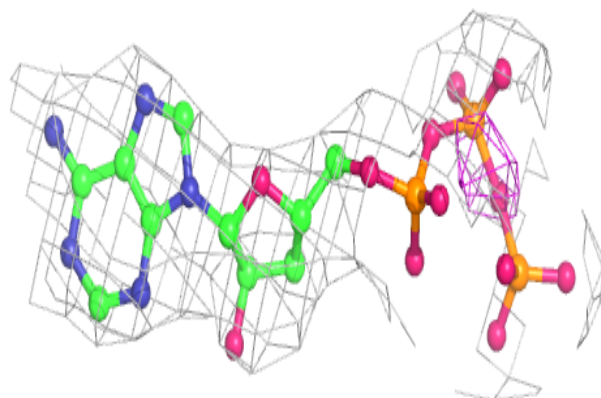


Electron density around 3AT C 905:

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

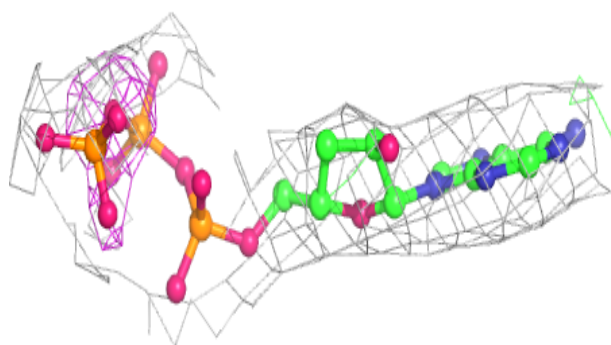
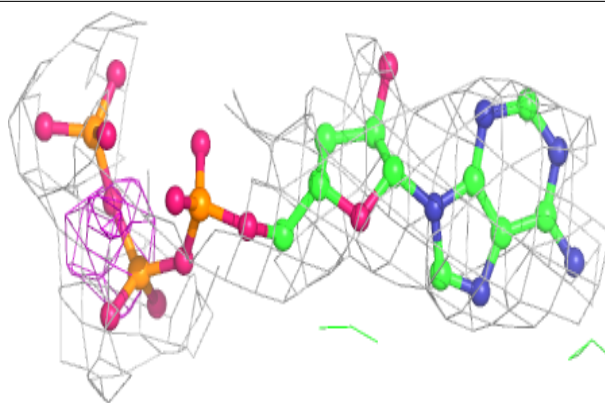
**Electron density around 3AT F 908:**

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

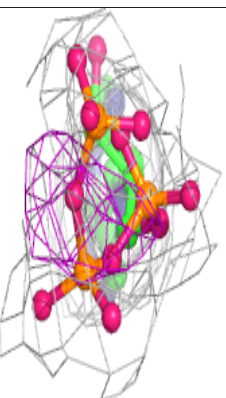
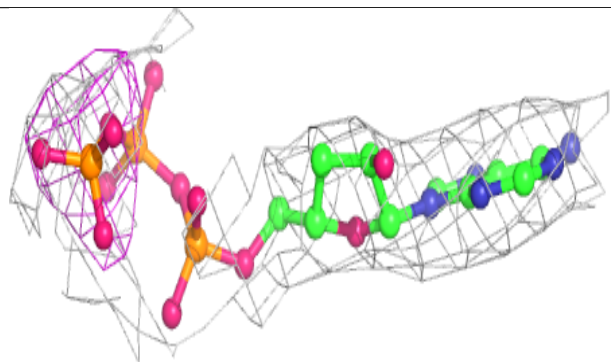
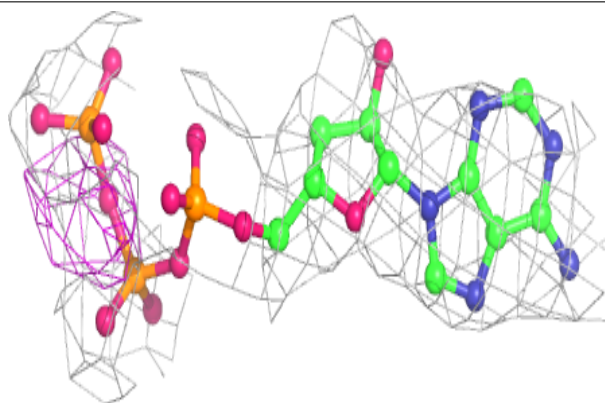


Electron density around 3AT E 907:

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

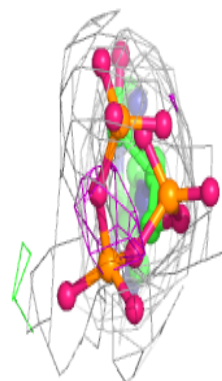
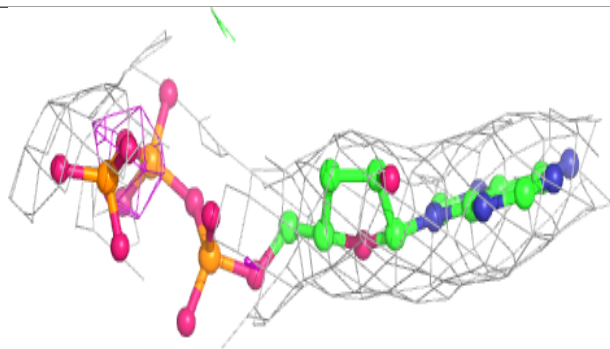
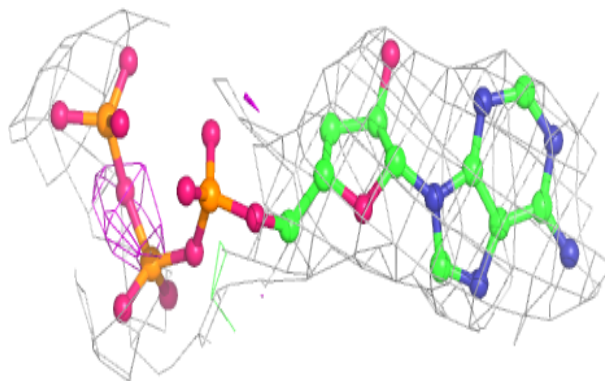
**Electron density around 3AT B 904:**

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



Electron density around 3AT D 906:

$2mF_o-DF_c$ (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.