



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 02:03 AM UTC

PDB ID : 3CF1 / pdb_00003cf1
Title : Structure of P97/vcp in complex with ADP/ADP.alfx
Authors : Davies, J.M.; Delabarre, B.; Brunger, A.T.; Weis, W.I.
Deposited on : 2008-03-01
Resolution : 4.40 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 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)
Xtrriage (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

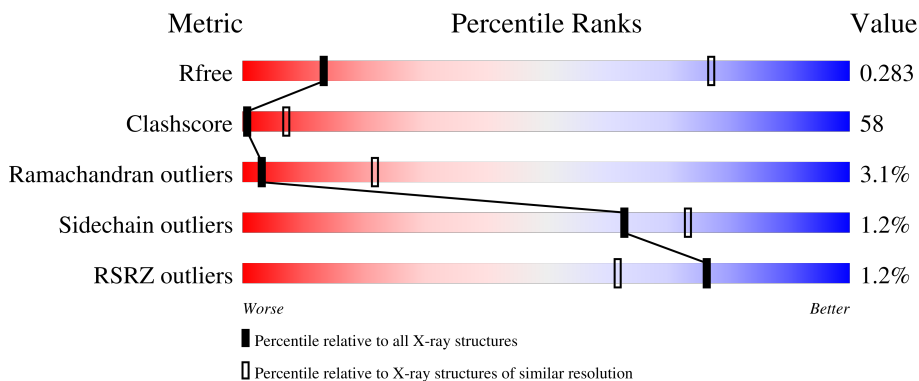
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 4.40 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	1088 (4.90-3.90)
Clashscore	190562	1135 (4.90-3.90)
Ramachandran outliers	187476	1026 (4.90-3.90)
Sidechain outliers	187428	1010 (4.90-3.90)
RSRZ outliers	180081	1084 (4.90-3.90)

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	806	 28% 57% 11%
1	B	806	 29% 55% 10%
1	C	806	 27% 57% 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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	AF3	A	915	-	-	X	-
3	AF3	B	915	-	-	X	-
3	AF3	C	915	-	-	X	-

2 Entry composition [i](#)

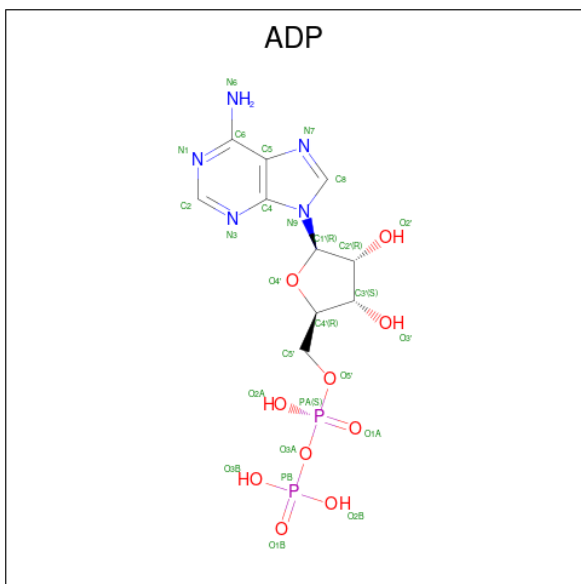
There are 3 unique types of molecules in this entry. The entry contains 17126 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Transitional endoplasmic reticulum ATPase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	719	Total 5634	C 3547	N 990	O 1067	S 30	0	0	0
1	B	723	Total 5659	C 3561	N 996	O 1072	S 30	0	0	0
1	C	723	Total 5659	C 3561	N 996	O 1072	S 30	0	0	0

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



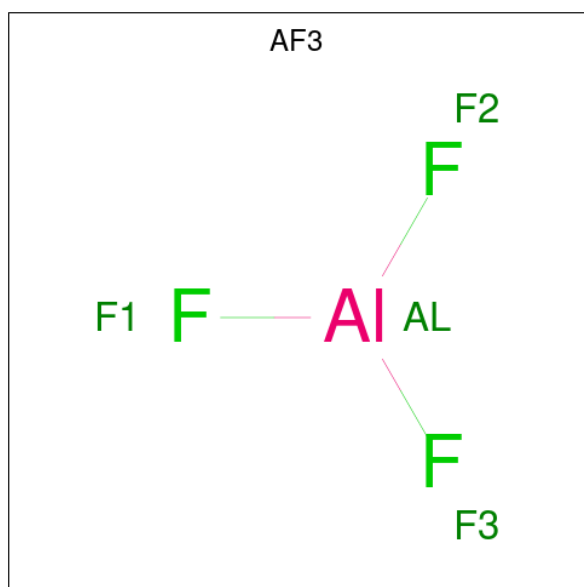
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
2	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
2	B	1	Total 27	C 10	N 5	O 10	P 2	0	0

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

- Molecule 3 is ALUMINUM FLUORIDE (CCD ID: AF3) (formula: AlF_3).

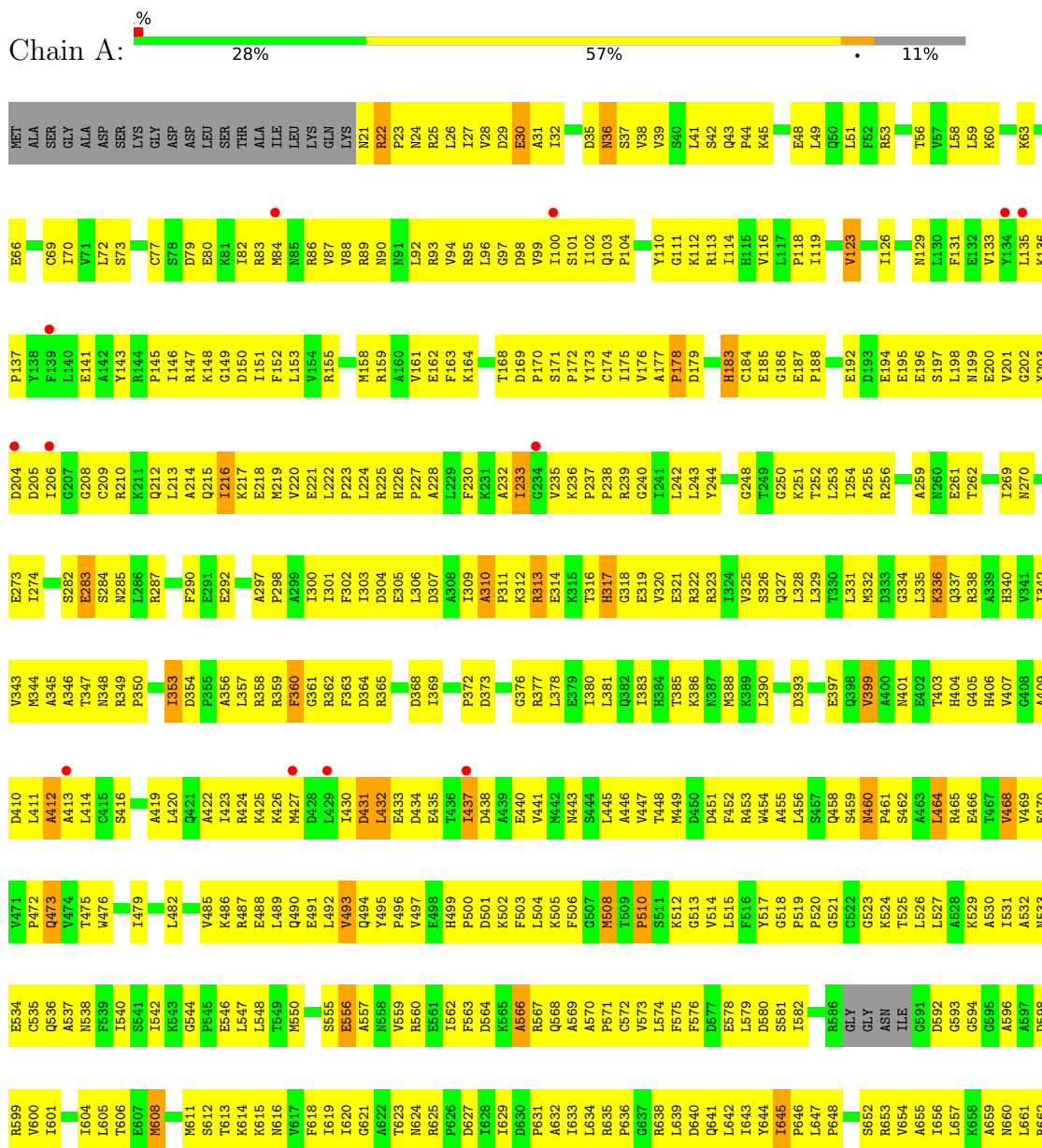


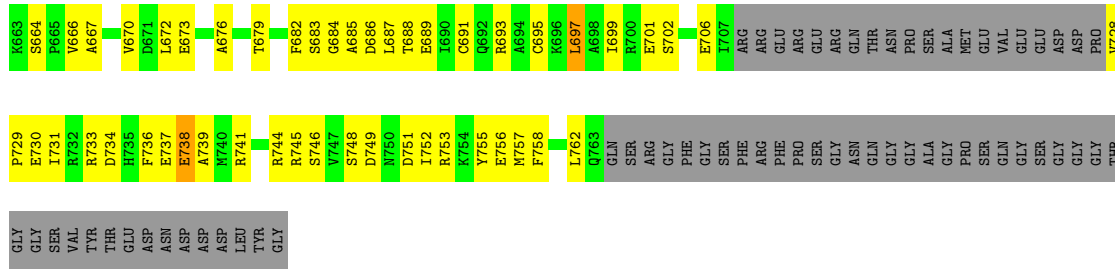
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf	
			Total	F			
3	A	1	Total	Al	F	0	0
			4	1	3		
3	B	1	Total	Al	F	0	0
			4	1	3		
3	C	1	Total	Al	F	0	0
			4	1	3		

3 Residue-property plots

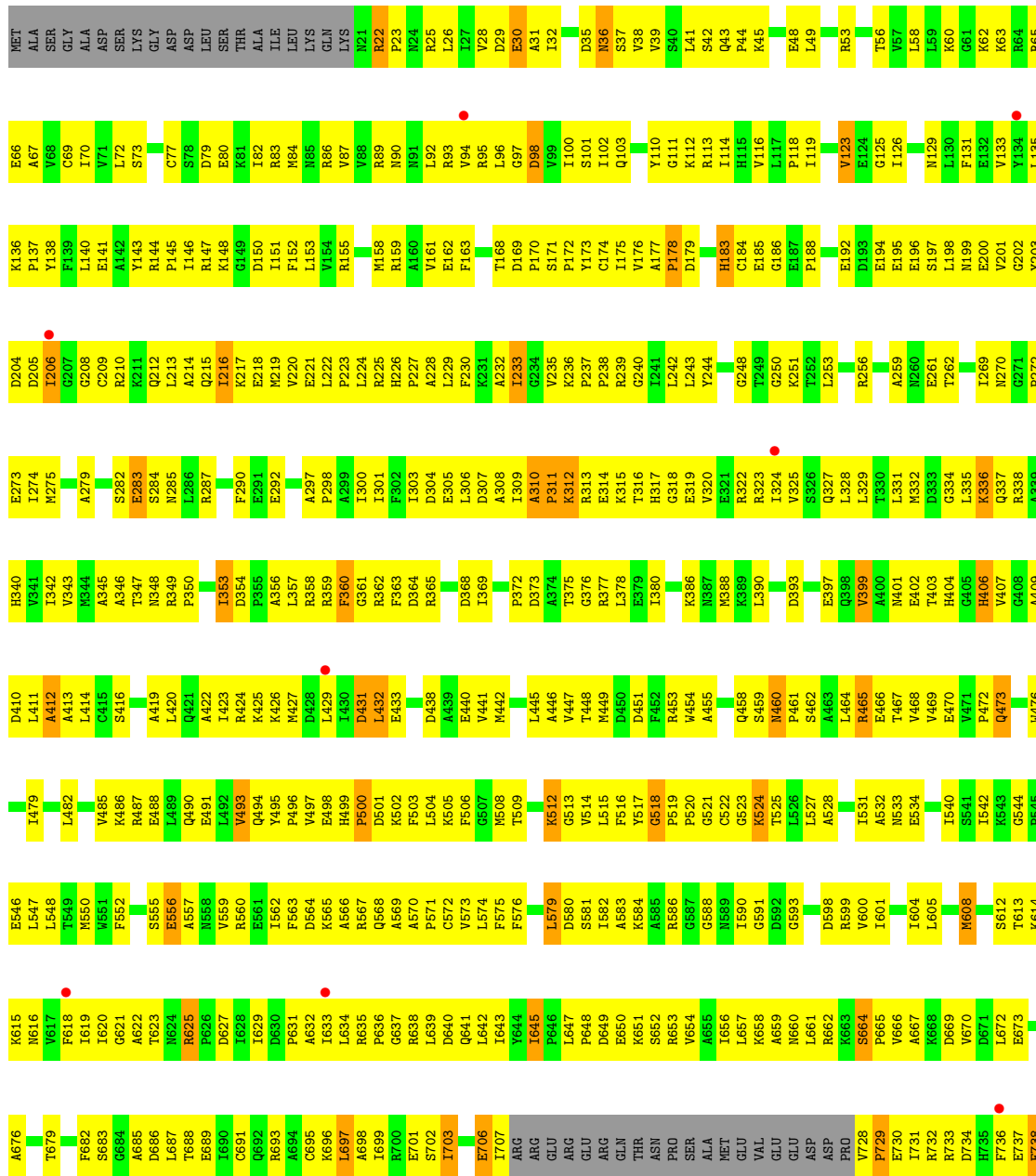
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Transitional endoplasmic reticulum ATPase





• Molecule 1: Transitional endoplasmic reticulum ATPase



A739	ALA
A740	GLY
R741	GLY
R745	ALA
S748	ASP
D749	LYS
N750	ASP
D751	ASP
I752	ASP
R753	LEU
K754	SER
Y755	THR
E756	ALA
M757	ILE
F758	LEU
L762	LYS
Q763	GLN
GLN	SER
SER	ARG
GLY	GLY
PHE	PHE
GLY	GLY
GLY	GLY
ALA	ALA
GLY	GLY
PRO	PRO
SER	SER
GLN	GLN
GLY	GLY
GLY	GLY
ALA	ALA
GLY	GLY
THR	THR
GLY	GLY
SER	SER
VAL	VAL
TYR	TYR
GLU	GLU
ASP	ASP
ASN	ASN
ASP	ASP
ASP	ASP
ASP	ASP

LEU
TYR
GLY

• Molecule 1: Transitional endoplasmic reticulum ATPase



MET	N21	E48	T56
ALA	R22	L41	V57
SER	P23	S42	L58
GLY	N24	Q43	L59
ASP	R25	P44	K60
LYS	L26	K45	G61
LYS	L27	E48	K62
GLN	L28	L49	K63
GLN	L29	L49	K64
SER	L30	L49	R65

E66	M129	E195	K136
C69	L130	E196	
I70	S197	L198	
V71	F131	L198	
L72	F132	N199	
S73	V133	E200	
C77	Y134	V201	
D78	K62	Y203	
S79	K63		
R80	K64		
A81	K65		
I82			
R83			
M84			
N85			
R86			
V87			
V88			
R89			
N90			
P91			
L92			
R93			
V94			
R95			
L96			
D97			
G98			
E99			
V99			
I100			
S101			
I102			
Q103			
Y110			
G111			
K112			
R113			
I114			
H115			
V116			
L117			
P118			
I119			
V123			
G125			
I126			

P137	M158	E192	Y203
Y138	R159	E195	
E141	A160	E196	
A142	V161	S197	
R144	E162	L198	
P145	E163	N199	
L146	K164	E200	
R147	T168	V201	
K148	D169	Y203	
ASP	D170		
LEU	A171		
D150	S171		
D151	P172		
I151	Y173		
F152	I175		
L153	I175		
V154	V176		
R155	A177		
M158	P178		
R159	D179		
A160	H183		
V161	C184		
E162	E185		
F163	E186		
K164	E187		
T168	P188		
D169	I189		
A171	E192		
S171	E194		
P172	E195		
Y173	E196		
I175	L198		
V176	S197		
G240	F131		
A177	N199		
P178	E200		
D179	V201		
H183	Y203		
C184			
E185			
E186			
E187			
P188			
I189			
E192			
E194			
E195			
E196			
L198			
S197			
F131			
N199			
E200			
V201			
Y203			

B204	L229	L254	L269
D205	F230	A255	L268
G207	R231	R256	L268
L206	A232	R256	L268
E207	L233	L243	L268
G208	I233	Y244	L268
C209	G234	G245	L268
R210	V235	P246	L268
R211	V235	G248	L268
Q212	R236	T249	L268
L213	P237	I324	L268
A214	R238	G250	L268
S284	R239	K251	L268
Q215	E314	Q327	L268
N285	K315	L328	L268
L286	G240	L329	L268
K217	L241	L329	L268
E218	L242	T330	L268
M219	L243	A259	L268
L153	L243	R256	L268
V154	Y244	M332	L268
R155	G245	M332	L268
M158	P246	D333	L268
R159	G248	G334	L268
A160	T249	L335	L268
V161	I324	K336	L268
E162	I324	Q337	L268
E163	G318	M401	L268
K164	L317	L402	L268
T168	L317	L402	L268
D169	L317	L402	L268
A171	L317	L402	L268
S171	L317	L402	L268
P172	L317	L402	L268
Y173	L317	L402	L268
I175	L317	L402	L268
V176	L317	L402	L268
A177	L317	L402	L268
P178	L317	L402	L268
D179	L317	L402	L268
H183	L317	L402	L268
C184	L317	L402	L268
E185	L317	L402	L268
E186	L317	L402	L268
E187	L317	L402	L268
P188	L317	L402	L268
I189	L317	L402	L268
E192	L317	L402	L268
E194	L317	L402	L268
E195	L317	L402	L268
E196	L317	L402	L268
L198	L317	L402	L268
S197	L317	L402	L268
F131	L317	L402	L268
N199	L317	L402	L268
E200	L317	L402	L268
V201	L317	L402	L268
Y203	L317	L402	L268

N270	L306	L329	R338
G271	D307	L330	R338
P272	A308	L331	R338
E273	I309	M332	R338
I274	L310	D333	R338
A279	A310	G334	R338
S282	R311	L335	R338
E283	R311	K336	R338
S284	R313	Q337	R338
S284	R313	L328	R338
N285	E314	L329	R338
L286	K315	L329	R338
R287	T316	L329	R338
E291	R317	L329	R338
E292	L317	L329	R338
A297	L317	L329	R338
P298	L317	L329	R338
A299	L317	L329	R338
I300	L317	L329	R338
I301	L317	L329	R338
P227	L317	L329	R338
F163	L317	L329	R338
A228	L317	L329	R338
L229	L317	L329	R338
F230	L317	L329	R338
R231	L317	L329	R338
A232	L317	L329	R338
L233	L317	L329	R338
G234	L317	L329	R338
V235	L317	L329	R338
R236	L317	L329	R338
P237	L317	L329	R338
R238	L317	L329	R338
R239	L317	L329	R338
G240	L317	L329	R338
L241	L317	L329	R338
L242	L317	L329	R338
L243	L317	L329	R338
Y244	L317	L329	R338
G245	L317	L329	R338
P246	L317	L329	R338
G248	L317	L329	R338
T249	L317	L329	R338
I324	L317	L329	R338
G250	L317	L329	R338
K251	L317	L329	R338
T252	L317	L329	R338
L253	L317	L329	R338
L254	L317	L329	R338
A255	L317	L329	R338
R256	L317	L329	R338
M332	L317	L329	R338
D333	L317	L329	R338
G334	L317	L329	R338
L335	L317	L329	R338
K336	L317	L329	R338
Q337	L317	L329	R338
L402	L317	L329	R338
L402	L317	L329	R338
L402	L317	L329	R338
L402	L317	L329	R338

A339	L365	L402	T403
H340	D368	L402	T403
Y341	I369	L402	T403
I342	F360	L402	T403
G343	G361	L402	T403
M344	R362	L402	T403
A345	F363	L402	T403
A346	D364	L402	T403
T347	R365	L402	T403
N348	D368	L402	T403
R349	I369	L402	T403
S284	F360	L402	T403
N285	G361	L402	T403
L286	R362	L402	T403
R287	F363	L402	T403
E291	D364	L402	T403
E292	R365	L402	T403
A297	D368	L402	T403
P298	I369	L402	T403
A299	F360	L402	T403
I300	G361	L402	T403
I301	R362	L402	T403
F302	F363	L402	T403
I303	D364	L402	T403
L306	R365	L402	T403
D307	D368	L402	T403
A308	I369	L402	T403
I309	F360	L402	T403
A310	G361	L402	T403
R311	R362	L402	T403
R313	D373	L402	T403
E314	A374	L402	T403
K315	S375	L402	T403
T316	R377	L402	T403
R317	L378	L402	T403
G318	E379	L402	T403
L329	L380	L402	T403
T330	L381	L402	T403
A259	Q382	L402	T403
R256	L383	L402	T403
M332	L383	L402	T403
D333	K386	L402	T403
G334	N387	L402	T403
L335	M388	L402	T403
K336	K388	L402	T403
Q337	L390	L402	T403
L328	L390	L402	T403
L329	A455	L402	T403
T330	Q458	L402	T403
A259	S459	L402	T403
R256	M460	L402	T403
M332	P461	L402	T403
D333	S462	L402	T403
G334	A463	L402	T403
L335	L464	L402	T403
K336	M401	L402	T403
Q337	E402	L402	T403
L402	L464	L402	T403
L402	R465	L402	T403
L402	E466	L402	T403

H404	L482	L402	E466
G405	E483	L402	E466
H406	M500	L402	E466
V407	D484	L402	E466
G408	M501	L402	E466
A409	K486	L402	E466
D410	R487	L402	E466
L411	E488	L402	E466
A412	E488	L402	E466
A413	E488	L402	E466
L414	E488	L402	E466
C415	E488	L402	E466
S416	E488	L402	E466
A419	E488	L402	E466
L420	E488	L402	E466
D421	E488	L402	E466
L423	E488	L402	E466
R424	E488	L402	E466
K425	E488	L402	E466
K426	E488	L402	E466
M427	E488	L402	E466
L428	E488	L402	E466
L430	E488	L402	E466
D431	E488	L402	E466
L432	E488	L402	E466
E433	E488	L402	E466
E435	E488	L402	E466
T436	E488	L402	E466
D438	E488	L402	E466
A439	E488	L402	E466
E440	E488	L402	E466
V441	E488	L402	E466
M44			

GLY
SER
VAL
TYR
THR
GLU
ASP
ASN
ASP
ASP
ASP
LEU
TYR
GLY

4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	162.66Å 178.02Å 321.14Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.87 – 4.40 29.87 – 4.40	Depositor EDS
% Data completeness (in resolution range)	82.2 (29.87-4.40) 81.9 (29.87-4.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.04 (at 4.45Å)	Xtrriage
Refinement program	CNS	Depositor
R, R_{free}	0.229 , 0.286 0.233 , 0.283	Depositor DCC
R_{free} test set	1874 reflections (6.67%)	wwPDB-VP
Wilson B-factor (Å ²)	176.9	Xtrriage
Anisotropy	0.325	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 286.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	17126	wwPDB-VP
Average B, all atoms (Å ²)	272.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.36% 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: AF3, 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	0.51	0/5724	0.96	23/7727 (0.3%)
1	B	0.53	2/5751 (0.0%)	0.96	26/7767 (0.3%)
1	C	0.52	0/5751	0.94	20/7767 (0.3%)
All	All	0.52	2/17226 (0.0%)	0.95	69/23261 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	308	ALA	CA-CB	-7.62	1.40	1.53
1	B	625	ARG	CD-NE	-7.27	1.36	1.46

The worst 5 of 69 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	431	ASP	N-CA-C	14.77	132.75	109.86
1	B	706	GLU	N-CA-C	12.16	126.92	111.24
1	C	433	GLU	N-CA-C	9.77	125.16	112.26
1	A	430	ILE	N-CA-C	8.86	119.69	111.45
1	A	63	LYS	N-CA-C	-8.71	102.21	112.92

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	5634	0	5705	697	0
1	B	5659	0	5731	696	0
1	C	5659	0	5731	671	0
2	A	54	0	24	8	0
2	B	54	0	24	14	0
2	C	54	0	24	11	0
3	A	4	0	0	2	0
3	B	4	0	0	9	0
3	C	4	0	0	2	0
All	All	17126	0	17239	1999	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 58.

The worst 5 of 1999 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:A:427:MET:HG3	1:A:431:ASP:CB	1.69	1.22
1:A:464:LEU:HD11	1:A:466:GLU:HB2	1.22	1.17
1:A:203:TYR:O	1:A:206:ILE:HG12	1.49	1.13
1:A:427:MET:HG3	1:A:431:ASP:HB2	1.20	1.09
1:A:427:MET:HE3	1:A:441:VAL:HG11	1.33	1.09

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	711/806 (88%)	536 (75%)	155 (22%)	20 (3%)	4	24
1	B	719/806 (89%)	548 (76%)	148 (21%)	23 (3%)	3	21
1	C	719/806 (89%)	533 (74%)	163 (23%)	23 (3%)	3	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
All	All	2149/2418 (89%)	1617 (75%)	466 (22%)	66 (3%)	3	22

5 of 66 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	360	PHE
1	B	360	PHE
1	C	360	PHE
1	A	185	GLU
1	A	353	ILE

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	612/678 (90%)	605 (99%)	7 (1%)	65	74
1	B	615/678 (91%)	607 (99%)	8 (1%)	61	72
1	C	615/678 (91%)	607 (99%)	8 (1%)	61	72
All	All	1842/2034 (91%)	1819 (99%)	23 (1%)	63	73

5 of 23 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	738	GLU
1	C	434	ASP
1	C	283	GLU
1	C	473	GLN
1	A	738	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 45 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	589	ASN
1	C	285	ASN

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Mol	Chain	Res	Type
1	B	641	GLN
1	C	90	ASN
1	C	348	ASN

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](#)

9 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	AF3	A	915	-	0,3,3	-	-	-		
2	ADP	A	807	-	28,29,29	1.78	4 (14%)	43,45,45	1.93	7 (16%)
2	ADP	B	900	-	28,29,29	1.70	5 (17%)	43,45,45	1.98	9 (20%)
3	AF3	B	915	-	0,3,3	-	-	-		
3	AF3	C	915	-	0,3,3	-	-	-		
2	ADP	C	807	-	28,29,29	1.94	5 (17%)	43,45,45	1.87	7 (16%)
2	ADP	C	900	-	28,29,29	1.74	4 (14%)	43,45,45	1.97	7 (16%)
2	ADP	A	900	-	28,29,29	1.87	5 (17%)	43,45,45	1.85	5 (11%)
2	ADP	B	807	-	28,29,29	1.92	6 (21%)	43,45,45	1.93	7 (16%)

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
2	ADP	A	807	-	-	5/16/32/32	0/3/3/3
2	ADP	B	900	-	-	4/16/32/32	0/3/3/3
2	ADP	C	807	-	-	5/16/32/32	0/3/3/3
2	ADP	C	900	-	-	5/16/32/32	0/3/3/3
2	ADP	A	900	-	-	5/16/32/32	0/3/3/3
2	ADP	B	807	-	-	5/16/32/32	0/3/3/3

The worst 5 of 29 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	807	ADP	C5-N7	-5.91	1.28	1.39
2	C	900	ADP	C5-N7	-5.85	1.28	1.39
2	A	900	ADP	C5-N7	-5.72	1.28	1.39
2	B	807	ADP	C5-N7	-5.58	1.28	1.39
2	A	807	ADP	C5-N7	-5.36	1.29	1.39

The worst 5 of 42 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	807	ADP	N3-C2-N1	-7.26	117.58	128.58
2	B	900	ADP	N3-C2-N1	-6.90	118.13	128.58
2	C	900	ADP	N3-C2-N1	-6.82	118.26	128.58
2	A	807	ADP	N3-C2-N1	-6.72	118.41	128.58
2	B	807	ADP	N3-C2-N1	-6.57	118.64	128.58

There are no chirality outliers.

5 of 29 torsion outliers are listed below:

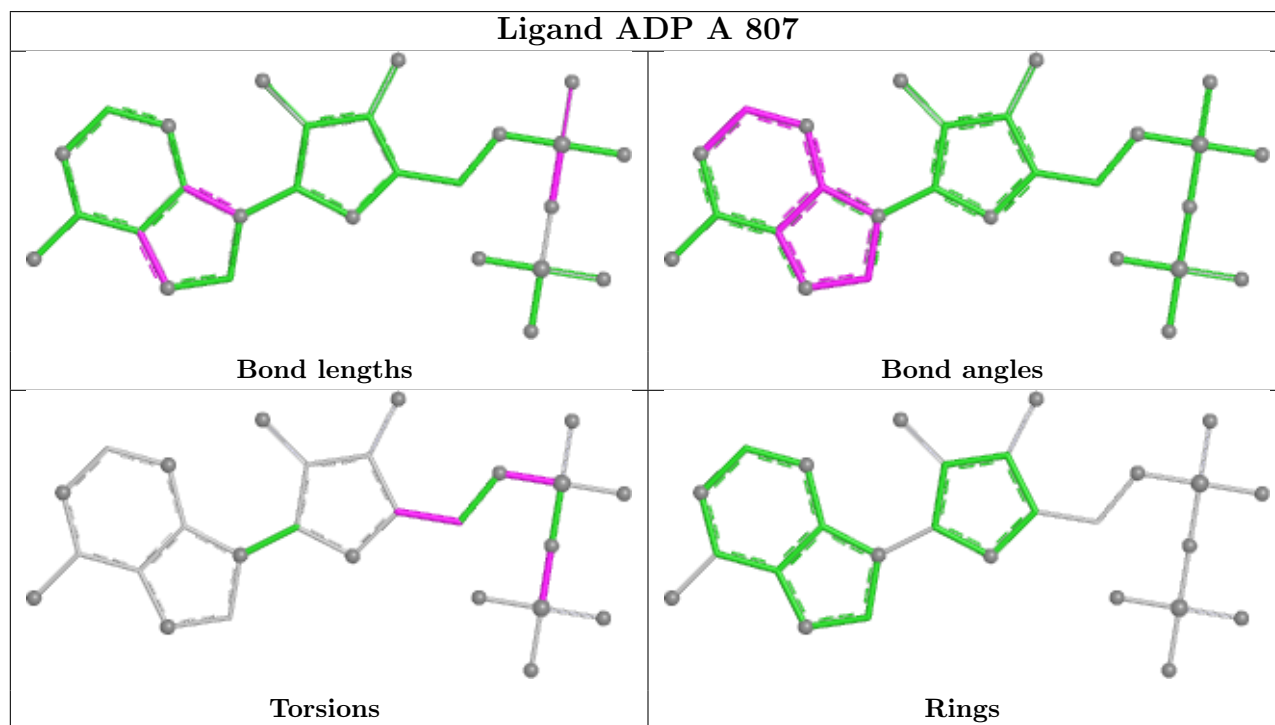
Mol	Chain	Res	Type	Atoms
2	A	807	ADP	C5'-O5'-PA-O1A
2	A	807	ADP	C5'-O5'-PA-O2A
2	A	807	ADP	C5'-O5'-PA-O3A
2	A	900	ADP	C5'-O5'-PA-O1A
2	A	900	ADP	C5'-O5'-PA-O2A

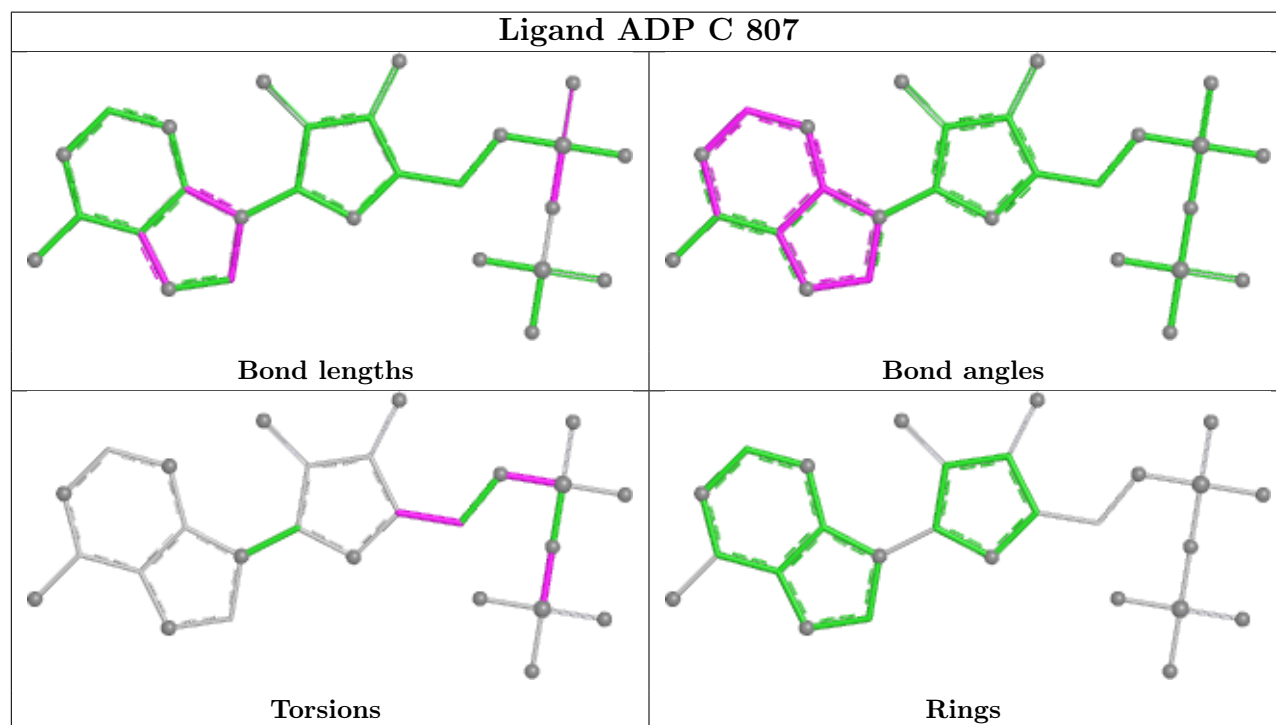
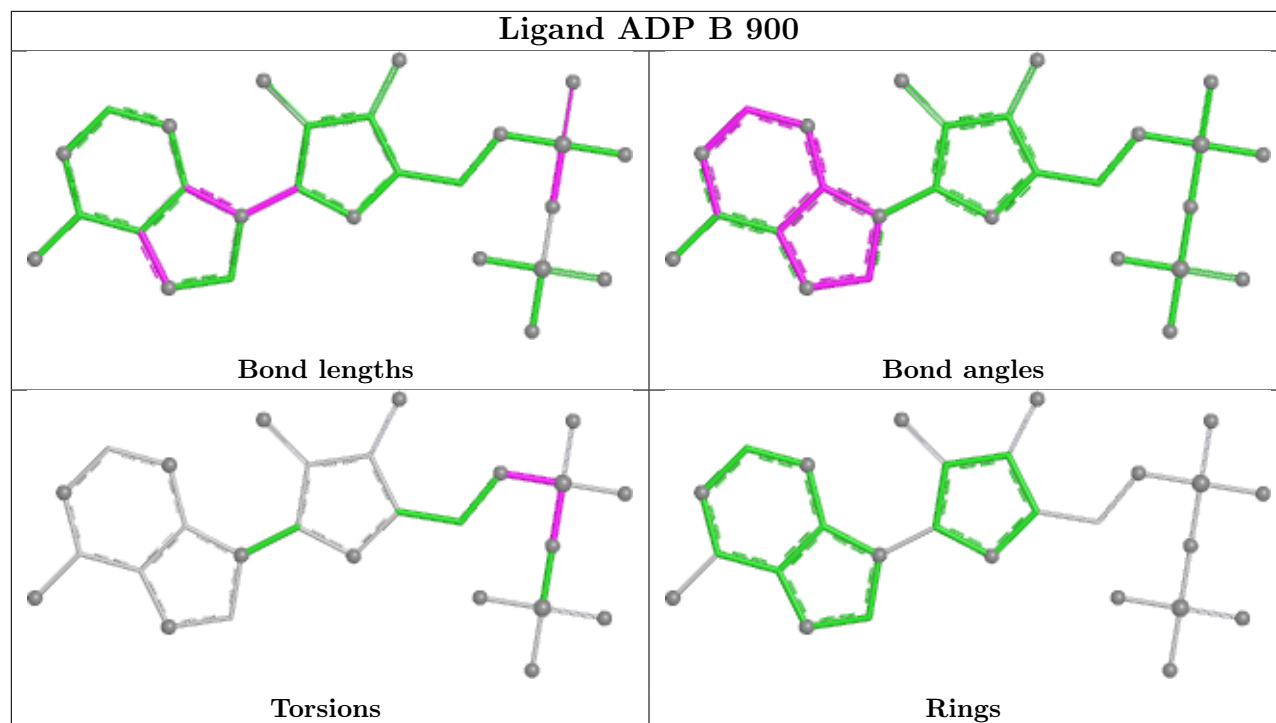
There are no ring outliers.

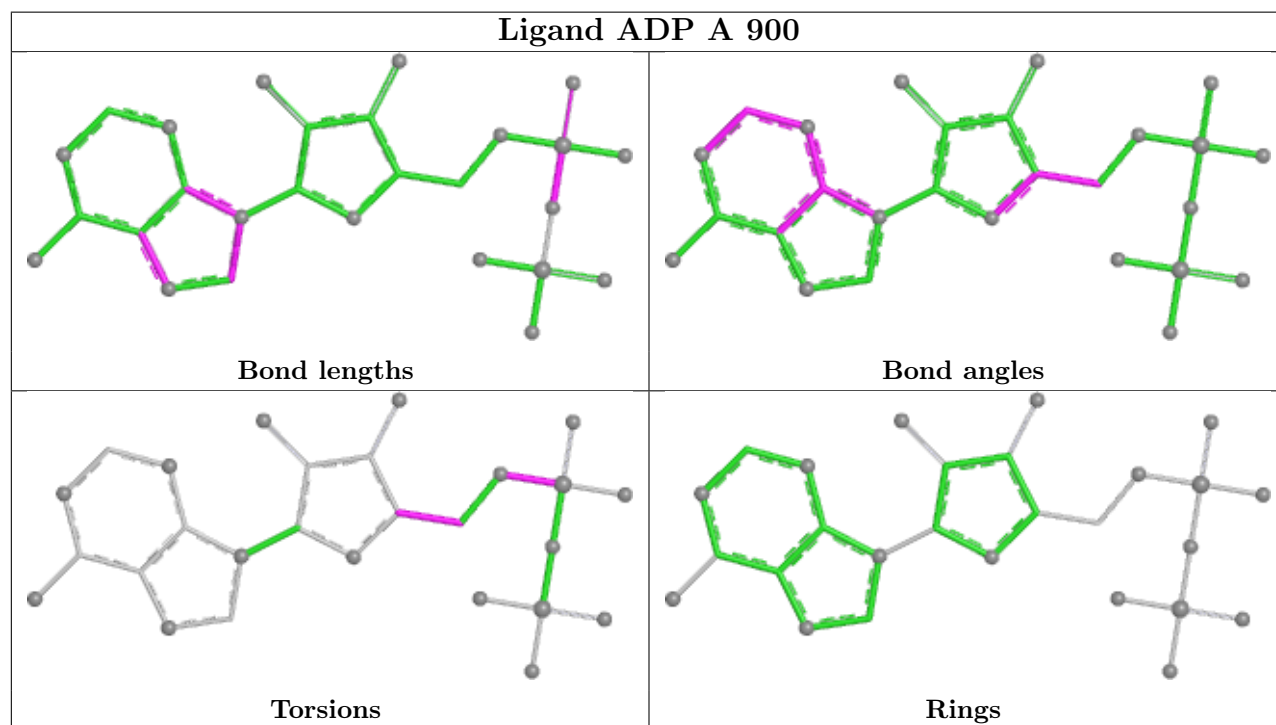
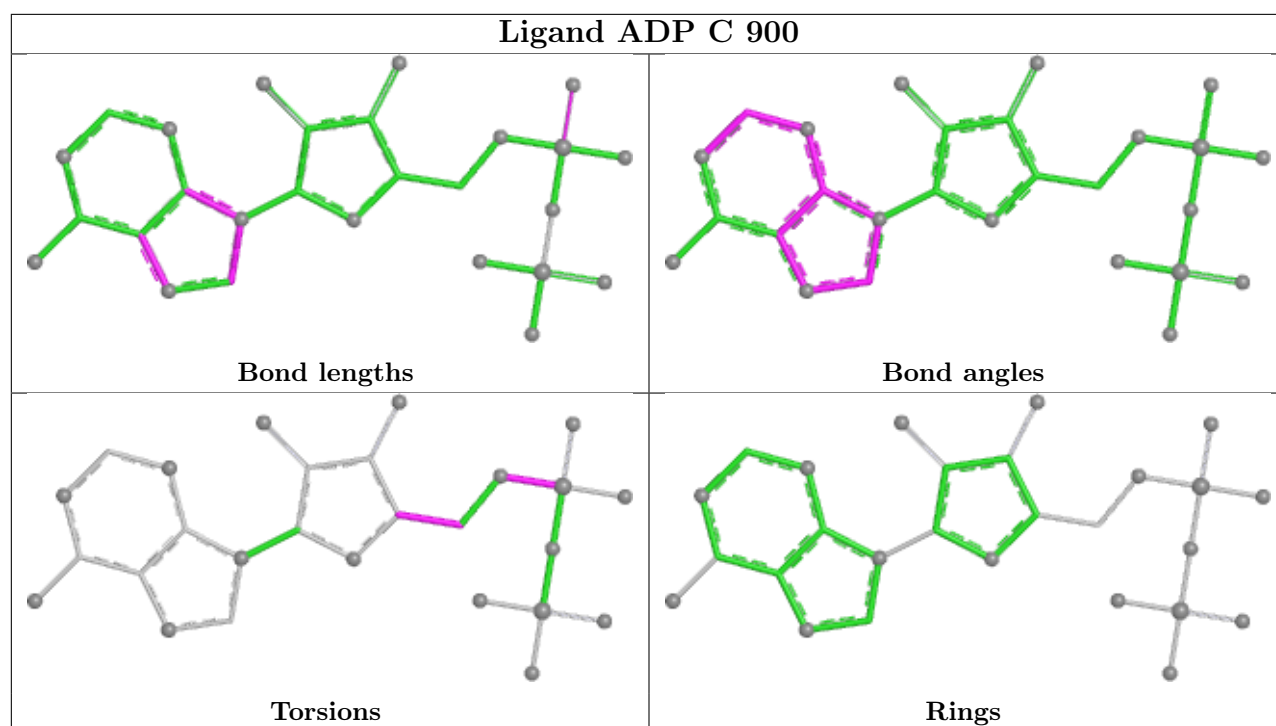
9 monomers are involved in 39 short contacts:

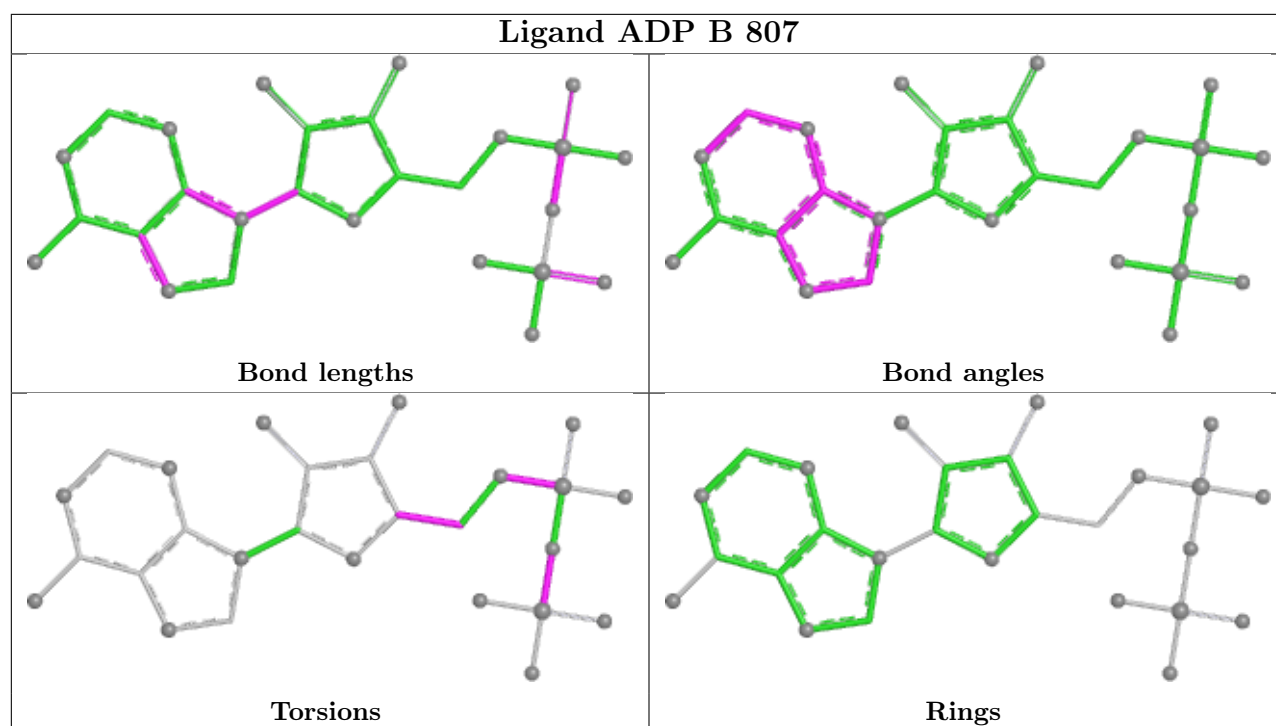
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	915	AF3	2	0
2	A	807	ADP	4	0
2	B	900	ADP	8	0
3	B	915	AF3	9	0
3	C	915	AF3	2	0
2	C	807	ADP	7	0
2	C	900	ADP	4	0
2	A	900	ADP	4	0
2	B	807	ADP	6	0

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	719/806 (89%)	-0.02	12 (1%) 69 55	50, 267, 356, 574	0
1	B	723/806 (89%)	-0.05	8 (1%) 78 63	49, 264, 348, 571	0
1	C	723/806 (89%)	0.01	7 (0%) 79 64	51, 266, 367, 616	0
All	All	2165/2418 (89%)	-0.02	27 (1%) 76 62	49, 266, 360, 616	0

The worst 5 of 27 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	736	PHE	5.2
1	C	206	ILE	3.9
1	B	736	PHE	3.8
1	C	672	LEU	3.4
1	B	206	ILE	3.3

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](#)

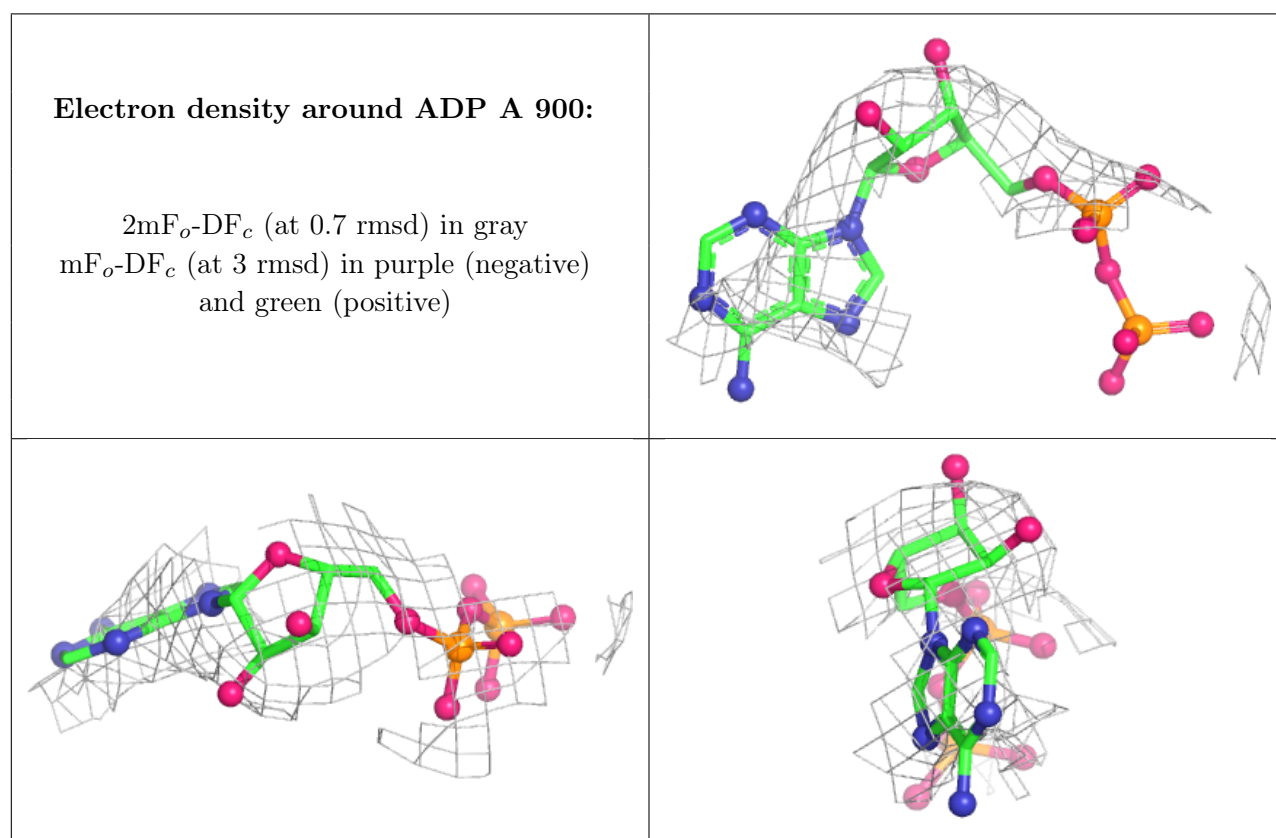
There are no oligosaccharides in this entry.

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.

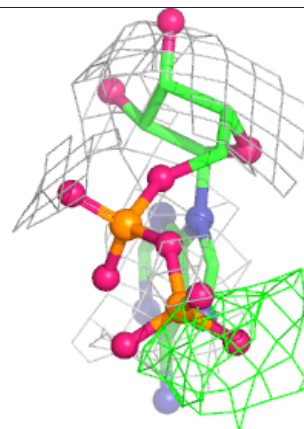
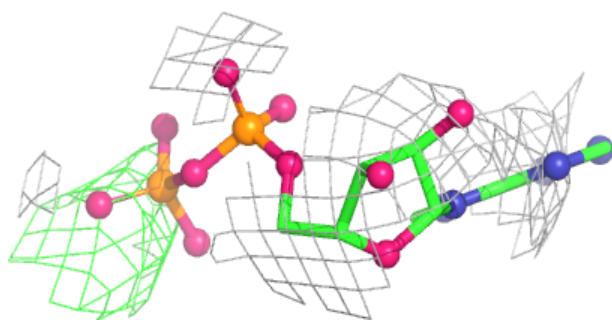
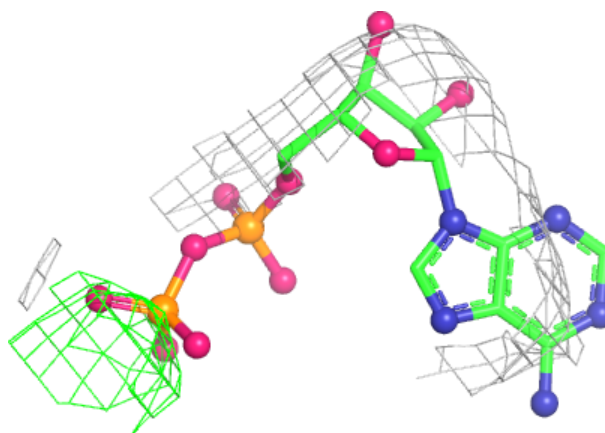
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	AF3	C	915	4/4	0.75	0.23	306,306,306,306	0
3	AF3	A	915	4/4	0.86	0.15	306,306,306,306	0
3	AF3	B	915	4/4	0.90	0.11	306,306,306,306	0
2	ADP	A	900	27/27	0.90	0.09	306,306,306,306	0
2	ADP	C	900	27/27	0.93	0.12	306,306,306,306	0
2	ADP	B	900	27/27	0.94	0.09	306,306,306,306	0
2	ADP	B	807	27/27	0.95	0.13	306,306,306,306	0
2	ADP	A	807	27/27	0.95	0.13	306,306,306,306	0
2	ADP	C	807	27/27	0.96	0.11	306,306,306,306	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.

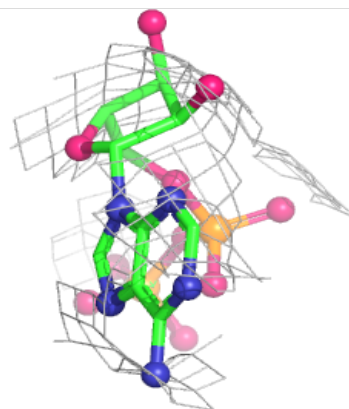
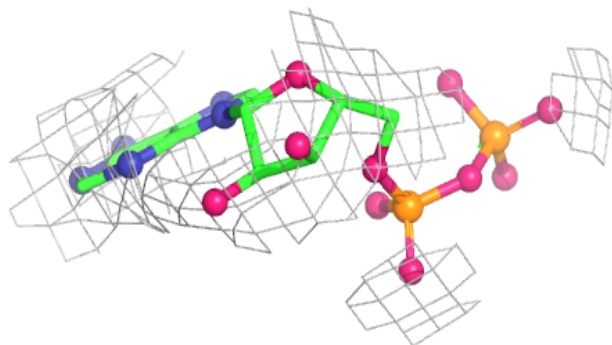
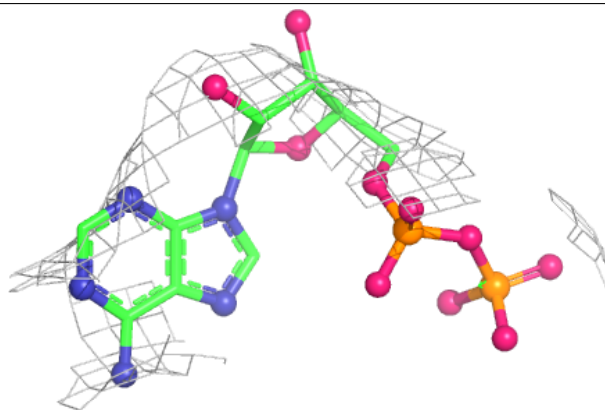


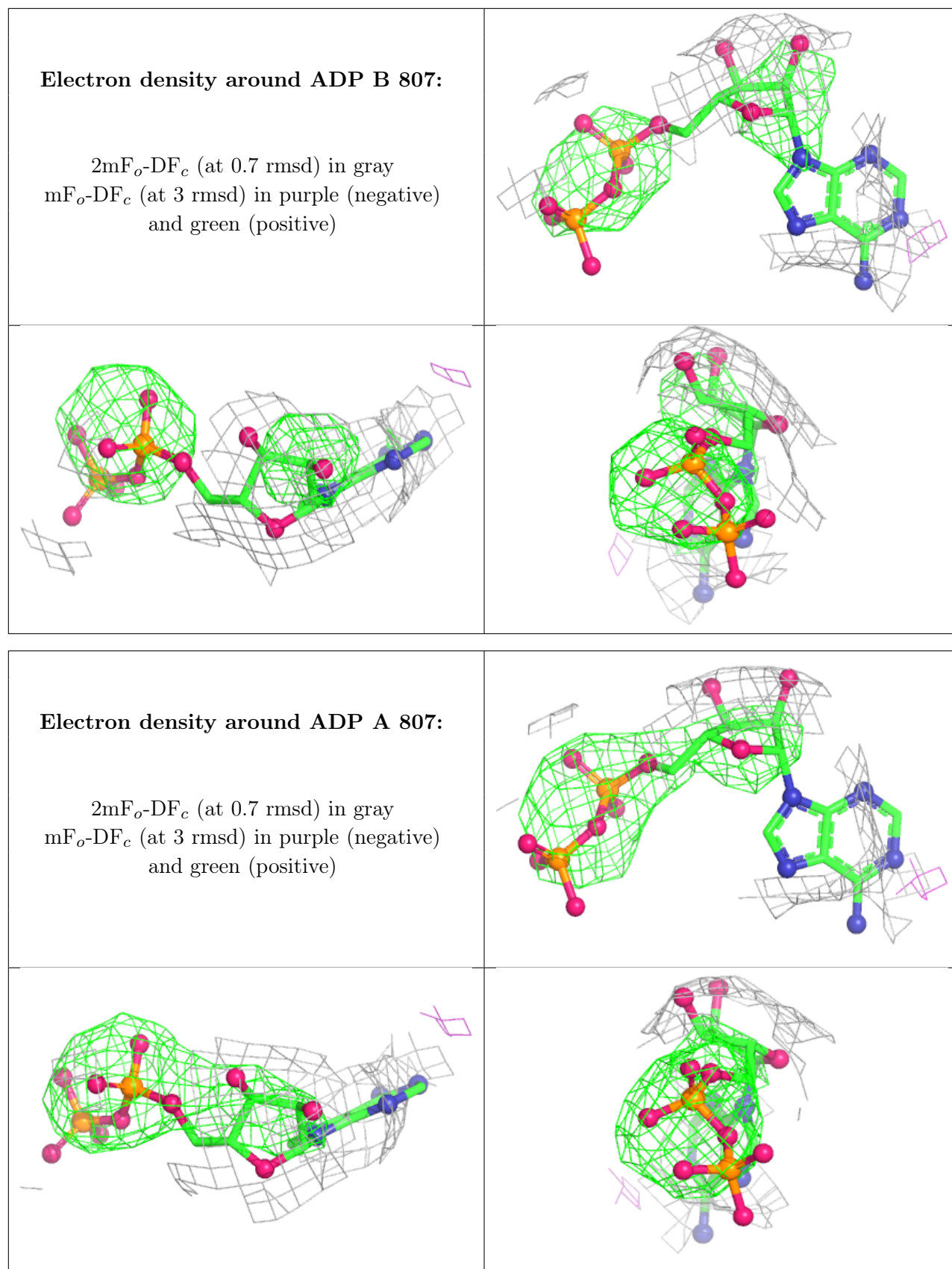
Electron density around ADP C 900:

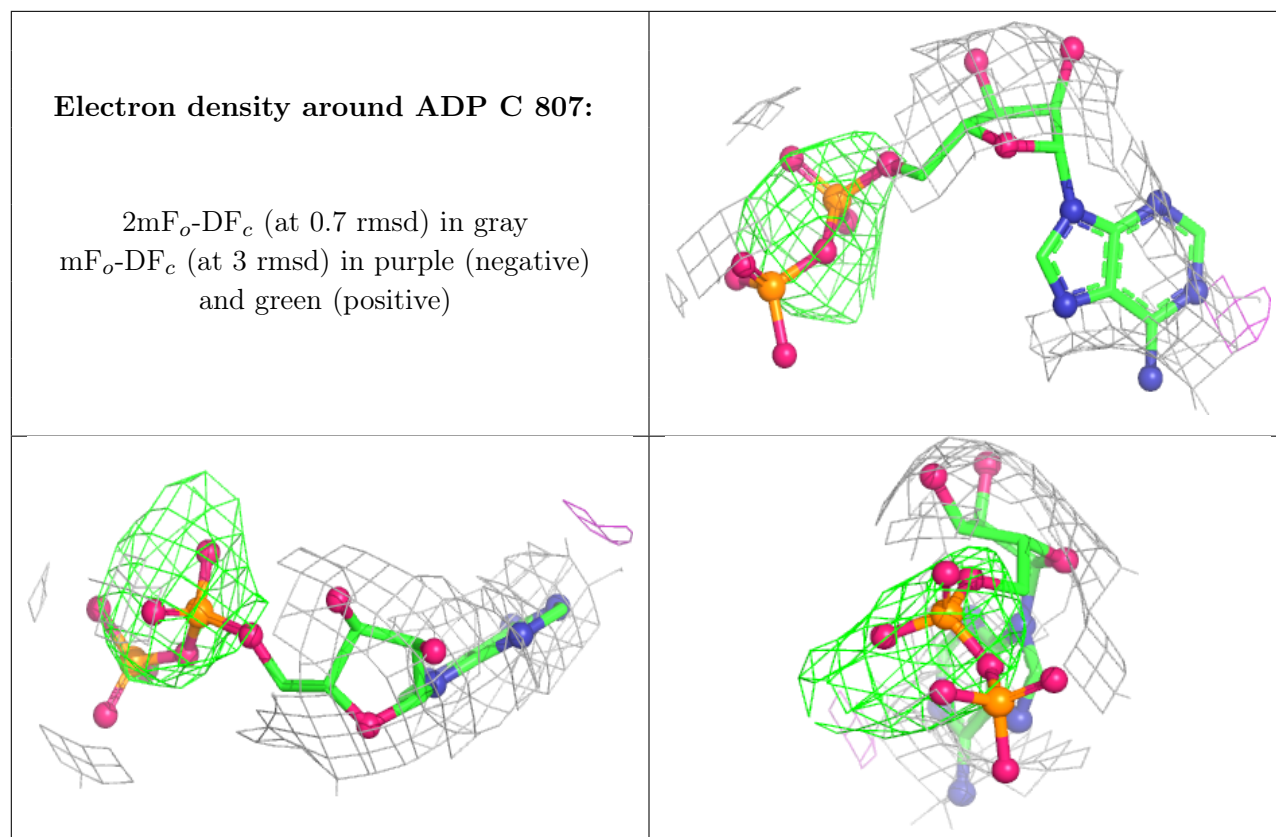
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around ADP B 900:**

$2mF_o-DF_c$ (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.