



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 01:58 PM UTC

PDB ID : 3KFE / pdb_00003kfe
Title : Crystal structures of a group II chaperonin from *Methanococcus maripaludis*
Authors : Pereira, J.H.; Ralston, C.Y.; Douglas, N.; Meyer, D.; Knee, K.M.; Goulet, D.R.; King, J.A.; Frydman, J.; Adams, P.D.
Deposited on : 2009-10-27
Resolution : 3.50 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)
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

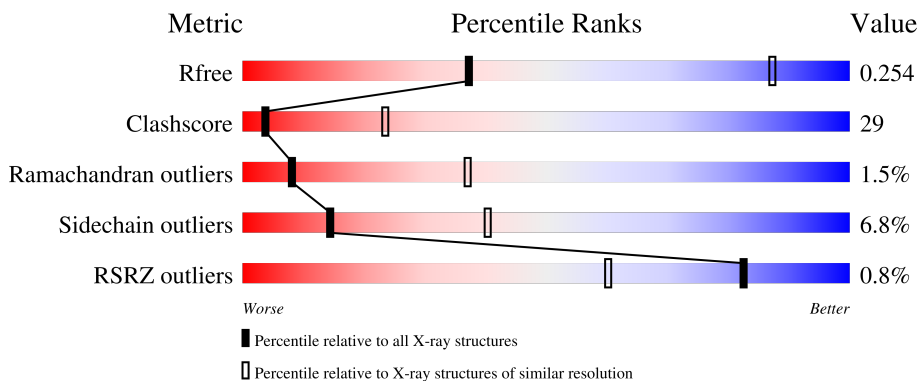
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	1085 (3.54-3.46)
Clashscore	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)
RSRZ outliers	180081	1084 (3.54-3.46)

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	521	49% 39% 7%
1	B	521	50% 39% 7%
1	C	521	49% 40% 5% 7%
1	D	521	49% 38% 6% 7%
1	E	521	48% 40% 5% 7%

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Mol	Chain	Length	Quality of chain
1	F	521	<p>% 49% 39% 5% 7%</p>
1	G	521	<p>% 50% 39% 7%</p>
1	H	521	<p>% 50% 39% 7%</p>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	SO4	A	546	-	-	X	-
4	SO4	B	546	-	-	X	-
4	SO4	C	546	-	-	X	-
4	SO4	D	546	-	-	X	-
4	SO4	E	546	-	-	X	-
4	SO4	F	546	-	-	X	-
4	SO4	G	546	-	-	X	-
4	SO4	H	546	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 29296 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 Chaperonin.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	487	3629	2249	631	725	24	0	0	0
1	B	487	3629	2249	631	725	24	0	0	0
1	C	487	3629	2249	631	725	24	0	0	0
1	D	487	3629	2249	631	725	24	0	0	0
1	E	487	3629	2249	631	725	24	0	0	0
1	F	487	3629	2249	631	725	24	0	0	0
1	G	487	3629	2249	631	725	24	0	0	0
1	H	487	3629	2249	631	725	24	0	0	0

There are 184 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ILE	deletion	UNP Q877G8
A	?	-	LYS	deletion	UNP Q877G8
A	?	-	GLU	deletion	UNP Q877G8
A	?	-	THR	deletion	UNP Q877G8
A	?	-	ASP	deletion	UNP Q877G8
A	?	-	ALA	deletion	UNP Q877G8
A	?	-	GLU	deletion	UNP Q877G8
A	?	-	ILE	deletion	UNP Q877G8
A	?	-	ARG	deletion	UNP Q877G8
A	?	-	ILE	deletion	UNP Q877G8
A	?	-	THR	deletion	UNP Q877G8
A	?	-	ASP	deletion	UNP Q877G8
A	?	-	PRO	deletion	UNP Q877G8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	LYS	deletion	UNP Q877G8
A	?	-	LEU	deletion	UNP Q877G8
A	?	-	MET	deletion	UNP Q877G8
A	?	-	GLU	deletion	UNP Q877G8
A	?	-	PHE	deletion	UNP Q877G8
A	?	-	ILE	deletion	UNP Q877G8
A	264	THR	GLN	engineered mutation	UNP Q877G8
A	265	ALA	GLU	engineered mutation	UNP Q877G8
A	266	SER	GLU	engineered mutation	UNP Q877G8
A	267	GLU	LYS	engineered mutation	UNP Q877G8
B	?	-	ILE	deletion	UNP Q877G8
B	?	-	LYS	deletion	UNP Q877G8
B	?	-	GLU	deletion	UNP Q877G8
B	?	-	THR	deletion	UNP Q877G8
B	?	-	ASP	deletion	UNP Q877G8
B	?	-	ALA	deletion	UNP Q877G8
B	?	-	GLU	deletion	UNP Q877G8
B	?	-	ILE	deletion	UNP Q877G8
B	?	-	ARG	deletion	UNP Q877G8
B	?	-	ILE	deletion	UNP Q877G8
B	?	-	THR	deletion	UNP Q877G8
B	?	-	ASP	deletion	UNP Q877G8
B	?	-	PRO	deletion	UNP Q877G8
B	?	-	LYS	deletion	UNP Q877G8
B	?	-	LEU	deletion	UNP Q877G8
B	?	-	MET	deletion	UNP Q877G8
B	?	-	GLU	deletion	UNP Q877G8
B	?	-	PHE	deletion	UNP Q877G8
B	?	-	ILE	deletion	UNP Q877G8
B	264	THR	GLN	engineered mutation	UNP Q877G8
B	265	ALA	GLU	engineered mutation	UNP Q877G8
B	266	SER	GLU	engineered mutation	UNP Q877G8
B	267	GLU	LYS	engineered mutation	UNP Q877G8
C	?	-	ILE	deletion	UNP Q877G8
C	?	-	LYS	deletion	UNP Q877G8
C	?	-	GLU	deletion	UNP Q877G8
C	?	-	THR	deletion	UNP Q877G8
C	?	-	ASP	deletion	UNP Q877G8
C	?	-	ALA	deletion	UNP Q877G8
C	?	-	GLU	deletion	UNP Q877G8
C	?	-	ILE	deletion	UNP Q877G8
C	?	-	ARG	deletion	UNP Q877G8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	ILE	deletion	UNP Q877G8
C	?	-	THR	deletion	UNP Q877G8
C	?	-	ASP	deletion	UNP Q877G8
C	?	-	PRO	deletion	UNP Q877G8
C	?	-	LYS	deletion	UNP Q877G8
C	?	-	LEU	deletion	UNP Q877G8
C	?	-	MET	deletion	UNP Q877G8
C	?	-	GLU	deletion	UNP Q877G8
C	?	-	PHE	deletion	UNP Q877G8
C	?	-	ILE	deletion	UNP Q877G8
C	264	THR	GLN	engineered mutation	UNP Q877G8
C	265	ALA	GLU	engineered mutation	UNP Q877G8
C	266	SER	GLU	engineered mutation	UNP Q877G8
C	267	GLU	LYS	engineered mutation	UNP Q877G8
D	?	-	ILE	deletion	UNP Q877G8
D	?	-	LYS	deletion	UNP Q877G8
D	?	-	GLU	deletion	UNP Q877G8
D	?	-	THR	deletion	UNP Q877G8
D	?	-	ASP	deletion	UNP Q877G8
D	?	-	ALA	deletion	UNP Q877G8
D	?	-	GLU	deletion	UNP Q877G8
D	?	-	ILE	deletion	UNP Q877G8
D	?	-	ARG	deletion	UNP Q877G8
D	?	-	ILE	deletion	UNP Q877G8
D	?	-	THR	deletion	UNP Q877G8
D	?	-	ASP	deletion	UNP Q877G8
D	?	-	PRO	deletion	UNP Q877G8
D	?	-	LYS	deletion	UNP Q877G8
D	?	-	LEU	deletion	UNP Q877G8
D	?	-	MET	deletion	UNP Q877G8
D	?	-	GLU	deletion	UNP Q877G8
D	?	-	PHE	deletion	UNP Q877G8
D	?	-	ILE	deletion	UNP Q877G8
D	264	THR	GLN	engineered mutation	UNP Q877G8
D	265	ALA	GLU	engineered mutation	UNP Q877G8
D	266	SER	GLU	engineered mutation	UNP Q877G8
D	267	GLU	LYS	engineered mutation	UNP Q877G8
E	?	-	ILE	deletion	UNP Q877G8
E	?	-	LYS	deletion	UNP Q877G8
E	?	-	GLU	deletion	UNP Q877G8
E	?	-	THR	deletion	UNP Q877G8
E	?	-	ASP	deletion	UNP Q877G8

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Chain	Residue	Modelled	Actual	Comment	Reference
E	?	-	ALA	deletion	UNP Q877G8
E	?	-	GLU	deletion	UNP Q877G8
E	?	-	ILE	deletion	UNP Q877G8
E	?	-	ARG	deletion	UNP Q877G8
E	?	-	ILE	deletion	UNP Q877G8
E	?	-	THR	deletion	UNP Q877G8
E	?	-	ASP	deletion	UNP Q877G8
E	?	-	PRO	deletion	UNP Q877G8
E	?	-	LYS	deletion	UNP Q877G8
E	?	-	LEU	deletion	UNP Q877G8
E	?	-	MET	deletion	UNP Q877G8
E	?	-	GLU	deletion	UNP Q877G8
E	?	-	PHE	deletion	UNP Q877G8
E	?	-	ILE	deletion	UNP Q877G8
E	264	THR	GLN	engineered mutation	UNP Q877G8
E	265	ALA	GLU	engineered mutation	UNP Q877G8
E	266	SER	GLU	engineered mutation	UNP Q877G8
E	267	GLU	LYS	engineered mutation	UNP Q877G8
F	?	-	ILE	deletion	UNP Q877G8
F	?	-	LYS	deletion	UNP Q877G8
F	?	-	GLU	deletion	UNP Q877G8
F	?	-	THR	deletion	UNP Q877G8
F	?	-	ASP	deletion	UNP Q877G8
F	?	-	ALA	deletion	UNP Q877G8
F	?	-	GLU	deletion	UNP Q877G8
F	?	-	ILE	deletion	UNP Q877G8
F	?	-	ARG	deletion	UNP Q877G8
F	?	-	ILE	deletion	UNP Q877G8
F	?	-	THR	deletion	UNP Q877G8
F	?	-	ASP	deletion	UNP Q877G8
F	?	-	PRO	deletion	UNP Q877G8
F	?	-	LYS	deletion	UNP Q877G8
F	?	-	LEU	deletion	UNP Q877G8
F	?	-	MET	deletion	UNP Q877G8
F	?	-	GLU	deletion	UNP Q877G8
F	?	-	PHE	deletion	UNP Q877G8
F	?	-	ILE	deletion	UNP Q877G8
F	264	THR	GLN	engineered mutation	UNP Q877G8
F	265	ALA	GLU	engineered mutation	UNP Q877G8
F	266	SER	GLU	engineered mutation	UNP Q877G8
F	267	GLU	LYS	engineered mutation	UNP Q877G8
G	?	-	ILE	deletion	UNP Q877G8

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Chain	Residue	Modelled	Actual	Comment	Reference
G	?	-	LYS	deletion	UNP Q877G8
G	?	-	GLU	deletion	UNP Q877G8
G	?	-	THR	deletion	UNP Q877G8
G	?	-	ASP	deletion	UNP Q877G8
G	?	-	ALA	deletion	UNP Q877G8
G	?	-	GLU	deletion	UNP Q877G8
G	?	-	ILE	deletion	UNP Q877G8
G	?	-	ARG	deletion	UNP Q877G8
G	?	-	ILE	deletion	UNP Q877G8
G	?	-	THR	deletion	UNP Q877G8
G	?	-	ASP	deletion	UNP Q877G8
G	?	-	PRO	deletion	UNP Q877G8
G	?	-	LYS	deletion	UNP Q877G8
G	?	-	LEU	deletion	UNP Q877G8
G	?	-	MET	deletion	UNP Q877G8
G	?	-	GLU	deletion	UNP Q877G8
G	?	-	PHE	deletion	UNP Q877G8
G	?	-	ILE	deletion	UNP Q877G8
G	264	THR	GLN	engineered mutation	UNP Q877G8
G	265	ALA	GLU	engineered mutation	UNP Q877G8
G	266	SER	GLU	engineered mutation	UNP Q877G8
G	267	GLU	LYS	engineered mutation	UNP Q877G8
H	?	-	ILE	deletion	UNP Q877G8
H	?	-	LYS	deletion	UNP Q877G8
H	?	-	GLU	deletion	UNP Q877G8
H	?	-	THR	deletion	UNP Q877G8
H	?	-	ASP	deletion	UNP Q877G8
H	?	-	ALA	deletion	UNP Q877G8
H	?	-	GLU	deletion	UNP Q877G8
H	?	-	ILE	deletion	UNP Q877G8
H	?	-	ARG	deletion	UNP Q877G8
H	?	-	ILE	deletion	UNP Q877G8
H	?	-	THR	deletion	UNP Q877G8
H	?	-	ASP	deletion	UNP Q877G8
H	?	-	PRO	deletion	UNP Q877G8
H	?	-	LYS	deletion	UNP Q877G8
H	?	-	LEU	deletion	UNP Q877G8
H	?	-	MET	deletion	UNP Q877G8
H	?	-	GLU	deletion	UNP Q877G8
H	?	-	PHE	deletion	UNP Q877G8
H	?	-	ILE	deletion	UNP Q877G8
H	264	THR	GLN	engineered mutation	UNP Q877G8

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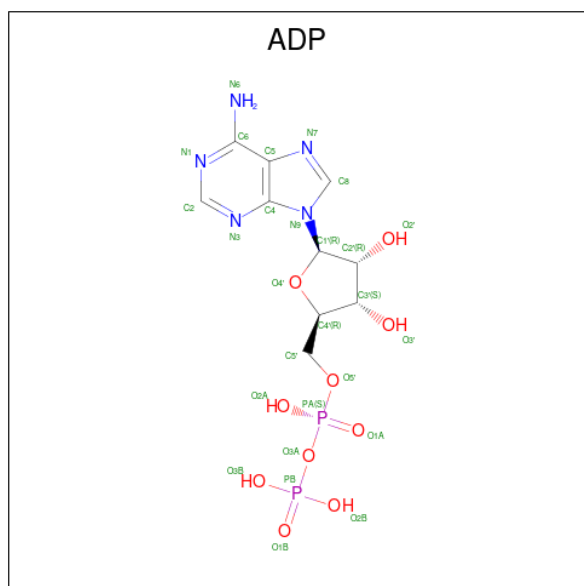
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Chain	Residue	Modelled	Actual	Comment	Reference
H	265	ALA	GLU	engineered mutation	UNP Q877G8
H	266	SER	GLU	engineered mutation	UNP Q877G8
H	267	GLU	LYS	engineered mutation	UNP Q877G8

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

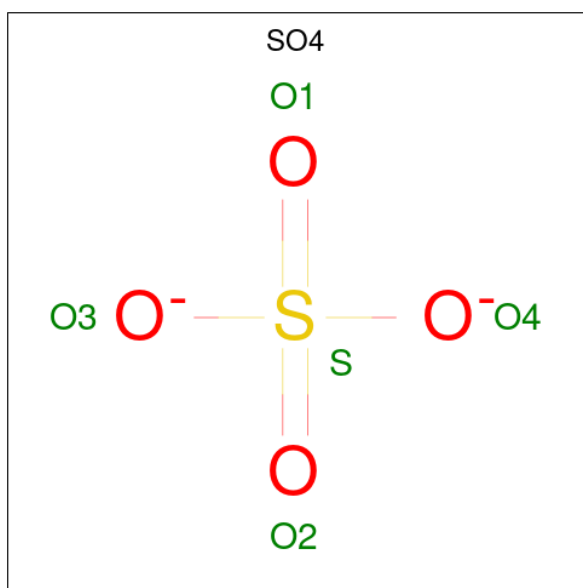
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Mg 1 1	0	0
2	B	1	Total Mg 1 1	0	0
2	C	1	Total Mg 1 1	0	0
2	D	1	Total Mg 1 1	0	0
2	E	1	Total Mg 1 1	0	0
2	F	1	Total Mg 1 1	0	0
2	G	1	Total Mg 1 1	0	0
2	H	1	Total Mg 1 1	0	0

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	P		
3	A	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	B	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	C	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	D	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	E	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	F	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	G	1	Total 27	C 10	N 5	O 10	P 2	0	0
3	H	1	Total 27	C 10	N 5	O 10	P 2	0	0

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O S		
4	A	1	Total 5	O S 4 1	0	0
4	B	1	Total 5	O S 4 1	0	0
4	C	1	Total 5	O S 4 1	0	0
4	D	1	Total 5	O S 4 1	0	0

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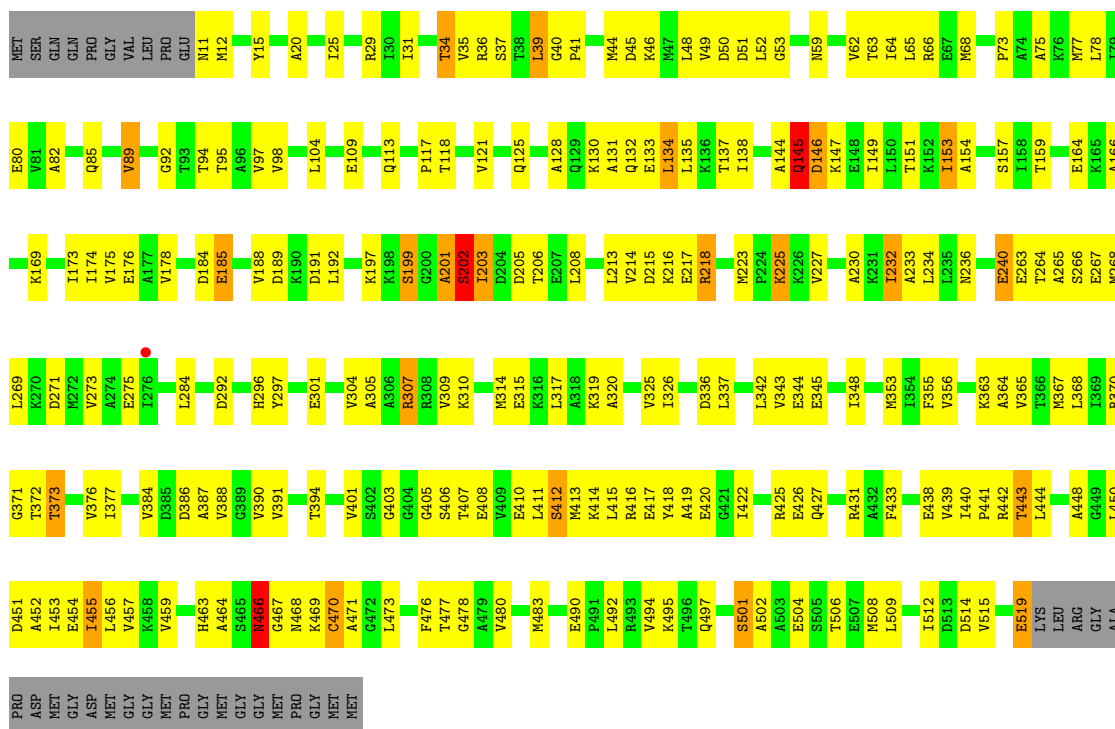
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	E	1	Total 5	O 4	S 1	0	0
4	F	1	Total 5	O 4	S 1	0	0
4	G	1	Total 5	O 4	S 1	0	0
4	H	1	Total 5	O 4	S 1	0	0

3 Residue-property plots [i](#)

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: Chaperonin

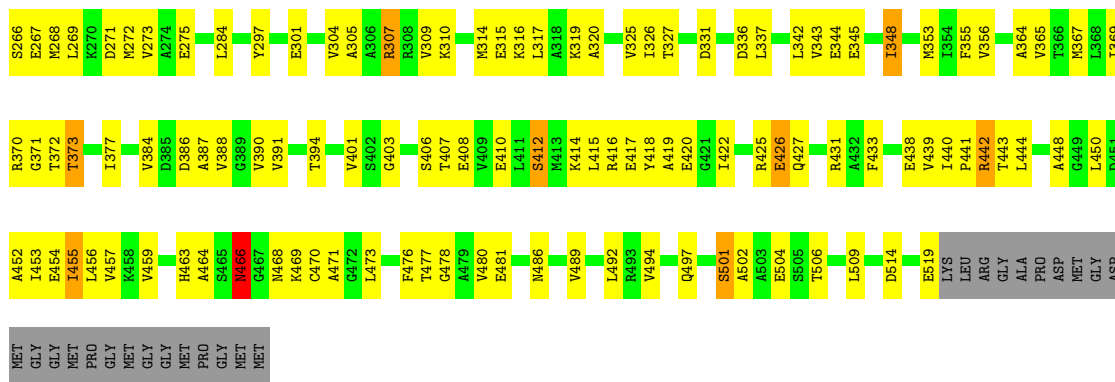
Chain A: 



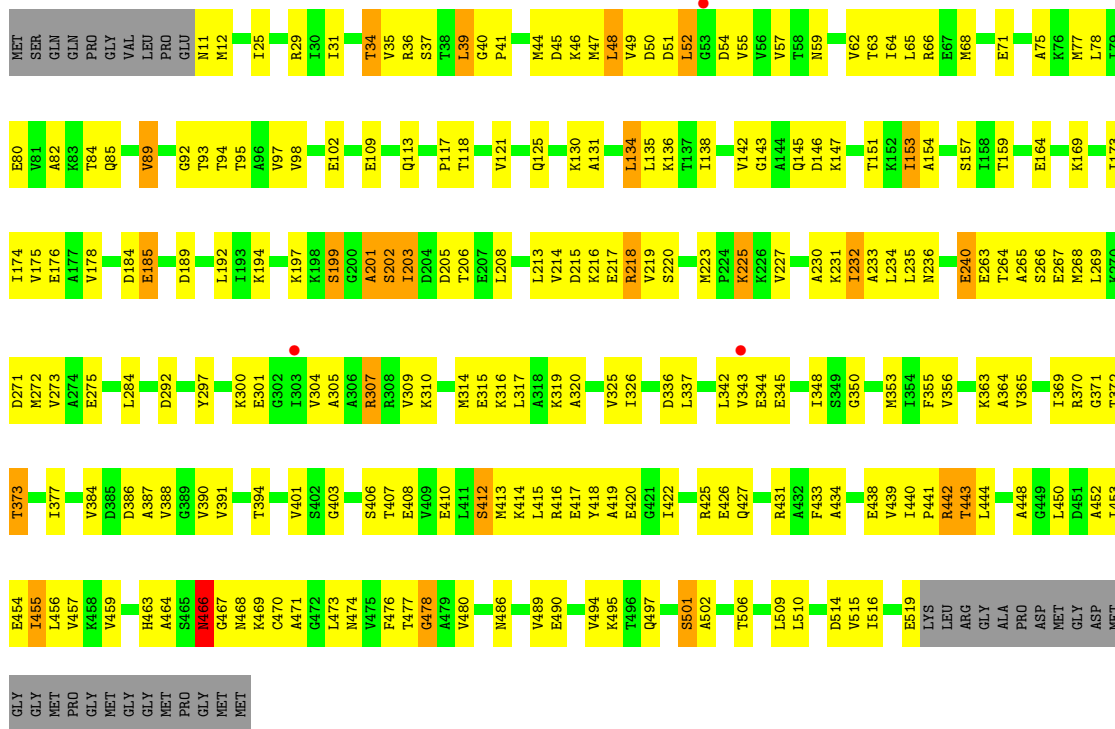
- Molecule 1: Chaperonin

Chain B: 

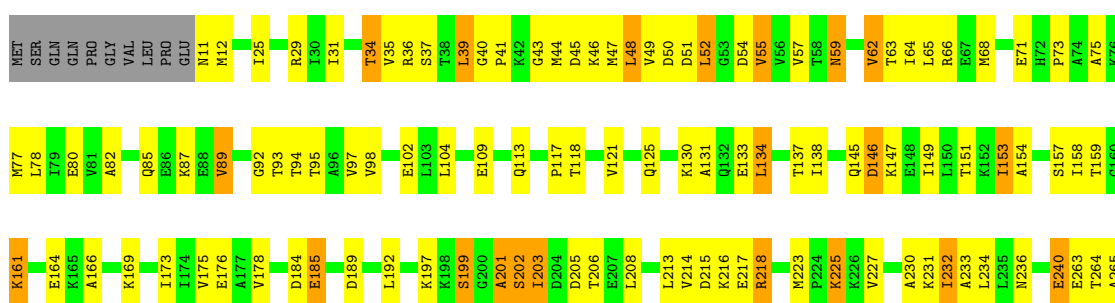


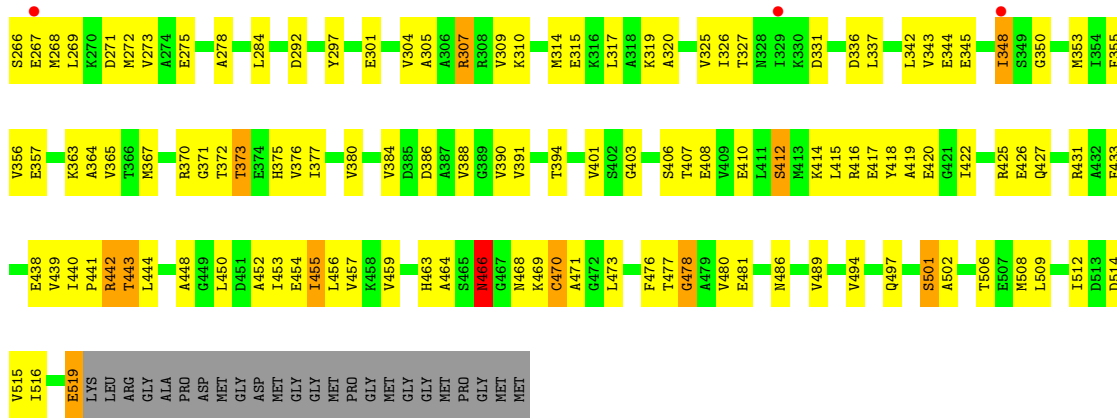


● Molecule 1: Chaperonin

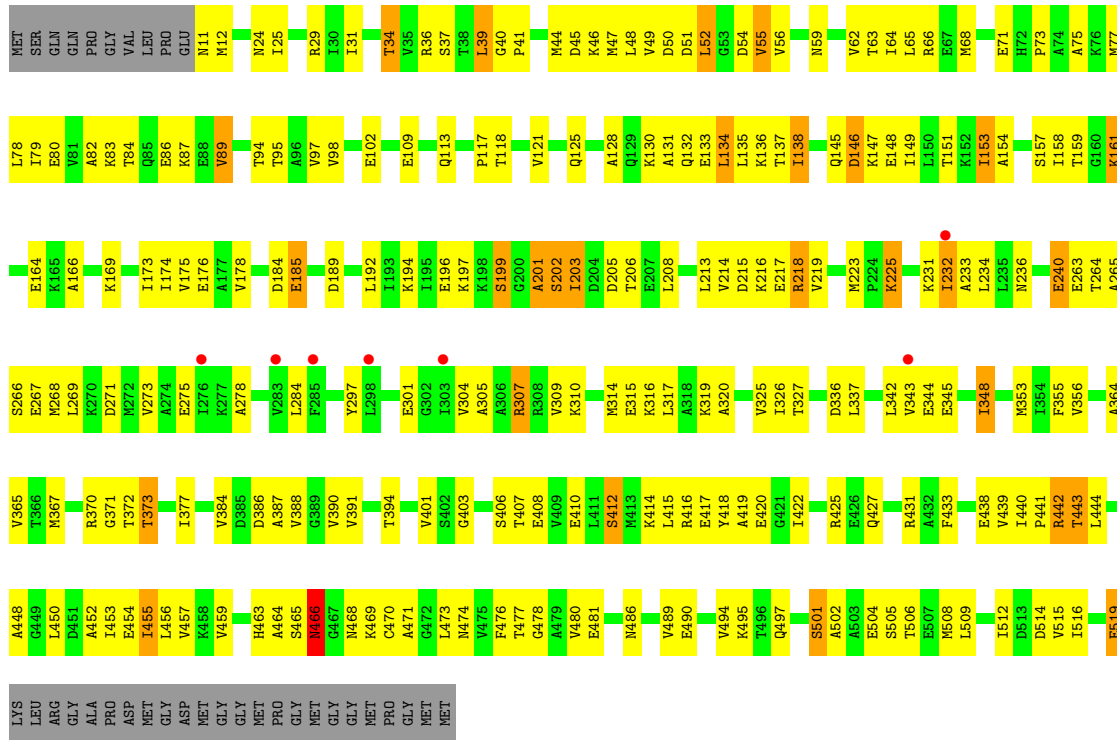


● Molecule 1: Chaperonin

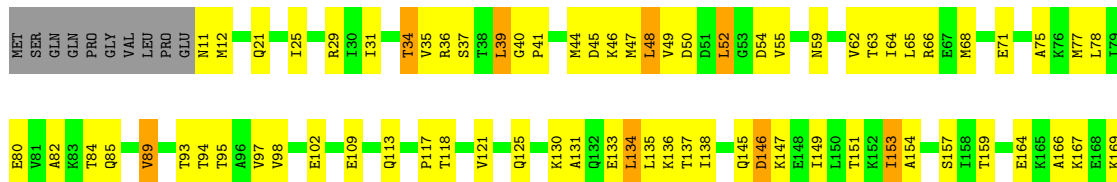




• Molecule 1: Chaperonin



• Molecule 1: Chaperonin



PRO	L450	K367	A265	A166	E80
ASP	D451	R370	S266	K167	V81
MET	A452	G371	E267	E168	A82
GLY	I453	K372	M268	K169	F83
ASP	E454	T373	L269	I173	T84
MET	I455	T374	K270	I174	Q85
GLY	L456	V376	D271	V175	V89
GLY	V457	I377	M272	E176	G92
MET	K458	V384	A274	A177	T93
PRO	V459	D385	E275	V178	T94
GLY	H463	D386	A278	D184	T95
MET	A464	D387	L284	E185	A96
GLY	S465	V388	Y297	V188	V97
MET	G467	G389	E301	D189	V98
PRO	N468	V390	E304	L192	E102
GLY	N469	V391	V304	K197	E109
MET	K470	T394	A305	K198	Q113
MET	C470	G398	A306	S199	P117
MET	A471	V401	R307	G200	T118
	G472	T407	R308	A201	T121
	L473	E408	K310	S202	Q125
	F476	V409	M314	I203	V121
	T477	E410	E315	D204	Q128
	G478	E411	E316	T205	K130
	A479	L411	K316	D206	A131
	V480	S412	L317	T207	Q132
	V489	M413	A318	E207	E133
	E490	K414	K319	L208	L134
	L492	L415	A320	L213	I138
	R493	R416	A325	V214	A139
	V494	E417	V325	V215	Q145
	K495	Y418	I326	D216	D146
	T496	A419	I327	E217	K147
	Q497	E420	D336	R218	E148
	S501	G421	L337	V219	I149
	A502	I422	M223	S220	L150
	E504	R425	L342	M229	T151
	S505	E426	V343	K230	K152
	T506	Q427	E344	K231	I153
	E507	R431	E345	K232	A154
	M508	A432	F348	T227	M155
	L509	F433	M353	T228	T156
	L510	E438	F354	V229	S157
	R511	V439	V356	I229	I158
	I512	I440	E357	A230	T159
	D513	P441	K363	K231	G160
	D514	P442	A364	K232	E164
	E519	R443	V365	T234	K165
	LEU	L444	E263	L234	
	ARG	T443	E264	L235	
	GLY	L444	T264	L236	
	ALA	A448		I236	
		G449		M236	

4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	261.45Å 161.92Å 147.37Å 90.00° 124.12° 90.00°	Depositor
Resolution (Å)	54.49 – 3.50 54.49 – 3.50	Depositor EDS
% Data completeness (in resolution range)	77.1 (54.49-3.50) 86.4 (54.49-3.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.63 (at 3.49Å)	Xtrriage
Refinement program	PHENIX (phenix.refine)	Depositor
R, R_{free}	0.232 , 0.269 0.226 , 0.254	Depositor DCC
R_{free} test set	2797 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	86.5	Xtrriage
Anisotropy	0.264	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 98.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.42$, $\langle L^2 \rangle = 0.25$	Xtrriage
Estimated twinning fraction	0.053 for -h-2*1,-k,l	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	29296	wwPDB-VP
Average B, all atoms (Å ²)	124.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.91% 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: ADP, SO4, 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	0.68	1/3649 (0.0%)	0.97	7/4911 (0.1%)
1	B	0.69	3/3649 (0.1%)	0.97	9/4911 (0.2%)
1	C	0.68	0/3649	0.97	5/4911 (0.1%)
1	D	0.64	0/3649	0.97	9/4911 (0.2%)
1	E	0.68	0/3649	0.96	5/4911 (0.1%)
1	F	0.65	0/3649	0.96	6/4911 (0.1%)
1	G	0.62	1/3649 (0.0%)	0.96	5/4911 (0.1%)
1	H	0.60	0/3649	0.94	4/4911 (0.1%)
All	All	0.66	5/29192 (0.0%)	0.96	50/39288 (0.1%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	1
1	C	0	1
1	D	0	1
1	E	0	1
1	F	0	1
1	G	0	1
1	H	0	1
All	All	0	9

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	72	HIS	CG-CD2	11.31	1.48	1.35
1	A	145	GLN	CA-C	-6.51	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	72	HIS	CB-CG	-6.08	1.41	1.50
1	B	72	HIS	ND1-CE1	-5.87	1.26	1.32
1	G	202	SER	CA-C	5.45	1.55	1.52

The worst 5 of 50 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	202	SER	N-CA-C	9.35	122.89	108.30
1	C	202	SER	N-CA-C	8.90	122.19	108.30
1	G	202	SER	N-CA-C	8.89	122.17	108.30
1	F	202	SER	N-CA-C	8.53	121.61	108.30
1	B	202	SER	N-CA-C	8.39	121.39	108.30

There are no chirality outliers.

5 of 9 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	201	ALA	Peptide
1	A	202	SER	Peptide
1	B	201	ALA	Peptide
1	C	201	ALA	Peptide
1	D	201	ALA	Peptide

5.2 Too-close contacts [i](#)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3629	0	3762	208	5
1	B	3629	0	3762	215	1
1	C	3629	0	3762	227	3
1	D	3629	0	3762	246	0
1	E	3629	0	3762	235	3
1	F	3629	0	3762	214	3
1	G	3629	0	3762	221	4
1	H	3629	0	3762	224	1
2	A	1	0	0	0	0
2	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	1	0	0	0	0
2	D	1	0	0	0	0
2	E	1	0	0	0	0
2	F	1	0	0	0	0
2	G	1	0	0	0	0
2	H	1	0	0	0	0
3	A	27	0	12	5	0
3	B	27	0	12	6	0
3	C	27	0	12	7	0
3	D	27	0	12	6	0
3	E	27	0	12	6	0
3	F	27	0	12	6	0
3	G	27	0	12	6	0
3	H	27	0	12	6	0
4	A	5	0	0	3	0
4	B	5	0	0	4	0
4	C	5	0	0	5	0
4	D	5	0	0	4	0
4	E	5	0	0	4	0
4	F	5	0	0	4	0
4	G	5	0	0	4	0
4	H	5	0	0	4	0
All	All	29296	0	30192	1710	10

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 29.

The worst 5 of 1710 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:H:39:LEU:HD23	1:H:444:LEU:CD2	1.71	1.21
1:G:39:LEU:HD23	1:G:444:LEU:CD2	1.73	1.18
1:D:39:LEU:HD23	1:D:444:LEU:CD2	1.74	1.17
1:F:39:LEU:HD23	1:F:444:LEU:CD2	1.71	1.17
1:C:39:LEU:HD23	1:C:444:LEU:CD2	1.74	1.16

The worst 5 of 10 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:A:144:ALA:O	1:C:185:GLU:OE2[4_556]	1.91	0.29
1:E:148:GLU:OE1	1:G:130:LYS:NZ[4_445]	1.99	0.21
1:A:451:ASP:OD1	1:G:425:ARG:NH2[2_556]	2.03	0.17
1:A:425:ARG:NH2	1:G:451:ASP:OD1[2_556]	2.05	0.15
1:E:465:SER:OG	1:F:176:GLU:OE2[4_445]	2.05	0.15

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	485/521 (93%)	424 (87%)	53 (11%)	8 (2%)	7	36
1	B	485/521 (93%)	423 (87%)	55 (11%)	7 (1%)	9	38
1	C	485/521 (93%)	422 (87%)	56 (12%)	7 (1%)	9	38
1	D	485/521 (93%)	423 (87%)	54 (11%)	8 (2%)	7	36
1	E	485/521 (93%)	426 (88%)	52 (11%)	7 (1%)	9	38
1	F	485/521 (93%)	427 (88%)	50 (10%)	8 (2%)	7	36
1	G	485/521 (93%)	424 (87%)	54 (11%)	7 (1%)	9	38
1	H	485/521 (93%)	425 (88%)	52 (11%)	8 (2%)	7	36
All	All	3880/4168 (93%)	3394 (88%)	426 (11%)	60 (2%)	8	37

5 of 60 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	SER
1	C	203	ILE
1	D	146	ASP
1	D	199	SER
1	E	199	SER

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	388/413 (94%)	362 (93%)	26 (7%)	15	41
1	B	388/413 (94%)	364 (94%)	24 (6%)	16	43
1	C	388/413 (94%)	362 (93%)	26 (7%)	15	41
1	D	388/413 (94%)	359 (92%)	29 (8%)	12	37
1	E	388/413 (94%)	359 (92%)	29 (8%)	12	37
1	F	388/413 (94%)	362 (93%)	26 (7%)	15	41
1	G	388/413 (94%)	363 (94%)	25 (6%)	16	42
1	H	388/413 (94%)	363 (94%)	25 (6%)	16	42
All	All	3104/3304 (94%)	2894 (93%)	210 (7%)	14	40

5 of 210 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	E	185	GLU
1	F	218	ARG
1	H	264	THR
1	E	231	LYS
1	E	466	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 22 such sidechains are listed below:

Mol	Chain	Res	Type
1	E	361	HIS
1	G	145	GLN
1	F	361	HIS
1	G	361	HIS
1	C	145	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 24 ligands modelled in this entry, 8 are monoatomic - leaving 16 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
3	ADP	D	545	2	28,29,29	1.44	6 (21%)	43,45,45	2.18	12 (27%)
3	ADP	G	545	2	28,29,29	1.49	5 (17%)	43,45,45	2.02	13 (30%)
4	SO4	A	546	2	4,4,4	0.29	0	6,6,6	0.22	0
4	SO4	C	546	2	4,4,4	0.26	0	6,6,6	0.23	0
4	SO4	D	546	2	4,4,4	0.31	0	6,6,6	0.36	0
4	SO4	F	546	2	4,4,4	0.22	0	6,6,6	0.27	0
3	ADP	A	545	2	28,29,29	1.51	5 (17%)	43,45,45	2.00	13 (30%)
4	SO4	H	546	2	4,4,4	0.32	0	6,6,6	0.25	0
4	SO4	G	546	2	4,4,4	0.26	0	6,6,6	0.25	0
3	ADP	F	545	2	28,29,29	1.43	6 (21%)	43,45,45	2.07	13 (30%)
3	ADP	C	545	2	28,29,29	1.40	6 (21%)	43,45,45	2.19	12 (27%)
4	SO4	E	546	2	4,4,4	0.34	0	6,6,6	0.35	0
4	SO4	B	546	2	4,4,4	0.24	0	6,6,6	0.33	0
3	ADP	E	545	2	28,29,29	1.38	6 (21%)	43,45,45	2.02	12 (27%)
3	ADP	B	545	2	28,29,29	1.49	6 (21%)	43,45,45	2.11	10 (23%)
3	ADP	H	545	2	28,29,29	1.55	5 (17%)	43,45,45	2.06	13 (30%)

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
3	ADP	D	545	2	-	5/16/32/32	0/3/3/3
3	ADP	G	545	2	-	5/16/32/32	0/3/3/3
3	ADP	A	545	2	-	5/16/32/32	0/3/3/3
3	ADP	F	545	2	-	5/16/32/32	0/3/3/3
3	ADP	C	545	2	-	5/16/32/32	0/3/3/3
3	ADP	E	545	2	-	5/16/32/32	0/3/3/3
3	ADP	B	545	2	-	5/16/32/32	0/3/3/3
3	ADP	H	545	2	-	5/16/32/32	0/3/3/3

The worst 5 of 45 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	545	ADP	C5-C4	4.47	1.47	1.39
3	H	545	ADP	C5-C4	4.37	1.46	1.39
3	B	545	ADP	C5-C4	4.19	1.46	1.39
3	E	545	ADP	C5-C4	4.11	1.46	1.39
3	A	545	ADP	C5-C4	4.08	1.46	1.39

The worst 5 of 98 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	545	ADP	C5-C4-N3	-6.67	117.53	126.72
3	B	545	ADP	C5-C4-N3	-6.09	118.33	126.72
3	D	545	ADP	C5-C4-N3	-6.02	118.43	126.72
3	F	545	ADP	C5-C4-N3	-5.55	119.08	126.72
3	E	545	ADP	C5-C4-N3	-5.43	119.24	126.72

There are no chirality outliers.

5 of 40 torsion outliers are listed below:

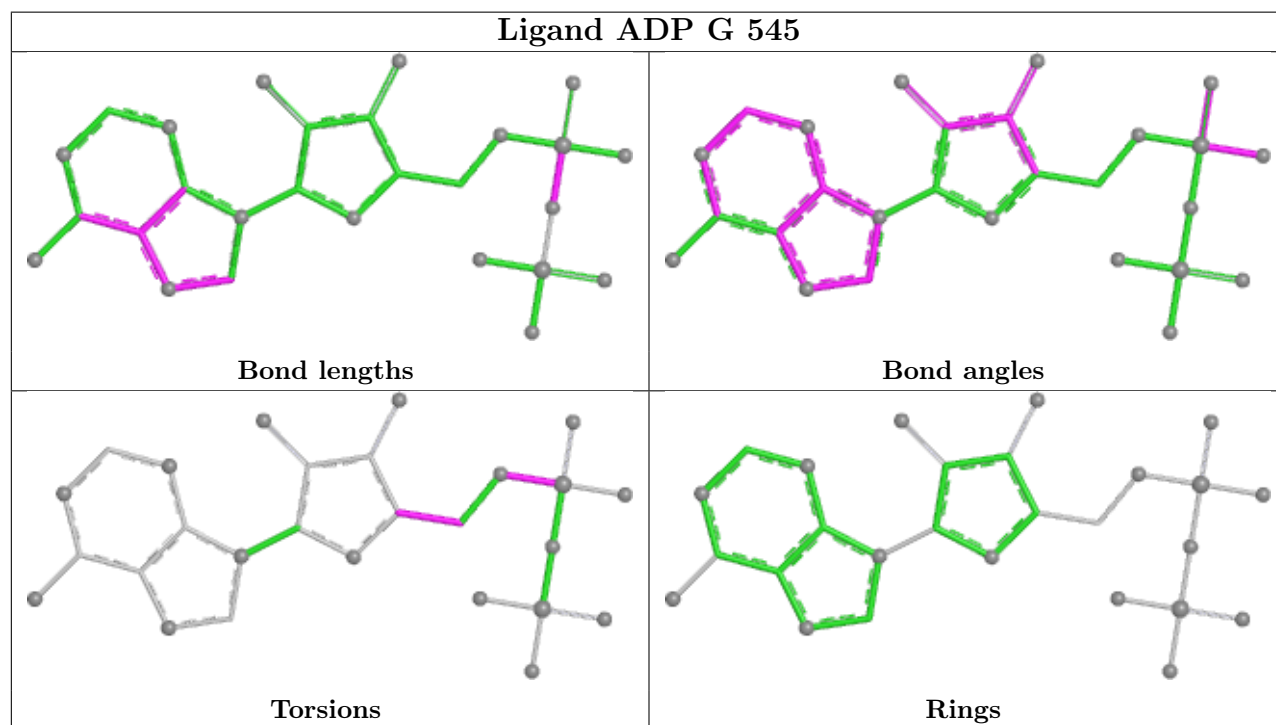
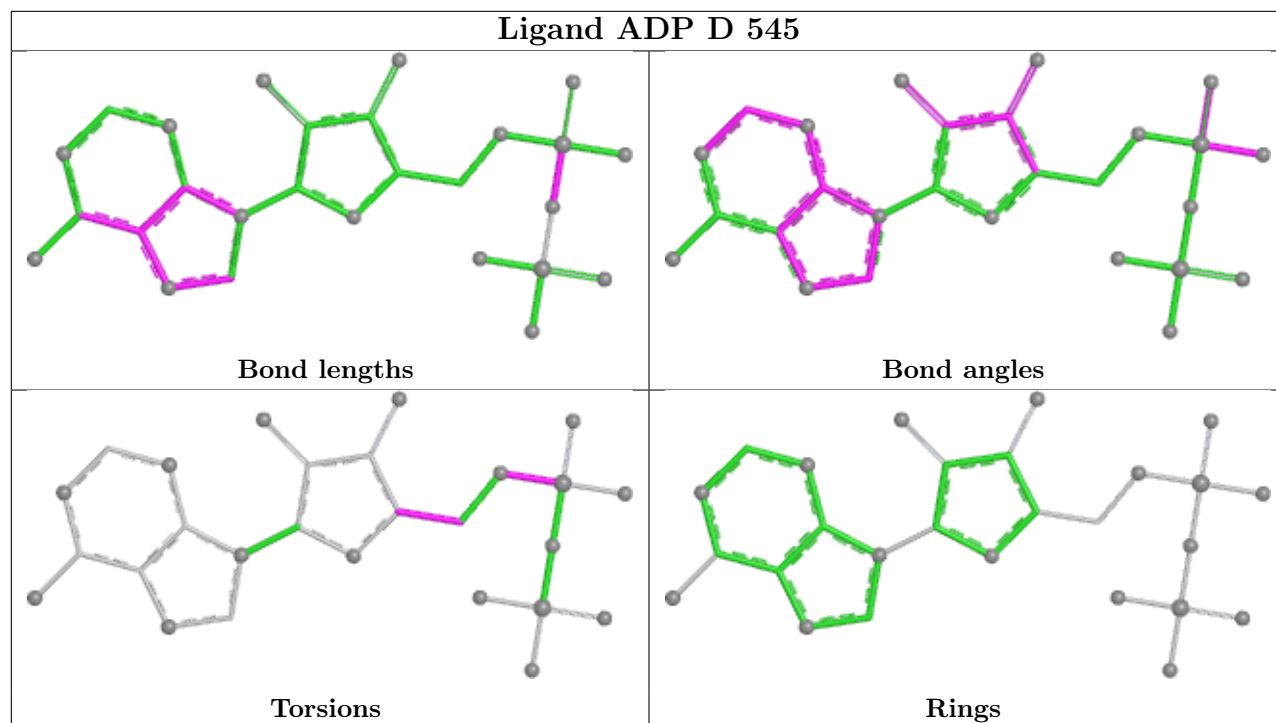
Mol	Chain	Res	Type	Atoms
3	A	545	ADP	C5'-O5'-PA-O1A
3	A	545	ADP	C5'-O5'-PA-O2A
3	A	545	ADP	C5'-O5'-PA-O3A
3	B	545	ADP	C5'-O5'-PA-O1A
3	B	545	ADP	C5'-O5'-PA-O2A

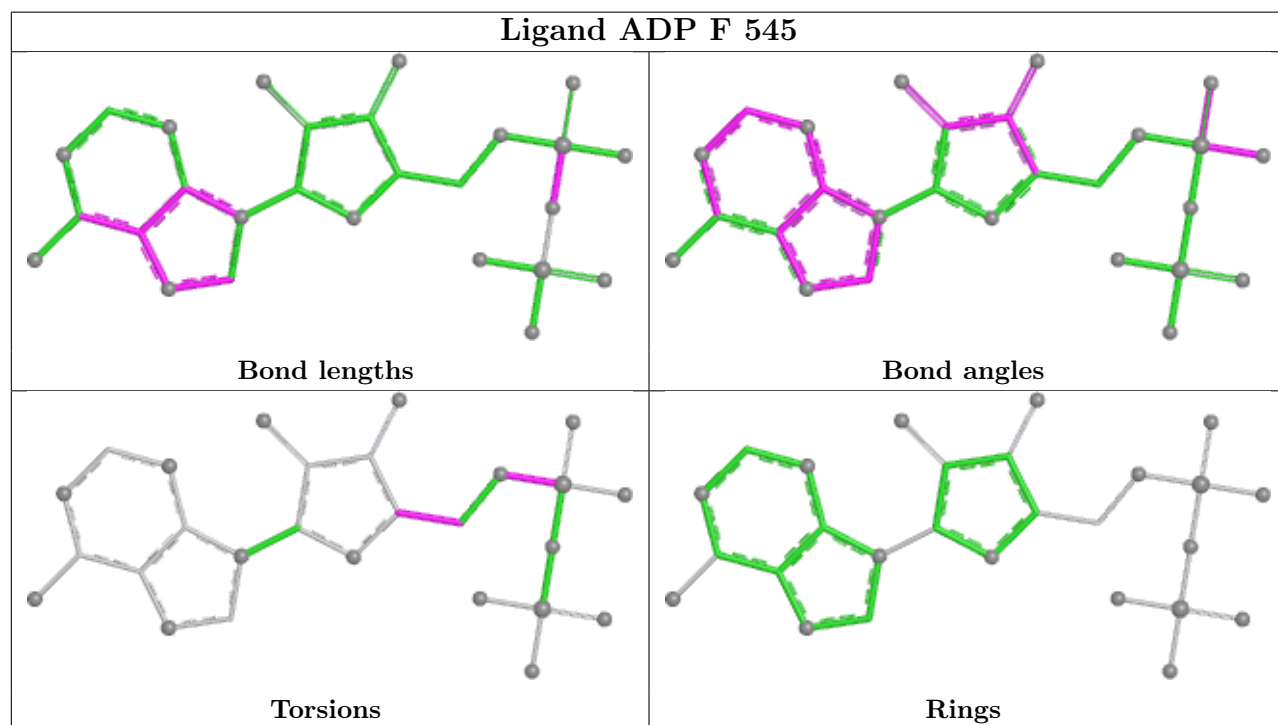
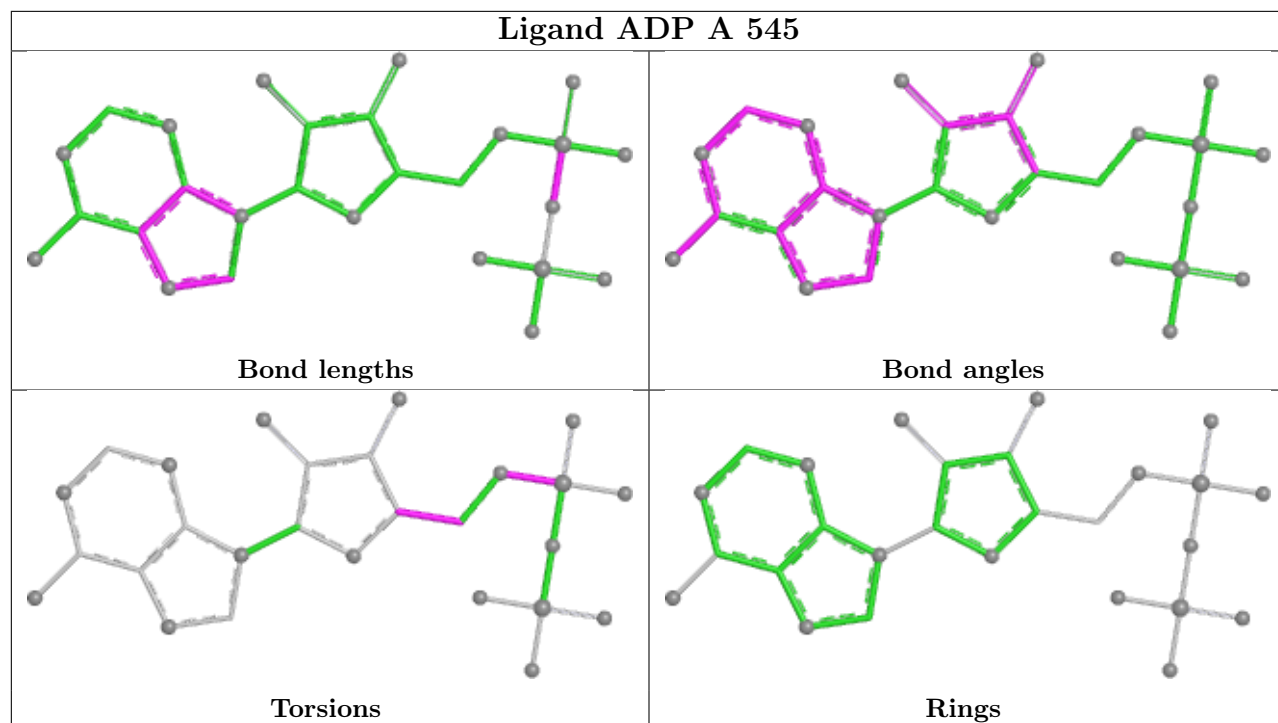
There are no ring outliers.

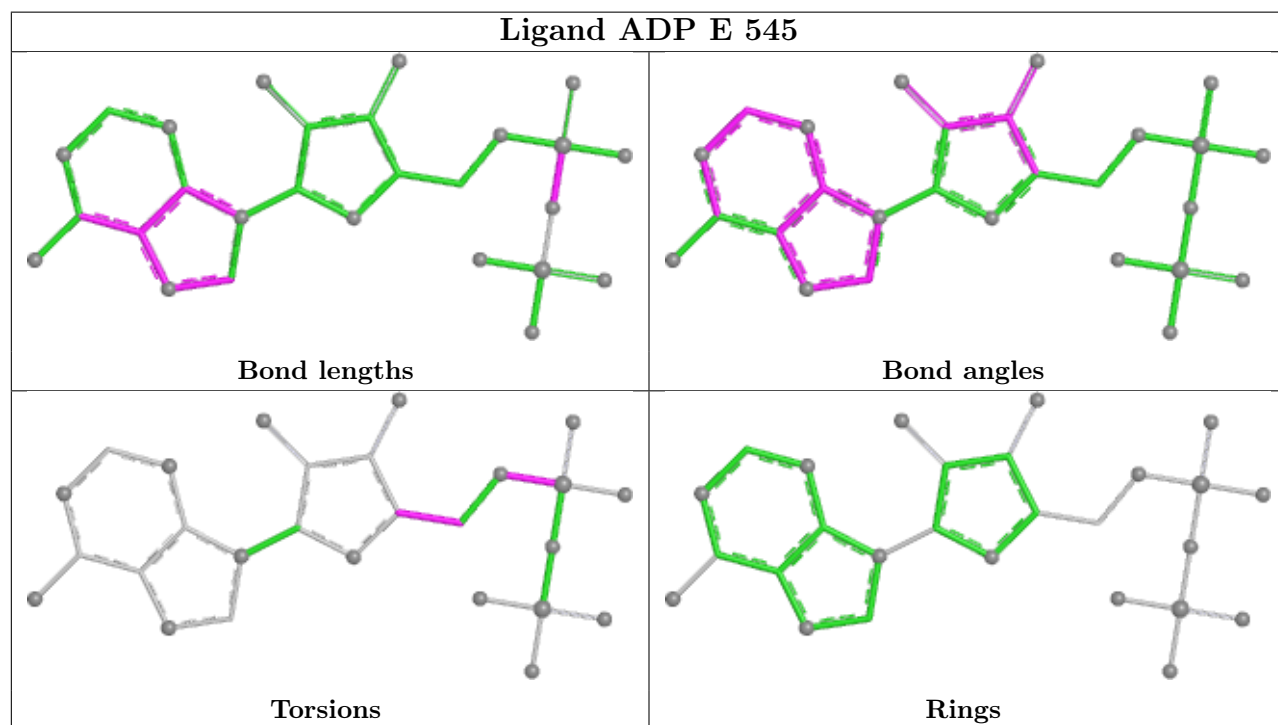
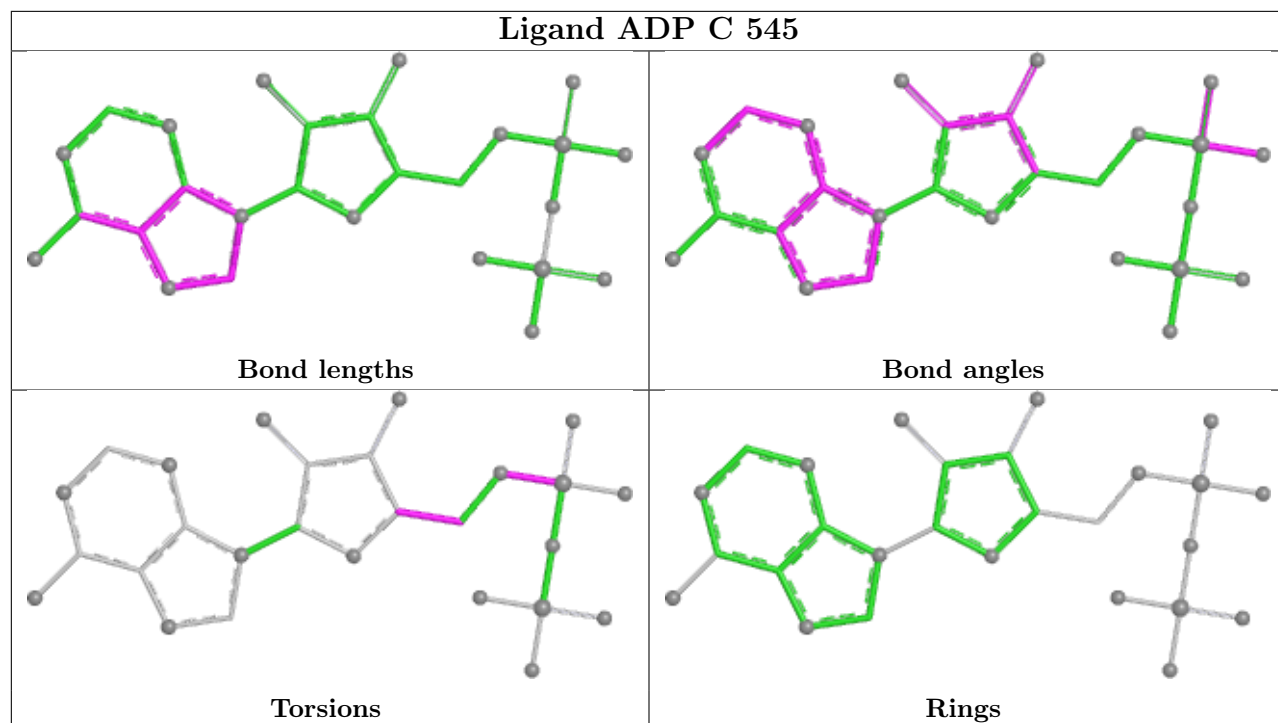
16 monomers are involved in 48 short contacts:

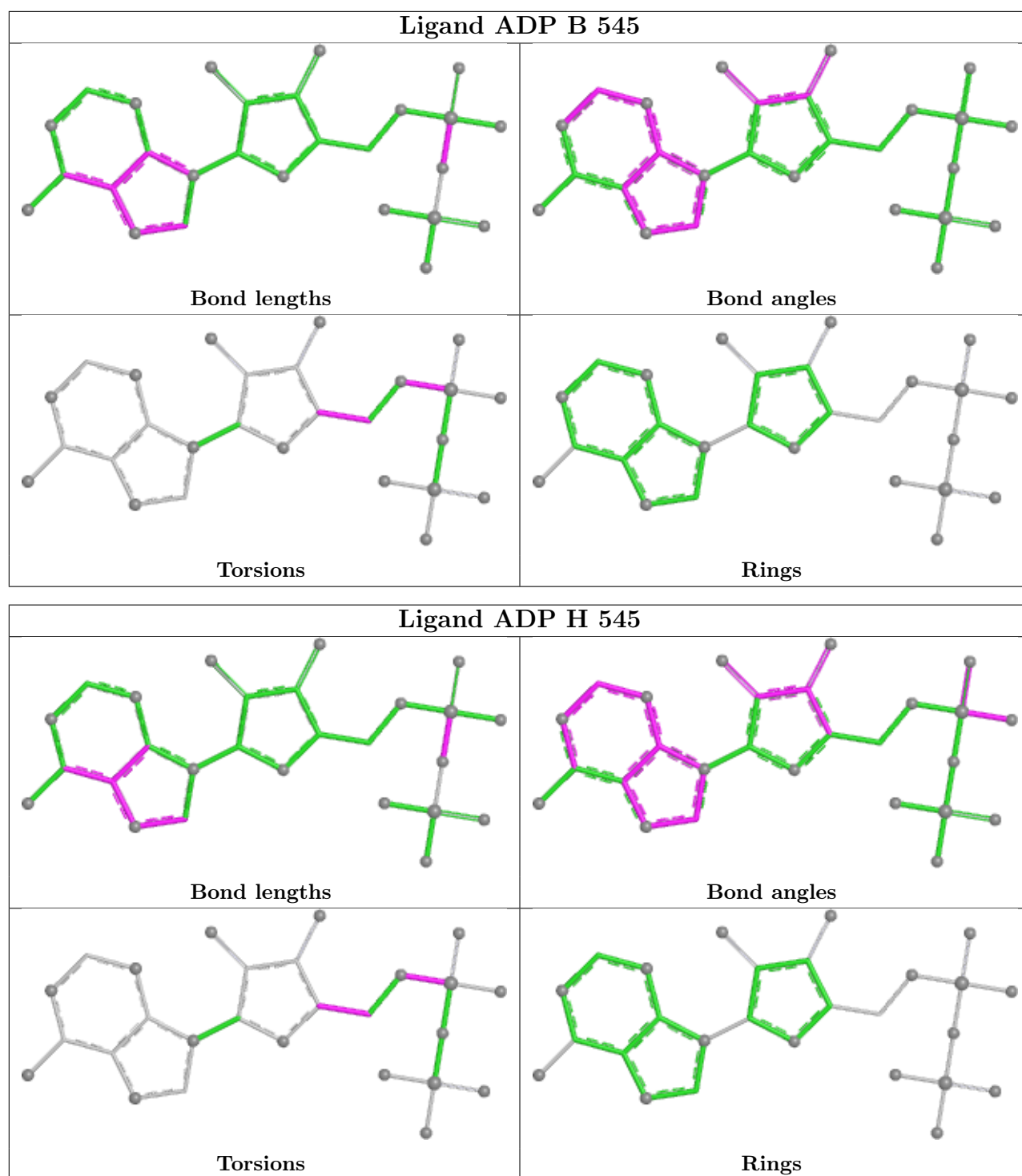
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	D	545	ADP	6	0
3	G	545	ADP	6	0
4	A	546	SO4	3	0
4	C	546	SO4	5	0
4	D	546	SO4	4	0
4	F	546	SO4	4	0
3	A	545	ADP	5	0
4	H	546	SO4	4	0
4	G	546	SO4	4	0
3	F	545	ADP	6	0
3	C	545	ADP	7	0
4	E	546	SO4	4	0
4	B	546	SO4	4	0
3	E	545	ADP	6	0
3	B	545	ADP	6	0
3	H	545	ADP	6	0

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

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	487/521 (93%)	-0.09	1 (0%) 91 82	26, 88, 242, 287	0
1	B	487/521 (93%)	-0.15	1 (0%) 91 82	38, 90, 196, 247	0
1	C	487/521 (93%)	-0.10	3 (0%) 85 65	39, 88, 282, 341	0
1	D	487/521 (93%)	-0.08	3 (0%) 85 65	42, 103, 243, 287	0
1	E	487/521 (93%)	0.02	7 (1%) 73 48	34, 94, 252, 294	0
1	F	487/521 (93%)	0.01	5 (1%) 79 56	41, 100, 258, 295	0
1	G	487/521 (93%)	0.02	5 (1%) 79 56	41, 122, 245, 291	0
1	H	487/521 (93%)	0.07	5 (1%) 79 56	64, 127, 229, 274	0
All	All	3896/4168 (93%)	-0.04	30 (0%) 82 60	26, 102, 250, 341	0

The worst 5 of 30 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	343	VAL	5.0
1	H	53	GLY	4.2
1	G	239	ILE	4.1
1	E	232	ILE	4.1
1	E	298	LEU	3.8

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

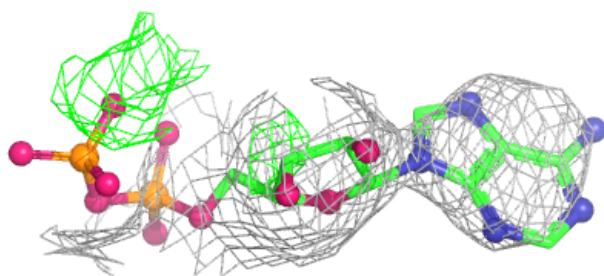
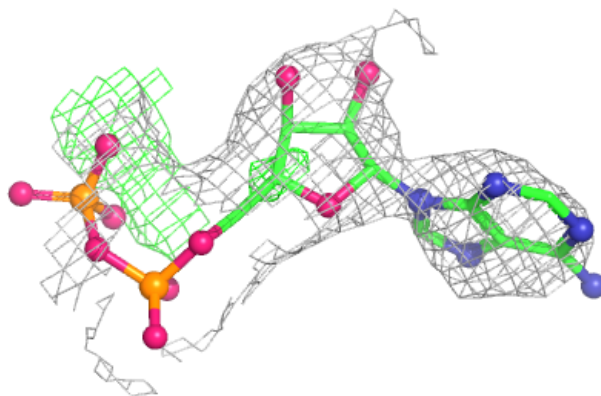
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	MG	G	544	1/1	0.89	0.12	111,111,111,111	0
2	MG	B	544	1/1	0.93	0.18	58,58,58,58	0
3	ADP	H	545	27/27	0.93	0.10	72,100,114,124	0
2	MG	C	544	1/1	0.94	0.10	57,57,57,57	0
3	ADP	E	545	27/27	0.95	0.09	49,70,86,98	0
3	ADP	G	545	27/27	0.95	0.08	71,99,116,122	0
2	MG	H	544	1/1	0.95	0.10	111,111,111,111	0
4	SO4	B	546	5/5	0.95	0.08	59,71,88,107	0
4	SO4	E	546	5/5	0.95	0.07	65,72,99,100	0
4	SO4	H	546	5/5	0.95	0.05	96,104,122,137	0
2	MG	E	544	1/1	0.96	0.06	55,55,55,55	0
3	ADP	A	545	27/27	0.96	0.08	38,59,78,83	0
4	SO4	A	546	5/5	0.96	0.06	76,81,105,106	0
3	ADP	B	545	27/27	0.96	0.09	47,65,83,90	0
4	SO4	C	546	5/5	0.96	0.08	71,78,107,110	0
4	SO4	D	546	5/5	0.96	0.06	66,71,89,100	0
3	ADP	C	545	27/27	0.96	0.07	46,68,88,95	0
2	MG	D	544	1/1	0.96	0.10	92,92,92,92	0
2	MG	A	544	1/1	0.97	0.05	65,65,65,65	0
3	ADP	D	545	27/27	0.97	0.08	66,89,104,118	0
2	MG	F	544	1/1	0.97	0.08	83,83,83,83	0
4	SO4	F	546	5/5	0.97	0.08	100,101,134,137	0
4	SO4	G	546	5/5	0.97	0.06	75,90,123,124	0
3	ADP	F	545	27/27	0.97	0.07	45,69,88,95	0

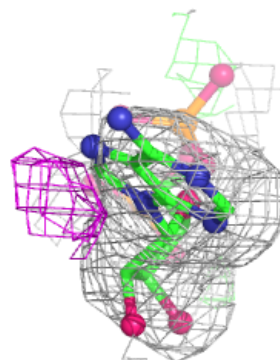
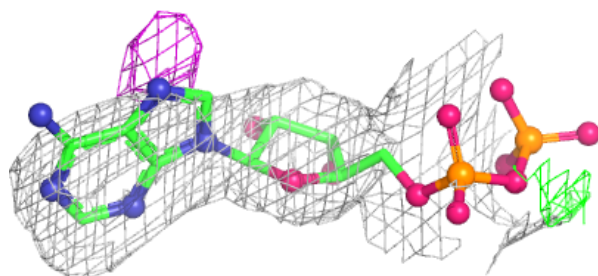
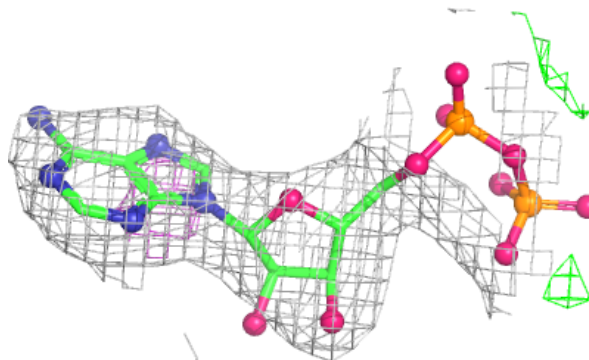
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP H 545:

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

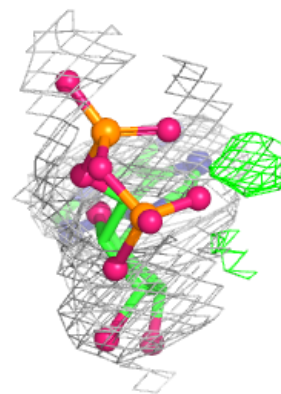
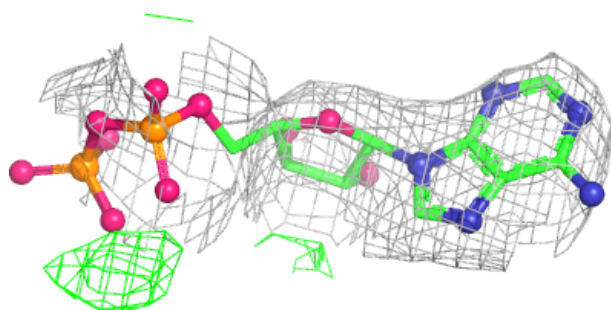
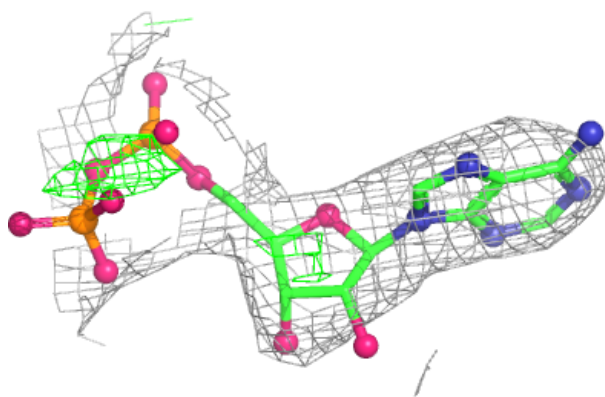
**Electron density around ADP E 545:**

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

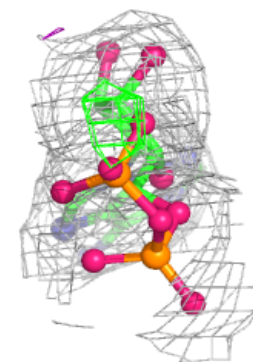
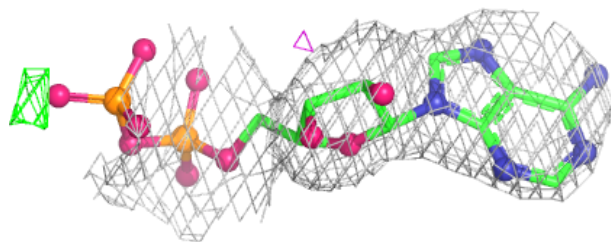
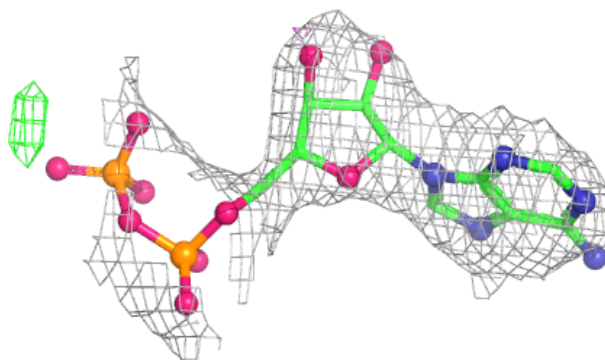


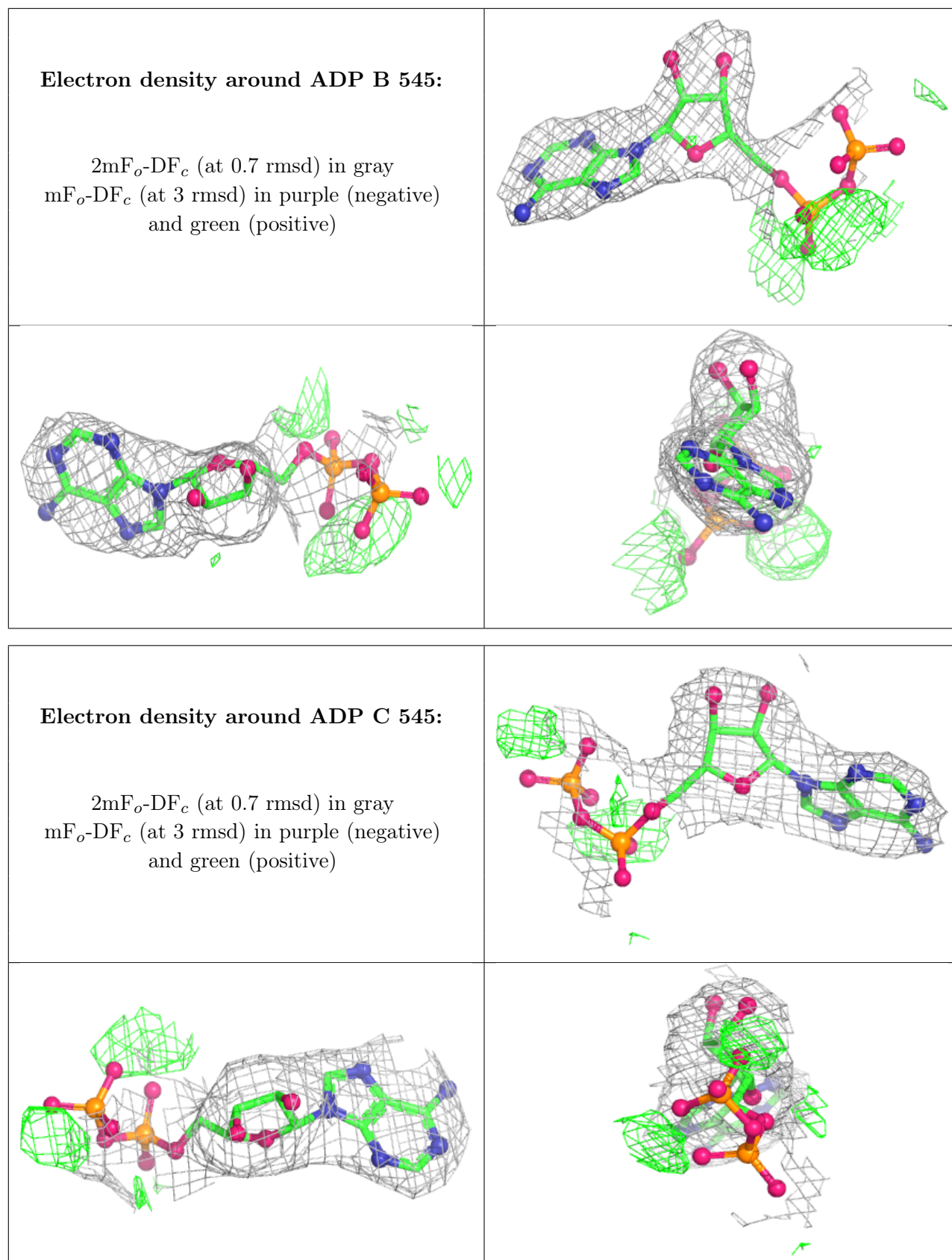
Electron density around ADP G 545:

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

**Electron density around ADP A 545:**

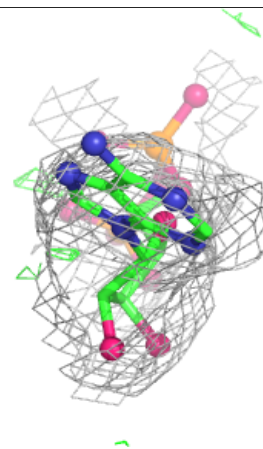
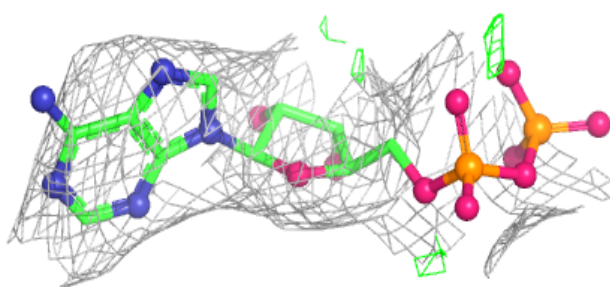
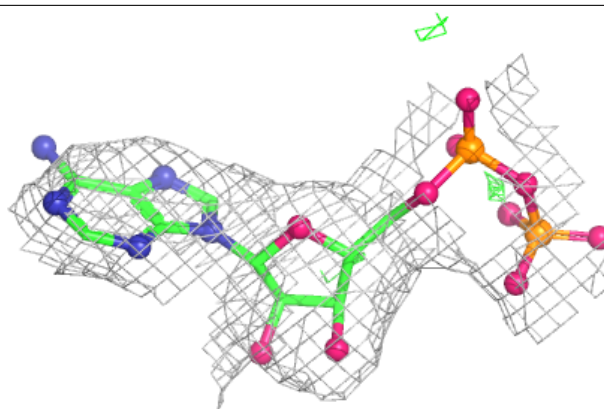
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



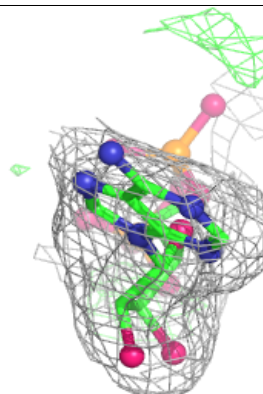
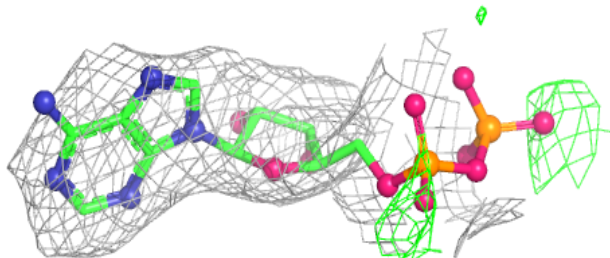
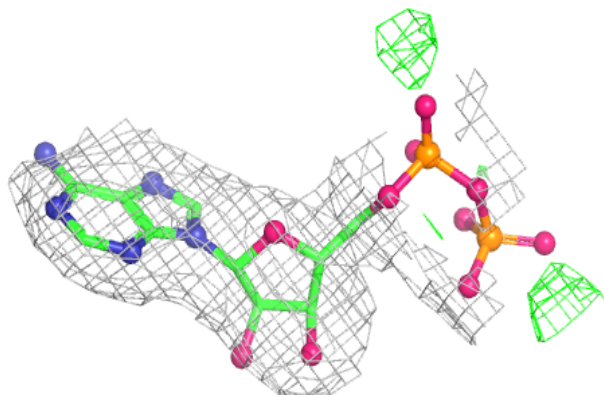


Electron density around ADP D 545:

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

**Electron density around ADP F 545:**

$2mF_o-DF_c$ (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.