



wwPDB X-ray Structure Validation Summary Report ⓘ

May 22, 2020 – 11:47 pm BST

PDB ID : 1PF9
Title : GroEL-GroES-ADP
Authors : Chaudhry, C.; Farr, G.W.; Todd, M.J.; Rye, H.S.; Brunger, A.T.; Adams, P.D.; Horwich, A.L.; Sigler, P.B.
Deposited on : 2003-05-24
Resolution : 2.99 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

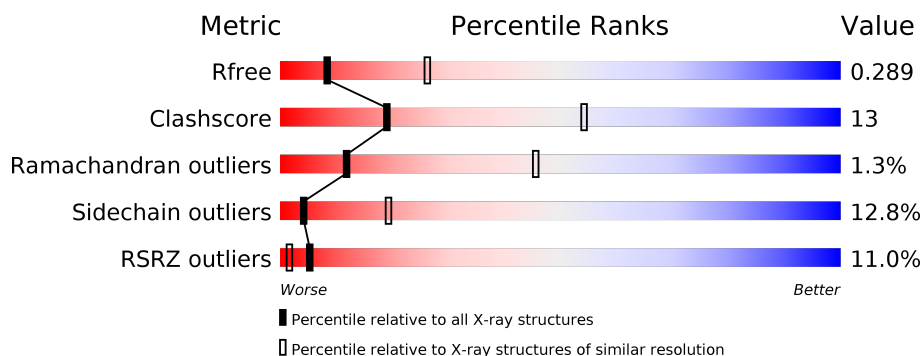
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.99 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	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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	524	
1	B	524	
1	C	524	
1	D	524	
1	E	524	
1	F	524	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
1	G	524	
1	H	524	
1	I	524	
1	J	524	
1	K	524	
1	L	524	
1	M	524	
1	N	524	
2	O	97	
2	P	97	
2	Q	97	
2	R	97	
2	S	97	
2	T	97	
2	U	97	

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 59283 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 groEL protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	B	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	C	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	D	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	E	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	F	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	G	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	H	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	I	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	J	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	K	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	L	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	M	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			
1	N	524	Total	C	N	O	S	0	0	0
			3856	2397	665	774	20			

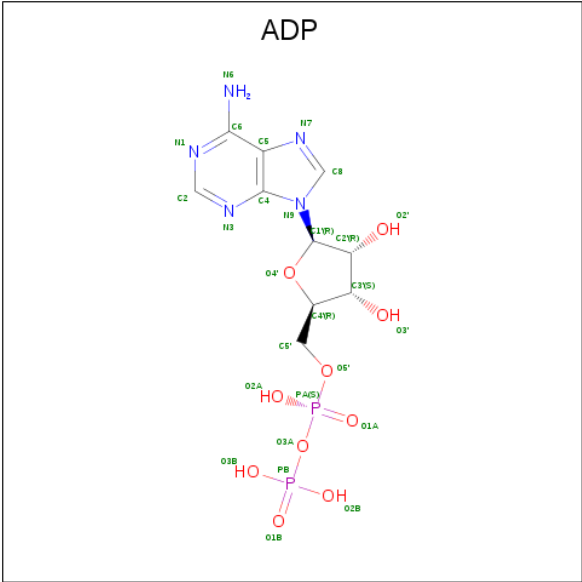
- Molecule 2 is a protein called groES protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	97	Total	C	N	O	S	0	0	0
			728	454	127	145	2			
2	P	97	Total	C	N	O	S	0	0	0
			728	454	127	145	2			
2	Q	97	Total	C	N	O	S	0	0	0
			728	454	127	145	2			
2	R	97	Total	C	N	O	S	0	0	0
			728	454	127	145	2			
2	S	97	Total	C	N	O	S	0	0	0
			728	454	127	145	2			
2	T	97	Total	C	N	O	S	0	0	0
			728	454	127	145	2			
2	U	97	Total	C	N	O	S	0	0	0
			728	454	127	145	2			

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

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

- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

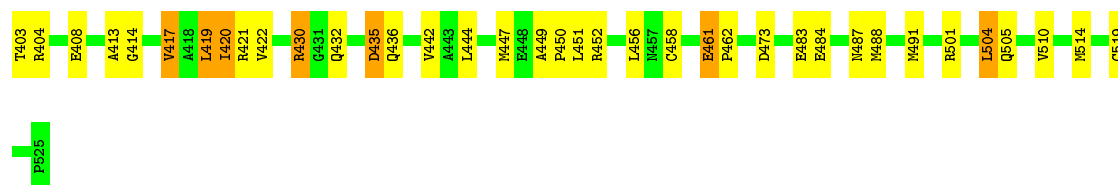
- Molecule 5 is water.

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

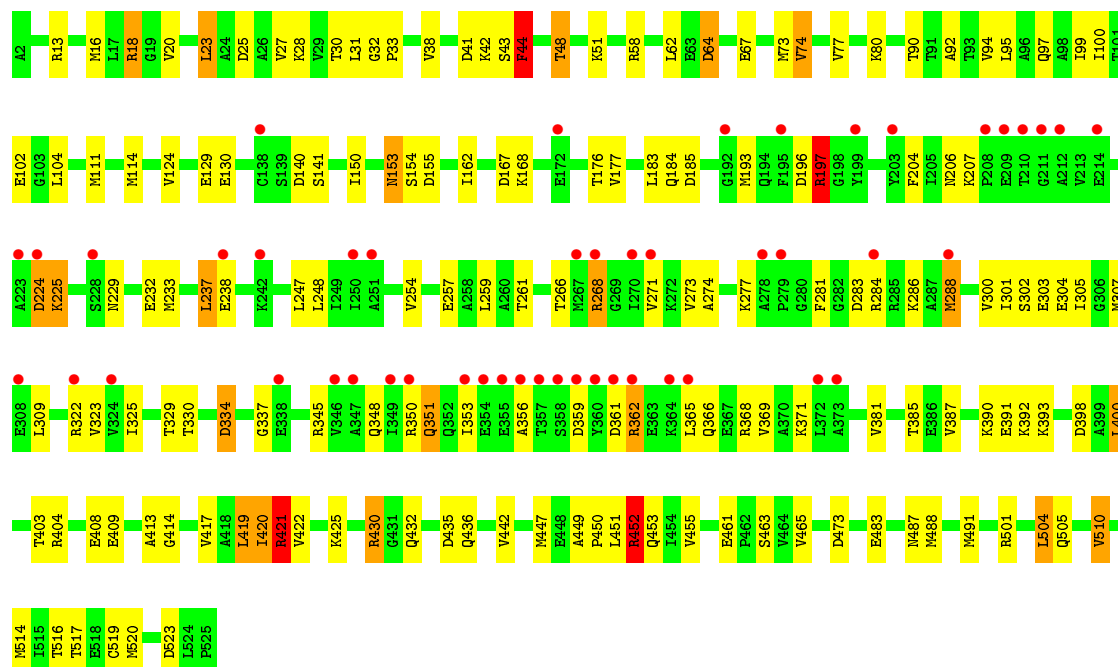
Continued on next page...

Continued from previous page...

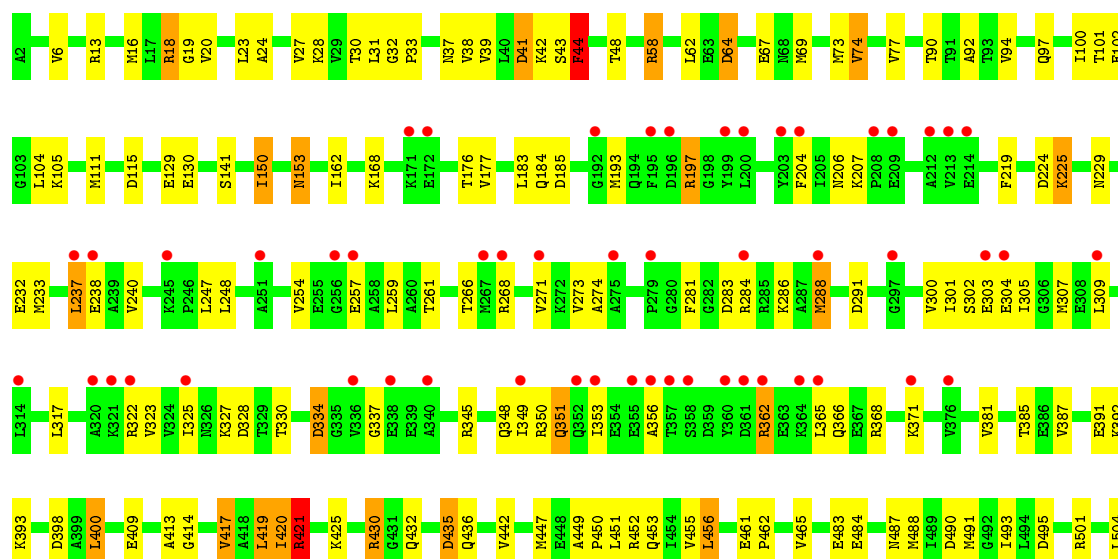
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	F	1	Total	O	0	0
			1	1		
5	G	1	Total	O	0	0
			1	1		



- Molecule 1: groEL protein

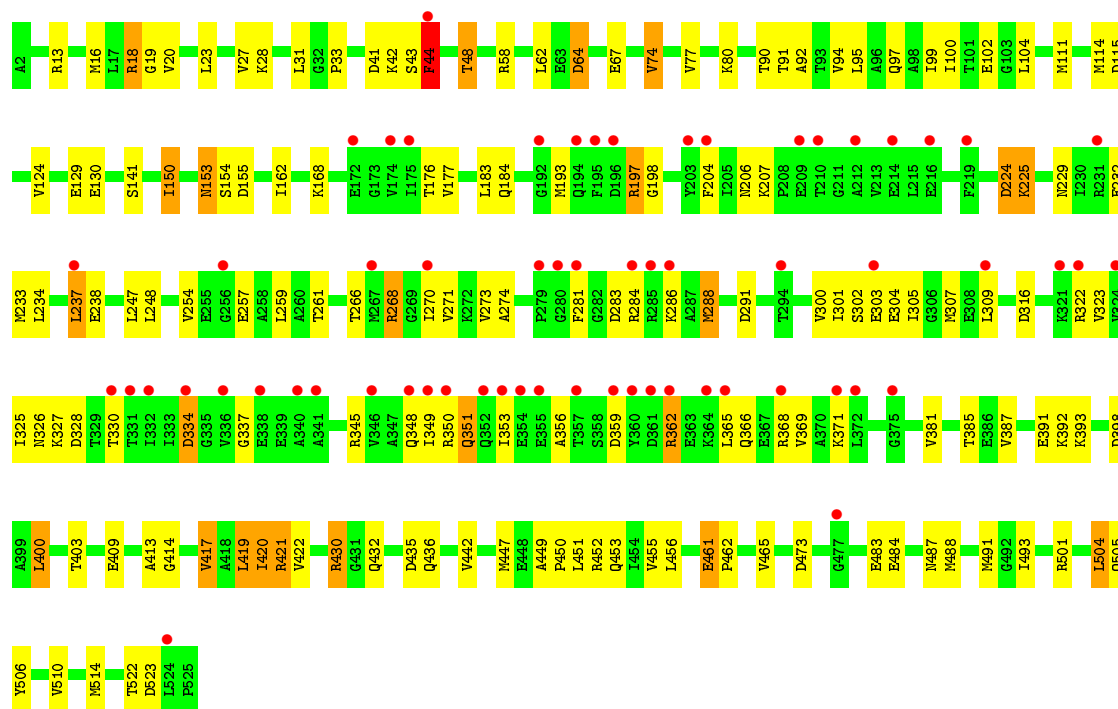


- Molecule 1: groEL protein

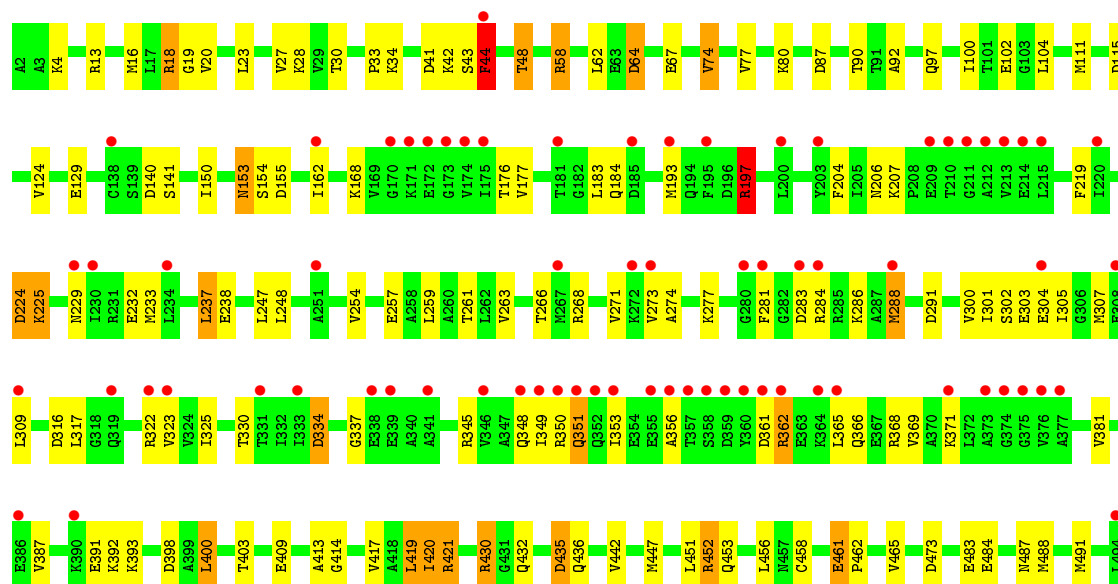


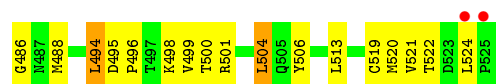


• Molecule 1: groEL protein

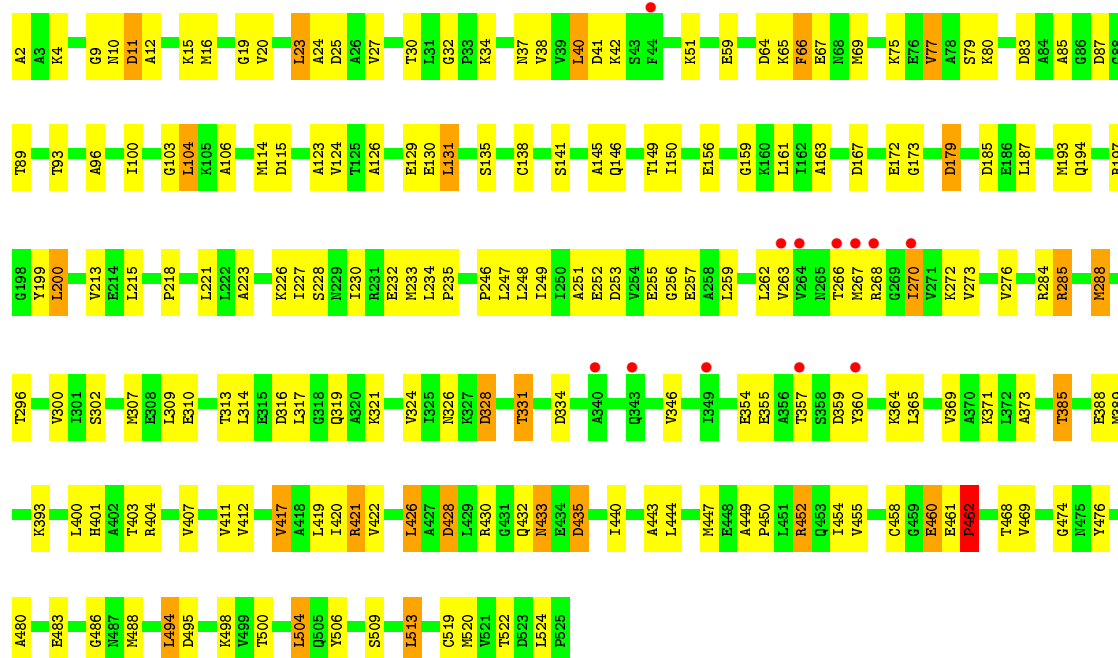


• Molecule 1: groEL protein

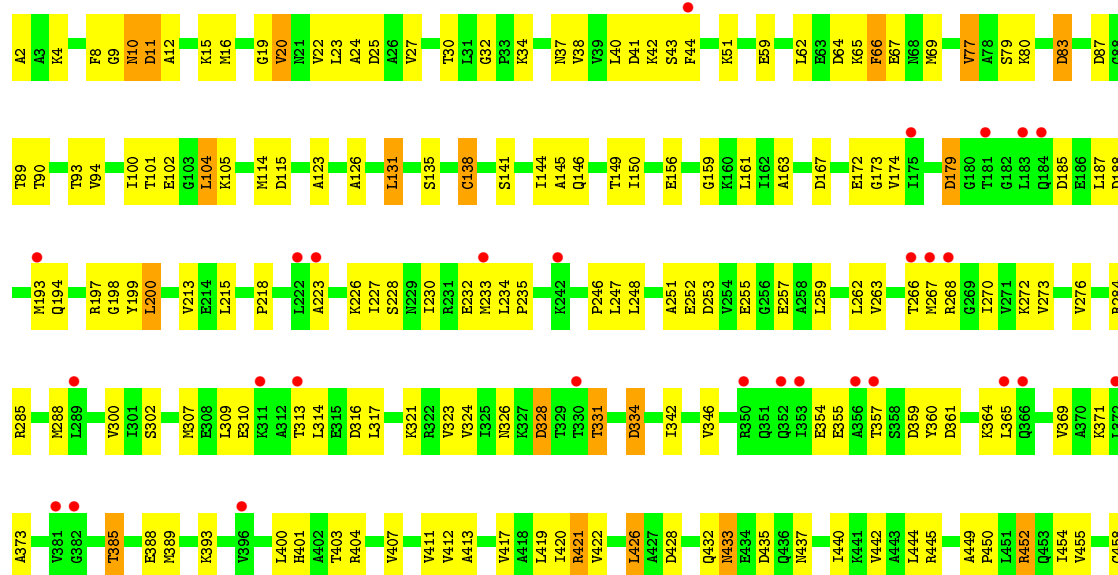


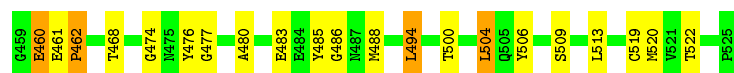


• Molecule 1: groEL protein

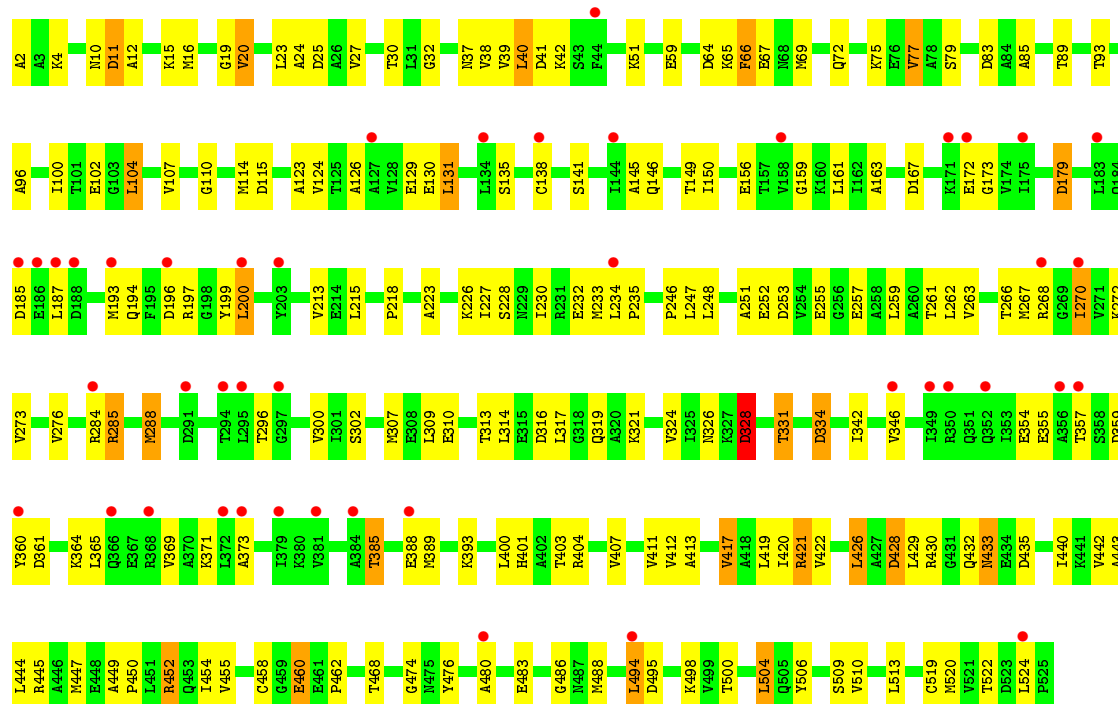


• Molecule 1: groEL protein

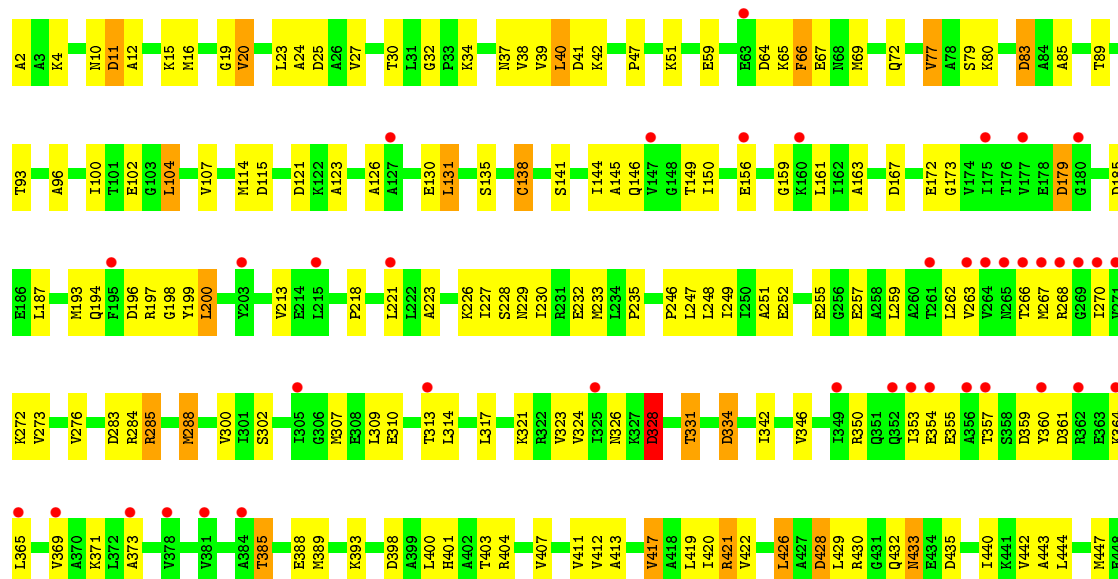


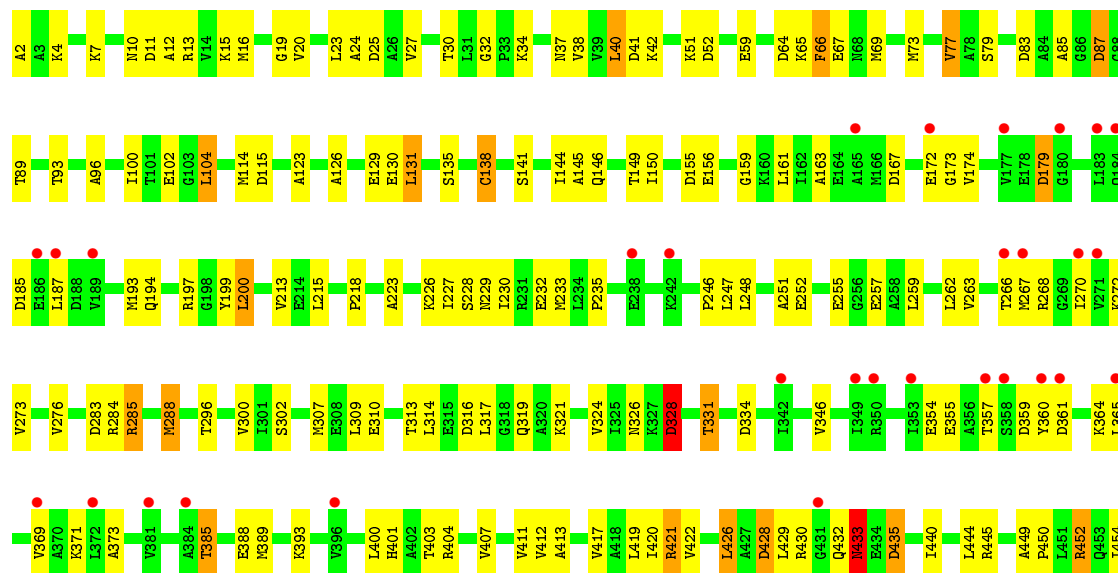


• Molecule 1: groEL protein



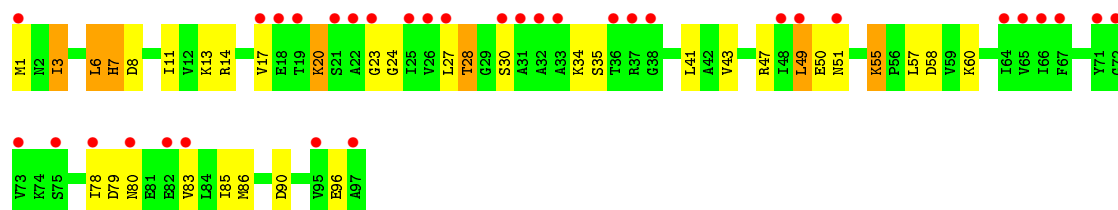
• Molecule 1: groEL protein



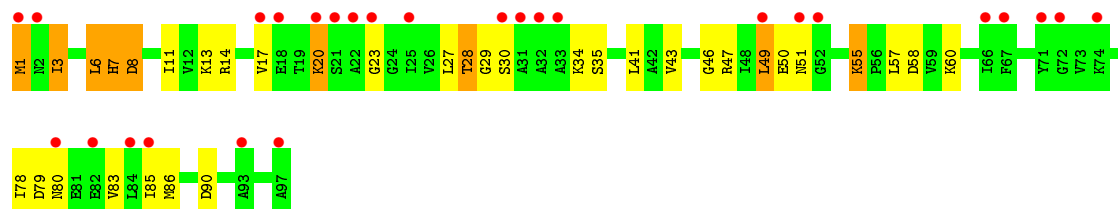




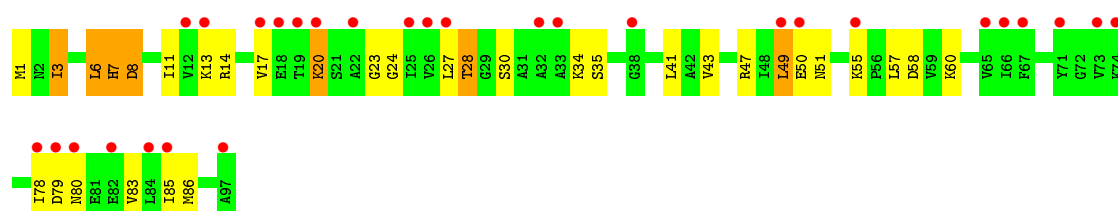
- Molecule 2: groES protein



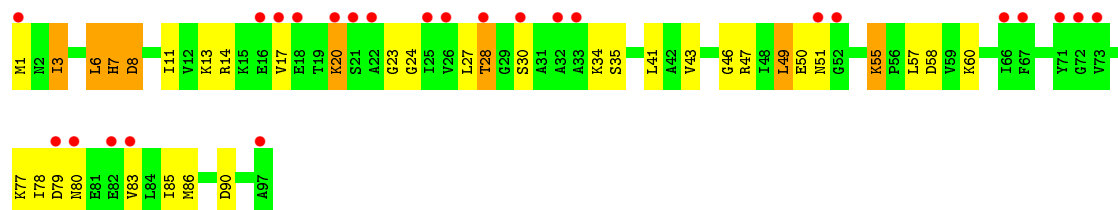
- Molecule 2: groES protein



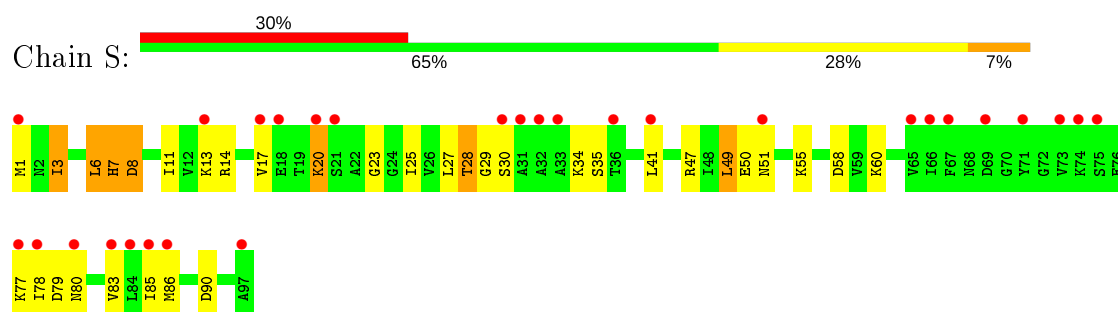
- Molecule 2: groES protein



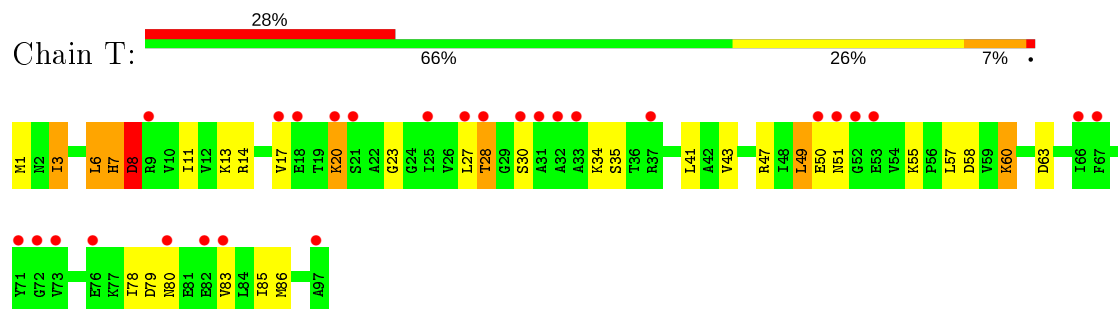
- Molecule 2: groES protein



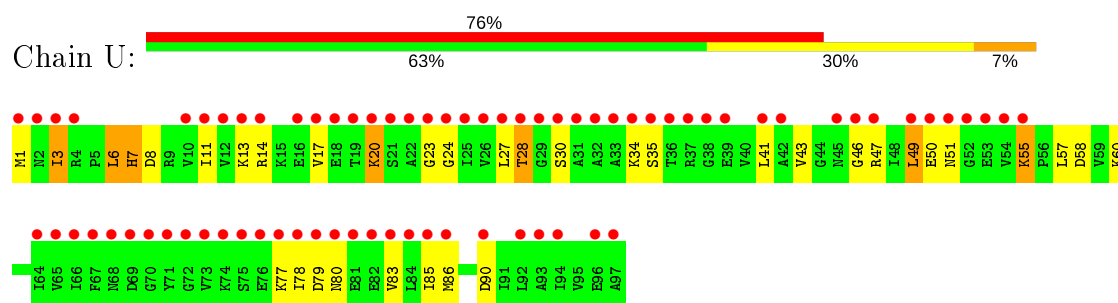
- Molecule 2: groES protein



- Molecule 2: groES protein



- Molecule 2: groES protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	255.26Å 265.25Å 184.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.16 – 2.99 40.07 – 2.99	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.16-2.99) 96.7 (40.07-2.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 3.01Å)	Xtriage
Refinement program	REFMAC refmac_5.1.24 24/04/2001	Depositor
R, R_{free}	0.269 , 0.287 0.272 , 0.289	Depositor DCC
R_{free} test set	12081 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	50.3	Xtriage
Anisotropy	0.614	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 58.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.003 for k,h,-l	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	59283	wwPDB-VP
Average B, all atoms (Å ²)	7.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.22% 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: MG, ADP

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.67	0/3884	0.90	18/5243 (0.3%)
1	B	0.60	0/3884	0.95	18/5243 (0.3%)
1	C	0.64	0/3884	0.91	20/5243 (0.4%)
1	D	0.66	1/3884 (0.0%)	0.90	17/5243 (0.3%)
1	E	0.57	0/3884	0.86	15/5243 (0.3%)
1	F	0.55	0/3884	0.86	17/5243 (0.3%)
1	G	0.64	0/3884	0.91	20/5243 (0.4%)
1	H	0.59	0/3884	0.85	14/5243 (0.3%)
1	I	0.64	0/3884	0.86	15/5243 (0.3%)
1	J	0.61	0/3884	0.87	18/5243 (0.3%)
1	K	0.54	0/3884	0.83	17/5243 (0.3%)
1	L	0.51	0/3884	0.87	20/5243 (0.4%)
1	M	0.59	0/3884	0.90	20/5243 (0.4%)
1	N	0.59	0/3884	0.85	17/5243 (0.3%)
2	O	0.37	0/732	0.73	3/983 (0.3%)
2	P	0.37	0/732	0.73	4/983 (0.4%)
2	Q	0.38	0/732	0.73	2/983 (0.2%)
2	R	0.41	0/732	0.74	4/983 (0.4%)
2	S	0.39	0/732	0.74	4/983 (0.4%)
2	T	0.39	0/732	0.74	3/983 (0.3%)
2	U	0.38	0/732	0.72	3/983 (0.3%)
All	All	0.59	1/59500 (0.0%)	0.87	269/80283 (0.3%)

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	N	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	130	GLU	CD-OE1	5.35	1.31	1.25

The worst 5 of 269 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	231	ARG	NE-CZ-NH1	-19.37	110.61	120.30
1	B	231	ARG	NE-CZ-NH2	18.28	129.44	120.30
1	L	268	ARG	NE-CZ-NH2	14.85	127.72	120.30
1	M	268	ARG	NE-CZ-NH2	14.77	127.68	120.30
1	M	268	ARG	NE-CZ-NH1	-14.67	112.97	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	N	433	ASN	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	3856	0	3976	105	0
1	B	3856	0	3976	99	0
1	C	3856	0	3976	109	0
1	D	3856	0	3976	115	0
1	E	3856	0	3976	104	0
1	F	3856	0	3976	99	0
1	G	3856	0	3976	113	0
1	H	3856	0	3976	107	0
1	I	3856	0	3976	104	0
1	J	3856	0	3976	106	0
1	K	3856	0	3976	110	0
1	L	3856	0	3976	112	0
1	M	3856	0	3976	115	0
1	N	3856	0	3976	111	0
2	O	728	0	762	20	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	P	728	0	762	21	0
2	Q	728	0	762	18	0
2	R	728	0	762	17	0
2	S	728	0	762	19	0
2	T	728	0	762	15	0
2	U	728	0	762	17	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
4	A	27	0	12	2	0
4	B	27	0	12	2	0
4	C	27	0	12	2	0
4	D	27	0	12	3	0
4	E	27	0	12	1	0
4	F	27	0	12	1	0
4	G	27	0	12	3	0
5	A	1	0	0	1	0
5	B	1	0	0	1	0
5	C	1	0	0	1	0
5	D	1	0	0	1	0
5	E	1	0	0	0	0
5	F	1	0	0	0	0
5	G	1	0	0	1	0
All	All	59283	0	61082	1567	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 13.

The worst 5 of 1567 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:114:MET:CE	1:E:114:MET:SD	2.05	1.45
1:C:73:MET:SD	1:C:73:MET:CE	2.05	1.42
1:C:18:ARG:HG2	1:C:18:ARG:HH11	1.07	1.19
1:G:18:ARG:HH11	1:G:18:ARG:HG2	1.07	1.17
1:D:432:GLN:NE2	1:D:436:GLN:HE22	1.47	1.13

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	522/524 (100%)	485 (93%)	33 (6%)	4 (1%)	19	57
1	B	522/524 (100%)	484 (93%)	33 (6%)	5 (1%)	15	53
1	C	522/524 (100%)	484 (93%)	34 (6%)	4 (1%)	19	57
1	D	522/524 (100%)	485 (93%)	32 (6%)	5 (1%)	15	53
1	E	522/524 (100%)	489 (94%)	29 (6%)	4 (1%)	19	57
1	F	522/524 (100%)	490 (94%)	27 (5%)	5 (1%)	15	53
1	G	522/524 (100%)	481 (92%)	36 (7%)	5 (1%)	15	53
1	H	522/524 (100%)	481 (92%)	36 (7%)	5 (1%)	15	53
1	I	522/524 (100%)	483 (92%)	32 (6%)	7 (1%)	12	45
1	J	522/524 (100%)	480 (92%)	38 (7%)	4 (1%)	19	57
1	K	522/524 (100%)	479 (92%)	38 (7%)	5 (1%)	15	53
1	L	522/524 (100%)	483 (92%)	34 (6%)	5 (1%)	15	53
1	M	522/524 (100%)	480 (92%)	37 (7%)	5 (1%)	15	53
1	N	522/524 (100%)	483 (92%)	35 (7%)	4 (1%)	19	57
2	O	95/97 (98%)	77 (81%)	13 (14%)	5 (5%)	2	11
2	P	95/97 (98%)	77 (81%)	13 (14%)	5 (5%)	2	11
2	Q	95/97 (98%)	76 (80%)	13 (14%)	6 (6%)	1	7
2	R	95/97 (98%)	77 (81%)	13 (14%)	5 (5%)	2	11
2	S	95/97 (98%)	77 (81%)	13 (14%)	5 (5%)	2	11
2	T	95/97 (98%)	76 (80%)	13 (14%)	6 (6%)	1	7
2	U	95/97 (98%)	76 (80%)	14 (15%)	5 (5%)	2	11
All	All	7973/8015 (100%)	7303 (92%)	566 (7%)	104 (1%)	12	45

5 of 104 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	PHE
1	B	44	PHE
1	C	44	PHE
1	D	44	PHE
1	E	44	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	404/404 (100%)	359 (89%)	45 (11%)	6	25
1	B	404/404 (100%)	358 (89%)	46 (11%)	5	24
1	C	404/404 (100%)	356 (88%)	48 (12%)	5	22
1	D	404/404 (100%)	357 (88%)	47 (12%)	5	23
1	E	404/404 (100%)	358 (89%)	46 (11%)	5	24
1	F	404/404 (100%)	357 (88%)	47 (12%)	5	23
1	G	404/404 (100%)	354 (88%)	50 (12%)	4	20
1	H	404/404 (100%)	347 (86%)	57 (14%)	3	16
1	I	404/404 (100%)	349 (86%)	55 (14%)	3	17
1	J	404/404 (100%)	349 (86%)	55 (14%)	3	17
1	K	404/404 (100%)	347 (86%)	57 (14%)	3	16
1	L	404/404 (100%)	348 (86%)	56 (14%)	3	16
1	M	404/404 (100%)	347 (86%)	57 (14%)	3	16
1	N	404/404 (100%)	349 (86%)	55 (14%)	3	17
2	O	80/80 (100%)	70 (88%)	10 (12%)	4	20
2	P	80/80 (100%)	70 (88%)	10 (12%)	4	20
2	Q	80/80 (100%)	70 (88%)	10 (12%)	4	20
2	R	80/80 (100%)	69 (86%)	11 (14%)	3	17
2	S	80/80 (100%)	69 (86%)	11 (14%)	3	17

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	T	80/80 (100%)	70 (88%)	10 (12%)	4	20
2	U	80/80 (100%)	69 (86%)	11 (14%)	3	17
All	All	6216/6216 (100%)	5422 (87%)	794 (13%)	4	19

5 of 794 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	300	VAL
1	J	37	ASN
2	P	6	LEU
1	H	385	THR
1	I	187	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 135 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	153	ASN
1	H	436	GLN
2	P	68	ASN
1	G	265	ASN
1	H	21	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 14 ligands modelled in this entry, 7 are monoatomic - leaving 7 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	ADP	A	700	3	24,29,29	1.30	4 (16%)	29,45,45	2.23	10 (34%)
4	ADP	B	701	3	24,29,29	1.44	4 (16%)	29,45,45	2.20	8 (27%)
4	ADP	E	704	3	24,29,29	1.31	3 (12%)	29,45,45	2.12	8 (27%)
4	ADP	G	706	3	24,29,29	1.28	1 (4%)	29,45,45	2.20	8 (27%)
4	ADP	D	703	3	24,29,29	1.53	5 (20%)	29,45,45	2.27	11 (37%)
4	ADP	F	705	3	24,29,29	1.16	2 (8%)	29,45,45	2.02	7 (24%)
4	ADP	C	702	3	24,29,29	1.25	3 (12%)	29,45,45	2.37	10 (34%)

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	ADP	A	700	3	-	4/12/32/32	0/3/3/3
4	ADP	B	701	3	-	4/12/32/32	0/3/3/3
4	ADP	E	704	3	-	4/12/32/32	0/3/3/3
4	ADP	G	706	3	-	4/12/32/32	0/3/3/3
4	ADP	D	703	3	-	4/12/32/32	0/3/3/3
4	ADP	F	705	3	-	4/12/32/32	0/3/3/3
4	ADP	C	702	3	-	4/12/32/32	0/3/3/3

The worst 5 of 22 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	706	ADP	C2-N3	4.43	1.39	1.32
4	B	701	ADP	C2-N3	4.17	1.38	1.32
4	D	703	ADP	C2-N3	3.88	1.38	1.32
4	A	700	ADP	C2-N3	3.77	1.38	1.32
4	E	704	ADP	C2-N3	3.74	1.38	1.32

The worst 5 of 62 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	703	ADP	N3-C2-N1	-6.41	118.65	128.68
4	A	700	ADP	N3-C2-N1	-6.04	119.24	128.68
4	F	705	ADP	N3-C2-N1	-5.75	119.69	128.68
4	C	702	ADP	N3-C2-N1	-5.56	119.99	128.68
4	E	704	ADP	N3-C2-N1	-5.54	120.02	128.68

There are no chirality outliers.

5 of 28 torsion outliers are listed below:

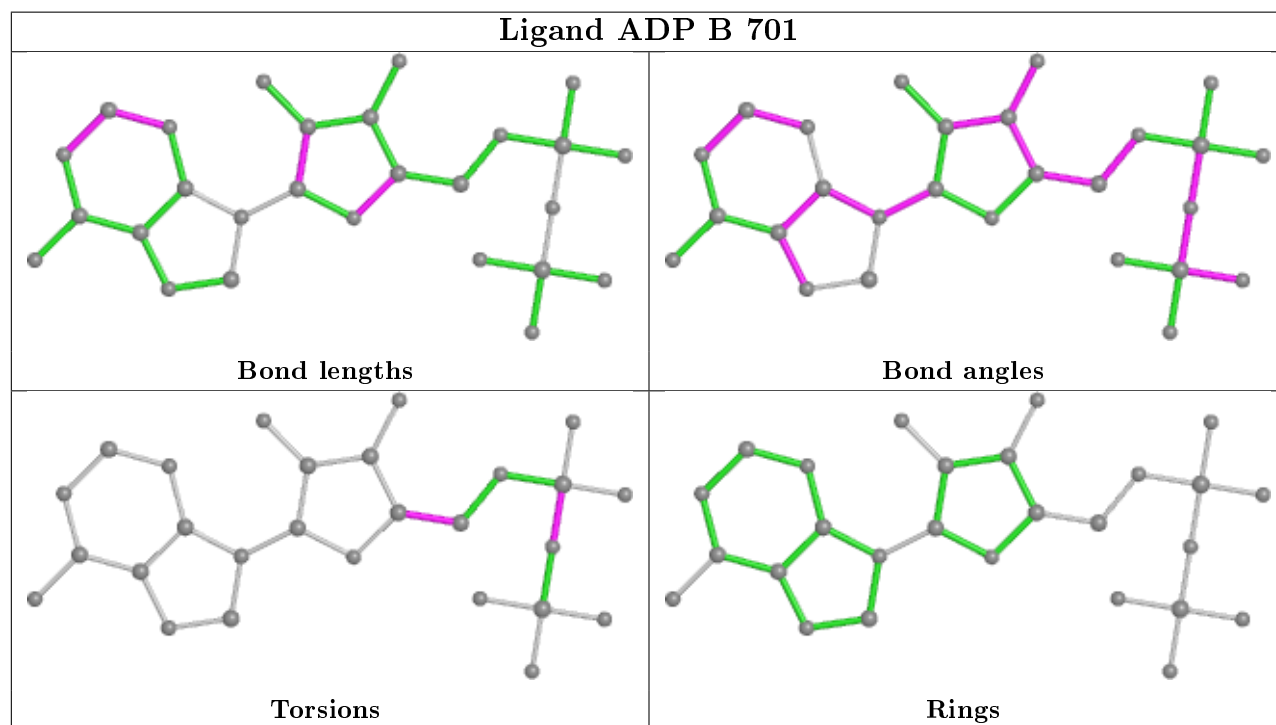
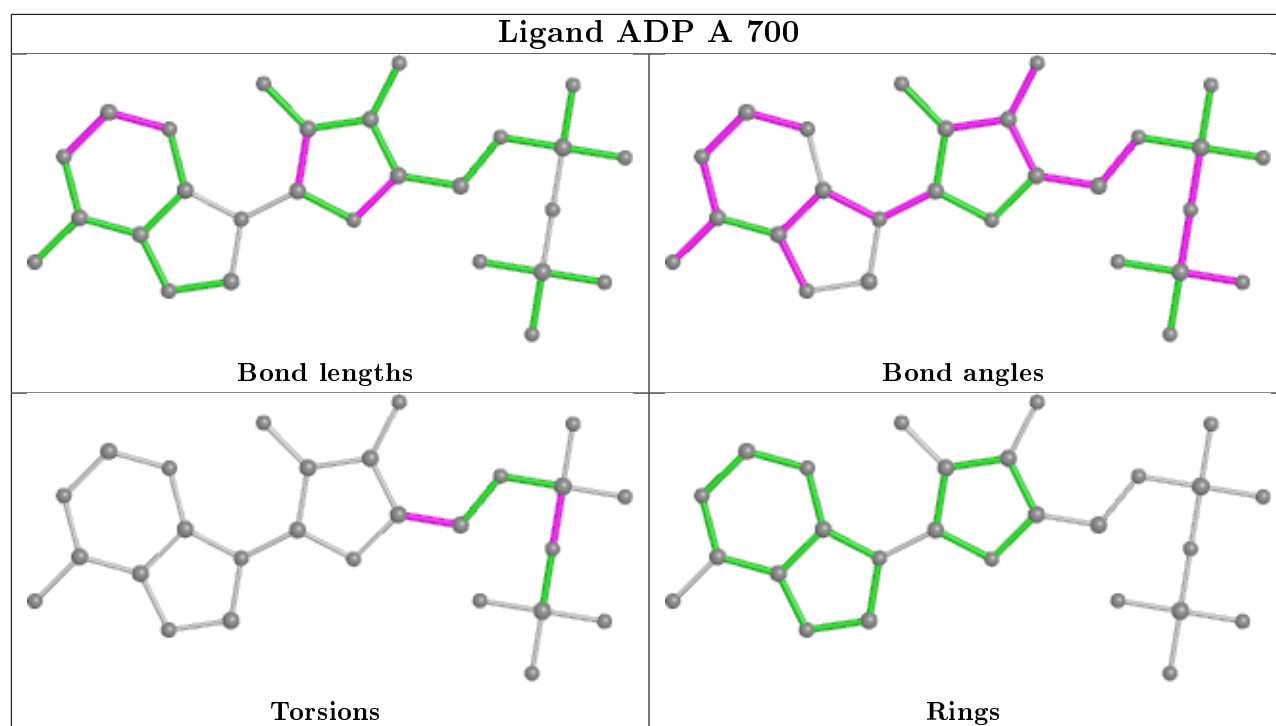
Mol	Chain	Res	Type	Atoms
4	B	701	ADP	O4'-C4'-C5'-O5'
4	A	700	ADP	O4'-C4'-C5'-O5'
4	E	704	ADP	O4'-C4'-C5'-O5'
4	G	706	ADP	O4'-C4'-C5'-O5'
4	G	706	ADP	C3'-C4'-C5'-O5'

There are no ring outliers.

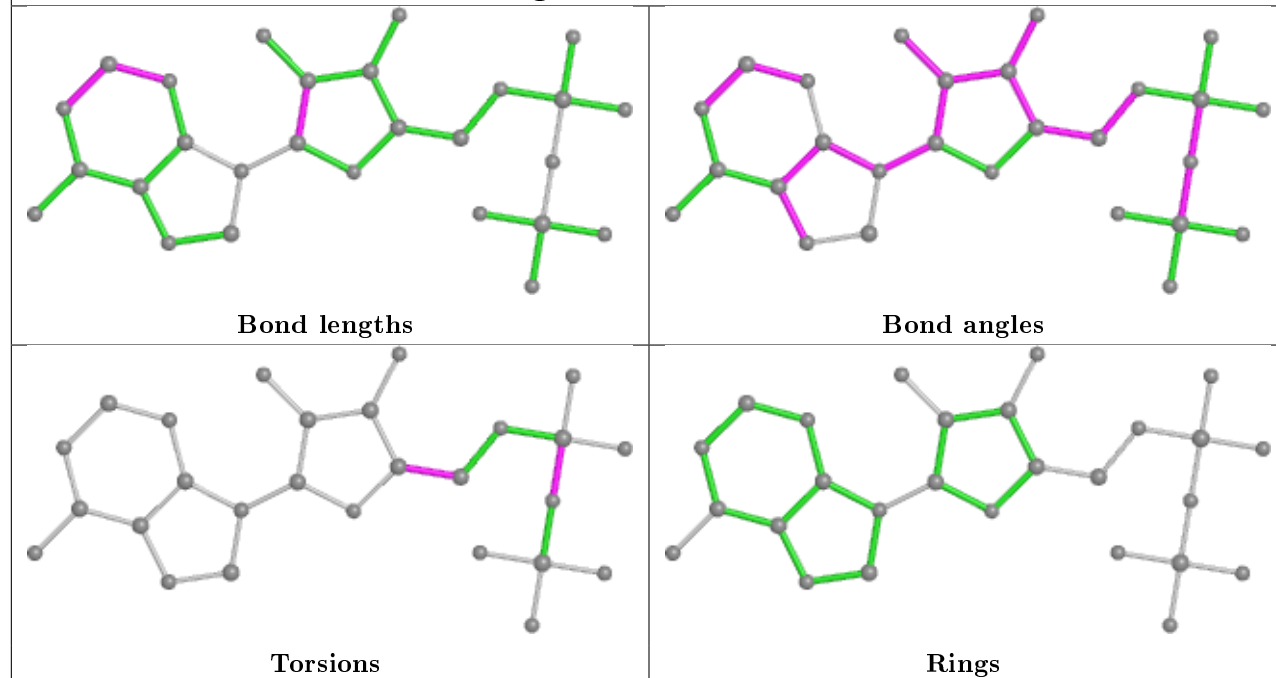
7 monomers are involved in 14 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	700	ADP	2	0
4	B	701	ADP	2	0
4	E	704	ADP	1	0
4	G	706	ADP	3	0
4	D	703	ADP	3	0
4	F	705	ADP	1	0
4	C	702	ADP	2	0

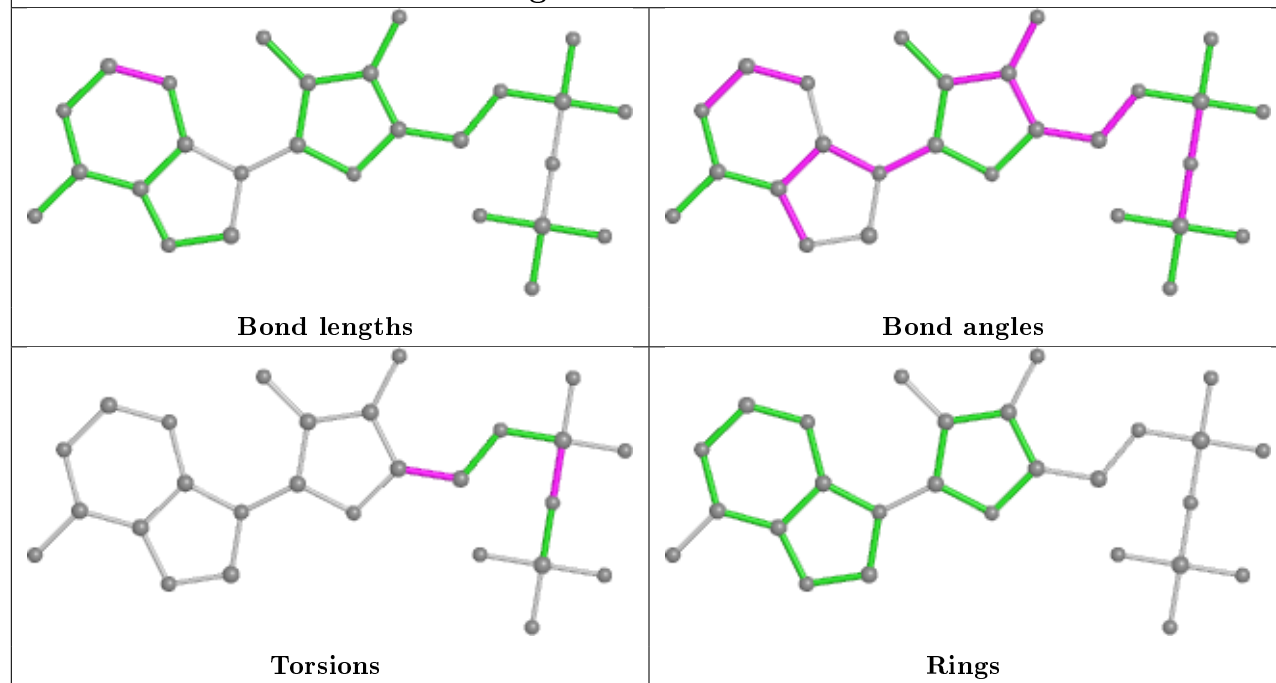
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



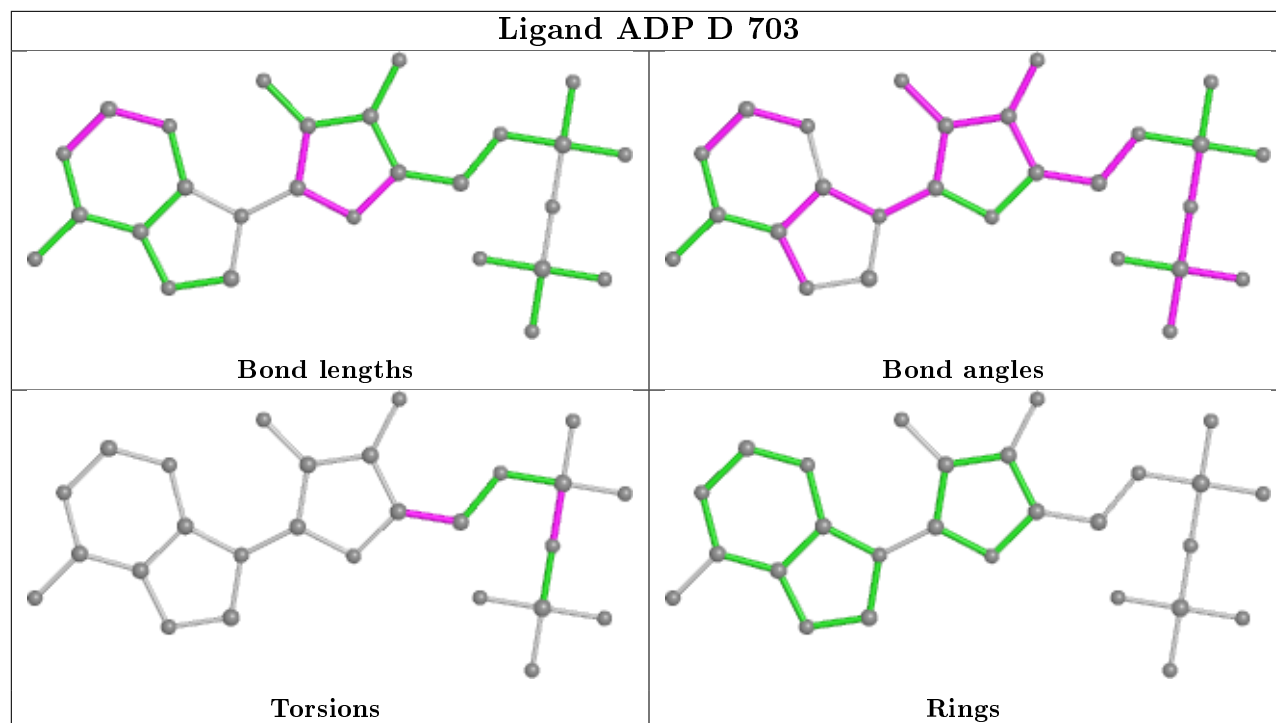
Ligand ADP E 704



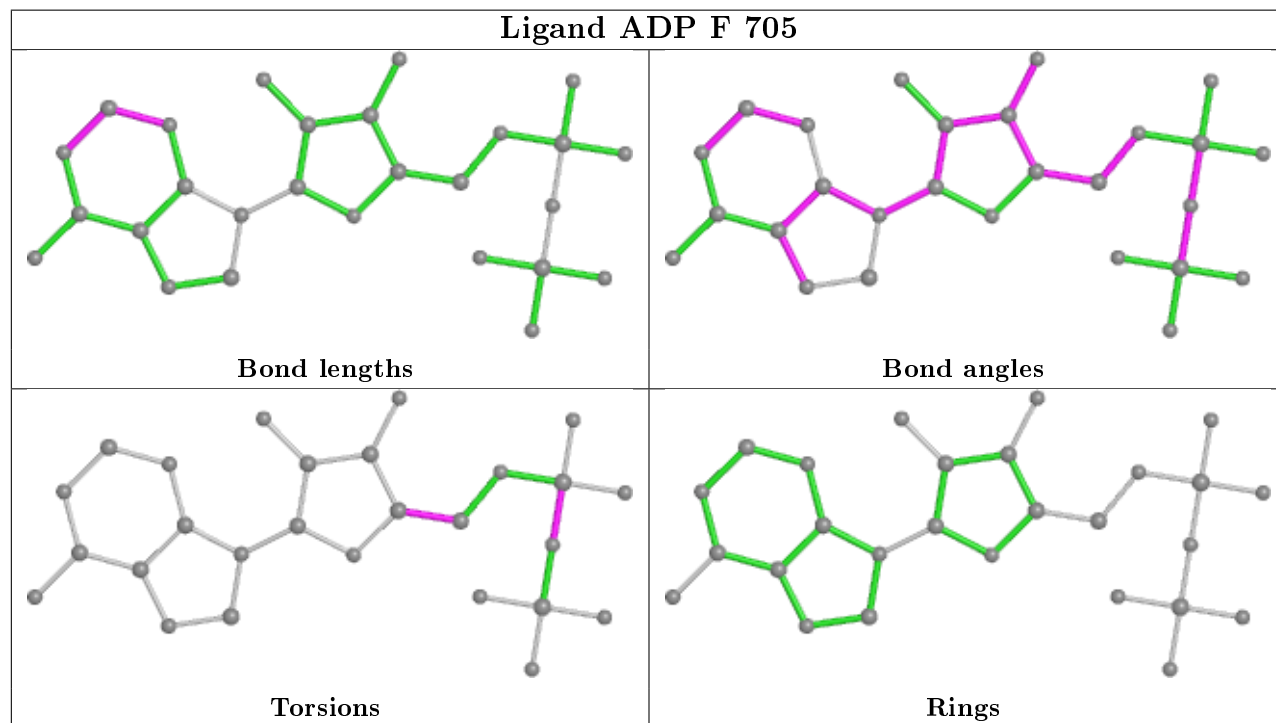
Ligand ADP G 706

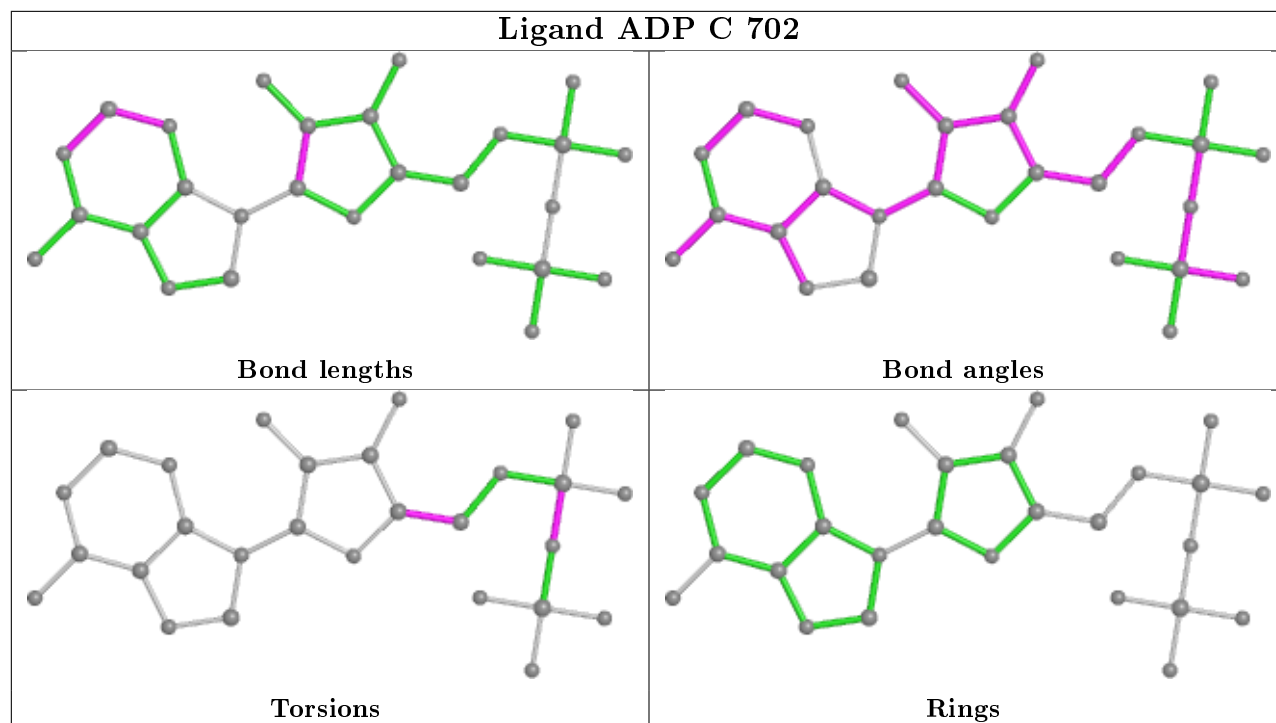


Ligand ADP D 703



Ligand ADP F 705





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	524/524 (100%)	0.60	58 (11%) 5 1	5, 7, 9, 10	0
1	B	524/524 (100%)	0.70	62 (11%) 4 1	5, 7, 9, 10	0
1	C	524/524 (100%)	0.49	49 (9%) 8 3	5, 7, 9, 10	0
1	D	524/524 (100%)	0.53	54 (10%) 6 2	5, 7, 9, 10	0
1	E	524/524 (100%)	0.79	62 (11%) 4 1	5, 7, 9, 10	0
1	F	524/524 (100%)	0.85	72 (13%) 3 1	5, 7, 9, 10	0
1	G	524/524 (100%)	0.68	65 (12%) 4 1	5, 7, 9, 10	0
1	H	524/524 (100%)	0.33	19 (3%) 42 17	6, 7, 9, 10	0
1	I	524/524 (100%)	0.30	12 (2%) 60 31	5, 7, 9, 10	0
1	J	524/524 (100%)	0.42	28 (5%) 26 10	5, 7, 9, 10	0
1	K	524/524 (100%)	0.58	44 (8%) 11 3	5, 7, 9, 10	0
1	L	524/524 (100%)	0.63	42 (8%) 12 4	5, 7, 9, 10	0
1	M	524/524 (100%)	0.48	35 (6%) 17 5	5, 7, 9, 10	0
1	N	524/524 (100%)	0.52	31 (5%) 22 7	5, 7, 9, 10	0
2	O	97/97 (100%)	1.73	34 (35%) 0 0	7, 7, 8, 8	0
2	P	97/97 (100%)	1.60	27 (27%) 0 0	7, 7, 8, 8	0
2	Q	97/97 (100%)	1.40	29 (29%) 0 0	7, 7, 8, 8	0
2	R	97/97 (100%)	1.50	25 (25%) 0 0	7, 7, 8, 8	0
2	S	97/97 (100%)	1.72	29 (29%) 0 0	7, 7, 8, 8	0
2	T	97/97 (100%)	1.55	27 (27%) 0 0	7, 7, 8, 8	0
2	U	97/97 (100%)	3.19	74 (76%) 0 0	7, 7, 8, 8	0
All	All	8015/8015 (100%)	0.67	878 (10%) 5 2	5, 7, 9, 10	0

The worst 5 of 878 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	361	ASP	16.6
1	F	361	ASP	10.5
1	E	361	ASP	10.2
1	A	361	ASP	9.9
1	G	199	TYR	9.5

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

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

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

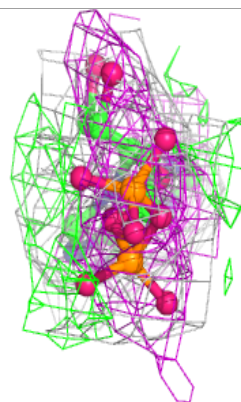
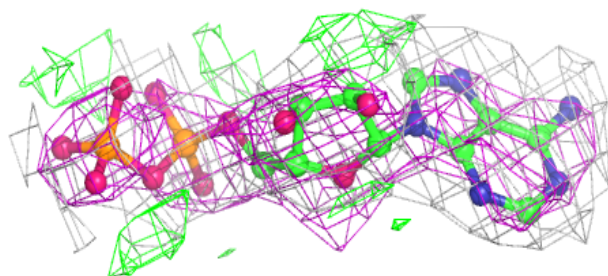
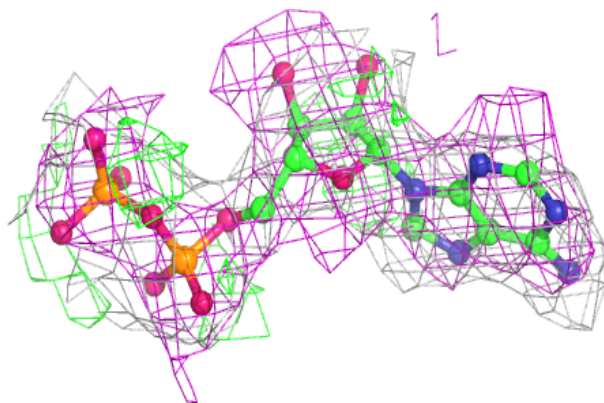
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	ADP	E	704	27/27	0.89	0.19	6,8,9,10	0
4	ADP	B	701	27/27	0.90	0.20	6,8,9,10	0
4	ADP	F	705	27/27	0.91	0.21	6,8,9,10	0
4	ADP	A	700	27/27	0.92	0.18	6,8,9,11	0
4	ADP	D	703	27/27	0.93	0.17	6,8,9,10	0
3	MG	B	602	1/1	0.94	0.21	2,2,2,2	0
4	ADP	G	706	27/27	0.94	0.15	6,8,9,10	0
3	MG	C	603	1/1	0.95	0.18	2,2,2,2	0
4	ADP	C	702	27/27	0.95	0.13	6,8,9,10	0
3	MG	A	601	1/1	0.96	0.28	2,2,2,2	0
3	MG	F	606	1/1	0.96	0.27	2,2,2,2	0
3	MG	D	604	1/1	0.97	0.32	2,2,2,2	0
3	MG	E	605	1/1	0.97	0.18	2,2,2,2	0
3	MG	G	607	1/1	0.98	0.20	2,2,2,2	0

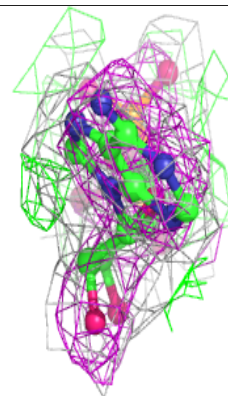
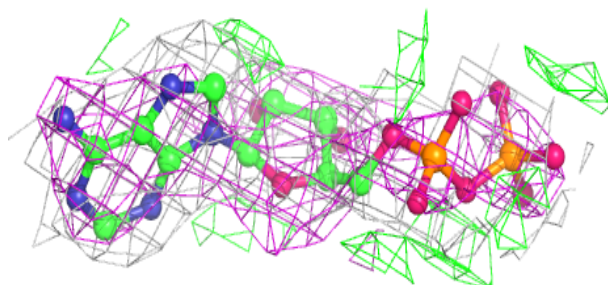
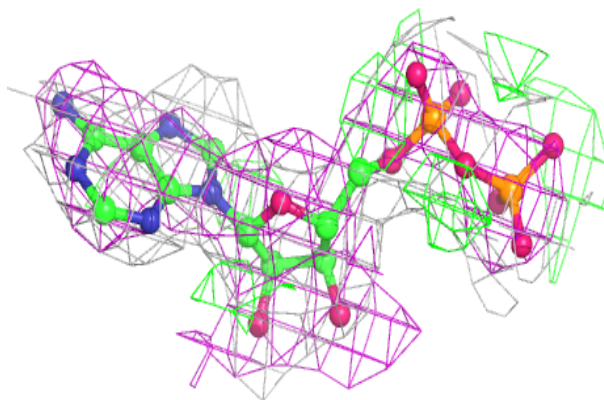
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ADP E 704:

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

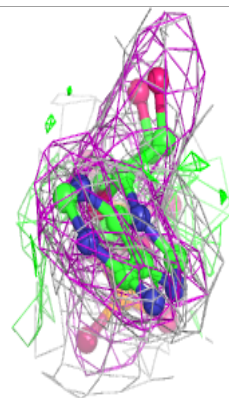
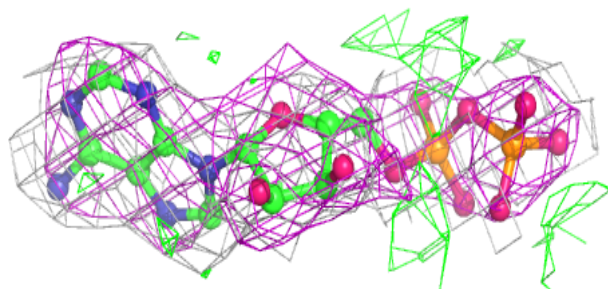
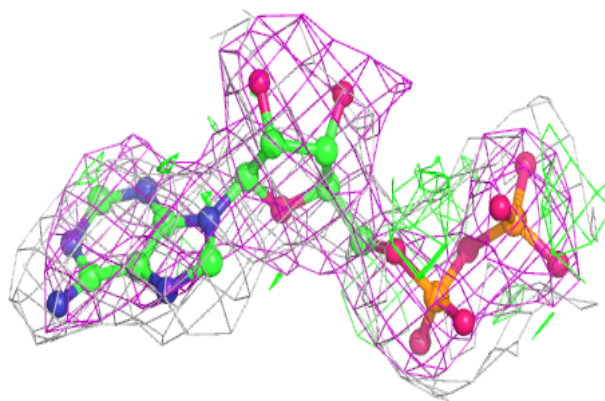
**Electron density around ADP B 701:**

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

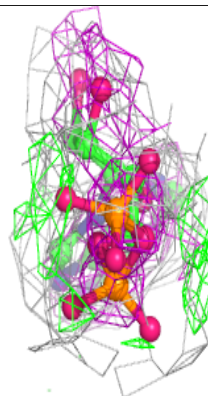
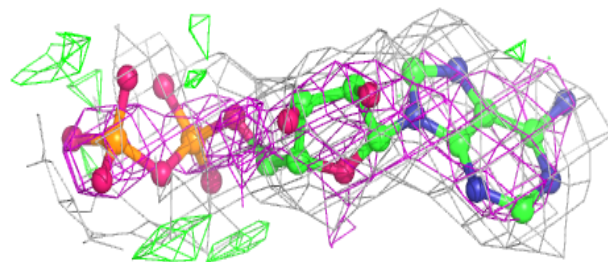
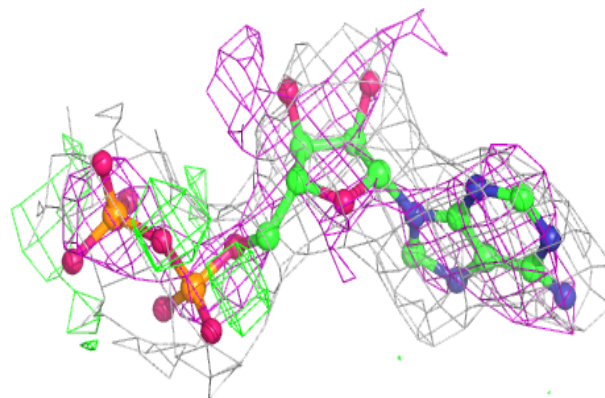


Electron density around ADP F 705:

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

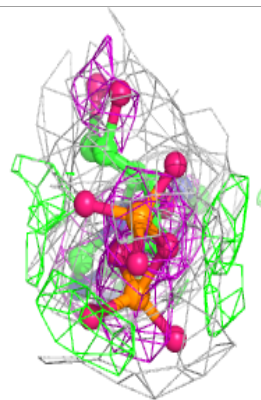
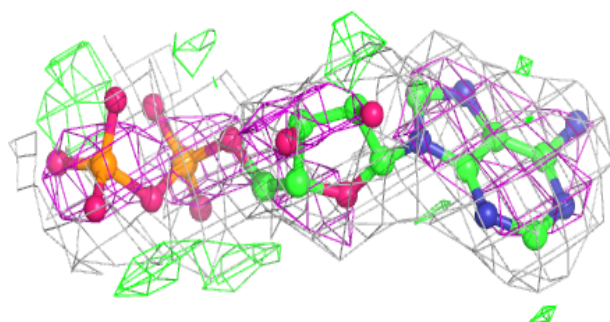
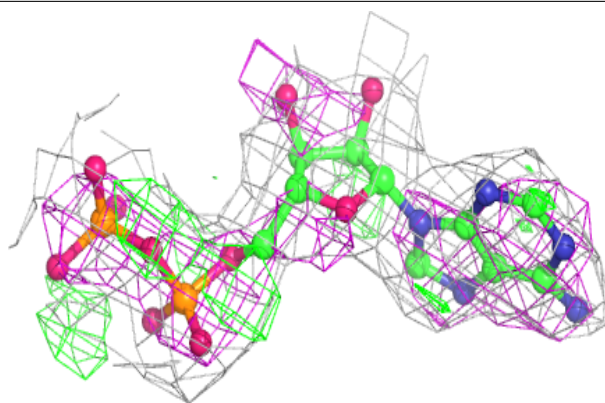
**Electron density around ADP A 700:**

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

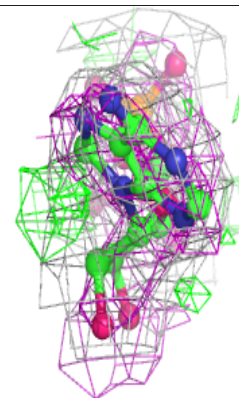
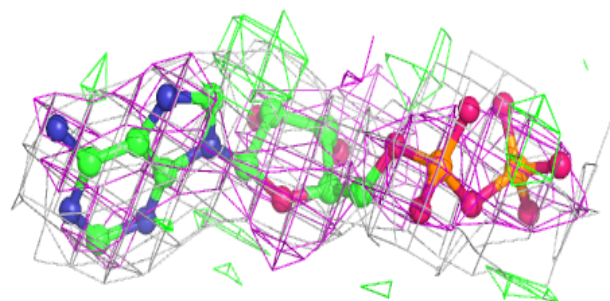
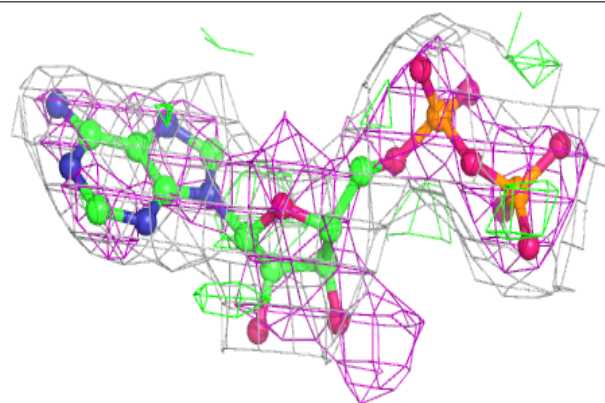


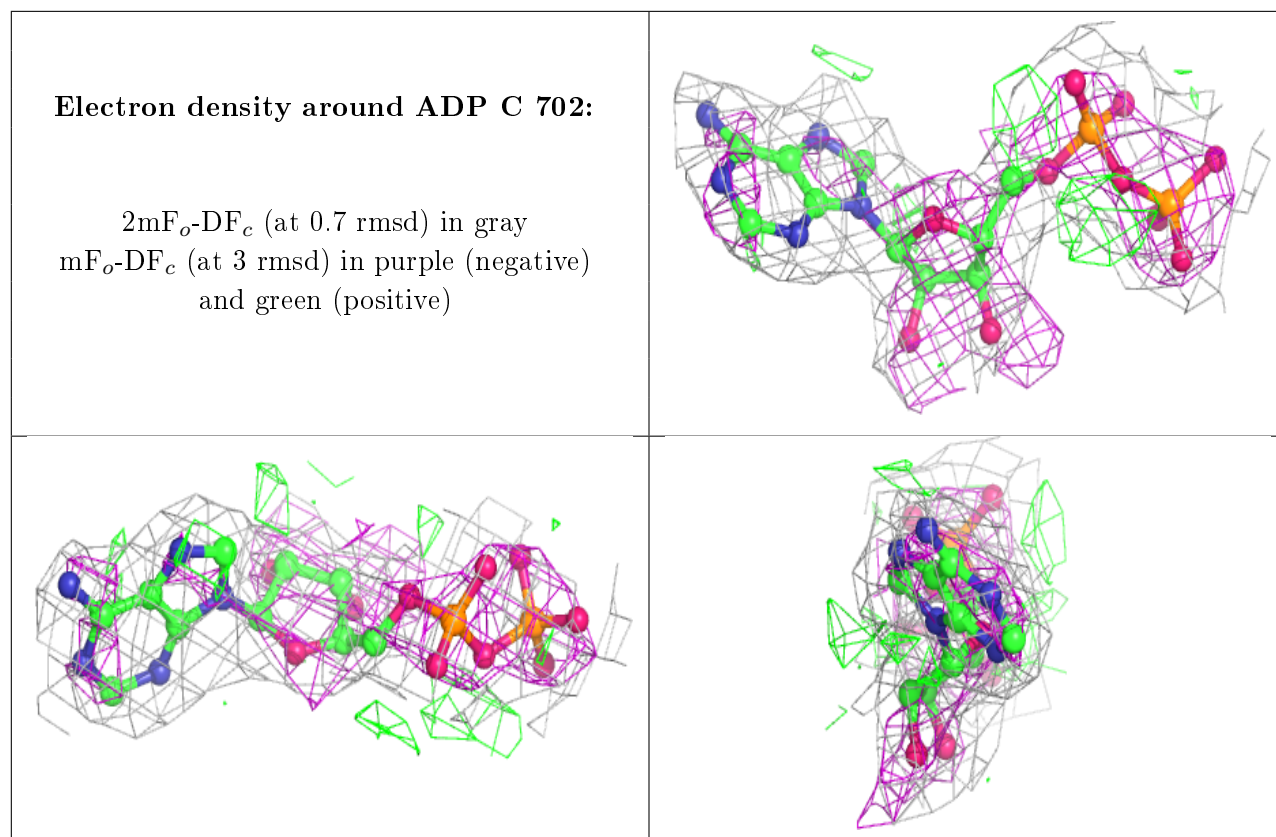
Electron density around ADP D 703:

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

**Electron density around ADP G 706:**

$2mF_o-DF_c$ (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.