



# wwPDB X-ray Structure Validation Summary Report ⓘ

Feb 15, 2017 – 07:50 pm GMT

PDB ID : 1AON  
Title : CRYSTAL STRUCTURE OF THE ASYMMETRIC CHAPERONIN COMPLEX GROEL/GROES/(ADP)7  
Authors : Xu, Z.; Horwich, A.L.; Sigler, P.B.  
Deposited on : 1997-07-08  
Resolution : 3.00 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

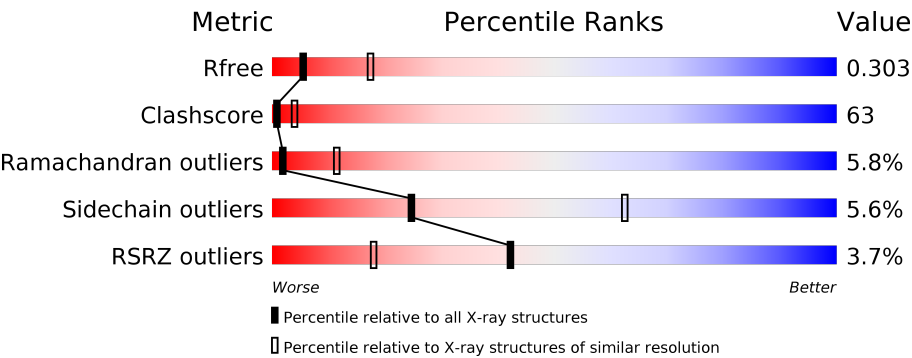
MolProbity	:	4.02b-467
Mogul	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk28620

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 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))
$R_{free}$	100719	1692 (3.00-3.00)
Clashscore	112137	2037 (3.00-3.00)
Ramachandran outliers	110173	1973 (3.00-3.00)
Sidechain outliers	110143	1976 (3.00-3.00)
RSRZ outliers	101464	1716 (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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	547	<div><div>3%</div><div><div></div><div>29%</div><div>58%</div><div>8%</div><div></div></div><div></div></div>
1	B	547	<div><div>3%</div><div><div></div><div>29%</div><div>58%</div><div>8%</div><div></div></div><div></div></div>
1	C	547	<div><div>3%</div><div><div></div><div>29%</div><div>57%</div><div>9%</div><div></div></div><div></div></div>
1	D	547	<div><div>3%</div><div><div></div><div>30%</div><div>58%</div><div>8%</div><div></div></div><div></div></div>
1	E	547	<div><div>6%</div><div><div></div><div>28%</div><div>59%</div><div>9%</div><div></div></div><div></div></div>
1	F	547	<div><div>5%</div><div><div></div><div>27%</div><div>60%</div><div>8%</div><div></div></div><div></div></div>

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Mol	Chain	Length	Quality of chain
1	G	547	
1	H	547	
1	I	547	
1	J	547	
1	K	547	
1	L	547	
1	M	547	
1	N	547	
2	O	97	
2	P	97	
2	Q	97	
2	R	97	
2	S	97	
2	T	97	
2	U	97	

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	ADP	A	1	-	-	-	X
4	ADP	B	1	-	-	-	X

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 58870 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	524	Total	C	N	O	S	0	0	0
			3808	2368	653	767	20			
1	B	524	Total	C	N	O	S	0	0	0
			3808	2368	653	767	20			
1	C	524	Total	C	N	O	S	0	0	0
			3808	2368	653	767	20			
1	D	524	Total	C	N	O	S	0	0	0
			3808	2368	653	767	20			
1	E	524	Total	C	N	O	S	0	0	0
			3808	2368	653	767	20			
1	F	524	Total	C	N	O	S	0	0	0
			3808	2368	653	767	20			
1	G	524	Total	C	N	O	S	0	0	0
			3808	2368	653	767	20			
1	H	524	Total	C	N	O	S	0	0	0
			3849	2394	662	773	20			
1	I	524	Total	C	N	O	S	0	0	0
			3849	2394	662	773	20			
1	J	524	Total	C	N	O	S	0	0	0
			3849	2394	662	773	20			
1	K	524	Total	C	N	O	S	0	0	0
			3849	2394	662	773	20			
1	L	524	Total	C	N	O	S	0	0	0
			3849	2394	662	773	20			
1	M	524	Total	C	N	O	S	0	0	0
			3849	2394	662	773	20			
1	N	524	Total	C	N	O	S	0	0	0
			3849	2394	662	773	20			

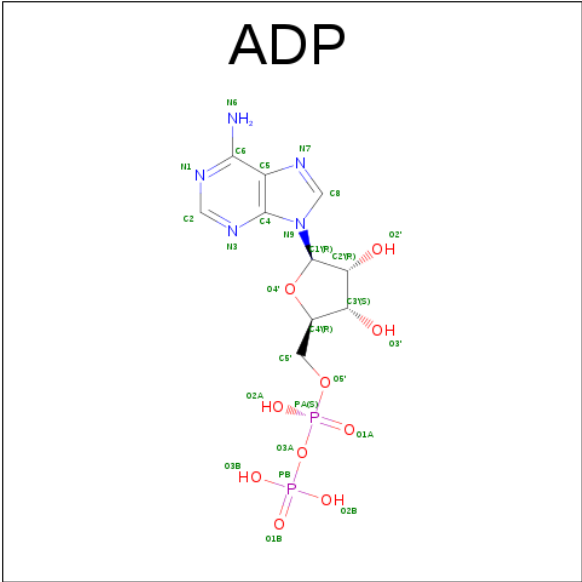
- Molecule 2 is a protein called GROEL/GROES COMPLEX.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	O	97	Total	C	N	O	S	0	0	0
			725	452	127	145	1			
2	P	97	Total	C	N	O	S	0	0	0
			725	452	127	145	1			
2	Q	97	Total	C	N	O	S	0	0	0
			725	452	127	145	1			
2	R	97	Total	C	N	O	S	0	0	0
			725	452	127	145	1			
2	S	97	Total	C	N	O	S	0	0	0
			725	452	127	145	1			
2	T	97	Total	C	N	O	S	0	0	0
			725	452	127	145	1			
2	U	97	Total	C	N	O	S	0	0	0
			725	452	127	145	1			

- 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		

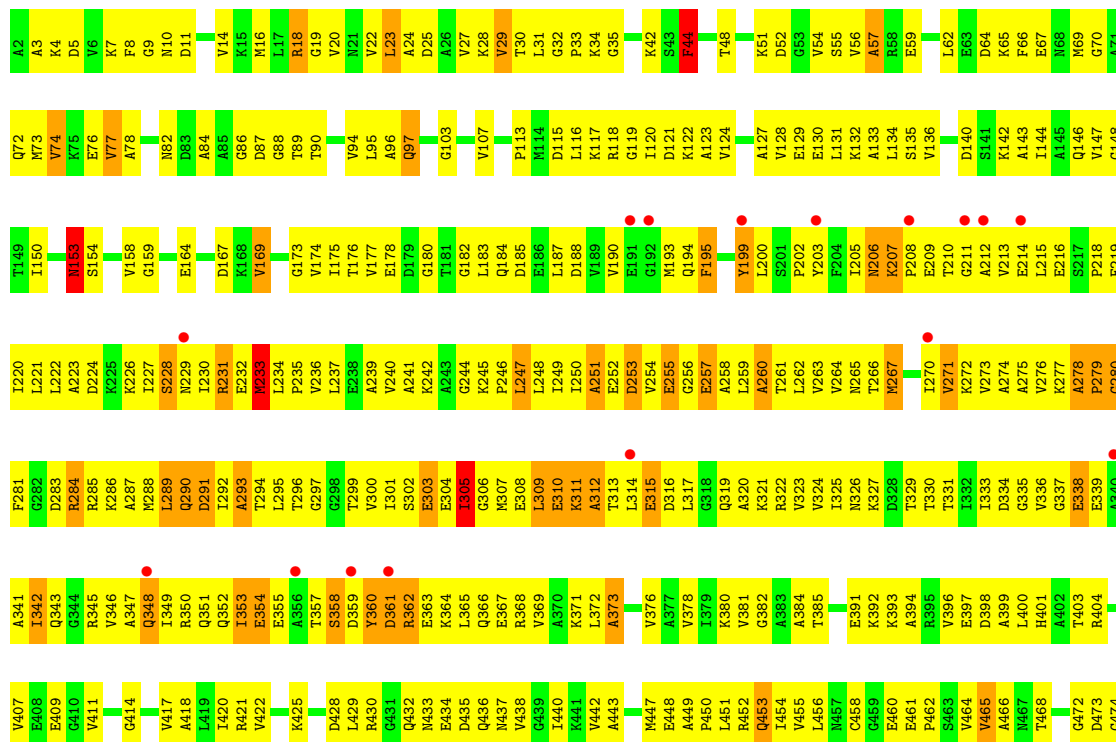
- Molecule 4 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C<sub>10</sub>H<sub>15</sub>N<sub>5</sub>O<sub>10</sub>P<sub>2</sub>).



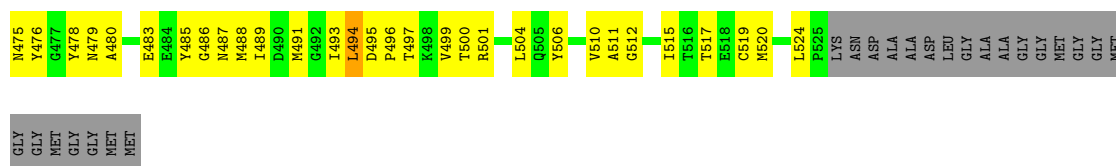
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	E	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
4	G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



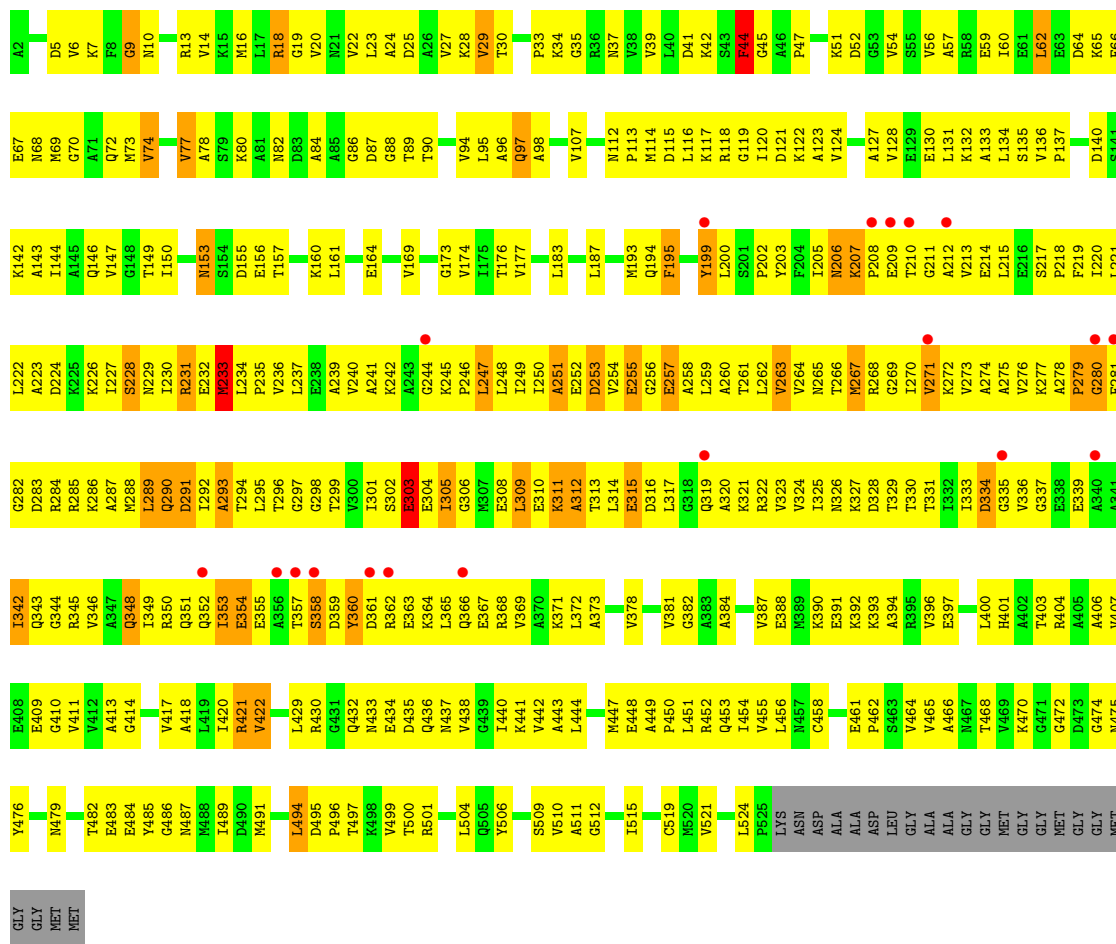
- Molecule 1: GROEL



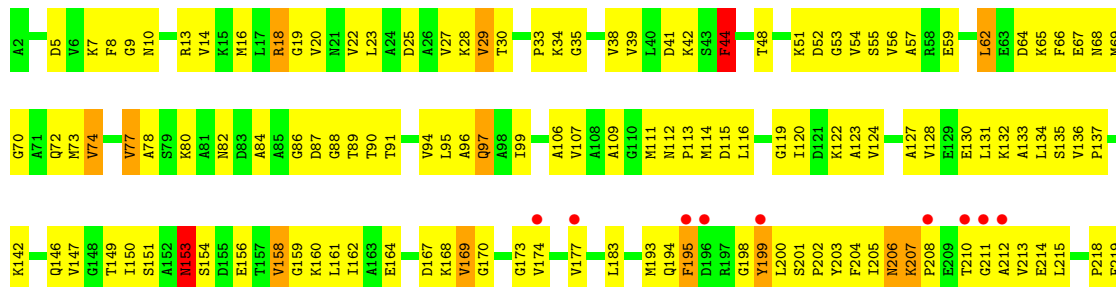




### • Molecule 1: GROEL

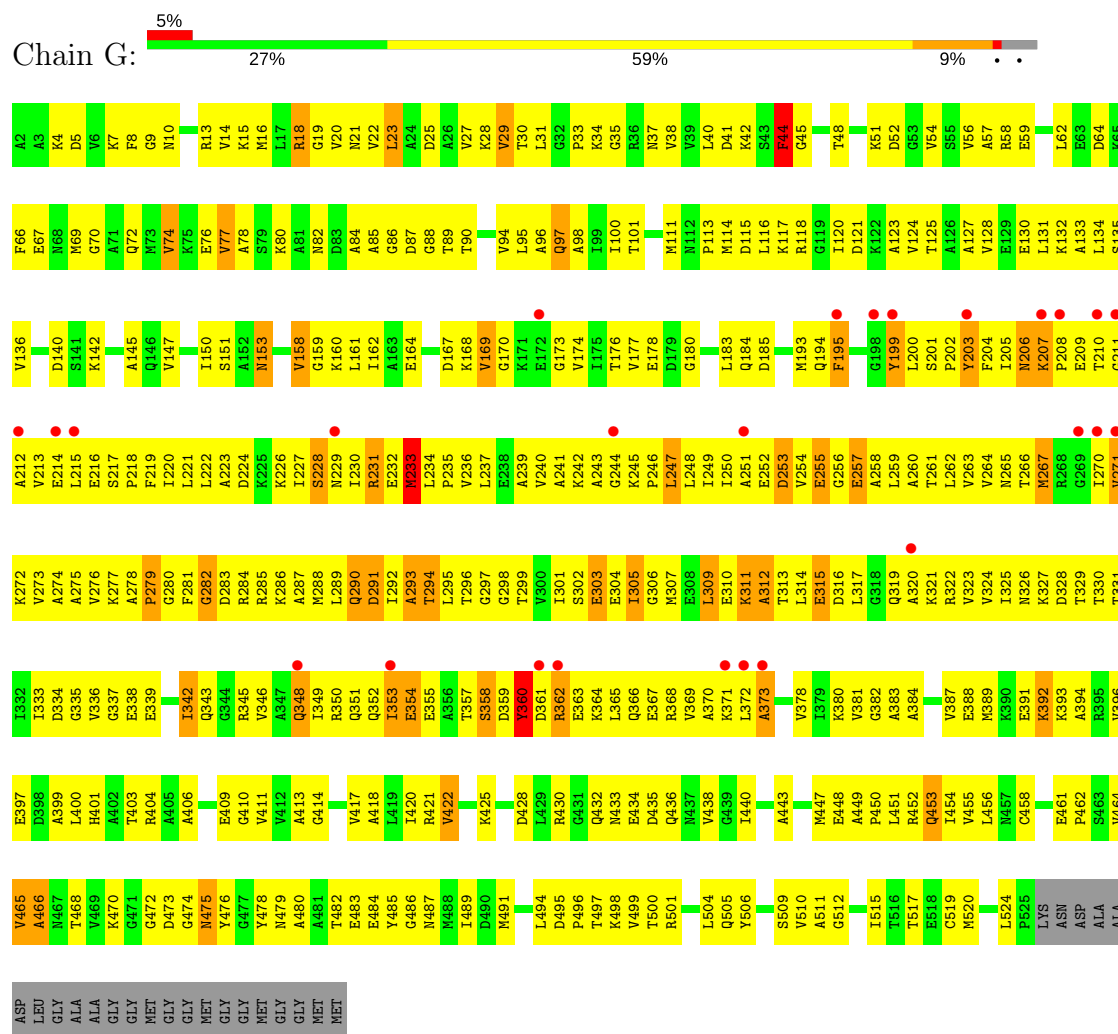


### • Molecule 1: GROEL

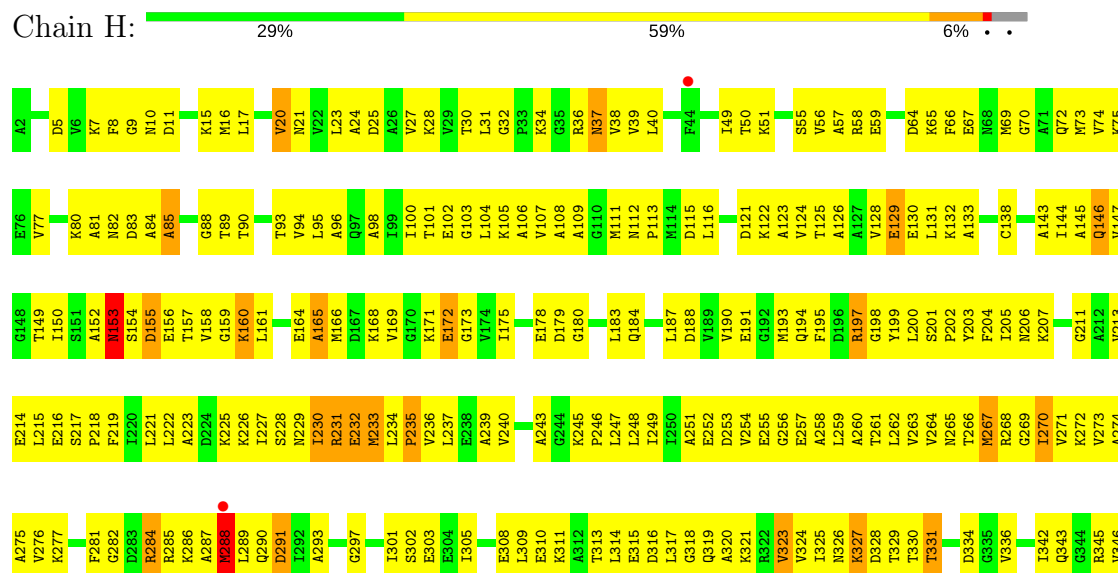




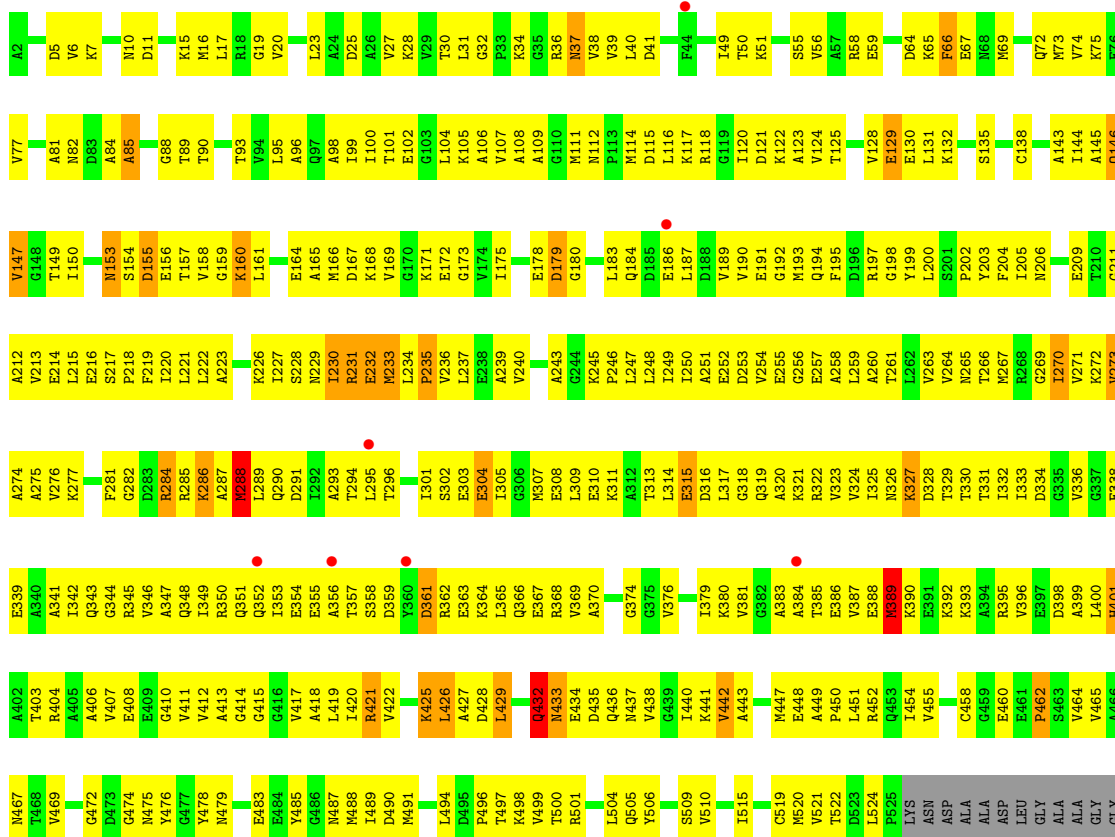
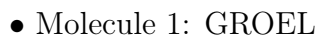
• Molecule 1: GROEL



• Molecule 1: GROEL



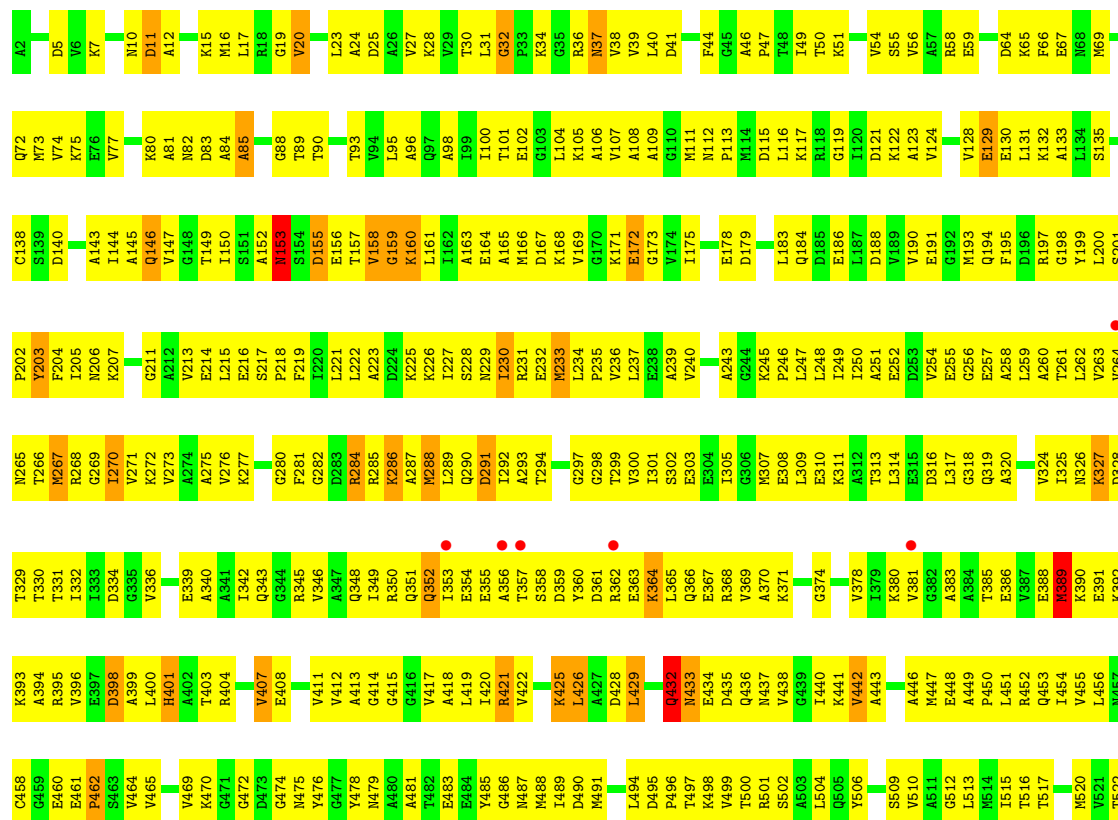


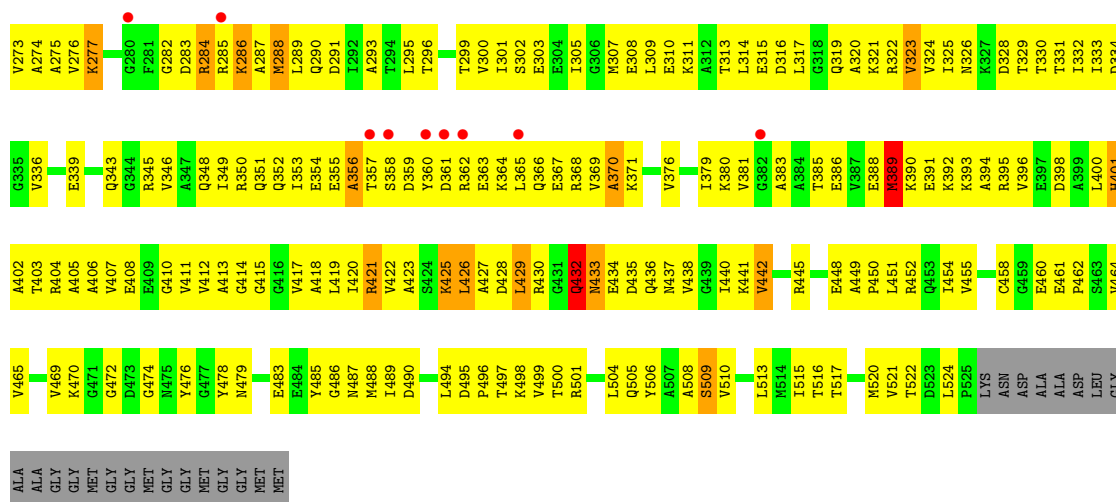


MET  
GLY  
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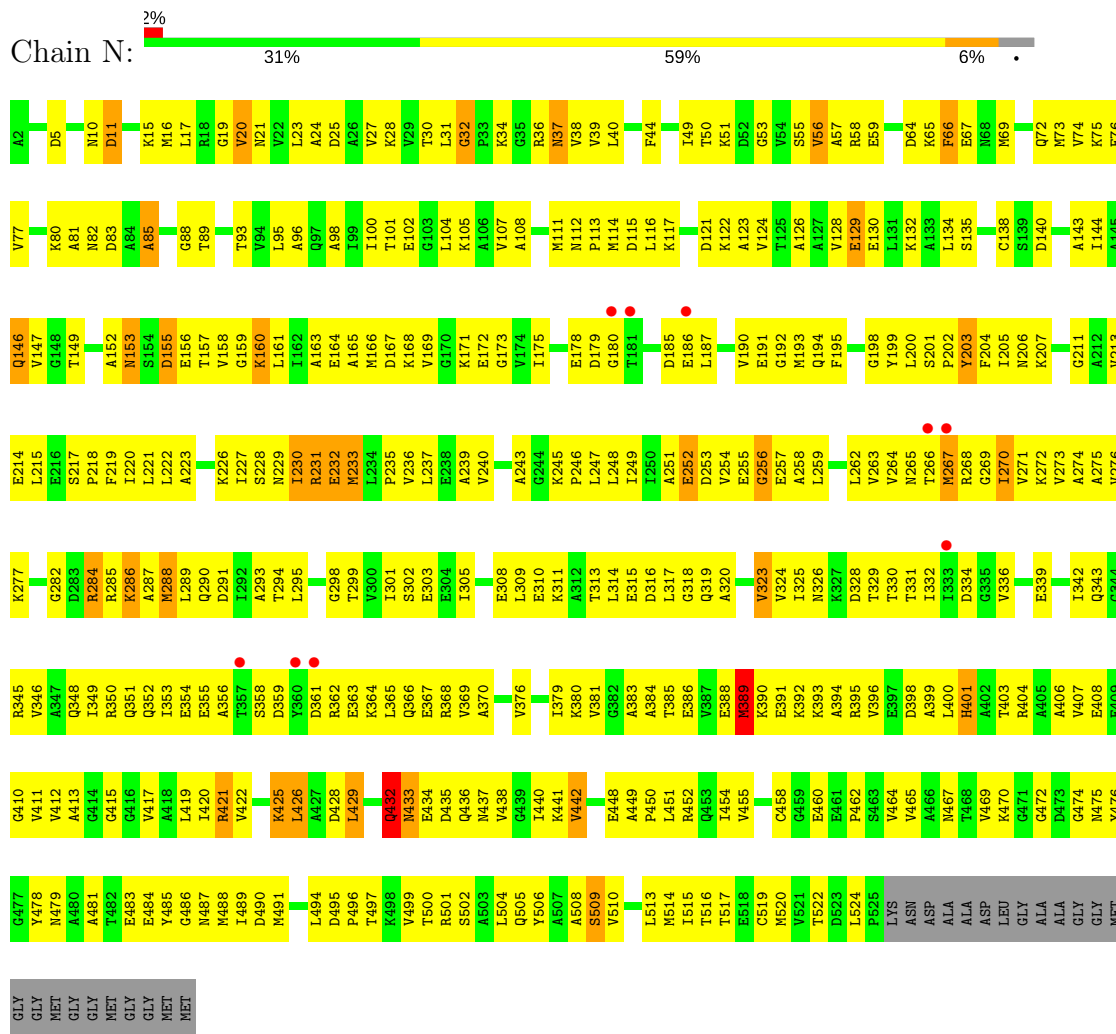
• Molecule 1: GROEL

Chain L: 27% 62% 6%



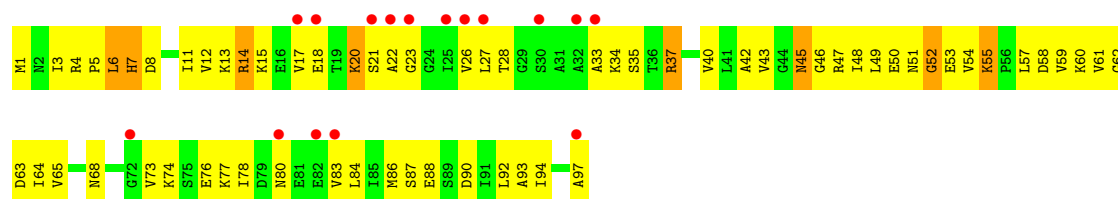


### • Molecule 1: GROEL

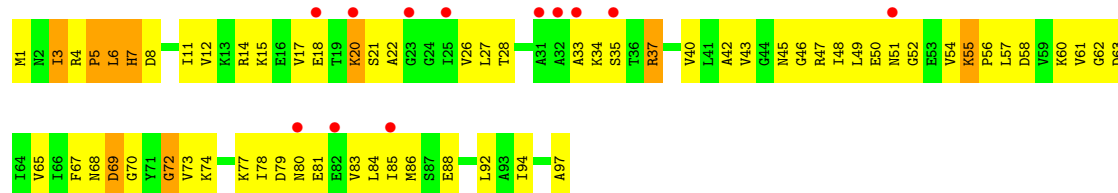


### • Molecule 2: GROEL/GROES COMPLEX

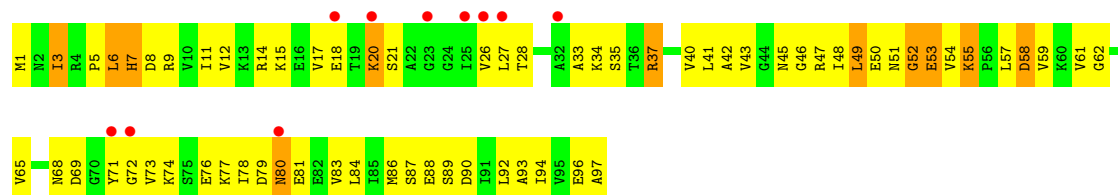




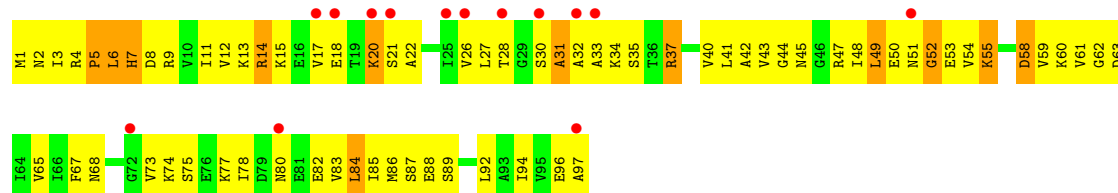
• Molecule 2: GROEL/GROES COMPLEX



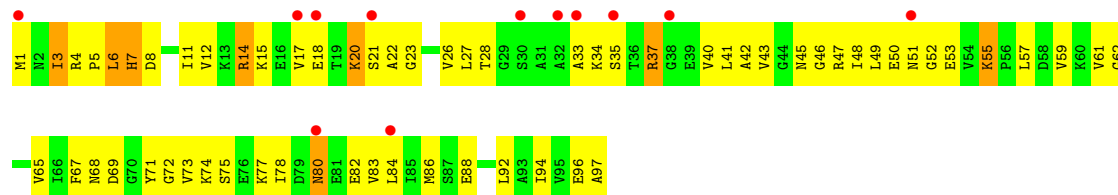
• Molecule 2: GROEL/GROES COMPLEX



• Molecule 2: GROEL/GROES COMPLEX

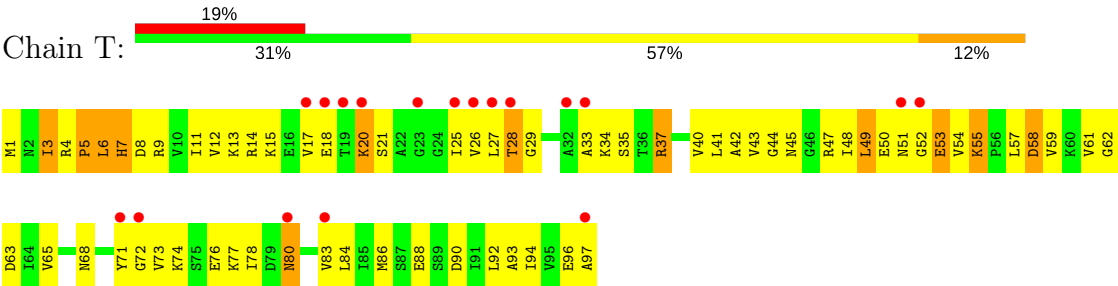


• Molecule 2: GROEL/GROES COMPLEX

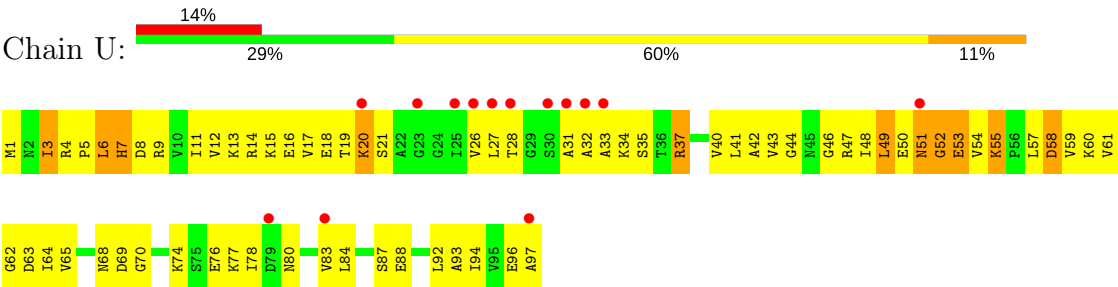


• Molecule 2: GROEL/GROES COMPLEX





● Molecule 2: GROEL/GROES COMPLEX



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	255.26Å 265.25Å 184.40Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.00 40.07 – 2.99	Depositor EDS
% Data completeness (in resolution range)	79.7 (40.00-3.00) 96.7 (40.07-2.99)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.12	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.25 (at 3.01Å)	Xtriage
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.248 , 0.291 0.266 , 0.303	Depositor DCC
$R_{free}$ test set	12040 reflections (4.98%)	DCC
Wilson B-factor (Å <sup>2</sup> )	50.3	Xtriage
Anisotropy	0.614	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 70.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.003 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	58870	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	61.0	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.52	0/3835	0.76	0/5186
1	B	0.52	0/3835	0.75	0/5186
1	C	0.52	0/3835	0.74	0/5186
1	D	0.53	0/3835	0.74	0/5186
1	E	0.52	0/3835	0.76	0/5186
1	F	0.52	0/3835	0.75	0/5186
1	G	0.52	0/3835	0.75	0/5186
1	H	0.48	0/3877	0.73	0/5236
1	I	0.49	0/3877	0.71	0/5236
1	J	0.47	0/3877	0.72	0/5236
1	K	0.47	0/3877	0.72	0/5236
1	L	0.46	0/3877	0.72	0/5236
1	M	0.47	0/3877	0.71	0/5236
1	N	0.48	0/3877	0.73	0/5236
2	O	0.39	0/729	0.68	0/980
2	P	0.36	0/729	0.68	0/980
2	Q	0.37	0/729	0.69	0/980
2	R	0.40	0/729	0.69	0/980
2	S	0.37	0/729	0.69	0/980
2	T	0.39	0/729	0.69	0/980
2	U	0.36	0/729	0.68	0/980
All	All	0.49	0/59087	0.73	0/79814

There are no bond length outliers.

There are no bond angle outliers.

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	3808	0	3890	563	1
1	B	3808	0	3890	513	0
1	C	3808	0	3890	525	0
1	D	3808	0	3890	527	0
1	E	3808	0	3890	537	0
1	F	3808	0	3890	556	0
1	G	3808	0	3890	535	0
1	H	3849	0	3965	479	0
1	I	3849	0	3965	439	0
1	J	3849	0	3965	444	1
1	K	3849	0	3965	479	0
1	L	3849	0	3965	504	0
1	M	3849	0	3965	486	0
1	N	3849	0	3965	435	0
2	O	725	0	755	119	0
2	P	725	0	755	98	0
2	Q	725	0	755	106	0
2	R	725	0	755	104	0
2	S	725	0	755	98	0
2	T	725	0	755	112	0
2	U	725	0	755	101	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	5	0
4	C	27	0	12	5	0
4	D	27	0	12	1	0
4	E	27	0	12	1	0
4	F	27	0	12	6	0
4	G	27	0	12	2	0
All	All	58870	0	60354	7568	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 63.

The worst 5 of 7568 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:G:233:MET:HA	1:G:310:GLU:HG3	1.20	1.19
1:F:322:ARG:HB3	1:F:333:ILE:HD12	1.24	1.18
1:B:228:SER:HA	1:B:255:GLU:HB2	1.27	1.13
1:D:214:GLU:HB3	1:D:322:ARG:HD3	1.30	1.13
2:O:55:LYS:H	2:O:55:LYS:HE2	1.15	1.12

All (1) 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:425:LYS:NZ	1:J:484:GLU:OE2[4_445]	2.13	0.07

## 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	522/547 (95%)	396 (76%)	92 (18%)	34 (6%)	1	8
1	B	522/547 (95%)	399 (76%)	94 (18%)	29 (6%)	2	12
1	C	522/547 (95%)	397 (76%)	88 (17%)	37 (7%)	1	6
1	D	522/547 (95%)	395 (76%)	95 (18%)	32 (6%)	2	10
1	E	522/547 (95%)	390 (75%)	98 (19%)	34 (6%)	1	8
1	F	522/547 (95%)	399 (76%)	93 (18%)	30 (6%)	2	12
1	G	522/547 (95%)	390 (75%)	98 (19%)	34 (6%)	1	8
1	H	522/547 (95%)	377 (72%)	115 (22%)	30 (6%)	2	12
1	I	522/547 (95%)	384 (74%)	113 (22%)	25 (5%)	2	16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	J	522/547 (95%)	387 (74%)	110 (21%)	25 (5%)	2	16
1	K	522/547 (95%)	376 (72%)	121 (23%)	25 (5%)	2	16
1	L	522/547 (95%)	372 (71%)	124 (24%)	26 (5%)	2	15
1	M	522/547 (95%)	383 (73%)	110 (21%)	29 (6%)	2	12
1	N	522/547 (95%)	384 (74%)	112 (22%)	26 (5%)	2	15
2	O	95/97 (98%)	69 (73%)	20 (21%)	6 (6%)	1	9
2	P	95/97 (98%)	65 (68%)	24 (25%)	6 (6%)	1	9
2	Q	95/97 (98%)	67 (70%)	21 (22%)	7 (7%)	1	6
2	R	95/97 (98%)	68 (72%)	18 (19%)	9 (10%)	1	3
2	S	95/97 (98%)	73 (77%)	16 (17%)	6 (6%)	1	9
2	T	95/97 (98%)	67 (70%)	20 (21%)	8 (8%)	1	4
2	U	95/97 (98%)	64 (67%)	25 (26%)	6 (6%)	1	9
All	All	7973/8337 (96%)	5902 (74%)	1607 (20%)	464 (6%)	2	11

5 of 464 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	29	VAL
1	A	44	PHE
1	A	233	MET
1	A	279	PRO
1	A	309	LEU

### 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	393/414 (95%)	369 (94%)	24 (6%)	22	59
1	B	393/414 (95%)	368 (94%)	25 (6%)	20	57
1	C	393/414 (95%)	369 (94%)	24 (6%)	22	59
1	D	393/414 (95%)	369 (94%)	24 (6%)	22	59

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	393/414 (95%)	368 (94%)	25 (6%)	20	57
1	F	393/414 (95%)	368 (94%)	25 (6%)	20	57
1	G	393/414 (95%)	367 (93%)	26 (7%)	19	55
1	H	403/414 (97%)	385 (96%)	18 (4%)	32	71
1	I	403/414 (97%)	383 (95%)	20 (5%)	28	67
1	J	403/414 (97%)	385 (96%)	18 (4%)	32	71
1	K	403/414 (97%)	387 (96%)	16 (4%)	36	74
1	L	403/414 (97%)	386 (96%)	17 (4%)	34	73
1	M	403/414 (97%)	386 (96%)	17 (4%)	34	73
1	N	403/414 (97%)	386 (96%)	17 (4%)	34	73
2	O	79/80 (99%)	73 (92%)	6 (8%)	15	48
2	P	79/80 (99%)	74 (94%)	5 (6%)	21	57
2	Q	79/80 (99%)	72 (91%)	7 (9%)	11	40
2	R	79/80 (99%)	70 (89%)	9 (11%)	7	27
2	S	79/80 (99%)	73 (92%)	6 (8%)	15	48
2	T	79/80 (99%)	71 (90%)	8 (10%)	9	33
2	U	79/80 (99%)	72 (91%)	7 (9%)	11	40
All	All	6125/6356 (96%)	5781 (94%)	344 (6%)	25	62

5 of 344 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	G	195	PHE
1	I	20	VAL
2	R	37	ARG
1	G	255	GLU
1	H	37	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 187 such sidechains are listed below:

Mol	Chain	Res	Type
1	G	82	ASN
1	H	433	ASN
2	Q	45	ASN
1	G	153	ASN

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Mol	Chain	Res	Type
1	G	432	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 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	1	3	25,29,29	0.69	0	24,45,45	1.03	1 (4%)
4	ADP	B	1	3	25,29,29	0.71	0	24,45,45	1.05	1 (4%)
4	ADP	C	1	3	25,29,29	0.69	0	24,45,45	1.01	1 (4%)
4	ADP	D	1	3	25,29,29	0.73	0	24,45,45	0.96	1 (4%)
4	ADP	E	1	3	25,29,29	0.70	0	24,45,45	1.23	1 (4%)
4	ADP	F	1	3	25,29,29	0.69	0	24,45,45	1.01	1 (4%)
4	ADP	G	1	3	25,29,29	0.70	0	24,45,45	1.02	1 (4%)

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	1	3	-	0/12/32/32	0/3/3/3
4	ADP	B	1	3	-	0/12/32/32	0/3/3/3
4	ADP	C	1	3	-	0/12/32/32	0/3/3/3
4	ADP	D	1	3	-	0/12/32/32	0/3/3/3
4	ADP	E	1	3	-	0/12/32/32	0/3/3/3
4	ADP	F	1	3	-	0/12/32/32	0/3/3/3
4	ADP	G	1	3	-	0/12/32/32	0/3/3/3

There are no bond length outliers.

The worst 5 of 7 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1	ADP	O3B-PB-O2B	2.04	115.82	107.61
4	C	1	ADP	O3B-PB-O2B	2.06	115.93	107.61
4	B	1	ADP	O3B-PB-O2B	2.09	116.03	107.61
4	A	1	ADP	O3B-PB-O2B	2.12	116.16	107.61
4	G	1	ADP	O3B-PB-O2B	2.15	116.29	107.61

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1	ADP	2	0
4	B	1	ADP	5	0
4	C	1	ADP	5	0
4	D	1	ADP	1	0
4	E	1	ADP	1	0
4	F	1	ADP	6	0
4	G	1	ADP	2	0

## 5.7 Other polymers ⓘ

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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	524/547 (95%)	0.11	18 (3%)	46	20	4, 43, 100, 100	0
1	B	524/547 (95%)	0.08	16 (3%)	49	22	6, 44, 100, 100	0
1	C	524/547 (95%)	0.03	16 (3%)	49	22	3, 44, 100, 100	0
1	D	524/547 (95%)	0.09	19 (3%)	43	18	5, 43, 100, 100	0
1	E	524/547 (95%)	0.18	31 (5%)	23	9	6, 46, 100, 100	0
1	F	524/547 (95%)	0.19	30 (5%)	24	9	6, 47, 100, 100	0
1	G	524/547 (95%)	0.11	26 (4%)	30	12	6, 44, 100, 100	0
1	H	524/547 (95%)	-0.07	2 (0%)	92	77	6, 61, 99, 100	0
1	I	524/547 (95%)	-0.07	1 (0%)	94	85	6, 61, 99, 100	0
1	J	524/547 (95%)	-0.03	5 (0%)	82	58	7, 61, 99, 100	0
1	K	524/547 (95%)	-0.01	7 (1%)	77	51	7, 63, 99, 100	0
1	L	524/547 (95%)	0.02	6 (1%)	80	55	9, 64, 99, 100	0
1	M	524/547 (95%)	0.03	11 (2%)	64	34	7, 63, 99, 100	0
1	N	524/547 (95%)	0.07	9 (1%)	70	42	6, 62, 99, 100	0
2	O	97/97 (100%)	0.92	16 (16%)	2	1	74, 96, 100, 100	0
2	P	97/97 (100%)	0.80	12 (12%)	4	2	71, 96, 100, 100	0
2	Q	97/97 (100%)	0.67	10 (10%)	7	3	71, 96, 100, 100	0
2	R	97/97 (100%)	0.84	14 (14%)	3	1	73, 96, 100, 100	0
2	S	97/97 (100%)	0.79	12 (12%)	4	2	72, 96, 100, 100	0
2	T	97/97 (100%)	0.89	18 (18%)	1	1	74, 96, 100, 100	0
2	U	97/97 (100%)	0.68	14 (14%)	3	1	73, 96, 100, 100	0
All	All	8015/8337 (96%)	0.12	293 (3%)	42	18	3, 64, 100, 100	0

The worst 5 of 293 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	212	ALA	5.6
1	F	211	GLY	5.1
1	A	361	ASP	5.0
2	T	27	LEU	4.9
2	O	33	ALA	4.8

## 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 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	ADP	B	1	27/27	0.89	0.29	3.27	13,34,39,49	0
4	ADP	A	1	27/27	0.92	0.29	2.19	14,31,39,48	0
4	ADP	C	1	27/27	0.93	0.26	2.00	16,31,38,47	0
4	ADP	G	1	27/27	0.94	0.26	1.73	15,31,39,49	0
4	ADP	D	1	27/27	0.92	0.26	1.72	11,31,36,48	0
4	ADP	F	1	27/27	0.90	0.26	1.05	20,35,41,47	0
4	ADP	E	1	27/27	0.90	0.26	1.02	8,32,39,50	0
3	MG	G	550	1/1	0.90	0.27	-	12,12,12,12	0
3	MG	A	550	1/1	0.92	0.33	-	2,2,2,2	0
3	MG	C	550	1/1	0.90	0.32	-	13,13,13,13	0
3	MG	B	550	1/1	0.93	0.28	-	14,14,14,14	0
3	MG	E	550	1/1	0.92	0.30	-	9,9,9,9	0
3	MG	F	550	1/1	0.82	0.35	-	13,13,13,13	0
3	MG	D	550	1/1	0.76	0.32	-	5,5,5,5	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.