



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 05:39 am GMT

PDB ID : 2XND  
Title : CRYSTAL STRUCTURE OF BOVINE F1-C8 SUB-COMPLEX OF ATP SYNTHASE  
Authors : Watt, I.N.; Montgomery, M.G.; Runswick, M.J.; Leslie, A.G.W.; Walker, J.E.  
Deposited on : 2010-08-02  
Resolution : 3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation 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) : recalc28949

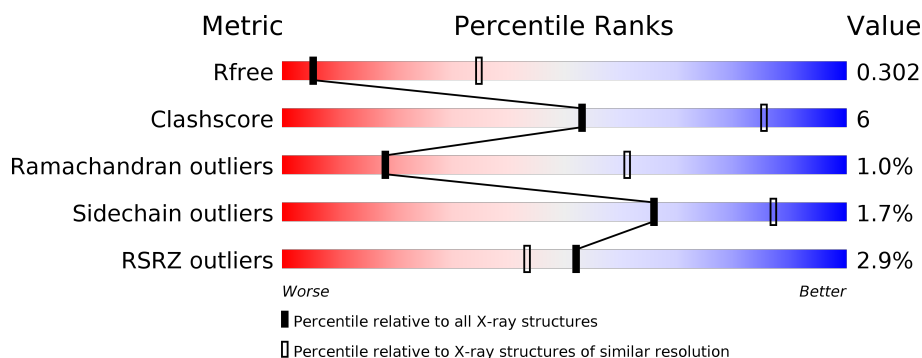
# 1 Overall quality at a glance

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))
$R_{free}$	100719	1195 (3.60-3.40)
Clashscore	112137	1322 (3.60-3.40)
Ramachandran outliers	110173	1283 (3.60-3.40)
Sidechain outliers	110143	1284 (3.60-3.40)
RSRZ outliers	101464	1226 (3.60-3.40)

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	492	
1	B	492	
1	C	492	
2	D	467	
2	E	467	
2	F	467	

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Mol	Chain	Length	Quality of chain
3	G	272	
4	H	131	
5	I	47	
6	J	72	
6	K	72	
6	L	72	
6	M	72	
6	N	72	
6	O	72	
6	P	72	
6	Q	72	

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
10	SO4	E	630	-	-	-	X
8	MG	D	601	-	-	-	X
8	MG	F	601	-	-	-	X

## 2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 28196 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 ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	492	Total	C	N	O	S	0	0	0
			3748	2360	661	715	12			
1	B	492	Total	C	N	O	S	0	0	0
			3748	2360	661	715	12			
1	C	492	Total	C	N	O	S	0	0	0
			3748	2360	661	715	12			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	481	GLY	SER	CLONING ARTIFACT	UNP P19483
B	481	GLY	SER	CLONING ARTIFACT	UNP P19483
C	481	GLY	SER	CLONING ARTIFACT	UNP P19483

- Molecule 2 is a protein called ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	467	Total	C	N	O	S	0	0	0
			3539	2243	601	684	11			
2	E	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			
2	F	466	Total	C	N	O	S	0	0	0
			3530	2238	600	681	11			

- Molecule 3 is a protein called ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	263	Total	C	N	O	S	0	0	0
			2051	1291	354	398	8			

- Molecule 4 is a protein called ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	131	Total	C	N	O	S	0	0	0
			970	609	164	195	2			

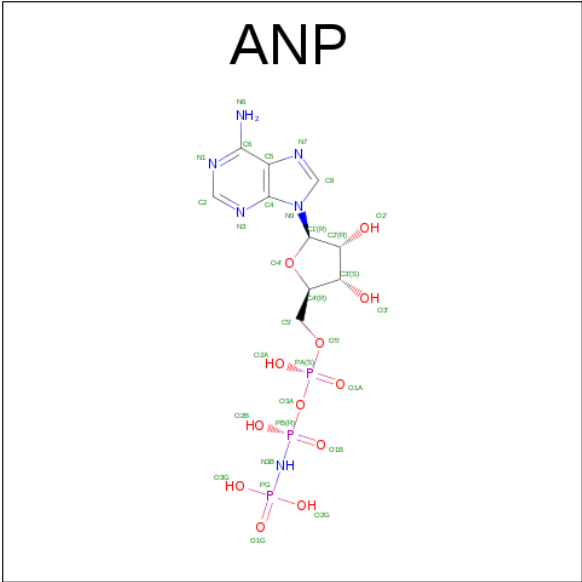
- Molecule 5 is a protein called ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	47	Total	C	N	O	S	0	0	0
			369	237	66	64	2			

- Molecule 6 is a protein called ATP SYNTHASE LIPID-BINDING PROTEIN, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	J	72	Total	C	N	O		0	0	0
			349	205	72	72				
6	K	72	Total	C	N	O		0	0	0
			349	205	72	72				
6	L	72	Total	C	N	O		0	0	0
			349	205	72	72				
6	M	72	Total	C	N	O		0	0	0
			349	205	72	72				
6	N	72	Total	C	N	O		0	0	0
			349	205	72	72				
6	O	72	Total	C	N	O		0	0	0
			349	205	72	72				
6	P	72	Total	C	N	O		0	0	0
			349	205	72	72				
6	Q	72	Total	C	N	O		0	0	0
			349	205	72	72				

- Molecule 7 is PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: C<sub>10</sub>H<sub>17</sub>N<sub>6</sub>O<sub>12</sub>P<sub>3</sub>).

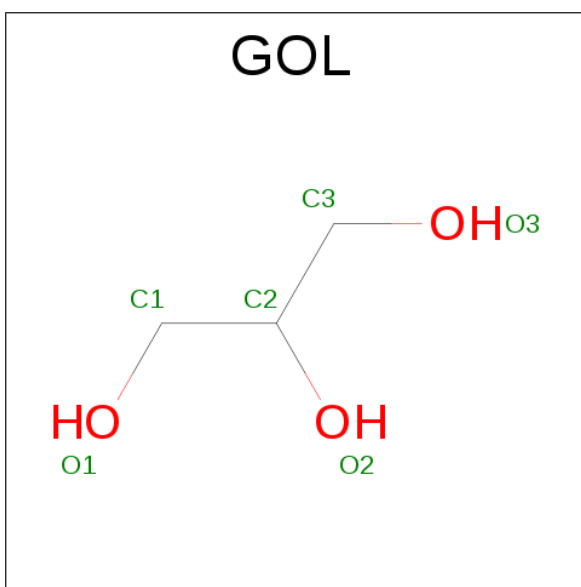


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
7	B	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
7	C	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
7	D	1	Total	C	N	O	P	0	0
			31	10	6	12	3		
7	F	1	Total	C	N	O	P	0	0
			31	10	6	12	3		

- Molecule 8 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

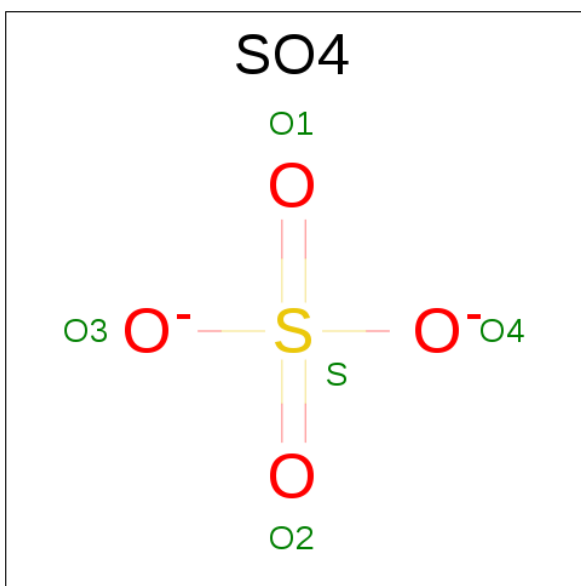
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Mg	0	0
			1	1		
8	A	1	Total	Mg	0	0
			1	1		
8	D	1	Total	Mg	0	0
			1	1		
8	C	1	Total	Mg	0	0
			1	1		
8	F	1	Total	Mg	0	0
			1	1		

- Molecule 9 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
9	B	1	Total	C	O	0	0
			6	3	3		

- Molecule 10 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).

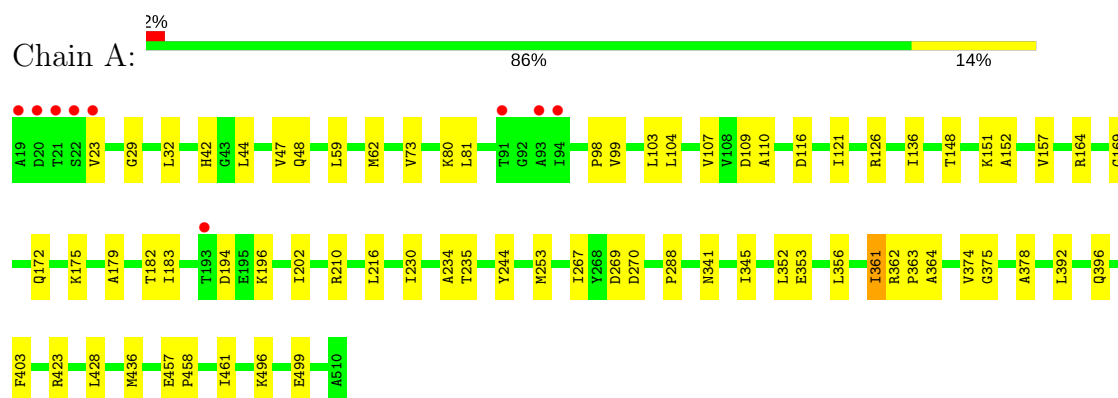


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
10	E	1	Total	O	S	0	0
			5	4	1		

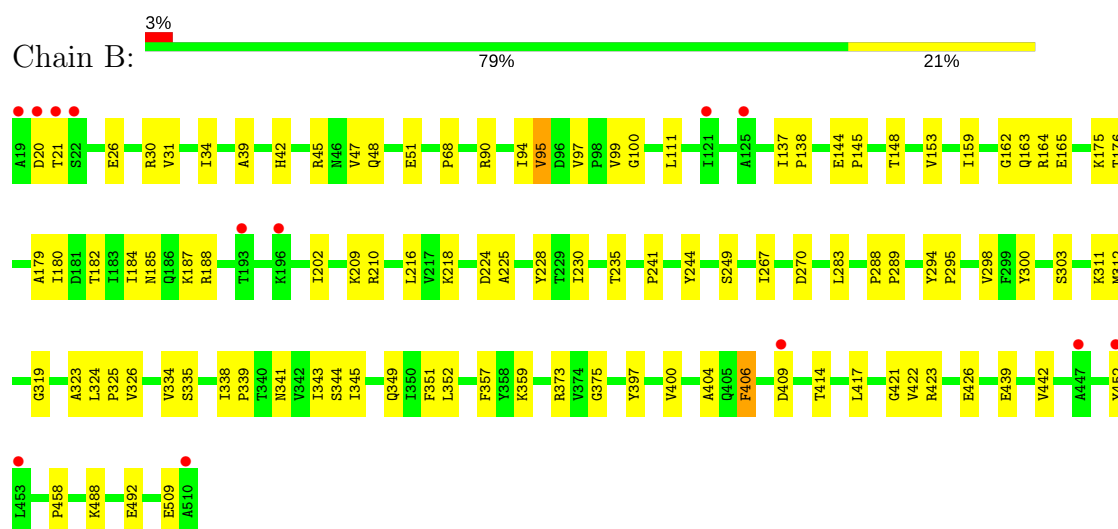
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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.

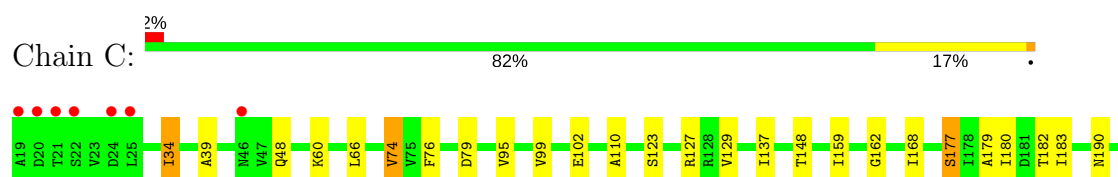
#### • Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL



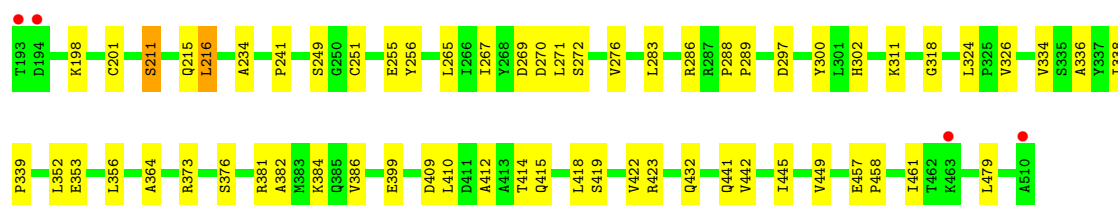
#### • Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL



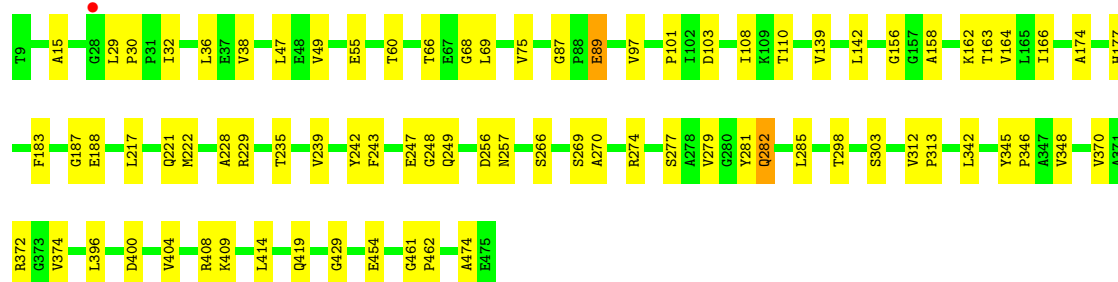
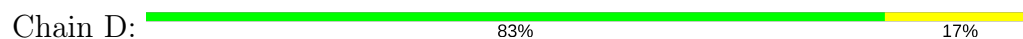
#### • Molecule 1: ATP SYNTHASE SUBUNIT ALPHA, MITOCHONDRIAL



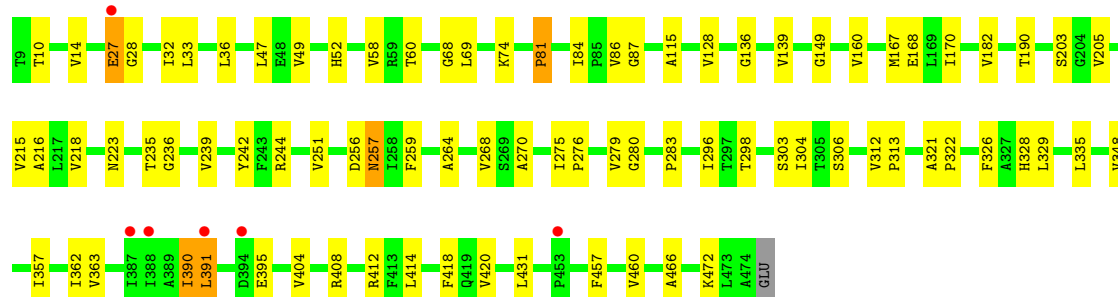
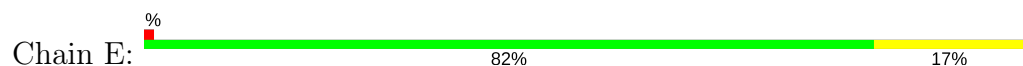




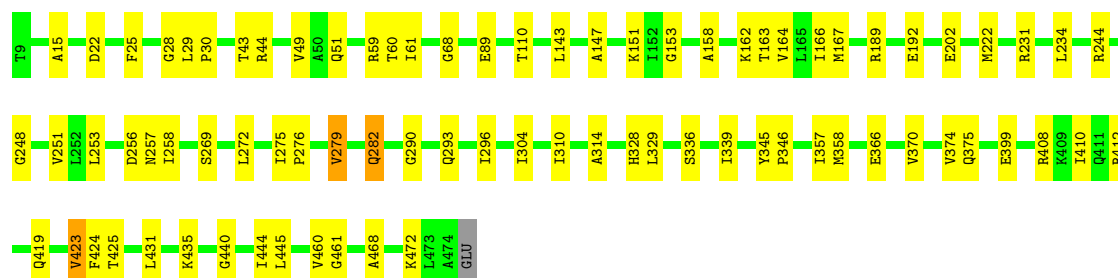
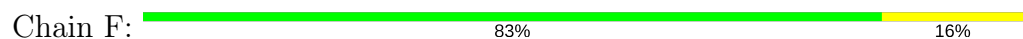
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL



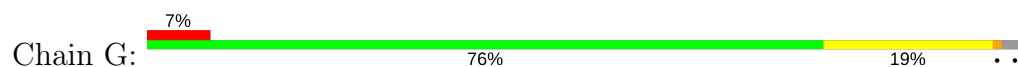
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

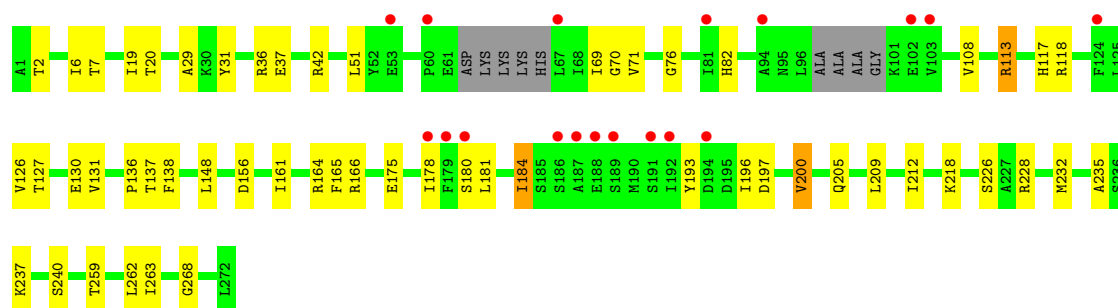


• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

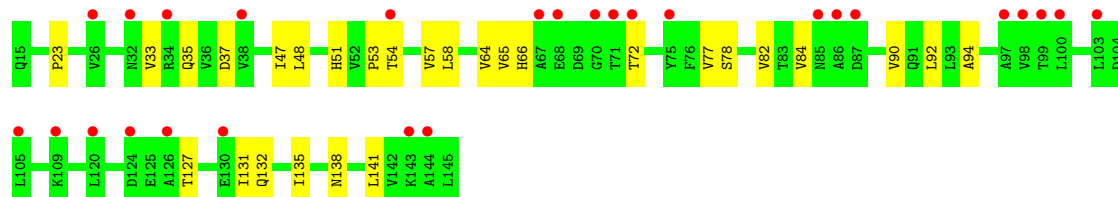
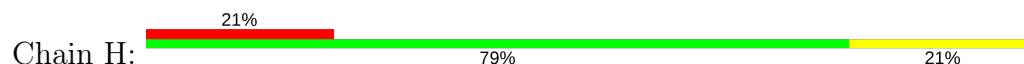


• Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL

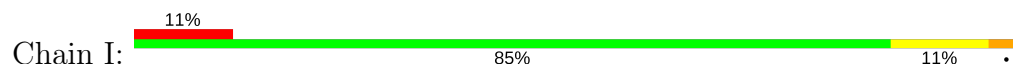




• Molecule 4: ATP SYNTHASE SUBUNIT DELTA, MITOCHONDRIAL



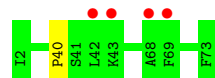
• Molecule 5: ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL



• Molecule 6: ATP SYNTHASE LIPID-BINDING PROTEIN, MITOCHONDRIAL



• Molecule 6: ATP SYNTHASE LIPID-BINDING PROTEIN, MITOCHONDRIAL



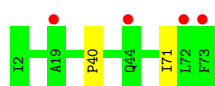
• Molecule 6: ATP SYNTHASE LIPID-BINDING PROTEIN, MITOCHONDRIAL



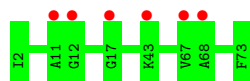
There are no outlier residues recorded for this chain.

• Molecule 6: ATP SYNTHASE LIPID-BINDING PROTEIN, MITOCHONDRIAL

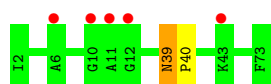




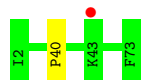
- Molecule 6: ATP SYNTHASE LIPID-BINDING PROTEIN, MITOCHONDRIAL



- Molecule 6: ATP SYNTHASE LIPID-BINDING PROTEIN, MITOCHONDRIAL



- Molecule 6: ATP SYNTHASE LIPID-BINDING PROTEIN, MITOCHONDRIAL



- Molecule 6: ATP SYNTHASE LIPID-BINDING PROTEIN, MITOCHONDRIAL



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	155.74Å 157.10Å 247.27Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	132.60 – 3.50 48.67 – 3.50	Depositor EDS
% Data completeness (in resolution range)	99.6 (132.60-3.50) 99.6 (48.67-3.50)	Depositor EDS
$R_{merge}$	0.26	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.80 (at 3.48Å)	Xtriage
Refinement program	REFMAC 5.5.0109	Depositor
R, $R_{free}$	0.261 , 0.304 0.262 , 0.302	Depositor DCC
$R_{free}$ test set	3855 reflections (5.28%)	DCC
Wilson B-factor (Å <sup>2</sup> )	76.6	Xtriage
Anisotropy	0.124	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 24.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.38$ , $\langle L^2 \rangle = 0.20$	Xtriage
Estimated twinning fraction	0.088 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.83	EDS
Total number of atoms	28196	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	83.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.41% of the height of the origin peak. No significant pseudotranslation is detected.*

<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: GOL, MG, ANP, SO4

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	0.33	0/3799	0.50	0/5126
1	B	0.33	0/3799	0.50	0/5126
1	C	0.33	0/3799	0.49	0/5126
2	D	0.33	0/3596	0.50	0/4879
2	E	0.32	0/3587	0.50	0/4867
2	F	0.33	0/3587	0.50	0/4867
3	G	0.32	0/2074	0.47	0/2785
4	H	0.35	0/982	0.49	0/1337
5	I	0.35	0/374	0.45	0/501
6	J	0.28	0/348	0.41	0/479
6	K	0.29	0/348	0.42	0/479
6	L	0.29	0/348	0.43	0/479
6	M	0.27	0/348	0.43	0/479
6	N	0.27	0/348	0.40	0/479
6	O	0.29	0/348	0.42	0/479
6	P	0.28	0/348	0.42	0/479
6	Q	0.28	0/348	0.43	0/479
All	All	0.32	0/28381	0.49	0/38446

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 [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	3748	0	3844	44	0
1	B	3748	0	3844	61	0
1	C	3748	0	3844	56	0
2	D	3539	0	3592	52	0
2	E	3530	0	3587	52	0
2	F	3530	0	3586	51	0
3	G	2051	0	2115	34	0
4	H	970	0	972	18	0
5	I	369	0	395	5	0
6	J	349	0	189	0	0
6	K	349	0	189	0	0
6	L	349	0	189	0	0
6	M	349	0	189	0	0
6	N	349	0	189	0	0
6	O	349	0	189	1	0
6	P	349	0	189	0	0
6	Q	349	0	189	0	0
7	A	31	0	13	1	0
7	B	31	0	13	1	0
7	C	31	0	13	2	0
7	D	31	0	13	3	0
7	F	31	0	13	4	0
8	A	1	0	0	0	0
8	B	1	0	0	0	0
8	C	1	0	0	0	0
8	D	1	0	0	0	0
8	F	1	0	0	0	0
9	B	6	0	8	0	0
10	E	5	0	0	0	0
All	All	28196	0	27364	343	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 6.

All (343) 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)
2:F:282:GLN:H	2:F:282:GLN:HE21	1.15	0.93
1:A:99:VAL:HG23	1:A:253:MET:HA	1.57	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:27:GLU:HG2	2:E:28:GLY:H	1.41	0.85
2:F:51:GLN:HE21	2:F:59:ARG:HD2	1.46	0.78
2:E:298:THR:HG23	2:E:303:SER:HB3	1.66	0.77
2:F:89:GLU:HB2	2:F:110:THR:HG22	1.67	0.75
2:E:257:ASN:HD21	2:E:259:PHE:HB3	1.54	0.72
1:A:403:PHE:HE1	3:G:19:ILE:HA	1.55	0.71
2:D:282:GLN:H	2:D:282:GLN:HE21	1.37	0.70
2:D:298:THR:HG23	2:D:303:SER:HA	1.73	0.70
1:C:423:ARG:HD2	1:C:461:ILE:HD11	1.72	0.70
1:A:341:ASN:O	1:A:345:ILE:HG12	1.92	0.69
1:A:44:LEU:O	1:A:47:VAL:HG22	1.94	0.68
1:C:179:ALA:O	1:C:183:ILE:HG12	1.92	0.68
1:C:419:SER:O	1:C:423:ARG:HG2	1.93	0.68
2:E:390:ILE:HG22	2:E:390:ILE:O	1.94	0.67
2:E:136:GLY:HA3	2:E:431:LEU:HD22	1.77	0.66
3:G:148:LEU:HD23	3:G:209:LEU:HD21	1.77	0.66
1:A:169:GLY:H	1:A:175:LYS:HD3	1.61	0.66
1:C:74:VAL:CG1	1:C:241:PRO:HB3	2.26	0.66
1:B:339:PRO:O	1:B:343:ILE:HG12	1.96	0.65
3:G:71:VAL:HA	3:G:108:VAL:HG12	1.78	0.65
3:G:156:ASP:HA	3:G:181:LEU:HD22	1.79	0.64
1:C:99:VAL:HG21	1:C:127:ARG:HB3	1.78	0.64
1:B:99:VAL:HG12	1:B:100:GLY:N	2.12	0.64
2:D:139:VAL:HG11	2:D:348:VAL:HB	1.80	0.63
1:C:48:GLN:HB3	2:D:68:GLY:HA2	1.80	0.63
1:C:168:ILE:HD11	1:C:339:PRO:HB3	1.79	0.63
1:B:343:ILE:HB	2:F:158:ALA:HB1	1.81	0.63
1:B:406:PHE:HB2	1:B:409:ASP:HB2	1.80	0.63
2:E:390:ILE:HG23	3:G:29:ALA:HB2	1.80	0.63
2:F:290:GLY:HA2	2:F:328:HIS:HE1	1.64	0.63
4:H:54:THR:H	4:H:84:VAL:HG23	1.64	0.62
2:D:188:GLU:O	2:D:221:GLN:HB3	1.99	0.62
2:F:419:GLN:HE21	2:F:431:LEU:HD13	1.65	0.62
1:C:441:GLN:O	1:C:445:ILE:HG12	2.01	0.61
2:E:390:ILE:CG2	2:E:390:ILE:O	2.48	0.61
2:D:29:LEU:HD12	2:D:30:PRO:HD2	1.81	0.61
4:H:47:ILE:HG21	4:H:84:VAL:HG11	1.82	0.61
3:G:197:ASP:HB2	3:G:200:VAL:HB	1.81	0.61
1:C:99:VAL:HG13	1:C:256:TYR:HB2	1.81	0.60
1:B:99:VAL:HG12	1:B:100:GLY:H	1.66	0.60
2:D:419:GLN:HA	2:D:429:GLY:HA3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:ARG:HG3	1:A:235:THR:HG21	1.83	0.60
1:B:218:LYS:HG3	2:E:128:VAL:HB	1.83	0.59
1:A:151:LYS:HD2	1:A:436:MET:SD	2.43	0.59
1:C:74:VAL:HG13	1:C:241:PRO:HB3	1.83	0.59
2:D:279:VAL:HG12	2:D:279:VAL:O	2.03	0.59
1:C:129:VAL:HG12	1:C:249:SER:HA	1.83	0.59
2:E:84:ILE:HG21	2:E:235:THR:HG23	1.84	0.58
1:A:179:ALA:HB1	1:A:267:ILE:HD13	1.85	0.58
2:F:147:ALA:HB2	2:F:357:ILE:HG13	1.85	0.58
1:B:283:LEU:HD21	1:B:289:PRO:HB3	1.84	0.58
1:A:59:LEU:HD11	1:A:81:LEU:HD13	1.84	0.58
1:C:34:ILE:HD11	1:C:79:ASP:HB2	1.84	0.58
2:E:408:ARG:O	2:E:412:ARG:HG2	2.04	0.58
2:F:162:LYS:HE3	2:F:257:ASN:HD21	1.69	0.58
2:D:139:VAL:HG13	2:D:414:LEU:HD22	1.86	0.57
2:D:183:PHE:HB3	2:D:217:LEU:HD23	1.86	0.57
2:F:189:ARG:HB2	2:F:192:GLU:HG3	1.85	0.57
2:E:167:MET:HA	2:E:170:ILE:HD12	1.85	0.57
1:B:162:GLY:HA3	1:B:311:LYS:HB2	1.86	0.57
3:G:178:ILE:HG22	3:G:180:SER:HB2	1.87	0.56
3:G:259:THR:O	3:G:263:ILE:HG12	2.04	0.56
1:C:179:ALA:HB1	1:C:267:ILE:HD13	1.85	0.56
1:B:34:ILE:HD13	1:B:39:ALA:HB2	1.87	0.56
1:B:439:GLU:HA	1:B:442:VAL:HG22	1.86	0.56
1:B:335:SER:O	2:F:314:ALA:HA	2.05	0.56
1:A:423:ARG:HG2	1:A:461:ILE:HD11	1.86	0.56
1:A:136:ILE:HD13	2:E:190:THR:HG23	1.87	0.56
1:B:344:SER:HA	7:F:600:ANP:O1G	2.04	0.56
2:F:253:LEU:HD23	2:F:296:ILE:HG23	1.87	0.56
3:G:37:GLU:HB3	3:G:218:LYS:HE3	1.87	0.56
1:B:148:THR:HA	1:B:182:THR:HG23	1.87	0.55
2:E:203:SER:HB2	2:E:420:VAL:HG13	1.87	0.55
1:C:183:ILE:HD11	1:C:267:ILE:HD11	1.88	0.55
2:F:244:ARG:O	2:F:248:GLY:HA2	2.06	0.55
4:H:58:LEU:HD13	4:H:77:VAL:HG11	1.87	0.55
1:B:422:VAL:O	1:B:426:GLU:HG2	2.07	0.55
1:A:169:GLY:N	1:A:175:LYS:HD3	2.22	0.55
2:F:163:THR:O	2:F:167:MET:HG2	2.06	0.54
2:F:49:VAL:HA	2:F:60:THR:HG22	1.88	0.54
3:G:20:THR:HG21	3:G:235:ALA:HB3	1.89	0.54
2:D:162:LYS:HE3	2:D:257:ASN:ND2	2.23	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:294:TYR:HD1	1:B:298:VAL:HG11	1.72	0.54
1:B:30:ARG:HB3	1:B:42:HIS:HB3	1.90	0.54
1:B:312:MET:HG2	1:B:319:GLY:O	2.07	0.54
1:B:241:PRO:HA	1:B:244:TYR:HB3	1.90	0.53
1:C:386:VAL:O	1:C:449:VAL:HG21	2.08	0.53
1:A:48:GLN:HB3	2:E:68:GLY:HA2	1.89	0.53
1:B:180:ILE:HG13	1:B:216:LEU:HD11	1.90	0.53
1:B:295:PRO:HG2	1:B:298:VAL:HG13	1.91	0.53
4:H:35:GLN:HG3	4:H:48:LEU:HG	1.91	0.53
1:A:148:THR:HA	1:A:182:THR:HG23	1.89	0.53
1:C:211:SER:O	1:C:215:GLN:HG2	2.08	0.53
1:A:110:ALA:HB2	1:A:234:ALA:HB2	1.90	0.52
2:D:49:VAL:HA	2:D:60:THR:HG22	1.91	0.52
1:B:47:VAL:HG12	1:B:90:ARG:HG2	1.89	0.52
2:D:89:GLU:HG3	2:D:110:THR:HA	1.90	0.52
2:D:404:VAL:O	2:D:408:ARG:HG3	2.09	0.52
1:C:183:ILE:HD12	1:C:201:CYS:SG	2.49	0.52
1:C:159:ILE:HD13	1:C:324:LEU:HD21	1.92	0.52
3:G:2:THR:O	3:G:6:ILE:HG12	2.09	0.51
1:B:179:ALA:HB1	1:B:267:ILE:HD13	1.92	0.51
1:B:423:ARG:HH21	1:B:458:PRO:HG3	1.74	0.51
2:E:49:VAL:HA	2:E:60:THR:HG22	1.92	0.51
2:D:97:VAL:HG21	2:D:228:ALA:HB1	1.92	0.51
1:C:272:SER:O	1:C:276:VAL:HG23	2.11	0.51
2:E:139:VAL:HG22	2:E:414:LEU:HB3	1.93	0.51
2:F:164:VAL:N	7:F:600:ANP:O1A	2.43	0.51
4:H:37:ASP:HB2	4:H:64:VAL:HB	1.93	0.51
3:G:127:THR:HB	5:I:45:VAL:HB	1.93	0.50
1:B:338:ILE:HB	1:B:339:PRO:HD3	1.92	0.50
4:H:58:LEU:HD11	4:H:92:LEU:HD11	1.93	0.50
2:F:425:THR:HG21	7:F:600:ANP:H2	1.93	0.50
1:A:183:ILE:HD11	1:A:267:ILE:CD1	2.42	0.50
1:A:103:LEU:HD23	1:A:121:ILE:HG21	1.93	0.49
2:E:182:VAL:HG22	2:E:216:ALA:HB3	1.94	0.49
1:A:352:LEU:HA	1:A:364:ALA:O	2.11	0.49
4:H:82:VAL:HB	4:H:92:LEU:HD13	1.94	0.49
2:E:312:VAL:HG13	2:E:322:PRO:HG3	1.94	0.49
4:H:84:VAL:HG12	4:H:90:VAL:HG22	1.95	0.49
1:C:60:LYS:O	1:C:76:PHE:HB2	2.12	0.49
1:A:353:GLU:HB2	1:A:356:LEU:HD12	1.95	0.49
1:C:457:GLU:HG2	1:C:458:PRO:HD2	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:LEU:O	2:D:15:ALA:HA	2.13	0.48
2:F:293:GLN:HA	2:F:296:ILE:HD12	1.96	0.48
2:F:25:PHE:HB2	2:F:29:LEU:HD12	1.96	0.48
2:F:251:VAL:HB	2:F:304:ILE:HG12	1.94	0.48
1:A:392:LEU:HG	1:A:396:GLN:HE21	1.77	0.48
1:B:180:ILE:O	1:B:184:ILE:HG12	2.13	0.48
2:D:370:VAL:O	2:D:374:VAL:HG23	2.13	0.48
2:E:27:GLU:CG	2:E:28:GLY:H	2.14	0.48
2:E:47:LEU:HB3	2:E:60:THR:HB	1.96	0.48
2:F:279:VAL:HG12	2:F:279:VAL:O	2.12	0.48
1:C:412:ALA:HA	1:C:415:GLN:HB2	1.95	0.48
1:A:152:ALA:HA	1:A:428:LEU:HD22	1.96	0.48
1:B:341:ASN:O	1:B:345:ILE:HG12	2.14	0.48
2:F:89:GLU:CB	2:F:110:THR:HG22	2.41	0.48
4:H:127:THR:O	4:H:131:ILE:HG12	2.14	0.48
2:D:142:LEU:HD21	2:D:374:VAL:HG21	1.95	0.47
1:B:99:VAL:CG1	1:B:100:GLY:N	2.77	0.47
2:E:32:ILE:O	2:E:33:LEU:HB2	2.14	0.47
1:A:107:VAL:HB	1:A:116:ASP:HB3	1.97	0.47
1:C:432:GLN:HE22	7:C:600:ANP:H2'	1.78	0.47
2:E:86:VAL:HG12	2:E:239:VAL:HA	1.96	0.47
2:F:15:ALA:HB3	2:F:22:ASP:HB2	1.96	0.47
1:B:303:SER:HB2	2:F:222:MET:HB2	1.96	0.47
2:D:139:VAL:HG21	2:D:346:PRO:HG2	1.95	0.47
2:F:345:TYR:HA	2:F:346:PRO:C	2.35	0.47
1:B:202:ILE:HG13	1:B:230:ILE:HB	1.95	0.47
2:D:101:PRO:HB3	2:D:108:ILE:HD11	1.97	0.47
3:G:71:VAL:HA	3:G:108:VAL:CG1	2.44	0.47
1:C:270:ASP:HB2	1:C:326:VAL:O	2.15	0.47
3:G:136:PRO:O	3:G:218:LYS:NZ	2.48	0.47
3:G:130:GLU:HB3	5:I:41:THR:HG22	1.97	0.47
1:B:175:LYS:HG2	1:B:352:LEU:HD12	1.97	0.47
1:B:48:GLN:HB2	1:B:51:GLU:HB2	1.97	0.47
1:B:97:VAL:HG11	1:B:249:SER:HB3	1.97	0.47
2:D:87:GLY:HA2	2:D:242:TYR:CE1	2.50	0.47
1:C:251:CYS:O	1:C:255:GLU:HG3	2.14	0.46
4:H:23:PRO:HD3	4:H:94:ALA:O	2.15	0.46
1:C:162:GLY:HA3	1:C:311:LYS:HB2	1.97	0.46
6:O:39:ASN:CB	6:O:40:PRO:HA	2.45	0.46
1:B:148:THR:HG21	1:B:153:VAL:HG11	1.96	0.46
1:B:414:THR:HA	1:B:417:LEU:HD12	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:190:ASN:HA	1:C:198:LYS:HD3	1.97	0.46
2:F:290:GLY:HA2	2:F:328:HIS:CE1	2.48	0.46
1:B:99:VAL:CG1	1:B:100:GLY:H	2.27	0.46
2:F:256:ASP:HA	2:F:257:ASN:HA	1.69	0.46
2:F:164:VAL:HG23	7:F:600:ANP:O1A	2.16	0.46
3:G:178:ILE:HD12	3:G:212:ILE:HG21	1.97	0.46
1:A:362:ARG:HH22	2:D:372:ARG:HD3	1.81	0.46
1:A:202:ILE:HG12	1:A:230:ILE:HB	1.98	0.46
1:A:457:GLU:HG2	1:A:458:PRO:HD2	1.97	0.46
2:F:61:ILE:HD11	2:F:272:LEU:HD11	1.97	0.46
3:G:164:ARG:HH21	3:G:166:ARG:HD3	1.80	0.46
1:B:357:PHE:C	1:B:359:LYS:H	2.18	0.46
2:E:259:PHE:CE1	2:E:313:PRO:HG3	2.49	0.46
1:A:98:PRO:HA	1:A:126:ARG:HG2	1.97	0.46
2:E:264:ALA:O	2:E:268:VAL:HG23	2.16	0.46
2:E:251:VAL:HB	2:E:304:ILE:HG12	1.98	0.46
3:G:113:ARG:O	3:G:117:HIS:HB2	2.16	0.46
1:A:374:VAL:HG12	1:A:378:ALA:HB2	1.98	0.46
1:A:80:LYS:HA	2:D:32:ILE:HB	1.97	0.46
1:C:289:PRO:HD2	3:G:268:GLY:HA2	1.97	0.46
1:B:225:ALA:HA	1:B:228:TYR:CE2	2.51	0.45
2:E:326:PHE:HA	2:E:329:LEU:HD12	1.97	0.45
2:E:357:ILE:HG22	2:E:362:ILE:HD13	1.97	0.45
2:F:275:ILE:HG22	2:F:276:PRO:HD2	1.98	0.45
1:A:288:PRO:HB2	2:E:270:ALA:O	2.16	0.45
2:D:89:GLU:HG3	2:D:110:THR:HG22	1.98	0.45
2:E:296:ILE:HG21	2:E:306:SER:HB2	1.98	0.45
1:B:209:LYS:HD2	2:E:328:HIS:HA	1.99	0.45
3:G:161:ILE:HG12	3:G:175:GLU:HG2	1.96	0.45
2:E:27:GLU:CD	2:E:27:GLU:H	2.20	0.45
2:F:468:ALA:O	2:F:472:LYS:HG2	2.17	0.45
5:I:37:THR:HG22	5:I:38:SER:H	1.81	0.45
1:A:32:LEU:HG	1:A:42:HIS:HB2	1.99	0.45
1:B:163:GLN:HG2	1:B:164:ARG:N	2.32	0.45
2:F:258:ILE:HG21	2:F:310:ILE:HG12	1.99	0.45
2:D:256:ASP:HA	2:D:257:ASN:HA	1.70	0.45
1:B:187:LYS:HE3	1:B:224:ASP:OD2	2.16	0.45
1:C:102:GLU:CD	1:C:123:SER:HA	2.38	0.45
2:F:374:VAL:HG23	2:F:445:LEU:HD11	1.99	0.45
2:E:81:PRO:HB2	2:E:115:ALA:HB1	1.99	0.45
2:E:218:VAL:HG21	2:E:236:GLY:HA2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:10:THR:HG21	2:E:74:LYS:HD2	1.99	0.45
2:F:282:GLN:H	2:F:282:GLN:NE2	1.98	0.45
2:D:269:SER:O	2:D:274:ARG:HD3	2.17	0.44
2:F:29:LEU:HD12	2:F:30:PRO:HD2	1.99	0.44
1:C:137:ILE:CD1	2:D:103:ASP:HA	2.47	0.44
1:A:29:GLY:HA3	1:A:42:HIS:O	2.18	0.44
1:A:104:LEU:HD23	1:A:230:ILE:HG13	1.99	0.44
1:A:99:VAL:CG2	1:A:253:MET:HA	2.38	0.44
2:D:163:THR:O	2:D:166:ILE:HG22	2.18	0.44
2:D:239:VAL:O	2:D:243:PHE:HD2	1.99	0.44
2:E:321:ALA:HB3	2:E:322:PRO:CD	2.47	0.44
2:F:51:GLN:HG3	2:F:59:ARG:HB3	2.00	0.44
3:G:137:THR:HG22	3:G:138:PHE:N	2.33	0.44
3:G:193:TYR:HA	4:H:53:PRO:HB2	1.99	0.44
1:C:336:ALA:HB3	1:C:339:PRO:HG2	1.99	0.44
2:E:460:VAL:HG21	2:E:466:ALA:HB2	2.00	0.44
2:E:36:LEU:HB2	2:E:47:LEU:HB2	2.00	0.44
1:A:183:ILE:HD11	1:A:267:ILE:HD12	2.00	0.44
1:B:94:ILE:O	1:B:95:VAL:C	2.56	0.44
1:C:148:THR:HA	1:C:182:THR:HG23	2.00	0.44
1:C:34:ILE:HD12	1:C:39:ALA:HB2	1.99	0.44
4:H:33:VAL:HG13	4:H:66:HIS:O	2.18	0.44
5:I:5:ARG:O	5:I:6:GLN:CB	2.65	0.44
1:C:338:ILE:HD13	1:C:338:ILE:HA	1.90	0.43
2:D:409:LYS:HG2	2:D:454:GLU:HA	1.99	0.43
2:E:244:ARG:HD3	2:E:304:ILE:HG13	2.00	0.43
2:E:280:GLY:HA2	3:G:262:LEU:CD2	2.48	0.43
1:B:185:ASN:O	1:B:188:ARG:HG2	2.18	0.43
1:C:288:PRO:HB2	2:D:270:ALA:HB1	1.99	0.43
1:C:297:ASP:HB2	1:C:300:TYR:HB3	2.00	0.43
2:D:312:VAL:HA	2:D:313:PRO:HD3	1.81	0.43
1:A:172:GLN:HA	7:A:600:ANP:N3B	2.33	0.43
1:C:110:ALA:HB2	1:C:234:ALA:HB2	1.99	0.43
2:D:38:VAL:HA	2:D:75:VAL:HG22	1.99	0.43
1:A:196:LYS:H	1:A:196:LYS:HG3	1.65	0.43
1:A:496:LYS:O	1:A:499:GLU:HG2	2.18	0.43
2:E:404:VAL:O	2:E:408:ARG:HG3	2.19	0.43
2:F:231:ARG:HA	2:F:234:LEU:HD12	1.99	0.43
1:C:271:LEU:HD13	1:C:302:HIS:CD2	2.54	0.43
1:C:283:LEU:HD21	1:C:289:PRO:HB3	1.99	0.43
2:D:158:ALA:HA	7:D:600:ANP:O3G	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:138:ASN:HA	4:H:141:LEU:HD12	2.00	0.43
1:A:362:ARG:HH22	2:D:372:ARG:CG	2.32	0.43
2:D:89:GLU:HG2	2:D:89:GLU:H	1.46	0.43
2:E:160:VAL:HG21	2:E:335:LEU:HB3	2.00	0.43
4:H:78:SER:HB3	5:I:22:VAL:HG21	2.01	0.43
1:B:164:ARG:HG3	1:B:323:ALA:HB3	1.99	0.43
2:D:281:TYR:HB3	2:D:285:LEU:HD12	2.00	0.43
1:C:373:ARG:HG2	7:D:600:ANP:O3'	2.19	0.43
1:C:180:ILE:HD11	1:C:216:LEU:HD12	2.01	0.43
1:C:311:LYS:NZ	1:C:318:GLY:O	2.52	0.43
1:A:362:ARG:NH2	2:D:372:ARG:HD3	2.34	0.43
1:B:288:PRO:HA	1:B:289:PRO:HD2	1.94	0.43
1:B:270:ASP:HB3	1:B:326:VAL:HB	2.00	0.43
1:C:399:GLU:HG3	2:D:342:LEU:HD13	2.00	0.43
2:E:256:ASP:HA	2:E:257:ASN:HA	1.62	0.43
1:C:269:ASP:HA	1:C:270:ASP:HA	1.77	0.42
2:F:258:ILE:CG2	2:F:310:ILE:HG12	2.49	0.42
2:D:266:SER:HB3	2:D:282:GLN:HE22	1.84	0.42
1:A:48:GLN:HA	2:E:69:LEU:O	2.20	0.42
1:B:48:GLN:HB3	2:F:68:GLY:HA2	2.01	0.42
1:B:180:ILE:HD11	1:B:216:LEU:HD21	2.01	0.42
2:F:163:THR:HA	2:F:166:ILE:HG22	2.02	0.42
2:E:395:GLU:HG3	3:G:36:ARG:NH2	2.33	0.42
1:C:286:ARG:HA	2:F:275:ILE:HD11	2.02	0.42
1:C:382:ALA:HB1	1:C:442:VAL:HG11	2.01	0.42
1:A:62:MET:O	1:A:73:VAL:HA	2.19	0.42
1:C:418:LEU:O	1:C:422:VAL:HG23	2.19	0.42
1:C:177:SER:OG	7:C:600:ANP:H8	2.20	0.42
3:G:31:TYR:CD1	3:G:226:SER:HB3	2.55	0.42
4:H:47:ILE:HG23	4:H:51:HIS:CB	2.50	0.42
4:H:47:ILE:HG12	4:H:84:VAL:HG11	2.00	0.42
2:D:36:LEU:HB2	2:D:47:LEU:HB2	2.02	0.42
2:F:410:ILE:HG13	2:F:444:ILE:HG21	2.01	0.42
4:H:65:VAL:O	4:H:72:THR:HG23	2.19	0.42
2:D:164:VAL:HG23	7:D:600:ANP:O1A	2.20	0.42
2:E:457:PHE:O	2:E:460:VAL:HG22	2.19	0.42
3:G:76:GLY:HA2	3:G:82:HIS:HE1	1.85	0.41
4:H:132:GLN:HA	4:H:135:ILE:HD12	2.01	0.41
2:F:151:LYS:HD3	2:F:328:HIS:O	2.20	0.41
3:G:42:ARG:NH2	3:G:165:PHE:O	2.53	0.41
1:C:265:LEU:HD11	1:C:324:LEU:HG	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:396:LEU:HD22	2:D:400:ASP:HB3	2.03	0.41
2:D:66:THR:HB	2:D:69:LEU:HD12	2.02	0.41
2:F:189:ARG:O	2:F:192:GLU:HB2	2.20	0.41
1:A:403:PHE:CE1	3:G:19:ILE:HA	2.43	0.41
1:B:176:THR:OG1	7:B:600:ANP:O2B	2.37	0.41
2:F:153:GLY:HA3	2:F:329:LEU:HD13	2.03	0.41
1:A:362:ARG:HA	1:A:363:PRO:C	2.41	0.41
1:B:397:TYR:CG	1:B:421:GLY:HA3	2.54	0.41
2:E:275:ILE:O	2:E:283:PRO:HG3	2.20	0.41
1:B:68:PRO:HD3	2:F:15:ALA:HB2	2.02	0.41
1:B:165:GLU:O	1:B:325:PRO:HD2	2.21	0.41
2:D:187:GLY:O	2:D:222:MET:HB3	2.20	0.41
2:F:336:SER:HB3	2:F:339:ILE:HG12	2.02	0.41
2:F:440:GLY:O	2:F:444:ILE:HD12	2.21	0.41
1:B:334:VAL:HG11	1:B:351:PHE:CE2	2.56	0.41
1:C:352:LEU:HA	1:C:364:ALA:O	2.21	0.41
1:C:376:SER:HB2	1:C:384:LYS:HG3	2.01	0.41
2:D:174:ALA:O	2:D:177:HIS:HB3	2.21	0.41
2:E:168:GLU:HG2	2:E:418:PHE:CD1	2.56	0.41
1:B:26:GLU:HA	1:B:45:ARG:HB2	2.03	0.41
1:B:45:ARG:HD3	1:B:45:ARG:HA	1.88	0.41
3:G:108:VAL:HG22	3:G:131:VAL:HG21	2.03	0.41
1:C:353:GLU:HB2	1:C:356:LEU:HD12	2.01	0.41
2:D:156:GLY:H	2:D:312:VAL:HG23	1.86	0.41
1:C:410:LEU:HB3	1:C:414:THR:HG23	2.03	0.41
2:D:247:GLU:O	2:D:249:GLN:N	2.52	0.41
2:D:461:GLY:HA3	2:D:462:PRO:HD2	1.95	0.41
2:E:52:HIS:CD2	2:E:58:VAL:HG12	2.56	0.41
2:F:269:SER:HB2	2:F:282:GLN:HB3	2.01	0.41
2:F:366:GLU:O	2:F:370:VAL:HG23	2.20	0.41
2:F:408:ARG:O	2:F:412:ARG:NH1	2.54	0.41
3:G:136:PRO:HG2	3:G:218:LYS:HZ2	1.85	0.41
1:B:97:VAL:HG12	1:B:111:LEU:O	2.21	0.41
1:B:159:ILE:HD13	1:B:324:LEU:HD21	2.02	0.41
1:B:210:ARG:HA	1:B:235:THR:HG21	2.02	0.41
2:E:275:ILE:HA	2:E:276:PRO:HD3	1.96	0.41
2:E:149:GLY:HA2	2:E:304:ILE:O	2.21	0.41
3:G:70:GLY:O	3:G:108:VAL:HG12	2.21	0.41
1:A:269:ASP:HA	1:A:270:ASP:HA	1.77	0.40
1:C:99:VAL:HG21	1:C:127:ARG:CB	2.49	0.40
2:E:139:VAL:HG11	2:E:348:VAL:HB	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:143:LEU:HD22	2:F:375:GLN:HG3	2.03	0.40
2:D:222:MET:HA	2:D:229:ARG:HD3	2.04	0.40
2:D:235:THR:O	2:D:239:VAL:HG23	2.22	0.40
2:D:345:TYR:HA	2:D:346:PRO:C	2.41	0.40
2:E:87:GLY:HA2	2:E:242:TYR:CE2	2.57	0.40
1:B:300:TYR:HA	1:B:303:SER:OG	2.21	0.40
1:B:343:ILE:HD13	1:B:349:GLN:HG2	2.02	0.40
3:G:181:LEU:HD23	3:G:184:ILE:HB	2.03	0.40
3:G:228:ARG:O	3:G:232:MET:HG2	2.22	0.40
3:G:237:LYS:HA	3:G:240:SER:HB2	2.03	0.40
1:B:137:ILE:N	1:B:138:PRO:CD	2.85	0.40
1:B:144:GLU:HA	1:B:145:PRO:HD3	1.89	0.40
1:C:381:ARG:H	1:C:381:ARG:HD2	1.87	0.40

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	490/492 (100%)	461 (94%)	25 (5%)	4 (1%)	22	65
1	B	490/492 (100%)	453 (92%)	29 (6%)	8 (2%)	11	50
1	C	490/492 (100%)	473 (96%)	16 (3%)	1 (0%)	51	85
2	D	465/467 (100%)	439 (94%)	22 (5%)	4 (1%)	20	63
2	E	464/467 (99%)	431 (93%)	28 (6%)	5 (1%)	17	59
2	F	464/467 (99%)	430 (93%)	27 (6%)	7 (2%)	12	52
3	G	257/272 (94%)	236 (92%)	20 (8%)	1 (0%)	38	77
4	H	129/131 (98%)	123 (95%)	6 (5%)	0	100	100
5	I	45/47 (96%)	40 (89%)	4 (9%)	1 (2%)	8	44
6	J	70/72 (97%)	62 (89%)	6 (9%)	2 (3%)	5	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	K	70/72 (97%)	64 (91%)	5 (7%)	1 (1%)	13	53
6	L	70/72 (97%)	57 (81%)	13 (19%)	0	100	100
6	M	70/72 (97%)	64 (91%)	4 (6%)	2 (3%)	5	38
6	N	70/72 (97%)	61 (87%)	9 (13%)	0	100	100
6	O	70/72 (97%)	64 (91%)	5 (7%)	1 (1%)	13	53
6	P	70/72 (97%)	64 (91%)	5 (7%)	1 (1%)	13	53
6	Q	70/72 (97%)	61 (87%)	7 (10%)	2 (3%)	5	38
All	All	3854/3903 (99%)	3583 (93%)	231 (6%)	40 (1%)	18	61

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	95	VAL
1	A	375	GLY
2	F	423	VAL
3	G	51	LEU
1	A	23	VAL
1	B	400	VAL
1	B	404	ALA
1	B	406	PHE
2	D	55	GLU
2	D	277	SER
2	D	474	ALA
2	E	391	LEU
2	E	472	LYS
2	F	28	GLY
2	F	44	ARG
2	F	358	MET
6	J	45	GLN
2	F	424	PHE
6	P	40	PRO
6	Q	44	GLN
1	A	194	ASP
1	B	31	VAL
1	B	373	ARG
1	B	452	TYR
5	I	6	GLN
6	O	39	ASN
2	E	223	ASN
1	A	361	ILE

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Mol	Chain	Res	Type
2	D	248	GLY
2	E	81	PRO
2	F	279	VAL
6	M	40	PRO
1	B	375	GLY
2	E	279	VAL
1	C	95	VAL
2	F	461	GLY
6	J	40	PRO
6	M	71	ILE
6	K	40	PRO
6	Q	40	PRO

### 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	397/397 (100%)	391 (98%)	6 (2%)	70	88
1	B	397/397 (100%)	392 (99%)	5 (1%)	73	90
1	C	397/397 (100%)	389 (98%)	8 (2%)	60	84
2	D	377/377 (100%)	375 (100%)	2 (0%)	91	96
2	E	376/377 (100%)	368 (98%)	8 (2%)	59	84
2	F	376/377 (100%)	369 (98%)	7 (2%)	62	85
3	G	225/230 (98%)	216 (96%)	9 (4%)	36	71
4	H	104/104 (100%)	103 (99%)	1 (1%)	80	91
5	I	38/38 (100%)	37 (97%)	1 (3%)	51	80
All	All	2687/2694 (100%)	2640 (98%)	47 (2%)	66	87

All (47) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	109	ASP
1	A	157	VAL

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Mol	Chain	Res	Type
1	A	164	ARG
1	A	216	LEU
1	A	244	TYR
1	A	361	ILE
1	B	20	ASP
1	B	21	THR
1	B	488	LYS
1	B	492	GLU
1	B	509	GLU
1	C	34	ILE
1	C	74	VAL
1	C	177	SER
1	C	211	SER
1	C	216	LEU
1	C	334	VAL
1	C	409	ASP
1	C	479	LEU
2	D	89	GLU
2	D	282	GLN
2	E	14	VAL
2	E	27	GLU
2	E	205	VAL
2	E	215	VAL
2	E	257	ASN
2	E	363	VAL
2	E	390	ILE
2	E	391	LEU
2	F	43	THR
2	F	202	GLU
2	F	282	GLN
2	F	399	GLU
2	F	423	VAL
2	F	435	LYS
2	F	460	VAL
3	G	7	THR
3	G	69	ILE
3	G	113	ARG
3	G	118	ARG
3	G	126	VAL
3	G	184	ILE
3	G	196	ILE
3	G	200	VAL

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Mol	Chain	Res	Type
3	G	205	GLN
4	H	57	VAL
5	I	37	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	379	GLN
1	A	396	GLN
1	A	432	GLN
1	A	471	HIS
1	B	113	ASN
1	B	415	GLN
1	B	432	GLN
1	B	471	HIS
1	C	215	GLN
1	C	432	GLN
2	D	130	GLN
2	D	282	GLN
2	D	367	HIS
2	E	257	ASN
2	E	263	GLN
2	F	51	GLN
2	F	112	GLN
2	F	194	ASN
2	F	221	GLN
2	F	282	GLN
2	F	328	HIS
2	F	379	GLN
2	F	419	GLN
2	F	443	GLN
3	G	123	GLN
3	G	234	ASN

### 5.3.3 RNA ⓘ

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 12 ligands modelled in this entry, 5 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	$\# Z  > 2$
7	ANP	A	600	8	29,33,33	3.61	7 (24%)	28,52,52	2.00	4 (14%)
7	ANP	B	600	8	29,33,33	3.53	7 (24%)	28,52,52	2.00	5 (17%)
9	GOL	B	701	-	5,5,5	0.32	0	5,5,5	0.29	0
7	ANP	C	600	8	29,33,33	3.57	7 (24%)	28,52,52	2.02	7 (25%)
7	ANP	D	600	8	29,33,33	3.63	7 (24%)	28,52,52	1.97	6 (21%)
10	SO4	E	630	-	4,4,4	0.16	0	6,6,6	0.10	0
7	ANP	F	600	8	29,33,33	3.49	6 (20%)	28,52,52	1.94	6 (21%)

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
7	ANP	A	600	8	-	0/13/38/38	0/3/3/3
7	ANP	B	600	8	-	0/13/38/38	0/3/3/3
9	GOL	B	701	-	-	0/4/4/4	0/0/0/0
7	ANP	C	600	8	-	0/13/38/38	0/3/3/3
7	ANP	D	600	8	-	0/13/38/38	0/3/3/3
10	SO4	E	630	-	-	0/0/0/0	0/0/0/0
7	ANP	F	600	8	-	0/13/38/38	0/3/3/3

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	A	600	ANP	PA-O1A	2.00	1.58	1.50
7	D	600	ANP	PA-O1A	2.03	1.58	1.50
7	A	600	ANP	C5-C4	2.05	1.45	1.40
7	B	600	ANP	PA-O1A	2.21	1.59	1.50
7	B	600	ANP	C5-C4	2.22	1.45	1.40
7	C	600	ANP	PA-O1A	2.23	1.59	1.50
7	D	600	ANP	C5-C4	2.35	1.45	1.40
7	C	600	ANP	C5-C4	2.48	1.46	1.40
7	F	600	ANP	C5-C4	2.50	1.46	1.40
7	A	600	ANP	PG-N3B	4.07	1.74	1.63
7	A	600	ANP	PB-N3B	4.08	1.74	1.63
7	F	600	ANP	PB-N3B	4.13	1.74	1.63
7	B	600	ANP	PB-N3B	4.15	1.74	1.63
7	F	600	ANP	PG-N3B	4.18	1.74	1.63
7	C	600	ANP	PG-N3B	4.20	1.74	1.63
7	C	600	ANP	PB-N3B	4.23	1.74	1.63
7	B	600	ANP	PG-N3B	4.27	1.74	1.63
7	D	600	ANP	PB-N3B	4.58	1.75	1.63
7	D	600	ANP	PG-N3B	4.68	1.75	1.63
7	D	600	ANP	C4-N3	5.79	1.44	1.35
7	F	600	ANP	C4-N3	5.80	1.44	1.35
7	A	600	ANP	C4-N3	6.06	1.44	1.35
7	C	600	ANP	C4-N3	6.29	1.44	1.35
7	B	600	ANP	C4-N3	6.30	1.44	1.35
7	B	600	ANP	PB-O1B	11.06	1.58	1.46
7	F	600	ANP	PG-O1G	11.08	1.58	1.46
7	D	600	ANP	PB-O1B	11.24	1.58	1.46
7	C	600	ANP	PB-O1B	11.33	1.59	1.46
7	F	600	ANP	PB-O1B	11.54	1.59	1.46
7	C	600	ANP	PG-O1G	11.60	1.59	1.46
7	B	600	ANP	PG-O1G	11.63	1.59	1.46
7	A	600	ANP	PG-O1G	11.77	1.59	1.46
7	A	600	ANP	PB-O1B	11.92	1.59	1.46
7	D	600	ANP	PG-O1G	12.13	1.59	1.46

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	A	600	ANP	N3-C2-N1	-7.29	122.51	128.86
7	B	600	ANP	N3-C2-N1	-7.25	122.55	128.86
7	C	600	ANP	N3-C2-N1	-6.96	122.80	128.86
7	D	600	ANP	N3-C2-N1	-6.95	122.80	128.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	F	600	ANP	N3-C2-N1	-6.04	123.60	128.86
7	F	600	ANP	PA-O3A-PB	-4.14	117.75	132.38
7	D	600	ANP	C4-C5-N7	-4.04	105.51	109.41
7	A	600	ANP	C4-C5-N7	-3.93	105.61	109.41
7	B	600	ANP	C4-C5-N7	-3.91	105.63	109.41
7	B	600	ANP	PA-O3A-PB	-3.69	119.35	132.38
7	F	600	ANP	C4-C5-N7	-3.65	105.88	109.41
7	C	600	ANP	C4-C5-N7	-3.64	105.89	109.41
7	C	600	ANP	PA-O3A-PB	-3.51	119.99	132.38
7	F	600	ANP	O1G-PG-N3B	-3.43	106.65	111.79
7	A	600	ANP	PA-O3A-PB	-3.26	120.86	132.38
7	C	600	ANP	O1B-PB-N3B	-3.04	107.25	111.79
7	D	600	ANP	O1B-PB-N3B	-2.94	107.39	111.79
7	D	600	ANP	PA-O3A-PB	-2.37	124.00	132.38
7	C	600	ANP	O1G-PG-N3B	-2.06	108.71	111.79
7	C	600	ANP	C4'-O4'-C1'	2.02	111.92	109.77
7	D	600	ANP	C4'-O4'-C1'	2.03	111.93	109.77
7	B	600	ANP	C2'-C3'-C4'	2.05	106.60	102.62
7	F	600	ANP	C4'-O4'-C1'	2.13	112.04	109.77
7	F	600	ANP	C2-N1-C6	2.36	122.89	118.77
7	A	600	ANP	C2-N1-C6	2.63	123.38	118.77
7	B	600	ANP	C2-N1-C6	2.71	123.51	118.77
7	C	600	ANP	C2-N1-C6	2.78	123.64	118.77
7	D	600	ANP	C2-N1-C6	2.97	123.97	118.77

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	600	ANP	1	0
7	B	600	ANP	1	0
7	C	600	ANP	2	0
7	D	600	ANP	3	0
7	F	600	ANP	4	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	492/492 (100%)	-0.25	9 (1%) 69 60	49, 67, 100, 111	0
1	B	492/492 (100%)	-0.09	13 (2%) 56 47	51, 72, 110, 128	0
1	C	492/492 (100%)	-0.22	11 (2%) 62 53	50, 72, 105, 107	0
2	D	467/467 (100%)	-0.32	1 (0%) 94 93	49, 69, 86, 104	0
2	E	466/467 (99%)	-0.17	6 (1%) 77 69	51, 74, 109, 125	0
2	F	466/467 (99%)	-0.35	0 100 100	53, 70, 87, 92	0
3	G	263/272 (96%)	0.36	18 (6%) 18 16	53, 115, 136, 141	0
4	H	131/131 (100%)	0.99	27 (20%) 1 1	138, 143, 150, 151	0
5	I	47/47 (100%)	0.69	5 (10%) 7 8	119, 125, 140, 140	0
6	J	72/72 (100%)	-0.21	0 100 100	127, 130, 135, 136	0
6	K	72/72 (100%)	0.04	4 (5%) 25 21	129, 132, 134, 135	0
6	L	72/72 (100%)	-0.16	0 100 100	129, 132, 137, 137	0
6	M	72/72 (100%)	-0.05	4 (5%) 25 21	118, 127, 135, 136	0
6	N	72/72 (100%)	0.39	6 (8%) 12 12	123, 126, 136, 137	0
6	O	72/72 (100%)	0.05	5 (6%) 18 15	123, 127, 137, 137	0
6	P	72/72 (100%)	-0.06	1 (1%) 75 67	128, 130, 132, 132	0
6	Q	72/72 (100%)	-0.12	1 (1%) 75 67	125, 126, 132, 133	0
All	All	3892/3903 (99%)	-0.11	111 (2%) 52 43	49, 76, 136, 151	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	191	SER	6.6
3	G	180	SER	5.9
6	N	11	ALA	5.9
4	H	86	ALA	5.8

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Mol	Chain	Res	Type	RSRZ
1	C	20	ASP	4.7
1	C	22	SER	4.7
1	B	20	ASP	4.3
4	H	100	LEU	4.3
1	C	21	THR	3.9
3	G	188	GLU	3.8
1	B	510	ALA	3.7
3	G	53	GLU	3.7
1	A	21	THR	3.7
1	B	19	ALA	3.6
5	I	6	GLN	3.6
1	A	22	SER	3.6
4	H	103	LEU	3.5
1	A	20	ASP	3.5
5	I	8	GLY	3.5
4	H	97	ALA	3.4
1	B	22	SER	3.4
6	N	12	GLY	3.4
5	I	30	PHE	3.3
1	A	193	THR	3.3
6	O	11	ALA	3.3
4	H	72	THR	3.2
6	Q	43	LYS	3.2
1	B	21	THR	3.2
1	B	409	ASP	3.2
2	E	391	LEU	3.1
6	N	68	ALA	3.1
1	B	196	LYS	3.0
3	G	187	ALA	3.0
4	H	85	ASN	3.0
2	E	387	ILE	3.0
4	H	75	TYR	3.0
3	G	179	PHE	2.9
3	G	103	VAL	2.9
6	O	10	GLY	2.9
4	H	71	THR	2.8
4	H	105	LEU	2.8
1	C	19	ALA	2.8
4	H	130	GLU	2.8
1	A	91	THR	2.8
1	A	19	ALA	2.8
4	H	143	LYS	2.8

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Mol	Chain	Res	Type	RSRZ
3	G	60	PRO	2.7
1	C	46	ASN	2.7
4	H	124	ASP	2.7
1	C	194	ASP	2.7
4	H	68	GLU	2.6
4	H	70	GLY	2.5
3	G	186	SER	2.5
4	H	38	VAL	2.5
4	H	98	VAL	2.5
6	K	68	ALA	2.5
3	G	67	LEU	2.5
3	G	178	ILE	2.5
3	G	94	ALA	2.5
1	C	463	LYS	2.5
1	C	24	ASP	2.5
6	M	73	PHE	2.5
1	B	452	TYR	2.5
6	K	43	LYS	2.5
6	N	43	LYS	2.5
2	E	394	ASP	2.4
6	M	19	ALA	2.4
4	H	99	THR	2.4
4	H	34	ARG	2.4
4	H	109	LYS	2.4
6	P	43	LYS	2.4
4	H	32	ASN	2.4
6	N	67	VAL	2.3
3	G	102	GLU	2.3
4	H	144	ALA	2.3
6	O	6	ALA	2.3
1	B	121	ILE	2.2
3	G	124	PHE	2.2
1	B	125	ALA	2.2
3	G	81	ILE	2.2
1	B	447	ALA	2.2
4	H	120	LEU	2.2
3	G	192	ILE	2.2
5	I	9	LEU	2.2
6	N	17	GLY	2.2
3	G	194	ASP	2.2
1	C	25	LEU	2.2
1	B	453	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	27	GLU	2.1
4	H	87	ASP	2.1
2	D	28	GLY	2.1
6	O	43	LYS	2.1
4	H	54	THR	2.1
6	M	44	GLN	2.1
2	E	453	PRO	2.1
6	K	42	LEU	2.1
1	A	23	VAL	2.1
4	H	126	ALA	2.1
6	O	12	GLY	2.1
6	K	69	PHE	2.1
5	I	46	LYS	2.1
4	H	67	ALA	2.1
4	H	26	VAL	2.1
6	M	72	LEU	2.1
1	C	193	THR	2.0
1	C	510	ALA	2.0
2	E	388	ILE	2.0
1	A	94	ILE	2.0
1	B	193	THR	2.0
3	G	189	SER	2.0
1	A	93	ALA	2.0

## 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( $\text{\AA}^2$ )	Q<0.9
8	MG	D	601	1/1	0.81	0.47	7.17	62,62,62,62	0
10	SO4	E	630	5/5	0.94	0.40	4.58	71,71,71,71	0
8	MG	F	601	1/1	0.97	0.33	4.04	56,56,56,56	0
7	ANP	B	600	31/31	0.90	0.27	1.22	54,59,61,61	0
7	ANP	D	600	31/31	0.94	0.24	0.63	62,63,67,68	0
7	ANP	C	600	31/31	0.91	0.26	0.52	59,62,64,64	0
7	ANP	F	600	31/31	0.96	0.25	0.34	55,60,61,62	0
7	ANP	A	600	31/31	0.95	0.21	-0.05	41,42,43,43	0
9	GOL	B	701	6/6	0.95	0.17	-1.54	42,43,43,43	0
8	MG	A	601	1/1	0.90	0.46	-	43,43,43,43	0
8	MG	C	601	1/1	0.96	0.90	-	60,60,60,60	0
8	MG	B	601	1/1	0.97	0.27	-	55,55,55,55	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.