



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:57 AM GMT

PDB ID : 2V7Q
Title : THE STRUCTURE OF F1-ATPASE INHIBITED BY I1-60HIS, A MONOMERIC FORM OF THE INHIBITOR PROTEIN, IF1.
Authors : Gledhill, J.R.; Montgomery, M.G.; Leslie, A.G.W.; Walker, J.E.
Deposited on : 2007-07-31
Resolution : 2.10 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
A user guide is available at
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
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) : trunk26865

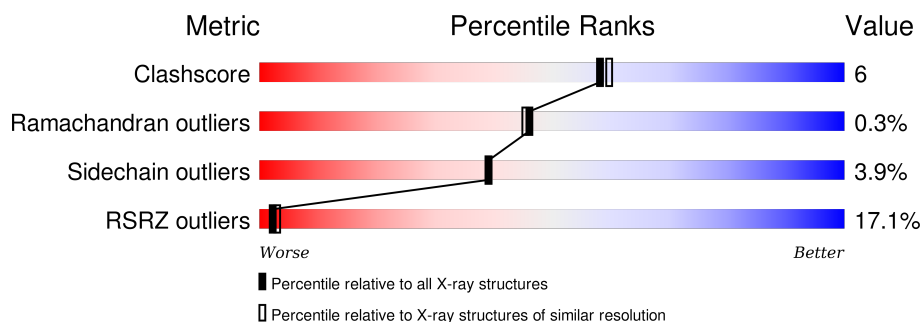
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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))
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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. 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	510	<div> <div>13%</div> <div>82%</div> <div>13%</div> <div>• 5%</div> </div>
1	B	510	<div> <div>17%</div> <div>81%</div> <div>11%</div> <div>• 6%</div> </div>
1	C	510	<div> <div>14%</div> <div>77%</div> <div>14%</div> <div>• 7%</div> </div>
2	D	482	<div> <div>7%</div> <div>85%</div> <div>11%</div> <div>• •</div> </div>
2	E	482	<div> <div>21%</div> <div>86%</div> <div>9%</div> <div>• •</div> </div>
2	F	482	<div> <div>8%</div> <div>87%</div> <div>9%</div> <div>• •</div> </div>
3	G	272	<div> <div>35%</div> <div>80%</div> <div>15%</div> <div>• •</div> </div>

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Mol	Chain	Length	Quality of chain
4	H	146	
5	I	50	
6	J	66	

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	PO4	E	1475	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 27418 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 HEART ISOFORM.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	0	0
			3715	2341	656	706	12			
1	B	479	Total	C	N	O	S	0	0	0
			3656	2303	647	694	12			
1	C	473	Total	C	N	O	S	0	0	0
			3607	2279	637	679	12			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	469	Total	C	N	O	S	0	0	0
			3558	2254	605	688	11			
2	E	465	Total	C	N	O	S	0	0	0
			3523	2234	599	679	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 GAMMA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	263	Total	C	N	O	S	0	0	0
			2054	1293	357	396	8			

- Molecule 4 is a protein called ATP SYNTHASE DELTA CHAIN.

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 EPSILON CHAIN.

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

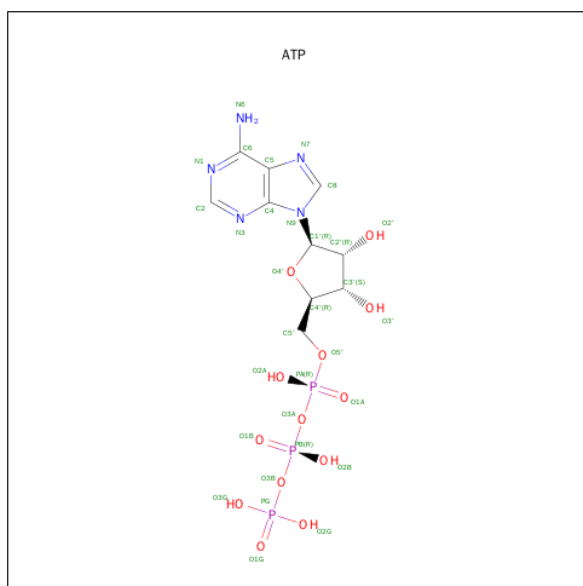
- Molecule 6 is a protein called ATPASE INHIBITOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	J	43	Total	C	N	O		0	0	0
			339	206	71	62				

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	61	HIS	-	EXPRESSION TAG	UNP P01096
J	62	HIS	-	EXPRESSION TAG	UNP P01096
J	63	HIS	-	EXPRESSION TAG	UNP P01096
J	64	HIS	-	EXPRESSION TAG	UNP P01096
J	65	HIS	-	EXPRESSION TAG	UNP P01096
J	66	HIS	-	EXPRESSION TAG	UNP P01096

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
7	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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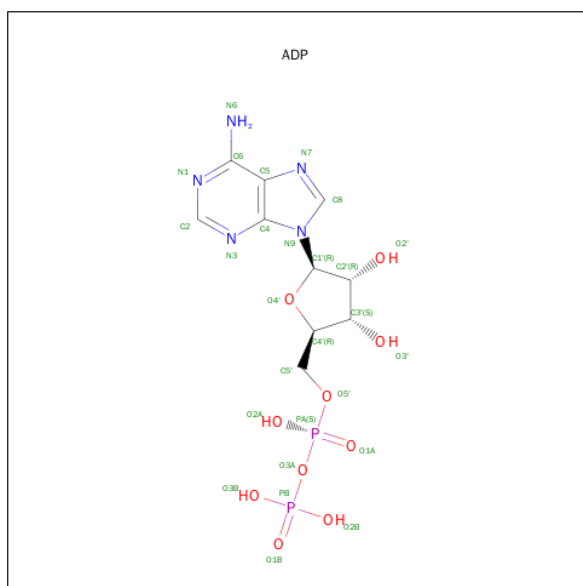
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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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

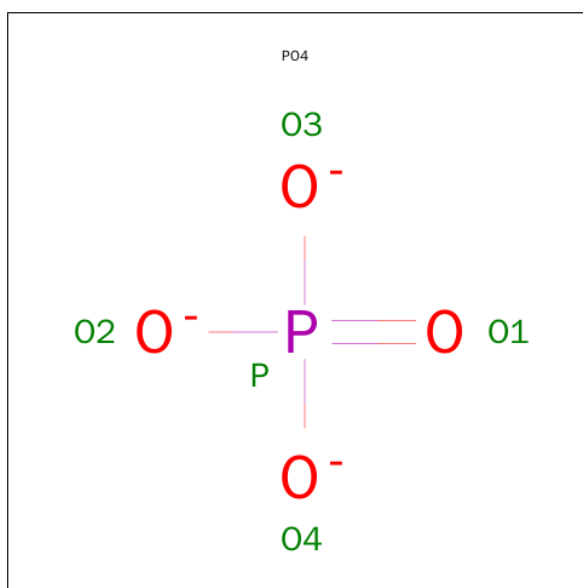
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	B	1	Total	Mg	0	0
			1	1		
8	A	1	Total	Mg	0	0
			1	1		
8	D	1	Total	Mg	0	0
			1	1		
8	C	1	Total	Mg	0	0
			1	1		
8	F	1	Total	Mg	0	0
			1	1		

- Molecule 9 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: C₁₀H₁₅N₅O₁₀P₂).



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

- Molecule 10 is PHOSPHATE ION (three-letter code: PO4) (formula: O₄P).



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

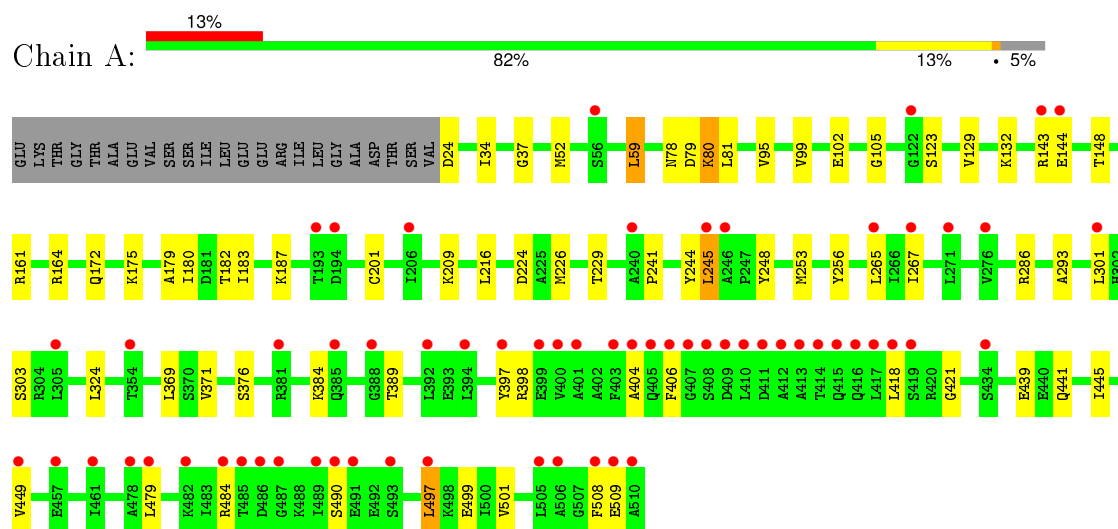
- Molecule 11 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
11	A	286	Total	O	0	0
			286	286		
11	B	294	Total	O	0	0
			294	294		
11	C	296	Total	O	0	0
			296	296		
11	D	367	Total	O	0	0
			367	367		
11	E	216	Total	O	0	0
			216	216		
11	F	316	Total	O	0	0
			316	316		
11	G	112	Total	O	0	0
			112	112		
11	H	27	Total	O	0	0
			27	27		
11	I	6	Total	O	0	0
			6	6		
11	J	20	Total	O	0	0
			20	20		

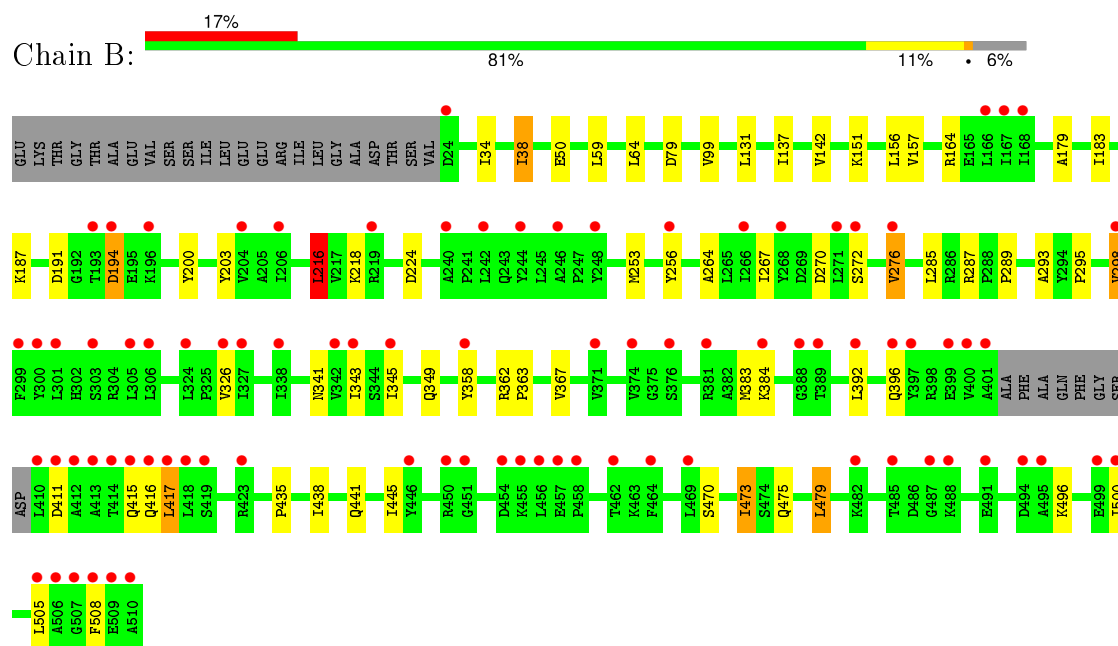
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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 HEART ISOFORM

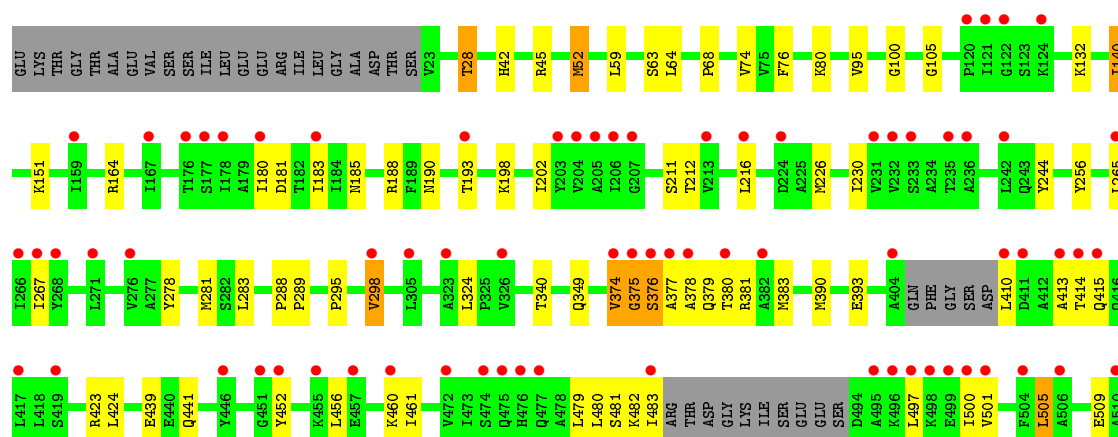


• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM




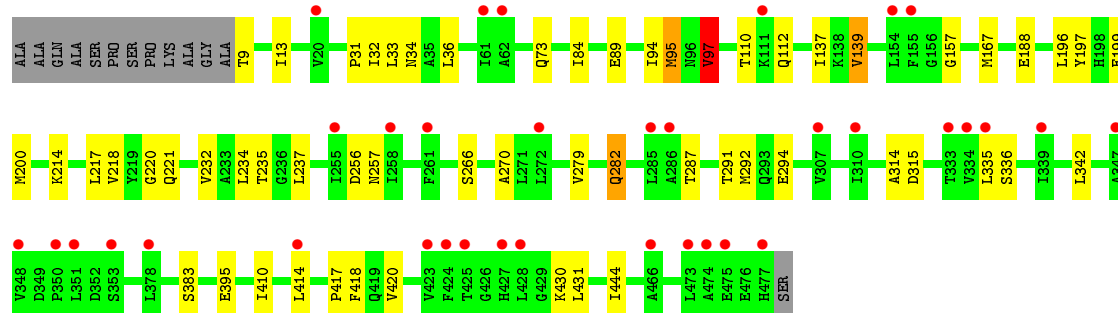
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM

Chain C: 




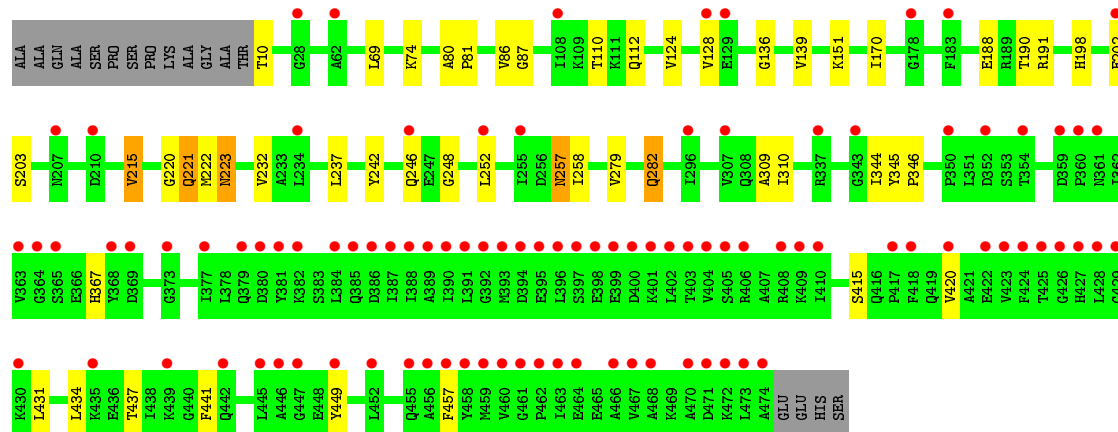
• Molecule 2: ATP SYNTHASE SUBUNIT BETA

Chain D: 




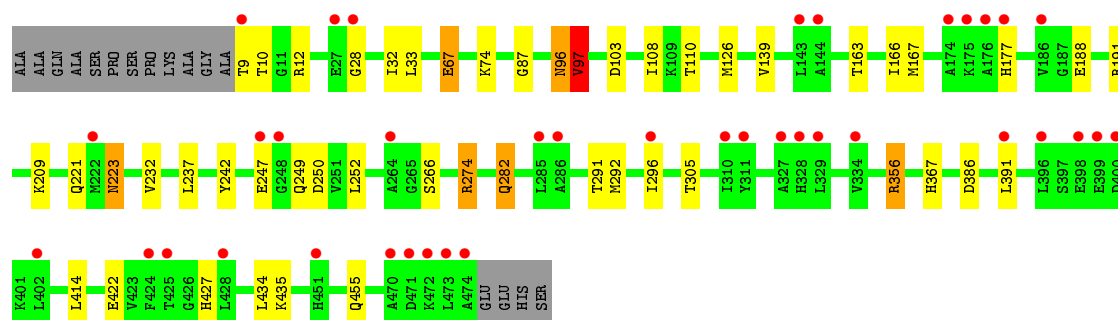
• Molecule 2: ATP SYNTHASE SUBUNIT BETA

Chain E: 

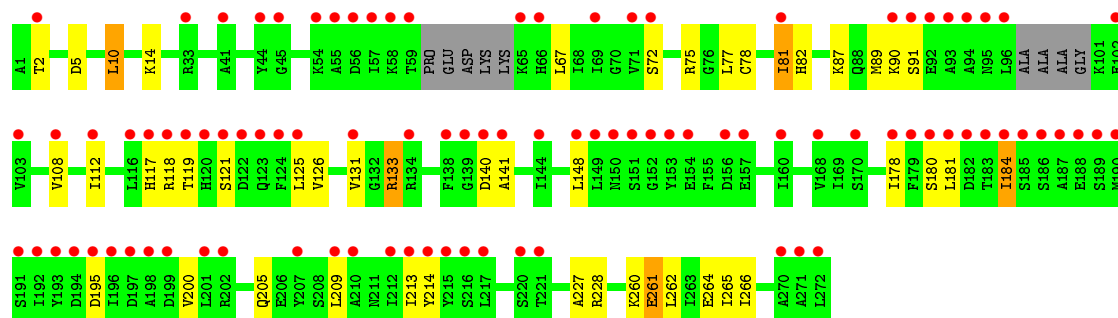
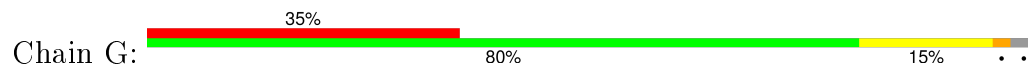


• Molecule 2: ATP SYNTHASE SUBUNIT BETA

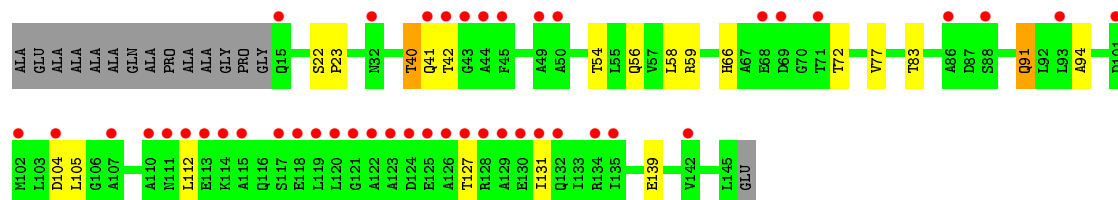
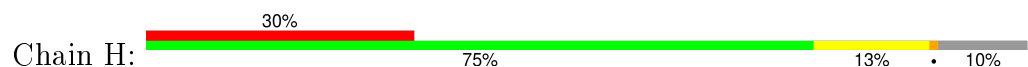
Chain F: 



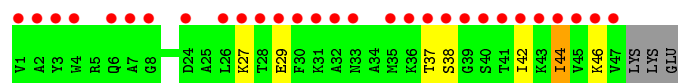
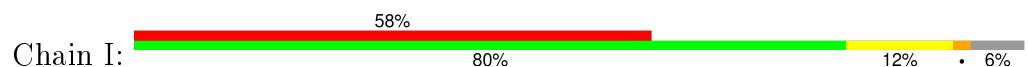
• Molecule 3: ATP SYNTHASE GAMMA CHAIN



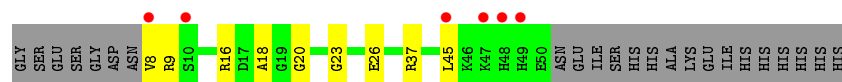
• Molecule 4: ATP SYNTHASE DELTA CHAIN



• Molecule 5: ATP SYNTHASE EPSILON CHAIN



• Molecule 6: ATPASE INHIBITOR



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	262.53Å 103.27Å 135.56Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	37.19 – 2.10 35.01 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.0 (37.19-2.10) 99.0 (35.01-2.10)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.89 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.190 , 0.245 0.195 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	31.9	Xtriage
Anisotropy	0.056	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 48.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.43$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 212299 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	27418	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: ATP, MG, PO4, 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	0.47	1/3766 (0.0%)	0.58	0/5080
1	B	0.44	0/3704	0.61	1/4995 (0.0%)
1	C	0.47	1/3655 (0.0%)	0.63	0/4930
2	D	0.47	0/3616	0.61	1/4906 (0.0%)
2	E	0.42	0/3580	0.57	0/4857
2	F	0.47	0/3587	0.61	2/4867 (0.0%)
3	G	0.38	0/2077	0.52	0/2787
4	H	0.38	0/982	0.53	0/1337
5	I	0.35	0/374	0.53	0/501
6	J	0.42	0/343	0.69	2/453 (0.4%)
All	All	0.45	2/25684 (0.0%)	0.59	6/34713 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	490	SER	CB-OG	9.72	1.54	1.42
1	C	482	LYS	C-N	7.17	1.50	1.34

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	97	VAL	CB-CA-C	-7.09	97.94	111.40
6	J	18	ALA	O-C-N	-6.80	111.64	123.20
1	B	216	LEU	CA-CB-CG	6.74	130.80	115.30
2	F	97	VAL	CB-CA-C	-5.82	100.35	111.40
6	J	18	ALA	CA-C-N	5.59	127.38	116.20
2	F	237	LEU	CA-CB-CG	5.50	127.94	115.30

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	3715	0	3812	42	0
1	B	3656	0	3763	35	0
1	C	3607	0	3717	60	0
2	D	3558	0	3605	44	0
2	E	3523	0	3580	33	0
2	F	3530	0	3586	52	0
3	G	2054	0	2122	40	0
4	H	970	0	972	10	0
5	I	369	0	395	7	0
6	J	339	0	333	5	0
7	A	31	0	12	2	0
7	B	31	0	12	0	0
7	C	31	0	12	0	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	D	27	0	12	0	0
9	F	27	0	12	0	0
10	E	5	0	0	0	0
11	A	286	0	0	4	0
11	B	294	0	0	4	0
11	C	296	0	0	7	0
11	D	367	0	0	3	0
11	E	216	0	0	1	0
11	F	316	0	0	10	0
11	G	112	0	0	3	0
11	H	27	0	0	0	0
11	I	6	0	0	0	0
11	J	20	0	0	0	0
All	All	27418	0	25945	303	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 (303) 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)
3:G:140:ASP:OD1	5:I:42:ILE:HG12	1.61	0.99
2:F:282:GLN:H	2:F:282:GLN:HE21	1.03	0.99
2:E:282:GLN:H	2:E:282:GLN:HE21	1.06	0.99
2:D:282:GLN:H	2:D:282:GLN:HE21	0.99	0.97
2:F:126:MET:HE3	11:F:2122:HOH:O	1.67	0.94
1:C:211:SER:HB3	2:F:126:MET:HE1	1.53	0.91
2:F:166:ILE:HG23	2:F:167:MET:CE	2.05	0.87
1:C:180:ILE:CD1	1:C:216:LEU:HD21	2.05	0.86
2:F:292:MET:SD	11:F:2222:HOH:O	2.37	0.81
1:C:211:SER:HB3	2:F:126:MET:CE	2.10	0.81
2:E:220:GLY:HA3	2:E:232:VAL:HG21	1.64	0.80
1:C:132:LYS:HD3	11:C:2106:HOH:O	1.81	0.79
3:G:89:MET:HE1	3:G:112:ILE:HD12	1.64	0.79
2:F:166:ILE:HG23	2:F:167:MET:HE2	1.66	0.78
1:C:52:MET:CE	1:C:76:PHE:HE1	1.96	0.77
1:C:180:ILE:HD11	1:C:216:LEU:HD21	1.68	0.76
2:F:292:MET:CE	2:F:296:ILE:HD11	2.16	0.76
2:F:209:LYS:HE2	2:F:209:LYS:HA	1.69	0.75
1:C:52:MET:CE	1:C:95:VAL:HG22	2.16	0.75
2:D:167:MET:CE	2:D:196:LEU:HD13	2.17	0.74
1:B:187:LYS:HE2	1:B:224:ASP:HB3	1.70	0.73
1:C:52:MET:HE2	1:C:76:PHE:HE1	1.54	0.73
1:C:52:MET:HE3	1:C:95:VAL:HG22	1.72	0.72
2:F:292:MET:HE2	2:F:296:ILE:HD11	1.70	0.71
1:A:52:MET:HG2	1:A:95:VAL:HG22	1.72	0.71
1:B:137:ILE:HG13	2:F:103:ASP:HA	1.72	0.71
1:C:340:THR:HG22	11:C:2231:HOH:O	1.91	0.71
1:A:99:VAL:HG23	1:A:253:MET:HA	1.73	0.71
2:F:166:ILE:HG23	2:F:167:MET:HE3	1.71	0.70
2:D:220:GLY:HA3	2:D:232:VAL:HG11	1.74	0.70
2:D:282:GLN:N	2:D:282:GLN:HE21	1.82	0.70
2:F:223:ASN:H	2:F:223:ASN:HD22	1.39	0.70
2:F:166:ILE:CG2	2:F:167:MET:HE3	2.22	0.69
2:F:282:GLN:H	2:F:282:GLN:NE2	1.85	0.68
2:D:287:THR:O	2:D:291:THR:HG23	1.93	0.68
1:B:156:LEU:HD13	1:B:367:VAL:HG13	1.73	0.68
3:G:78:CYS:HB3	11:G:2032:HOH:O	1.91	0.68
2:D:282:GLN:H	2:D:282:GLN:NE2	1.82	0.68
1:C:28:THR:HG22	11:C:2006:HOH:O	1.94	0.67
2:F:291:THR:HG21	11:F:2221:HOH:O	1.93	0.67
1:C:283:LEU:HD21	1:C:289:PRO:HB3	1.78	0.66
2:D:167:MET:HE2	2:D:196:LEU:HD13	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:126:MET:CE	11:F:2122:HOH:O	2.35	0.64
1:C:374:VAL:HG13	1:C:375:GLY:H	1.63	0.64
2:F:209:LYS:HA	2:F:209:LYS:CE	2.28	0.64
2:D:167:MET:HE1	2:D:196:LEU:HD13	1.80	0.63
2:E:223:ASN:H	2:E:223:ASN:HD22	1.45	0.63
2:D:200:MET:HE3	2:D:217:LEU:HD11	1.80	0.63
1:A:389:THR:HB	1:A:449:VAL:HG21	1.79	0.63
2:F:282:GLN:N	2:F:282:GLN:HE21	1.87	0.63
3:G:178:ILE:HG22	3:G:180:SER:HB2	1.81	0.63
1:B:295:PRO:O	1:B:298:VAL:HG22	1.99	0.63
1:A:180:ILE:HD11	1:A:216:LEU:HD21	1.82	0.62
2:E:257:ASN:HB2	2:E:309:ALA:O	2.00	0.62
2:F:12:ARG:HG2	2:F:74:LYS:HE2	1.82	0.61
2:E:203:SER:HB2	2:E:420:VAL:HG13	1.82	0.60
2:F:266:SER:HB3	2:F:282:GLN:HE22	1.65	0.60
2:F:249:GLN:HE21	2:F:249:GLN:HA	1.66	0.60
2:E:282:GLN:H	2:E:282:GLN:NE2	1.89	0.60
1:A:404:ALA:HB2	1:A:418:LEU:HD22	1.85	0.59
2:D:137:ILE:HD12	2:D:418:PHE:CE1	2.37	0.59
1:C:52:MET:HE2	1:C:76:PHE:CE1	2.36	0.59
1:C:340:THR:HG21	2:D:314:ALA:HB2	1.85	0.59
1:C:244:TYR:CB	1:C:281:MET:HE1	2.33	0.59
2:E:449:TYR:HB3	2:E:457:PHE:HZ	1.68	0.58
2:F:188:GLU:O	2:F:221:GLN:HB3	2.02	0.58
2:D:234:LEU:CD2	2:D:292:MET:HG3	2.34	0.58
1:A:78:ASN:HD21	1:A:80:LYS:HD3	1.69	0.58
1:A:376:SER:HB3	1:A:384:LYS:HE3	1.84	0.58
1:C:52:MET:CE	1:C:76:PHE:CE1	2.83	0.58
2:D:200:MET:CE	2:D:217:LEU:HD11	2.33	0.58
5:I:37:THR:HG22	5:I:38:SER:H	1.69	0.58
3:G:117:HIS:O	3:G:121:SER:HB2	2.03	0.58
1:C:52:MET:HE1	1:C:76:PHE:HE1	1.69	0.57
1:A:303:SER:HB2	2:E:222:MET:HG2	1.86	0.57
2:E:198:HIS:O	2:E:202:GLU:HG2	2.04	0.57
1:A:497:LEU:O	1:A:501:VAL:HG23	2.04	0.57
1:C:52:MET:HE1	1:C:95:VAL:HG22	1.86	0.56
2:F:96:ASN:HD22	2:F:96:ASN:C	2.08	0.56
1:B:289:PRO:HB2	1:B:293:ALA:HA	1.88	0.56
6:J:8:VAL:HG23	6:J:9:ARG:H	1.71	0.56
2:D:234:LEU:HD21	2:D:292:MET:HG3	1.87	0.56
1:A:187:LYS:HE3	1:A:224:ASP:HB3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:LYS:HD2	2:E:128:VAL:HB	1.88	0.55
1:B:183:ILE:HD11	1:B:267:ILE:HD13	1.88	0.55
2:D:139:VAL:HG13	2:D:414:LEU:HD22	1.87	0.55
4:H:127:THR:O	4:H:131:ILE:HG12	2.07	0.55
2:D:221:GLN:HA	2:D:221:GLN:HE21	1.72	0.54
2:D:97:VAL:HG22	11:D:2176:HOH:O	2.07	0.54
1:C:439:GLU:HG3	1:C:480:LEU:HB3	1.89	0.54
1:C:379:GLN:HG2	1:C:380:THR:H	1.73	0.54
1:C:380:THR:HG22	1:C:381:ARG:H	1.72	0.54
3:G:2:THR:HG23	3:G:5:ASP:H	1.73	0.54
4:H:104:ASP:HB2	5:I:27:LYS:HB3	1.89	0.54
2:F:249:GLN:NE2	2:F:249:GLN:HA	2.22	0.54
1:A:24:ASP:N	11:A:2002:HOH:O	2.41	0.54
1:C:180:ILE:HD12	1:C:216:LEU:HD21	1.86	0.53
2:D:395:GLU:CD	3:G:75:ARG:HD3	2.29	0.53
2:F:9:THR:N	11:F:2001:HOH:O	2.41	0.53
2:E:257:ASN:HD22	2:E:257:ASN:C	2.10	0.53
1:C:265:LEU:HD11	1:C:324:LEU:HG	1.90	0.53
2:F:97:VAL:HG22	11:F:2173:HOH:O	2.08	0.53
1:A:439:GLU:HG2	1:A:484:ARG:HB2	1.90	0.53
2:D:84:ILE:HD13	2:D:235:THR:HG23	1.91	0.52
2:D:157:GLY:HA3	2:D:315:ASP:OD1	2.09	0.52
2:D:89:GLU:HB2	2:D:110:THR:CG2	2.39	0.52
1:C:390:MET:HG3	1:C:424:LEU:HD13	1.90	0.52
1:B:496:LYS:O	1:B:500:ILE:HG12	2.09	0.52
1:C:376:SER:C	1:C:378:ALA:H	2.13	0.52
4:H:22:SER:HA	4:H:94:ALA:O	2.10	0.52
1:B:287:ARG:HD3	11:B:2219:HOH:O	2.08	0.52
2:E:136:GLY:HA3	2:E:431:LEU:HD12	1.91	0.52
4:H:58:LEU:HD13	4:H:77:VAL:HG11	1.93	0.51
2:E:170:ILE:HG21	2:E:215:VAL:HG22	1.92	0.51
1:C:151:LYS:HG2	1:C:441:GLN:HG2	1.92	0.51
2:D:188:GLU:O	2:D:221:GLN:HB3	2.11	0.51
1:C:202:ILE:HG12	1:C:230:ILE:HD12	1.93	0.51
2:F:252:LEU:HD23	2:F:305:THR:HB	1.93	0.51
1:C:45:ARG:NH2	1:C:68:PRO:O	2.22	0.51
1:B:358:TYR:HB3	11:B:2258:HOH:O	2.11	0.51
1:A:179:ALA:HB1	1:A:267:ILE:HG12	1.93	0.51
2:D:279:VAL:HG12	2:D:279:VAL:O	2.10	0.50
3:G:78:CYS:HB3	3:G:228:ARG:HG3	1.91	0.50
1:B:479:LEU:HG	1:B:496:LYS:HD3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:VAL:CG2	1:A:256:TYR:HB2	2.41	0.50
1:B:99:VAL:HG13	1:B:256:TYR:HB2	1.92	0.50
2:E:258:ILE:HG21	2:E:310:ILE:HG12	1.93	0.50
2:F:223:ASN:N	2:F:223:ASN:HD22	2.05	0.50
5:I:44:ILE:HD13	5:I:44:ILE:H	1.75	0.50
1:C:423:ARG:HD2	1:C:461:ILE:HD11	1.93	0.50
2:E:223:ASN:N	2:E:223:ASN:HD22	2.10	0.49
1:A:293:ALA:HB2	3:G:265:ILE:HD13	1.93	0.49
1:C:497:LEU:HA	1:C:500:ILE:HG22	1.93	0.49
1:C:52:MET:HE3	1:C:52:MET:HA	1.94	0.49
2:D:395:GLU:OE1	3:G:75:ARG:NH1	2.40	0.49
11:C:2234:HOH:O	3:G:2:THR:HG21	2.11	0.49
2:F:391:LEU:HD22	3:G:77:LEU:HD21	1.93	0.49
2:E:242:TYR:CD1	2:E:246:GLN:HG3	2.47	0.49
1:C:380:THR:HB	1:C:383:MET:HB3	1.95	0.49
2:E:86:VAL:O	2:E:110:THR:OG1	2.30	0.49
3:G:131:VAL:HG22	5:I:42:ILE:HD12	1.94	0.49
2:D:291:THR:HG21	11:D:2116:HOH:O	2.13	0.49
2:F:292:MET:HE1	2:F:296:ILE:HD11	1.90	0.49
2:F:139:VAL:HG23	11:F:2296:HOH:O	2.13	0.49
1:A:183:ILE:HD11	1:A:267:ILE:HD13	1.94	0.49
1:B:343:ILE:HG12	1:B:349:GLN:HG2	1.95	0.49
2:D:89:GLU:HB2	2:D:110:THR:HG22	1.95	0.49
1:A:102:GLU:HG3	1:A:123:SER:HA	1.94	0.49
1:A:175:LYS:HE3	7:A:1511:ATP:O1B	2.13	0.49
1:A:172:GLN:NE2	7:A:1511:ATP:O1G	2.41	0.48
1:B:392:LEU:HB2	11:B:2262:HOH:O	2.12	0.48
2:F:266:SER:HB3	2:F:282:GLN:NE2	2.27	0.48
2:E:203:SER:CB	2:E:420:VAL:HG13	2.43	0.48
1:B:411:ASP:HB3	1:B:415:GLN:HB2	1.94	0.48
3:G:75:ARG:O	3:G:82:HIS:HE1	1.97	0.48
1:B:272:SER:O	1:B:276:VAL:HG13	2.14	0.48
1:A:248:TYR:OH	1:A:301:LEU:HD12	2.13	0.48
2:D:97:VAL:HG13	2:D:232:VAL:HG13	1.95	0.48
1:A:143:ARG:HB2	11:A:2118:HOH:O	2.14	0.48
1:C:211:SER:HB3	2:F:126:MET:HE2	1.94	0.48
1:B:441:GLN:O	1:B:445:ILE:HG12	2.14	0.48
3:G:140:ASP:HB3	5:I:42:ILE:HG13	1.96	0.47
1:A:397:TYR:CG	1:A:421:GLY:HA3	2.49	0.47
2:D:395:GLU:OE2	3:G:75:ARG:HD3	2.15	0.47
1:C:379:GLN:HG2	1:C:380:THR:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:87:LYS:HA	3:G:90:LYS:HE2	1.97	0.47
3:G:75:ARG:NH2	3:G:228:ARG:HG2	2.29	0.47
1:A:201:CYS:O	1:A:229:THR:HA	2.14	0.47
1:B:34:ILE:HD11	1:B:79:ASP:HB2	1.97	0.47
3:G:2:THR:HG22	3:G:5:ASP:CG	2.35	0.47
1:C:452:TYR:HB3	1:C:505:LEU:HD12	1.97	0.47
2:D:94:ILE:HD11	2:D:197:TYR:CD1	2.50	0.47
2:F:166:ILE:CG2	2:F:167:MET:CE	2.81	0.47
1:A:369:LEU:HD21	6:J:8:VAL:HB	1.97	0.47
2:E:345:TYR:HA	2:E:346:PRO:C	2.35	0.47
3:G:2:THR:CG2	3:G:5:ASP:H	2.27	0.47
1:C:185:ASN:O	1:C:188:ARG:HG2	2.14	0.47
1:A:37:GLY:HA2	1:A:79:ASP:CG	2.35	0.47
3:G:81:ILE:HD13	3:G:227:ALA:CB	2.45	0.46
1:A:105:GLY:HA2	1:A:226:MET:O	2.15	0.46
3:G:10:LEU:HD22	3:G:14:LYS:HE3	1.97	0.46
3:G:262:LEU:O	3:G:266:ILE:HG12	2.15	0.46
2:E:344:ILE:HG23	2:E:415:SER:HB3	1.96	0.46
2:D:31:PRO:HD2	2:D:34:ASN:ND2	2.30	0.46
1:C:278:TYR:CE2	1:C:295:PRO:HG2	2.50	0.46
2:D:188:GLU:H	2:D:221:GLN:NE2	2.13	0.46
2:F:221:GLN:HE21	2:F:221:GLN:HA	1.81	0.46
1:C:295:PRO:HD2	1:C:298:VAL:HG13	1.97	0.46
1:B:38:ILE:HD11	1:B:64:LEU:HD23	1.97	0.46
2:E:257:ASN:ND2	2:E:257:ASN:C	2.70	0.46
2:E:367:HIS:CE1	2:E:434:LEU:HD11	2.51	0.46
2:D:13:ILE:HD12	2:D:73:GLN:HB3	1.98	0.46
3:G:89:MET:CE	3:G:112:ILE:HG23	2.46	0.45
2:F:163:THR:O	2:F:167:MET:HG2	2.17	0.45
2:E:188:GLU:O	2:E:221:GLN:HG3	2.17	0.45
2:E:437:THR:O	2:E:441:PHE:HD1	1.99	0.45
1:A:441:GLN:O	1:A:445:ILE:HG12	2.16	0.45
2:F:139:VAL:HG22	2:F:414:LEU:HB3	1.98	0.45
1:C:80:LYS:HG2	2:F:32:ILE:HG21	1.99	0.45
1:B:99:VAL:HG22	1:B:253:MET:HA	1.99	0.45
2:D:410:ILE:HG13	2:D:444:ILE:HG21	1.97	0.45
1:C:456:LEU:HD11	1:C:460:LYS:HD2	1.97	0.45
1:C:100:GLY:HA2	1:C:256:TYR:CZ	2.52	0.45
1:C:212:THR:HA	2:F:356:ARG:HH22	1.81	0.45
1:B:187:LYS:NZ	1:B:191:ASP:OD2	2.49	0.45
1:A:99:VAL:HG21	1:A:256:TYR:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:72:SER:CB	3:G:82:HIS:HD2	2.29	0.45
3:G:72:SER:HB2	3:G:82:HIS:HD2	1.82	0.45
1:A:479:LEU:HD11	1:A:497:LEU:HG	1.98	0.45
1:C:140:ILE:HD12	11:C:2110:HOH:O	2.16	0.45
4:H:41:GLN:HA	4:H:59:ARG:HG3	1.98	0.45
3:G:214:TYR:CE2	4:H:23:PRO:HB3	2.52	0.45
2:D:266:SER:HB3	2:D:282:GLN:HE22	1.82	0.44
2:E:87:GLY:HA2	2:E:242:TYR:CE2	2.53	0.44
3:G:133:ARG:HG3	11:G:2055:HOH:O	2.17	0.44
3:G:209:LEU:O	3:G:213:ILE:HG22	2.16	0.44
2:F:367:HIS:CE1	2:F:434:LEU:HD11	2.53	0.44
1:B:38:ILE:HD12	1:B:285:LEU:HD21	1.99	0.44
1:C:52:MET:HE3	1:C:52:MET:CA	2.47	0.44
1:A:209:LYS:HB2	2:D:294:GLU:OE1	2.18	0.44
2:F:274:ARG:NH2	11:F:2203:HOH:O	2.51	0.44
1:B:156:LEU:HD13	1:B:367:VAL:CG1	2.46	0.44
3:G:75:ARG:HG3	11:G:2032:HOH:O	2.18	0.44
1:C:244:TYR:CG	1:C:281:MET:HE1	2.52	0.44
2:D:214:LYS:HE3	11:D:2193:HOH:O	2.17	0.44
2:E:190:THR:OG1	2:E:221:GLN:HG2	2.18	0.44
6:J:20:GLY:O	6:J:23:GLY:N	2.51	0.44
1:C:52:MET:HE1	1:C:76:PHE:CE1	2.50	0.43
4:H:83:THR:HB	4:H:91:GLN:HG2	2.00	0.43
1:A:99:VAL:HG22	1:A:256:TYR:CB	2.48	0.43
1:C:42:HIS:HD2	11:C:2010:HOH:O	2.00	0.43
1:A:508:PHE:CD2	1:A:509:GLU:HG2	2.53	0.43
1:B:270:ASP:HB2	1:B:326:VAL:O	2.19	0.43
2:E:282:GLN:N	2:E:282:GLN:HE21	1.91	0.43
1:B:362:ARG:HA	1:B:363:PRO:C	2.38	0.43
2:F:87:GLY:HA2	2:F:242:TYR:CE2	2.53	0.43
1:C:481:SER:C	1:C:483:ILE:H	2.21	0.43
1:A:144:GLU:HB3	1:A:161:ARG:HD2	2.01	0.43
1:B:470:SER:O	1:B:473:ILE:HG22	2.19	0.43
11:A:2114:HOH:O	2:E:191:ARG:HG3	2.19	0.43
3:G:87:LYS:O	3:G:91:SER:HB2	2.19	0.43
2:D:95:MET:HG2	2:D:218:VAL:HG22	2.01	0.43
2:D:417:PRO:HG2	2:D:430:LYS:HG2	2.00	0.43
4:H:40:THR:OG1	4:H:56:GLN:CG	2.67	0.43
1:B:50:GLU:OE2	2:F:67:GLU:HG3	2.19	0.43
1:C:278:TYR:CD2	1:C:295:PRO:HG2	2.54	0.43
1:A:148:THR:HA	1:A:182:THR:HG23	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:108:ILE:HG22	2:F:110:THR:HG23	2.00	0.43
3:G:141:ALA:HB1	3:G:213:ILE:HG23	2.00	0.43
1:B:435:PRO:HG2	11:B:2063:HOH:O	2.18	0.43
1:C:190:ASN:HA	1:C:198:LYS:HG2	2.01	0.42
3:G:178:ILE:CG2	3:G:180:SER:HB2	2.47	0.42
2:D:221:GLN:HA	2:D:221:GLN:NE2	2.33	0.42
1:C:376:SER:C	1:C:378:ALA:N	2.72	0.42
1:A:397:TYR:CD1	1:A:421:GLY:HA3	2.54	0.42
1:B:383:MET:HG3	1:B:438:ILE:HD11	2.01	0.42
1:C:64:LEU:HD23	1:C:64:LEU:HA	1.86	0.42
1:B:341:ASN:O	1:B:345:ILE:HG13	2.19	0.42
2:D:342:LEU:HD11	6:J:16:ARG:HH21	1.83	0.42
2:F:139:VAL:HG21	11:F:2258:HOH:O	2.19	0.42
3:G:261:GLU:HG2	3:G:262:LEU:N	2.34	0.42
1:A:59:LEU:HD11	1:A:81:LEU:HD12	2.02	0.42
2:F:422:GLU:HG2	2:F:427:HIS:O	2.19	0.42
3:G:181:LEU:HD23	3:G:184:ILE:HB	2.01	0.42
2:E:248:GLY:HA3	11:E:2187:HOH:O	2.18	0.42
2:E:10:THR:HG21	2:E:74:LYS:HD2	2.01	0.42
1:A:265:LEU:HD11	1:A:324:LEU:HG	2.02	0.42
2:F:188:GLU:H	2:F:221:GLN:NE2	2.17	0.42
1:B:179:ALA:HB1	1:B:267:ILE:HG12	2.02	0.42
2:E:258:ILE:CG2	2:E:310:ILE:HG12	2.50	0.42
6:J:37:ARG:HA	6:J:37:ARG:HD3	1.80	0.42
1:B:203:TYR:CZ	1:B:216:LEU:HD21	2.55	0.42
1:C:105:GLY:HA2	1:C:226:MET:O	2.20	0.41
3:G:117:HIS:CE1	3:G:118:ARG:HG3	2.56	0.41
2:F:32:ILE:O	2:F:33:LEU:HB2	2.20	0.41
2:E:80:ALA:HB1	2:E:81:PRO:HD2	2.02	0.41
1:A:129:VAL:HG21	1:A:245:LEU:HD21	2.02	0.41
1:A:180:ILE:CD1	1:A:216:LEU:HD21	2.50	0.41
2:F:97:VAL:HG13	2:F:232:VAL:HB	2.01	0.41
1:A:78:ASN:OD1	1:A:80:LYS:HB3	2.20	0.41
1:C:288:PRO:HB2	2:D:270:ALA:HB1	2.02	0.41
1:C:375:GLY:O	1:C:377:ALA:N	2.53	0.41
3:G:140:ASP:CG	5:I:42:ILE:HG12	2.34	0.41
1:C:374:VAL:N	11:C:2256:HOH:O	2.50	0.41
2:F:177:HIS:HE1	2:F:250:ASP:HB3	1.85	0.41
2:F:435:LYS:HG2	11:F:2299:HOH:O	2.21	0.41
1:C:497:LEU:O	1:C:501:VAL:HG23	2.21	0.41
1:A:241:PRO:O	1:A:245:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:TYR:O	1:B:264:ALA:HA	2.21	0.41
4:H:66:HIS:HA	4:H:72:THR:HG22	2.03	0.41
2:D:97:VAL:HG13	2:D:232:VAL:CG1	2.51	0.41
2:E:69:LEU:HD23	2:E:69:LEU:HA	1.88	0.41
2:D:32:ILE:O	2:D:33:LEU:HB2	2.21	0.41
3:G:260:LYS:HE3	3:G:264:GLU:OE2	2.21	0.41
1:A:398:ARG:HD3	11:A:2239:HOH:O	2.20	0.40
1:C:183:ILE:HD11	1:C:267:ILE:HD13	2.03	0.40
3:G:72:SER:HB2	3:G:82:HIS:CD2	2.55	0.40
1:B:151:LYS:HB2	1:B:151:LYS:HE3	1.96	0.40
3:G:2:THR:HG22	3:G:5:ASP:OD2	2.22	0.40
1:C:413:ALA:C	1:C:415:GLN:H	2.25	0.40
1:B:396:GLN:HB3	1:B:417:LEU:HD11	2.02	0.40
4:H:40:THR:OG1	4:H:56:GLN:HG2	2.22	0.40
2:D:256:ASP:HA	2:D:257:ASN:HA	1.94	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	485/510 (95%)	472 (97%)	13 (3%)	0	100	100
1	B	475/510 (93%)	459 (97%)	15 (3%)	1 (0%)	52	53
1	C	467/510 (92%)	447 (96%)	16 (3%)	4 (1%)	21	15
2	D	467/482 (97%)	451 (97%)	16 (3%)	0	100	100
2	E	463/482 (96%)	448 (97%)	14 (3%)	1 (0%)	52	53
2	F	464/482 (96%)	452 (97%)	10 (2%)	2 (0%)	39	37
3	G	257/272 (94%)	244 (95%)	11 (4%)	2 (1%)	24	17
4	H	129/146 (88%)	122 (95%)	7 (5%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
5	I	45/50 (90%)	42 (93%)	2 (4%)	1 (2%)	8	3
6	J	41/66 (62%)	40 (98%)	1 (2%)	0	100	100
All	All	3293/3510 (94%)	3177 (96%)	105 (3%)	11 (0%)	46	45

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	374	VAL
1	B	194	ASP
2	F	247	GLU
5	I	29	GLU
3	G	148	LEU
1	C	376	SER
1	C	509	GLU
2	F	28	GLY
3	G	195	ASP
1	C	375	GLY
2	E	279	VAL

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	393/413 (95%)	381 (97%)	12 (3%)	47	50
1	B	388/413 (94%)	370 (95%)	18 (5%)	33	31
1	C	381/413 (92%)	365 (96%)	16 (4%)	36	35
2	D	379/386 (98%)	365 (96%)	14 (4%)	41	41
2	E	375/386 (97%)	364 (97%)	11 (3%)	50	53
2	F	376/386 (97%)	365 (97%)	11 (3%)	50	53
3	G	225/230 (98%)	213 (95%)	12 (5%)	28	25
4	H	104/109 (95%)	97 (93%)	7 (7%)	20	16
5	I	38/41 (93%)	36 (95%)	2 (5%)	28	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	J	30/50 (60%)	28 (93%)	2 (7%)	20	16
All	All	2689/2827 (95%)	2584 (96%)	105 (4%)	39	39

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ILE
1	A	59	LEU
1	A	80	LYS
1	A	132	LYS
1	A	164	ARG
1	A	244	TYR
1	A	245	LEU
1	A	286	ARG
1	A	371	VAL
1	A	406	PHE
1	A	497	LEU
1	A	499	GLU
1	B	38	ILE
1	B	59	LEU
1	B	131	LEU
1	B	142	VAL
1	B	157	VAL
1	B	164	ARG
1	B	194	ASP
1	B	216	LEU
1	B	276	VAL
1	B	298	VAL
1	B	384	LYS
1	B	416	GLN
1	B	417	LEU
1	B	473	ILE
1	B	475	GLN
1	B	479	LEU
1	B	505	LEU
1	B	508	PHE
1	C	28	THR
1	C	52	MET
1	C	59	LEU
1	C	63	SER
1	C	74	VAL
1	C	140	ILE

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Mol	Chain	Res	Type
1	C	164	ARG
1	C	181	ASP
1	C	193	THR
1	C	298	VAL
1	C	349	GLN
1	C	393	GLU
1	C	410	LEU
1	C	414	THR
1	C	479	LEU
1	C	505	LEU
2	D	9	THR
2	D	36	LEU
2	D	95	MET
2	D	97	VAL
2	D	112	GLN
2	D	139	VAL
2	D	199	GLU
2	D	237	LEU
2	D	282	GLN
2	D	335	LEU
2	D	336	SER
2	D	383	SER
2	D	420	VAL
2	D	431	LEU
2	E	112	GLN
2	E	124	VAL
2	E	139	VAL
2	E	151	LYS
2	E	215	VAL
2	E	221	GLN
2	E	223	ASN
2	E	237	LEU
2	E	252	LEU
2	E	257	ASN
2	E	282	GLN
2	F	10	THR
2	F	67	GLU
2	F	96	ASN
2	F	97	VAL
2	F	191	ARG
2	F	223	ASN
2	F	274	ARG

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Mol	Chain	Res	Type
2	F	282	GLN
2	F	356	ARG
2	F	386	ASP
2	F	455	GLN
3	G	10	LEU
3	G	67	LEU
3	G	81	ILE
3	G	108	VAL
3	G	119	THR
3	G	125	LEU
3	G	126	VAL
3	G	133	ARG
3	G	184	ILE
3	G	200	VAL
3	G	205	GLN
3	G	261	GLU
4	H	40	THR
4	H	42	THR
4	H	54	THR
4	H	91	GLN
4	H	105	LEU
4	H	112	LEU
4	H	139	GLU
5	I	44	ILE
5	I	46	LYS
6	J	26	GLU
6	J	45	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	48	GLN
1	A	405	GLN
1	B	65	ASN
1	B	172	GLN
1	B	475	GLN
1	C	48	GLN
1	C	263	HIS
1	C	330	GLN
1	C	349	GLN
2	D	24	GLN
2	D	112	GLN

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Mol	Chain	Res	Type
2	D	194	ASN
2	D	198	HIS
2	D	221	GLN
2	D	249	GLN
2	D	282	GLN
2	E	112	GLN
2	E	223	ASN
2	E	249	GLN
2	E	257	ASN
2	E	282	GLN
2	F	96	ASN
2	F	177	HIS
2	F	194	ASN
2	F	221	GLN
2	F	223	ASN
2	F	249	GLN
2	F	282	GLN
2	F	361	ASN
2	F	367	HIS
2	F	379	GLN
3	G	82	HIS
3	G	120	HIS
3	G	225	GLN
3	G	234	ASN
4	H	85	ASN
4	H	91	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 11 ligands modelled in this entry, 5 are monoatomic - leaving 6 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	ATP	A	1511	8	24,33,33	0.99	1 (4%)	31,52,52	1.86	4 (12%)
7	ATP	B	1511	8	24,33,33	1.04	1 (4%)	31,52,52	1.77	3 (9%)
7	ATP	C	1511	8	24,33,33	0.98	1 (4%)	31,52,52	1.91	4 (12%)
9	ADP	D	1478	8	22,29,29	1.11	2 (9%)	27,45,45	1.82	3 (11%)
10	PO4	E	1475	-	4,4,4	0.47	0	6,6,6	0.27	0
9	ADP	F	1475	8	22,29,29	1.01	1 (4%)	27,45,45	2.03	3 (11%)

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	ATP	A	1511	8	-	0/18/38/38	0/3/3/3
7	ATP	B	1511	8	-	0/18/38/38	0/3/3/3
7	ATP	C	1511	8	-	0/18/38/38	0/3/3/3
9	ADP	D	1478	8	-	0/12/32/32	0/3/3/3
10	PO4	E	1475	-	-	0/0/0/0	0/0/0/0
9	ADP	F	1475	8	-	0/12/32/32	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	D	1478	ADP	O4'-C1'	2.00	1.43	1.41
7	C	1511	ATP	C5-C4	3.02	1.47	1.40
9	F	1475	ADP	C5-C4	3.10	1.47	1.40
7	A	1511	ATP	C5-C4	3.24	1.47	1.40
9	D	1478	ADP	C5-C4	3.29	1.47	1.40
7	B	1511	ATP	C5-C4	3.29	1.47	1.40

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	F	1475	ADP	N3-C2-N1	-8.06	122.72	128.89
7	A	1511	ATP	N3-C2-N1	-7.67	123.02	128.89
7	B	1511	ATP	N3-C2-N1	-7.50	123.15	128.89
7	C	1511	ATP	N3-C2-N1	-7.06	123.49	128.89
9	D	1478	ADP	N3-C2-N1	-6.61	123.83	128.89
9	D	1478	ADP	C4-C5-N7	-3.73	106.05	109.48
9	F	1475	ADP	C2'-C1'-N9	-3.59	108.81	114.29
7	C	1511	ATP	C4-C5-N7	-3.56	106.21	109.48
7	A	1511	ATP	C4-C5-N7	-3.28	106.47	109.48
7	C	1511	ATP	C2'-C1'-N9	-3.19	109.42	114.29
9	F	1475	ADP	C4-C5-N7	-3.07	106.66	109.48
7	C	1511	ATP	O3A-PA-O5'	-2.75	95.65	102.94
7	B	1511	ATP	C4-C5-N7	-2.58	107.11	109.48
9	D	1478	ADP	C2'-C1'-N9	-2.35	110.70	114.29
7	A	1511	ATP	O3A-PA-O5'	-2.12	97.31	102.94
7	B	1511	ATP	C2'-C1'-N9	-2.09	111.10	114.29
7	A	1511	ATP	O2B-PB-O3B	2.23	115.21	105.09

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	A	1511	ATP	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	487/510 (95%)	0.88	64 (13%) 5 6	22, 34, 60, 86	0
1	B	479/510 (93%)	1.02	86 (17%) 2 2	21, 33, 70, 82	0
1	C	473/510 (92%)	0.88	73 (15%) 3 4	22, 32, 65, 87	0
2	D	469/482 (97%)	0.64	35 (7%) 17 23	21, 30, 47, 65	0
2	E	465/482 (96%)	1.31	99 (21%) 1 1	23, 40, 84, 89	0
2	F	466/482 (96%)	0.69	38 (8%) 14 20	22, 32, 59, 77	0
3	G	263/272 (96%)	1.82	95 (36%) 0 0	26, 53, 83, 93	0
4	H	131/146 (89%)	1.88	44 (33%) 0 1	36, 54, 75, 76	0
5	I	47/50 (94%)	3.05	29 (61%) 0 0	46, 60, 105, 108	0
6	J	43/66 (65%)	0.96	6 (13%) 4 5	12, 24, 56, 65	0
All	All	3323/3510 (94%)	1.04	569 (17%) 2 3	12, 35, 74, 108	0

All (569) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	510	ALA	13.7
1	C	377	ALA	11.6
1	B	410	LEU	11.3
2	E	387	ILE	9.7
4	H	123	ALA	9.6
2	E	384	LEU	9.0
2	E	474	ALA	8.5
2	E	394	ASP	8.4
3	G	191	SER	8.3
5	I	47	VAL	8.2
4	H	120	LEU	8.2
2	E	396	LEU	8.0
5	I	1	VAL	7.9

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Mol	Chain	Res	Type	RSRZ
4	H	121	GLY	7.9
3	G	184	ILE	7.6
3	G	183	THR	7.6
1	A	406	PHE	7.6
1	C	414	THR	7.5
4	H	122	ALA	7.5
1	B	414	THR	7.4
5	I	36	LYS	7.3
2	E	390	ILE	7.3
5	I	35	MET	7.2
2	E	389	ALA	7.1
3	G	94	ALA	7.1
5	I	40	SER	7.0
5	I	42	ILE	6.9
2	E	457	PHE	6.8
1	A	412	ALA	6.8
1	B	418	LEU	6.7
1	B	509	GLU	6.7
2	E	425	THR	6.6
3	G	56	ASP	6.6
3	G	181	LEU	6.6
1	C	376	SER	6.5
4	H	128	ARG	6.4
3	G	95	ASN	6.4
5	I	30	PHE	6.4
2	E	470	ALA	6.4
3	G	196	ILE	6.3
3	G	185	SER	6.3
2	E	395	GLU	6.2
3	G	122	ASP	6.1
2	E	427	HIS	6.1
1	A	411	ASP	6.0
2	E	405	SER	6.0
1	B	412	ALA	6.0
2	E	402	LEU	6.0
1	B	411	ASP	6.0
1	A	409	ASP	5.9
1	A	403	PHE	5.8
5	I	39	GLY	5.8
4	H	119	LEU	5.8
3	G	153	TYR	5.8
2	E	473	LEU	5.7

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Mol	Chain	Res	Type	RSRZ
3	G	188	GLU	5.7
3	G	96	LEU	5.7
4	H	124	ASP	5.6
3	G	212	ILE	5.5
1	A	418	LEU	5.5
3	G	189	SER	5.5
2	E	403	THR	5.5
4	H	42	THR	5.5
1	B	401	ALA	5.5
1	A	410	LEU	5.5
1	A	392	LEU	5.5
1	C	451	GLY	5.4
5	I	44	ILE	5.4
2	E	428	LEU	5.4
1	C	206	ILE	5.3
1	B	413	ALA	5.3
1	B	388	GLY	5.3
3	G	156	ASP	5.2
3	G	187	ALA	5.2
1	B	508	PHE	5.2
1	C	378	ALA	5.2
4	H	126	ALA	5.2
3	G	195	ASP	5.2
2	E	388	ILE	5.2
2	E	399	GLU	5.2
1	C	483	ILE	5.1
4	H	68	GLU	5.1
6	J	48	HIS	5.1
2	E	398	GLU	5.1
3	G	180	SER	5.0
2	E	393	MET	5.0
4	H	135	ILE	5.0
3	G	124	PHE	5.0
1	B	507	GLY	5.0
3	G	121	SER	5.0
3	G	108	VAL	4.9
3	G	118	ARG	4.9
1	A	408	SER	4.9
1	A	479	LEU	4.9
2	F	176	ALA	4.9
2	E	424	PHE	4.8
2	E	429	GLY	4.8

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Mol	Chain	Res	Type	RSRZ
2	E	472	LYS	4.8
3	G	71	VAL	4.8
1	C	404	ALA	4.8
2	E	456	ALA	4.8
2	E	409	LYS	4.8
1	B	376	SER	4.8
2	E	380	ASP	4.8
2	F	474	ALA	4.8
3	G	194	ASP	4.8
2	E	392	GLY	4.7
2	E	455	GLN	4.7
3	G	57	ILE	4.7
1	A	510	ALA	4.7
1	C	267	ILE	4.7
3	G	182	ASP	4.7
1	A	405	GLN	4.7
4	H	131	ILE	4.7
1	C	193	THR	4.7
5	I	28	THR	4.6
4	H	86	ALA	4.6
2	E	458	TYR	4.6
1	B	456	LEU	4.6
1	A	407	GLY	4.6
4	H	107	ALA	4.6
4	H	130	GLU	4.6
4	H	117	SER	4.6
5	I	7	ALA	4.5
2	E	447	GLY	4.5
3	G	213	ILE	4.5
3	G	179	PHE	4.5
1	B	416	GLN	4.5
4	H	71	THR	4.5
4	H	125	GLU	4.5
3	G	141	ALA	4.5
5	I	4	TRP	4.5
1	C	411	ASP	4.5
2	E	386	ASP	4.4
3	G	210	ALA	4.4
2	E	385	GLN	4.4
4	H	45	PHE	4.4
1	A	491	GLU	4.3
1	B	396	GLN	4.3

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Mol	Chain	Res	Type	RSRZ
1	A	490	SER	4.3
1	C	375	GLY	4.3
3	G	59	THR	4.3
1	B	487	GLY	4.3
2	E	464	GLU	4.3
2	E	365	SER	4.3
1	A	381	ARG	4.3
2	E	410	ILE	4.3
4	H	110	ALA	4.3
3	G	66	HIS	4.3
1	A	505	LEU	4.3
4	H	44	ALA	4.3
5	I	29	GLU	4.2
1	B	271	LEU	4.2
1	A	478	ALA	4.2
1	A	413	ALA	4.2
2	E	361	ASN	4.2
2	E	426	GLY	4.2
2	F	28	GLY	4.2
1	A	414	THR	4.1
2	E	210	ASP	4.1
2	E	422	GLU	4.1
2	F	473	LEU	4.1
1	A	486	ASP	4.1
1	B	389	THR	4.1
2	E	401	LYS	4.0
2	E	406	ARG	4.0
3	G	151	SER	4.0
3	G	55	ALA	4.0
3	G	209	LEU	4.0
2	F	424	PHE	4.0
4	H	113	GLU	3.9
6	J	49	HIS	3.9
3	G	186	SER	3.9
5	I	6	GLN	3.9
1	B	446	TYR	3.9
3	G	207	TYR	3.9
2	F	471	ASP	3.9
1	A	416	GLN	3.9
2	E	360	PRO	3.9
4	H	41	GLN	3.9
2	E	369	ASP	3.9

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Mol	Chain	Res	Type	RSRZ
1	A	385	GLN	3.8
1	A	404	ALA	3.8
2	D	475	GLU	3.8
2	E	373	GLY	3.8
2	F	402	LEU	3.8
4	H	93	LEU	3.8
3	G	138	PHE	3.8
4	H	88	SER	3.8
1	C	382	ALA	3.8
5	I	37	THR	3.8
1	A	415	GLN	3.8
1	B	342	VAL	3.8
3	G	125	LEU	3.8
1	C	374	VAL	3.8
1	C	460	LYS	3.7
3	G	214	TYR	3.7
5	I	43	LYS	3.7
2	D	473	LEU	3.7
2	E	418	PHE	3.7
3	G	149	LEU	3.7
3	G	65	LYS	3.7
1	B	495	ALA	3.7
2	E	460	VAL	3.7
4	H	118	GLU	3.7
2	F	175	LYS	3.7
1	B	419	SER	3.7
3	G	93	ALA	3.7
1	B	451	GLY	3.7
2	F	398	GLU	3.7
3	G	117	HIS	3.7
3	G	199	ASP	3.6
1	C	504	PHE	3.6
4	H	142	VAL	3.6
1	C	271	LEU	3.6
1	C	475	GLN	3.6
5	I	24	ASP	3.6
1	B	345	ILE	3.6
3	G	197	ASP	3.6
2	E	423	VAL	3.6
2	E	397	SER	3.5
1	B	298	VAL	3.5
3	G	148	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
3	G	272	LEU	3.5
2	F	470	ALA	3.5
2	E	404	VAL	3.5
1	B	305	LEU	3.5
2	F	247	GLU	3.5
1	B	415	GLN	3.5
1	B	454	ASP	3.5
2	E	207	ASN	3.5
6	J	10	SER	3.5
1	B	399	GLU	3.5
2	E	471	ASP	3.4
2	E	364	GLY	3.4
6	J	47	LYS	3.4
3	G	119	THR	3.4
1	C	121	ILE	3.4
1	C	476	HIS	3.4
1	C	495	ALA	3.4
2	D	477	HIS	3.4
3	G	102	GLU	3.4
1	B	24	ASP	3.4
2	D	339	ILE	3.4
3	G	144	ILE	3.4
3	G	215	TYR	3.4
1	A	401	ALA	3.3
2	F	329	LEU	3.3
2	E	439	LYS	3.3
1	C	266	ILE	3.3
2	D	334	VAL	3.3
1	B	324	LEU	3.3
3	G	217	LEU	3.3
1	C	499	GLU	3.3
1	B	358	TYR	3.3
1	C	205	ALA	3.3
2	E	466	ALA	3.2
3	G	154	GLU	3.2
3	G	103	VAL	3.2
5	I	45	VAL	3.2
1	C	122	GLY	3.2
2	E	379	GLN	3.2
1	C	500	ILE	3.2
2	D	425	THR	3.2
6	J	45	LEU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	206	ILE	3.2
2	E	28	GLY	3.2
1	C	413	ALA	3.1
5	I	41	THR	3.1
3	G	90	LYS	3.1
3	G	160	ILE	3.1
1	C	474	SER	3.1
2	E	391	LEU	3.1
2	E	382	LYS	3.1
1	A	271	LEU	3.1
1	A	449	VAL	3.1
1	A	509	GLU	3.1
3	G	92	GLU	3.1
4	H	114	LYS	3.1
2	E	381	TYR	3.0
2	E	445	LEU	3.0
3	G	131	VAL	3.0
3	G	152	GLY	3.0
2	D	310	ILE	3.0
3	G	170	SER	3.0
5	I	38	SER	3.0
1	A	497	LEU	3.0
3	G	72	SER	3.0
4	H	49	ALA	3.0
2	D	61	ILE	3.0
3	G	192	ILE	3.0
1	B	306	LEU	3.0
2	D	154	LEU	3.0
1	C	203	TYR	3.0
1	C	204	VAL	3.0
2	F	27	GLU	3.0
3	G	91	SER	3.0
4	H	111	ASN	3.0
1	C	410	LEU	2.9
4	H	15	GLN	2.9
2	F	399	GLU	2.9
1	B	506	ALA	2.9
2	E	446	ALA	2.9
1	C	224	ASP	2.9
2	D	111	LYS	2.9
5	I	27	LYS	2.9
5	I	31	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	C	497	LEU	2.9
3	G	150	ASN	2.9
1	B	194	ASP	2.9
2	E	463	ILE	2.9
1	B	392	LEU	2.9
1	B	204	VAL	2.9
1	C	326	VAL	2.9
3	G	123	GLN	2.9
1	C	323	ALA	2.9
1	A	193	THR	2.9
1	B	299	PHE	2.9
5	I	46	LYS	2.9
1	B	276	VAL	2.9
2	E	363	VAL	2.9
1	A	487	GLY	2.8
3	G	139	GLY	2.8
1	A	489	ILE	2.8
4	H	101	ASP	2.8
2	F	391	LEU	2.8
3	G	134	ARG	2.8
5	I	33	ASN	2.8
1	B	167	ILE	2.8
1	B	301	LEU	2.8
2	D	428	LEU	2.8
4	H	132	GLN	2.8
3	G	220	SER	2.8
3	G	271	ALA	2.8
2	E	255	ILE	2.8
2	E	452	LEU	2.8
3	G	2	THR	2.8
1	B	326	VAL	2.8
1	C	380	THR	2.8
3	G	202	ARG	2.8
1	A	56	SER	2.7
1	A	246	ALA	2.7
2	D	474	ALA	2.7
3	G	41	ALA	2.7
1	A	417	LEU	2.7
1	C	417	LEU	2.7
1	C	501	VAL	2.7
6	J	8	VAL	2.7
2	D	424	PHE	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	166	LEU	2.7
4	H	69	ASP	2.7
2	D	285	LEU	2.7
1	C	268	TYR	2.7
3	G	193	TYR	2.7
2	E	252	LEU	2.7
2	E	128	VAL	2.7
2	E	467	VAL	2.7
1	C	452	TYR	2.7
1	C	457	GLU	2.7
2	D	378	LEU	2.6
1	C	213	VAL	2.6
1	A	122	GLY	2.6
1	A	508	PHE	2.6
2	E	359	ASP	2.6
2	F	310	ILE	2.6
1	B	193	THR	2.6
2	E	307	VAL	2.6
1	A	419	SER	2.6
1	A	399	GLU	2.6
2	E	368	TYR	2.6
1	B	500	ILE	2.6
2	D	258	ILE	2.6
2	F	177	HIS	2.6
1	C	242	LEU	2.6
2	D	351	LEU	2.6
1	A	506	ALA	2.6
2	E	108	ILE	2.6
4	H	115	ALA	2.6
4	H	32	ASN	2.6
2	F	472	LYS	2.6
1	A	143	ARG	2.6
1	A	485	THR	2.6
1	C	176	THR	2.6
2	E	417	PRO	2.6
5	I	8	GLY	2.6
1	C	496	LYS	2.6
1	B	374	VAL	2.6
4	H	134	ARG	2.6
3	G	54	LYS	2.5
3	G	216	SER	2.5
1	C	235	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	301	LEU	2.5
4	H	102	MET	2.5
2	D	307	VAL	2.5
1	C	506	ALA	2.5
1	C	510	ALA	2.5
1	B	384	LYS	2.5
1	B	338	ILE	2.5
2	F	296	ILE	2.5
2	E	435	LYS	2.5
3	G	120	HIS	2.5
1	A	457	GLU	2.5
4	H	104	ASP	2.5
2	F	396	LEU	2.5
1	A	267	ILE	2.5
1	B	327	ILE	2.5
1	C	455	LYS	2.5
2	F	451	HIS	2.5
1	B	268	TYR	2.5
4	H	50	ALA	2.5
1	B	303	SER	2.5
1	C	419	SER	2.5
4	H	43	GLY	2.5
3	G	69	ILE	2.5
3	G	33	ARG	2.5
1	C	178	ILE	2.5
1	B	381	ARG	2.5
2	E	408	ARG	2.5
3	G	190	MET	2.4
2	F	286	ALA	2.4
2	E	400	ASP	2.4
1	B	300	TYR	2.4
2	D	155	PHE	2.4
1	C	305	LEU	2.4
2	E	462	PRO	2.4
1	A	461	ILE	2.4
1	B	494	ASP	2.4
2	F	311	TYR	2.4
2	D	335	LEU	2.4
2	F	222	MET	2.4
1	A	240	ALA	2.4
2	E	461	GLY	2.4
1	A	305	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	450	ARG	2.4
1	C	472	VAL	2.4
2	E	337	ARG	2.4
3	G	178	ILE	2.4
1	B	457	GLU	2.4
1	A	394	LEU	2.4
2	D	414	LEU	2.4
2	E	449	TYR	2.4
2	F	428	LEU	2.4
4	H	112	LEU	2.4
2	F	174	ALA	2.4
1	B	491	GLU	2.4
2	D	255	ILE	2.4
1	C	265	LEU	2.4
1	A	276	VAL	2.3
2	D	20	VAL	2.3
1	B	206	ILE	2.3
1	B	482	LYS	2.3
1	B	488	LYS	2.3
2	E	430	LYS	2.3
4	H	127	THR	2.3
1	B	244	TYR	2.3
1	B	256	TYR	2.3
2	F	186	VAL	2.3
2	D	466	ALA	2.3
2	E	202	GLU	2.3
2	E	296	ILE	2.3
3	G	140	ASP	2.3
1	A	482	LYS	2.3
1	A	265	LEU	2.3
2	F	285	LEU	2.3
2	E	343	GLY	2.3
2	E	352	ASP	2.3
1	B	196	LYS	2.3
1	C	167	ILE	2.3
1	C	183	ILE	2.3
1	A	354	THR	2.3
2	D	350	PRO	2.3
1	B	417	LEU	2.3
4	H	129	ALA	2.3
5	I	2	ALA	2.3
2	E	246	GLN	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	388	GLY	2.3
5	I	3	TYR	2.3
2	D	427	HIS	2.3
1	B	485	THR	2.3
1	C	120	PRO	2.3
2	F	9	THR	2.3
2	F	327	ALA	2.3
1	C	216	LEU	2.3
2	F	143	LEU	2.3
1	C	298	VAL	2.2
3	G	58	LYS	2.2
1	B	343	ILE	2.2
2	E	442	GLN	2.2
2	E	459	MET	2.2
1	A	194	ASP	2.2
1	A	400	VAL	2.2
2	D	348	VAL	2.2
2	E	420	VAL	2.2
2	E	377	ILE	2.2
2	D	353	SER	2.2
1	B	423	ARG	2.2
3	G	116	LEU	2.2
3	G	201	LEU	2.2
5	I	26	LEU	2.2
3	G	112	ILE	2.2
5	I	32	ALA	2.2
1	B	462	THR	2.2
3	G	221	THR	2.2
1	B	371	VAL	2.2
1	B	240	ALA	2.2
1	B	499	GLU	2.2
1	A	484	ARG	2.2
2	F	425	THR	2.2
1	C	232	VAL	2.2
2	D	286	ALA	2.2
3	G	198	ALA	2.2
1	B	168	ILE	2.2
2	E	354	THR	2.1
2	F	248	GLY	2.1
3	G	44	TYR	2.1
1	B	400	VAL	2.1
1	C	231	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	276	VAL	2.1
2	D	423	VAL	2.1
1	B	266	ILE	2.1
1	B	455	LYS	2.1
3	G	45	GLY	2.1
1	B	464	PHE	2.1
1	C	415	GLN	2.1
1	B	246	ALA	2.1
1	B	397	TYR	2.1
2	F	144	ALA	2.1
3	G	270	ALA	2.1
2	E	350	PRO	2.1
2	F	334	VAL	2.1
1	C	177	SER	2.1
1	A	245	LEU	2.1
1	A	144	GLU	2.1
2	F	400	ASP	2.1
1	B	248	TYR	2.1
1	C	446	TYR	2.1
1	B	219	ARG	2.1
1	C	159	ILE	2.1
1	A	397	TYR	2.1
1	A	434	SER	2.1
1	C	233	SER	2.1
1	C	180	ILE	2.1
3	G	81	ILE	2.1
1	B	242	LEU	2.1
1	B	505	LEU	2.1
2	E	129	GLU	2.1
2	F	328	HIS	2.1
3	G	157	GLU	2.1
1	C	236	ALA	2.1
1	C	498	LYS	2.1
2	E	62	ALA	2.1
2	E	468	ALA	2.1
2	D	261	PHE	2.1
2	E	183	PHE	2.1
3	G	168	VAL	2.1
2	D	272	LEU	2.0
2	E	234	LEU	2.0
1	C	207	GLY	2.0
1	A	493	SER	2.0

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Mol	Chain	Res	Type	RSRZ
2	D	62	ALA	2.0
2	D	347	ALA	2.0
2	F	264	ALA	2.0
2	D	333	THR	2.0
1	B	272	SER	2.0
1	B	469	LEU	2.0
1	C	477	GLN	2.0
1	B	458	PRO	2.0
2	E	178	GLY	2.0
1	C	124	LYS	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, 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	LLDF	B-factors(Å ²)	Q<0.9
10	PO4	E	1475	5/5	0.91	0.28	4.09	88,90,90,90	0
8	MG	D	1479	1/1	0.90	0.15	0.60	24,24,24,24	0
7	ATP	A	1511	31/31	0.95	0.14	-0.45	23,28,38,40	4
7	ATP	C	1511	31/31	0.97	0.14	-0.56	25,30,37,39	4
8	MG	F	1476	1/1	0.83	0.16	-0.68	27,27,27,27	0
7	ATP	B	1511	31/31	0.96	0.11	-1.13	23,34,37,44	0
9	ADP	F	1475	27/27	0.97	0.13	-1.23	27,32,37,41	0
9	ADP	D	1478	27/27	0.97	0.11	-1.26	22,29,33,36	0
8	MG	B	1512	1/1	0.83	0.18	-	27,27,27,27	0
8	MG	C	1512	1/1	0.85	0.13	-	29,29,29,29	0
8	MG	A	1512	1/1	0.82	0.18	-	27,27,27,27	0

6.5 Other polymers [i](#)

There are no such residues in this entry.