



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:45 PM GMT

PDB ID : 4YXW
Title : Bovine heart mitochondrial F1-ATPase inhibited by AMP-PNP and ADP in the presence of thiophosphate.
Authors : Bason, J.V.; Montgomery, M.G.; Leslie, A.G.W.; Walker, J.E.
Deposited on : 2015-03-23
Resolution : 3.10 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

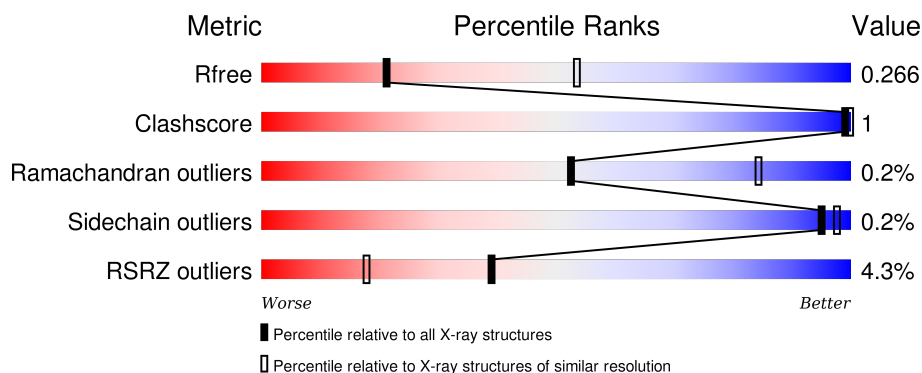
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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.



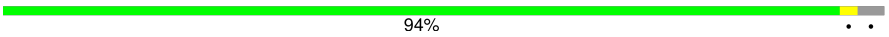


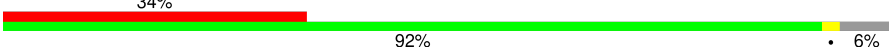
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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>%</div> <div>93%</div> <div>• •</div> </div>
1	B	510	<div> <div>4%</div> <div>93%</div> <div>• 6%</div> </div>
1	C	510	<div> <div>93%</div> <div>• •</div> </div>
2	D	482	<div> <div>94%</div> <div>• •</div> </div>
2	E	482	<div> <div>2%</div> <div>92%</div> <div>• 5%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	482	
3	G	273	
4	H	146	
5	I	50	

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	NA	F	503	-	-	-	X
8	CL	D	503	-	-	-	X

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 24827 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	489	Total	C	N	O	S	0	0	0
			3728	2349	658	709	12			
1	B	480	Total	C	N	O	S	0	0	0
			3663	2308	648	695	12			
1	C	488	Total	C	N	O	S	0	0	0
			3722	2346	657	707	12			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLU	GLN	variant	UNP P19483
A	481	GLY	SER	variant	UNP P19483
B	1	GLU	GLN	variant	UNP P19483
B	481	GLY	SER	variant	UNP P19483
C	1	GLU	GLN	variant	UNP P19483
C	481	GLY	SER	variant	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	458	Total	C	N	O	S	0	0	0
			3472	2201	592	669	10			
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	213	Total	C	N	O	S	0	0	0
			1654	1039	298	310	7			

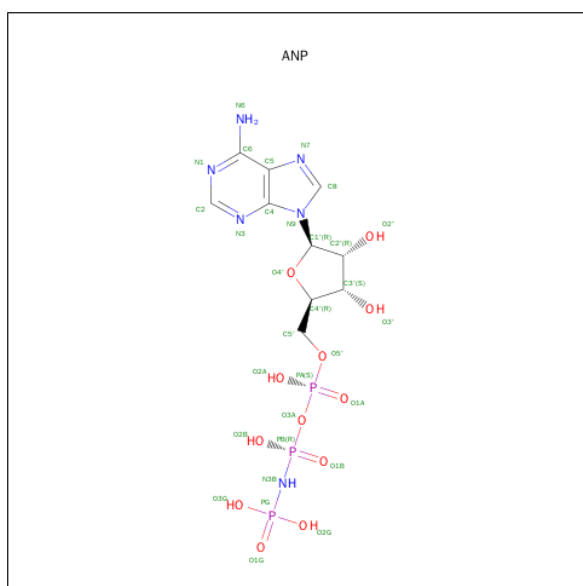
- Molecule 4 is a protein called ATP synthase subunit delta, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	128	Total	C	N	O	S	0	0	0
			946	594	160	190	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 PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



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

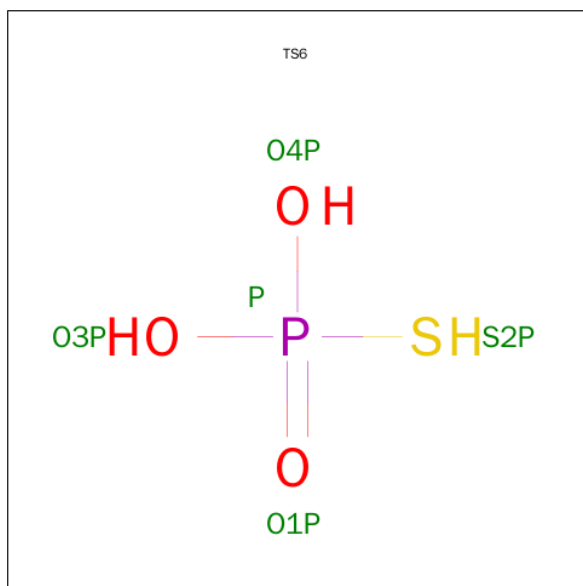
- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 8 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	D	1	Total Cl 1 1	0	0

- Molecule 9 is Monothiophosphate (three-letter code: TS6) (formula: H₃O₃PS).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
9	E	1	Total O P S 5 3 1 1	0	0

- Molecule 10 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
10	F	1	Total Na 1 1	0	0

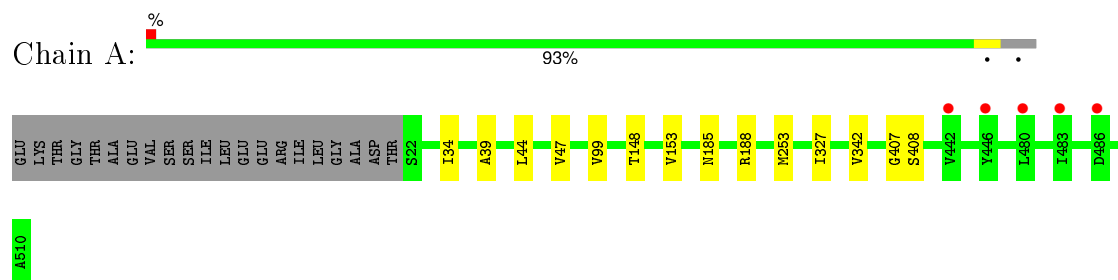
- Molecule 11 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
11	A	6	Total O 6 6	0	0
11	B	7	Total O 7 7	0	0
11	C	4	Total O 4 4	0	0
11	D	8	Total O 8 8	0	0
11	E	3	Total O 3 3	0	0
11	F	9	Total O 9 9	0	0

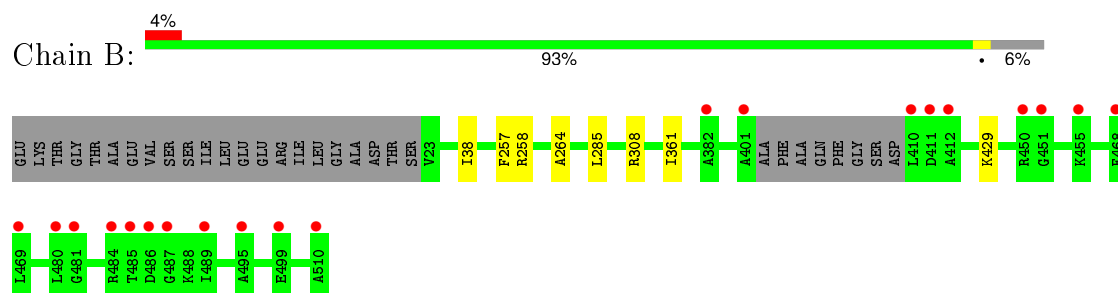
3 Residue-property plots [i](#)

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.

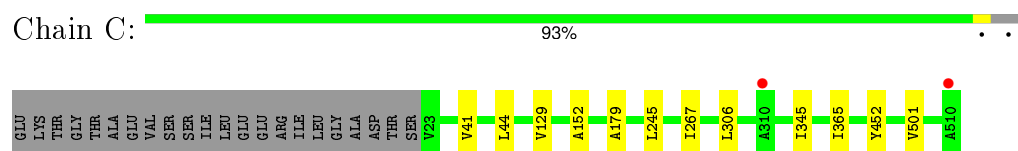
- Molecule 1: ATP synthase subunit alpha, mitochondrial



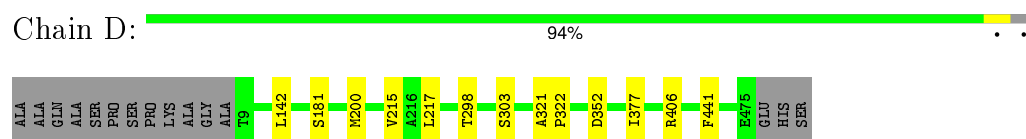
- Molecule 1: ATP synthase subunit alpha, mitochondrial



- Molecule 1: ATP synthase subunit alpha, mitochondrial

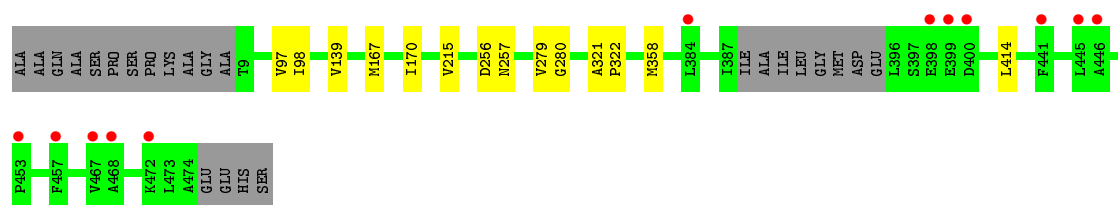


- Molecule 2: ATP synthase subunit beta, mitochondrial



- Molecule 2: ATP synthase subunit beta, mitochondrial





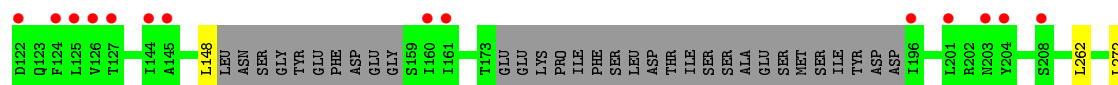
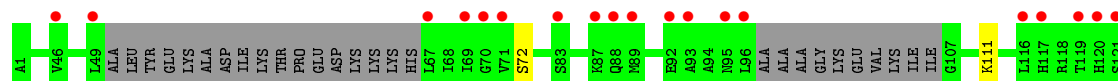
- Molecule 2: ATP synthase subunit beta, mitochondrial

Chain F: 94%



- Molecule 3: ATP synthase subunit gamma, mitochondrial

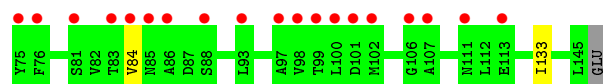
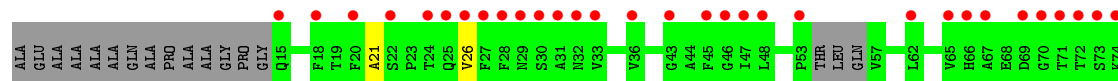
Chain G: 76%



ASP

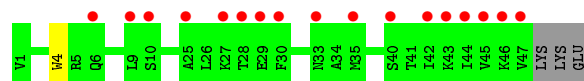
- Molecule 4: ATP synthase subunit delta, mitochondrial

Chain H: 85%



- Molecule 5: ATP synthase subunit epsilon, mitochondrial

Chain I: 92%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.35Å 123.05Å 261.28Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	76.50 – 3.10 76.52 – 3.10	Depositor EDS
% Data completeness (in resolution range)	94.2 (76.50-3.10) 94.2 (76.52-3.10)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.35 (at 3.13Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.226 , 0.273 0.224 , 0.266	Depositor DCC
R_{free} test set	3000 reflections (5.37%)	DCC
Wilson B-factor (Å ²)	62.7	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 22.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 58823 reflections (0.002%)	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	24827	wwPDB-VP
Average B, all atoms (Å ²)	76.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.80% 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: TS6, NA, MG, ANP, CL

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	0.35	0/3779	0.54	0/5098
1	B	0.35	0/3711	0.54	0/5005
1	C	0.35	0/3773	0.54	0/5090
2	D	0.35	0/3596	0.55	0/4879
2	E	0.35	0/3528	0.53	0/4786
2	F	0.35	0/3587	0.55	0/4867
3	G	0.37	0/1668	0.53	0/2234
4	H	0.36	0/957	0.47	0/1301
5	I	0.41	0/374	0.56	0/501
All	All	0.35	0/24973	0.54	0/33761

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	3728	0	3828	6	0
1	B	3663	0	3774	4	0
1	C	3722	0	3823	6	0
2	D	3539	0	3592	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	E	3472	0	3526	6	0
2	F	3530	0	3586	6	0
3	G	1654	0	1733	1	0
4	H	946	0	945	2	0
5	I	369	0	395	1	0
6	A	31	0	13	0	0
6	B	31	0	13	0	0
6	C	31	0	13	0	0
6	D	31	0	13	0	0
6	F	31	0	13	0	0
7	A	1	0	0	0	0
7	B	1	0	0	0	0
7	C	1	0	0	0	0
7	D	1	0	0	0	0
7	F	1	0	0	0	0
8	D	1	0	0	0	0
9	E	5	0	1	0	0
10	F	1	0	0	0	0
11	A	6	0	0	0	0
11	B	7	0	0	0	0
11	C	4	0	0	0	0
11	D	8	0	0	0	0
11	E	3	0	0	0	0
11	F	9	0	0	0	0
All	All	24827	0	25268	37	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 1.

All (37) 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:139:VAL:HG12	2:F:414:LEU:HD22	1.55	0.89
4:H:21:ALA:HB2	4:H:26:VAL:HG23	1.83	0.60
2:F:84:ILE:HD11	2:F:238:THR:HB	1.90	0.54
2:D:181:SER:HB2	2:D:215:VAL:HG22	1.92	0.51
2:E:97:VAL:HG13	2:E:98:ILE:HG23	1.93	0.51
1:B:361:ILE:HD13	1:B:429:LYS:HE2	1.93	0.50
1:A:34:ILE:HD13	1:A:39:ALA:HB2	1.93	0.49
2:D:200:MET:CE	2:D:217:LEU:HD21	2.43	0.47
1:C:41:VAL:HG11	1:C:44:LEU:HD12	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:452:TYR:CE2	1:C:501:VAL:HG21	2.50	0.46
2:D:200:MET:HE2	2:D:217:LEU:HD21	1.97	0.45
2:D:321:ALA:HB3	2:D:322:PRO:CD	2.46	0.44
1:A:44:LEU:O	1:A:47:VAL:HG22	2.17	0.44
1:C:152:ALA:HB3	1:C:365:ILE:HD12	2.00	0.44
1:A:99:VAL:HG13	1:A:253:MET:HA	2.00	0.44
2:D:142:LEU:HD22	2:D:441:PHE:CD2	2.53	0.43
2:D:298:THR:HG23	2:D:303:SER:HA	2.02	0.42
1:C:129:VAL:HG21	1:C:245:LEU:HD11	2.01	0.42
2:F:298:THR:HG23	2:F:303:SER:HA	2.01	0.42
2:E:167:MET:HA	2:E:170:ILE:HD12	2.01	0.42
2:E:256:ASP:HA	2:E:257:ASN:HA	1.89	0.42
2:F:321:ALA:HB3	2:F:322:PRO:CD	2.50	0.42
1:C:179:ALA:HB1	1:C:267:ILE:HD13	2.02	0.42
1:A:185:ASN:OD1	1:A:188:ARG:NH1	2.53	0.41
1:A:327:ILE:HD11	1:A:342:VAL:HG21	2.01	0.41
1:A:148:THR:HG21	1:A:153:VAL:HG11	2.02	0.41
2:F:359:ASP:O	2:F:363:VAL:HG22	2.21	0.40
2:E:280:GLY:HA2	3:G:262:LEU:CD2	2.52	0.40
1:C:306:LEU:HD12	1:C:345:ILE:HG21	2.03	0.40
2:D:377:ILE:HD11	2:D:406:ARG:HB2	2.02	0.40
1:B:258:ARG:NH1	1:B:308:ARG:O	2.55	0.40
2:F:374:VAL:HG13	2:F:410:ILE:HG21	2.02	0.40
2:E:139:VAL:HG12	2:E:414:LEU:HD22	2.02	0.40
1:B:38:ILE:CD1	1:B:285:LEU:HD21	2.51	0.40
1:B:257:PHE:HB2	1:B:264:ALA:HB2	2.04	0.40
2:E:321:ALA:HB3	2:E:322:PRO:CD	2.51	0.40
4:H:133:ILE:HD11	5:I:4:TRP:HB2	2.04	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	487/510 (96%)	476 (98%)	9 (2%)	2 (0%)	39	75
1	B	476/510 (93%)	463 (97%)	13 (3%)	0	100	100
1	C	486/510 (95%)	474 (98%)	12 (2%)	0	100	100
2	D	465/482 (96%)	442 (95%)	22 (5%)	1 (0%)	52	84
2	E	454/482 (94%)	431 (95%)	21 (5%)	2 (0%)	39	75
2	F	464/482 (96%)	443 (96%)	21 (4%)	0	100	100
3	G	203/273 (74%)	191 (94%)	11 (5%)	1 (0%)	34	72
4	H	124/146 (85%)	116 (94%)	8 (6%)	0	100	100
5	I	45/50 (90%)	40 (89%)	5 (11%)	0	100	100
All	All	3204/3445 (93%)	3076 (96%)	122 (4%)	6 (0%)	52	84

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	407	GLY
2	E	358	MET
2	D	352	ASP
1	A	408	SER
3	G	72	SER
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	395/412 (96%)	395 (100%)	0	100	100
1	B	389/412 (94%)	389 (100%)	0	100	100
1	C	394/412 (96%)	394 (100%)	0	100	100
2	D	377/386 (98%)	377 (100%)	0	100	100
2	E	370/386 (96%)	369 (100%)	1 (0%)	94	97
2	F	376/386 (97%)	376 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	G	180/231 (78%)	177 (98%)	3 (2%)	68	89
4	H	101/109 (93%)	100 (99%)	1 (1%)	82	93
5	I	38/41 (93%)	38 (100%)	0	100	100
All	All	2620/2775 (94%)	2615 (100%)	5 (0%)	95	97

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	E	215	VAL
3	G	111	LYS
3	G	148	LEU
3	G	272	LEU
4	H	84	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
2	D	419	GLN
2	E	112	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 7 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
6	ANP	A	600	7	27,33,33	2.05	7 (25%)	30,52,52	2.28	7 (23%)
6	ANP	B	600	7	27,33,33	2.04	7 (25%)	30,52,52	2.26	7 (23%)
6	ANP	C	600	7	27,33,33	2.02	8 (29%)	30,52,52	2.12	6 (20%)
6	ANP	D	600	7	27,33,33	2.08	8 (29%)	30,52,52	2.11	6 (20%)
9	TS6	E	603	-	2,4,4	2.52	1 (50%)	3,6,6	1.27	0
6	ANP	F	600	7	27,33,33	2.05	8 (29%)	30,52,52	2.31	9 (30%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	ANP	A	600	7	-	0/12/38/38	0/3/3/3
6	ANP	B	600	7	-	0/12/38/38	0/3/3/3
6	ANP	C	600	7	-	0/12/38/38	0/3/3/3
6	ANP	D	600	7	-	0/12/38/38	0/3/3/3
9	TS6	E	603	-	-	0/0/0/0	0/0/0/0
6	ANP	F	600	7	-	0/12/38/38	0/3/3/3

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	E	603	TS6	P-O3P	-3.07	1.48	1.56
6	F	600	ANP	PG-O2G	-2.10	1.50	1.56
6	D	600	ANP	PG-O2G	-2.08	1.50	1.56
6	C	600	ANP	PG-O3G	-2.03	1.51	1.56
6	D	600	ANP	PG-O3G	-2.01	1.51	1.56
6	A	600	ANP	C2-N3	2.01	1.35	1.32
6	D	600	ANP	O4'-C1'	2.01	1.43	1.41
6	B	600	ANP	PB-O3A	2.03	1.61	1.59
6	C	600	ANP	PB-O3A	2.04	1.61	1.59
6	C	600	ANP	C2-N3	2.05	1.35	1.32
6	B	600	ANP	C2-N3	2.06	1.35	1.32
6	F	600	ANP	PB-O3A	2.13	1.61	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	A	600	ANP	PB-O3A	2.15	1.61	1.59
6	F	600	ANP	O4'-C1'	2.16	1.43	1.41
6	D	600	ANP	C5-C4	3.13	1.47	1.40
6	B	600	ANP	C5-C4	3.16	1.47	1.40
6	A	600	ANP	C5-C4	3.25	1.47	1.40
6	F	600	ANP	C5-C4	3.27	1.47	1.40
6	C	600	ANP	C5-C4	3.38	1.48	1.40
6	C	600	ANP	PB-O1B	3.72	1.50	1.46
6	A	600	ANP	PB-O1B	3.92	1.50	1.46
6	B	600	ANP	PB-O1B	4.04	1.50	1.46
6	F	600	ANP	PB-N3B	4.10	1.74	1.63
6	F	600	ANP	PB-O1B	4.13	1.50	1.46
6	F	600	ANP	PG-N3B	4.23	1.74	1.63
6	D	600	ANP	PG-O1G	4.26	1.51	1.46
6	C	600	ANP	PG-O1G	4.27	1.51	1.46
6	B	600	ANP	PB-N3B	4.28	1.74	1.63
6	C	600	ANP	PB-N3B	4.29	1.74	1.63
6	C	600	ANP	PG-N3B	4.29	1.74	1.63
6	B	600	ANP	PG-N3B	4.30	1.74	1.63
6	A	600	ANP	PG-N3B	4.32	1.74	1.63
6	F	600	ANP	PG-O1G	4.43	1.51	1.46
6	D	600	ANP	PB-N3B	4.43	1.75	1.63
6	A	600	ANP	PB-N3B	4.49	1.75	1.63
6	D	600	ANP	PB-O1B	4.49	1.51	1.46
6	B	600	ANP	PG-O1G	4.54	1.51	1.46
6	D	600	ANP	PG-N3B	4.55	1.75	1.63
6	A	600	ANP	PG-O1G	4.56	1.51	1.46

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	600	ANP	N3-C2-N1	-7.96	122.80	128.89
6	B	600	ANP	N3-C2-N1	-7.94	122.82	128.89
6	F	600	ANP	N3-C2-N1	-7.91	122.84	128.89
6	D	600	ANP	N3-C2-N1	-7.71	122.99	128.89
6	C	600	ANP	N3-C2-N1	-7.61	123.07	128.89
6	A	600	ANP	O1G-PG-N3B	-5.73	103.11	111.90
6	B	600	ANP	O1G-PG-N3B	-5.15	104.00	111.90
6	C	600	ANP	O1G-PG-N3B	-4.64	104.78	111.90
6	F	600	ANP	O1G-PG-N3B	-4.29	105.31	111.90
6	D	600	ANP	C2'-C1'-N9	-4.26	107.78	114.29
6	F	600	ANP	PA-O3A-PB	-3.36	121.41	132.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	600	ANP	PA-O3A-PB	-3.33	121.49	132.67
6	F	600	ANP	C4-C5-N7	-3.21	106.53	109.48
6	C	600	ANP	PA-O3A-PB	-3.20	121.95	132.67
6	A	600	ANP	C4-C5-N7	-3.13	106.60	109.48
6	A	600	ANP	PA-O3A-PB	-3.09	122.31	132.67
6	B	600	ANP	C4-C5-N7	-3.07	106.65	109.48
6	F	600	ANP	O1B-PB-N3B	-3.07	107.19	111.90
6	D	600	ANP	PA-O3A-PB	-2.99	122.63	132.67
6	C	600	ANP	C4-C5-N7	-2.98	106.73	109.48
6	F	600	ANP	C2'-C1'-N9	-2.90	109.86	114.29
6	D	600	ANP	C4-C5-N7	-2.89	106.82	109.48
6	B	600	ANP	O1B-PB-N3B	-2.64	107.86	111.90
6	A	600	ANP	O1B-PB-N3B	-2.60	107.91	111.90
6	F	600	ANP	C2-N1-C6	2.07	122.46	118.77
6	C	600	ANP	O3G-PG-O2G	2.16	113.99	107.58
6	A	600	ANP	O3G-PG-O2G	2.19	114.07	107.58
6	B	600	ANP	O3G-PG-O2G	2.27	114.30	107.58
6	F	600	ANP	O3G-PG-O2G	2.56	115.17	107.58
6	D	600	ANP	O3G-PG-O2G	2.59	115.25	107.58
6	C	600	ANP	O2B-PB-O1B	3.51	117.33	110.00
6	A	600	ANP	O2B-PB-O1B	3.56	117.44	110.00
6	D	600	ANP	O2B-PB-O1B	3.71	117.75	110.00
6	B	600	ANP	O2B-PB-O1B	3.78	117.89	110.00
6	F	600	ANP	O2B-PB-O1B	4.31	119.00	110.00

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	489/510 (95%)	-0.11	5 (1%) 84 69	42, 66, 108, 144	0
1	B	480/510 (94%)	-0.10	20 (4%) 40 19	38, 59, 135, 163	0
1	C	488/510 (95%)	-0.24	2 (0%) 93 85	42, 61, 97, 142	0
2	D	467/482 (96%)	-0.32	0 100 100	43, 61, 88, 109	0
2	E	458/482 (95%)	-0.12	12 (2%) 59 35	37, 72, 139, 158	0
2	F	466/482 (96%)	-0.34	1 (0%) 95 91	39, 58, 97, 125	0
3	G	213/273 (78%)	0.84	33 (15%) 3 1	47, 115, 157, 174	0
4	H	128/146 (87%)	1.69	50 (39%) 0 0	92, 141, 175, 191	0
5	I	47/50 (94%)	1.59	17 (36%) 0 0	90, 134, 161, 172	0
All	All	3236/3445 (93%)	-0.03	140 (4%) 39 18	37, 66, 139, 191	0

All (140) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	I	47	VAL	10.4
5	I	29	GLU	7.1
4	H	69	ASP	6.5
4	H	83	THR	6.4
4	H	101	ASP	6.3
4	H	27	PHE	5.5
3	G	160	ILE	5.5
4	H	75	TYR	4.9
3	G	196	ILE	4.9
3	G	89	MET	4.7
4	H	86	ALA	4.6
4	H	26	VAL	4.6
3	G	125	LEU	4.4
4	H	25	GLN	4.3
4	H	71	THR	4.0

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Mol	Chain	Res	Type	RSRZ
3	G	116	LEU	3.9
4	H	32	ASN	3.9
2	E	472	LYS	3.9
5	I	46	LYS	3.8
3	G	201	LEU	3.8
4	H	66	HIS	3.7
4	H	45	PHE	3.7
4	H	76	PHE	3.7
4	H	67	ALA	3.7
4	H	30	SER	3.7
3	G	92	GLU	3.7
4	H	31	ALA	3.6
4	H	29	ASN	3.5
4	H	46	GLY	3.5
3	G	127	THR	3.4
4	H	107	ALA	3.4
1	B	486	ASP	3.4
2	E	445	LEU	3.4
3	G	122	ASP	3.3
2	E	446	ALA	3.3
3	G	69	ILE	3.2
5	I	25	ALA	3.2
4	H	106	GLY	3.2
1	B	410	LEU	3.2
1	B	484	ARG	3.1
1	B	412	ALA	3.1
4	H	70	GLY	3.1
4	H	15	GLN	3.1
5	I	40	SER	3.0
5	I	44	ILE	3.0
1	B	469	LEU	3.0
4	H	28	PHE	3.0
4	H	33	VAL	3.0
4	H	85	ASN	3.0
3	G	119	THR	3.0
4	H	102	MET	3.0
4	H	111	ASN	3.0
3	G	96	LEU	2.9
1	B	455	LYS	2.9
5	I	9	LEU	2.9
4	H	43	GLY	2.9
4	H	72	THR	2.9

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Mol	Chain	Res	Type	RSRZ
3	G	117	HIS	2.8
4	H	22	SER	2.8
4	H	73	SER	2.8
1	B	489	ILE	2.8
3	G	88	GLN	2.8
2	E	468	ALA	2.8
5	I	45	VAL	2.8
3	G	70	GLY	2.7
2	E	398	GLU	2.7
1	B	411	ASP	2.7
5	I	30	PHE	2.7
4	H	62	LEU	2.7
4	H	98	VAL	2.7
3	G	120	HIS	2.6
2	E	457	PHE	2.6
4	H	99	THR	2.5
4	H	100	LEU	2.5
5	I	42	ILE	2.5
2	E	399	GLU	2.5
1	B	487	GLY	2.4
1	B	485	THR	2.4
3	G	95	ASN	2.4
4	H	48	LEU	2.4
5	I	28	THR	2.4
3	G	93	ALA	2.4
1	B	499	GLU	2.4
2	E	467	VAL	2.4
1	B	495	ALA	2.4
4	H	53	PRO	2.3
3	G	67	LEU	2.3
3	G	124	PHE	2.3
4	H	84	VAL	2.3
3	G	83	SER	2.3
1	B	382	ALA	2.3
4	H	18	PHE	2.3
3	G	121	SER	2.3
4	H	88	SER	2.3
1	B	451	GLY	2.3
4	H	93	LEU	2.3
1	B	468	PHE	2.2
1	B	480	LEU	2.2
2	E	384	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
3	G	208	SER	2.2
3	G	49	LEU	2.2
3	G	203	ASN	2.2
1	B	450	ARG	2.2
1	A	446	TYR	2.2
1	A	442	VAL	2.2
4	H	97	ALA	2.2
2	F	9	THR	2.2
3	G	71	VAL	2.2
3	G	126	VAL	2.2
3	G	161	ILE	2.2
5	I	33	ASN	2.2
1	B	481	GLY	2.2
1	C	310	ALA	2.2
1	B	510	ALA	2.1
4	H	65	VAL	2.1
1	A	486	ASP	2.1
2	E	453	PRO	2.1
5	I	6	GLN	2.1
3	G	144	ILE	2.1
5	I	10	SER	2.1
4	H	20	PHE	2.1
4	H	47	ILE	2.1
5	I	43	LYS	2.1
3	G	46	VAL	2.1
2	E	441	PHE	2.1
3	G	204	TYR	2.1
1	B	401	ALA	2.1
1	C	510	ALA	2.1
4	H	81	SER	2.1
1	A	480	LEU	2.1
4	H	74	LYS	2.1
3	G	145	ALA	2.0
5	I	35	MET	2.0
3	G	87	LYS	2.0
5	I	27	LYS	2.0
2	E	400	ASP	2.0
4	H	113	GLU	2.0
4	H	36	VAL	2.0
1	A	483	ILE	2.0
4	H	24	THR	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	NA	F	503	1/1	0.78	0.56	8.16	61,61,61,61	0
8	CL	D	503	1/1	0.71	0.26	2.99	76,76,76,76	0
9	TS6	E	603	5/5	0.84	0.21	0.66	100,107,108,109	0
6	ANP	D	600	31/31	0.95	0.18	-0.29	48,49,55,55	0
6	ANP	B	600	31/31	0.95	0.17	-0.41	51,57,59,59	0
6	ANP	F	600	31/31	0.97	0.15	-1.01	47,58,68,69	0
6	ANP	C	600	31/31	0.96	0.15	-1.32	47,53,55,55	0
7	MG	D	601	1/1	0.96	0.14	-1.66	55,55,55,55	0
6	ANP	A	600	31/31	0.96	0.14	-1.71	47,52,56,56	0
7	MG	F	601	1/1	0.94	0.10	-3.36	48,48,48,48	0
7	MG	B	601	1/1	0.96	0.08	-	53,53,53,53	0
7	MG	C	601	1/1	0.85	0.16	-	49,49,49,49	0
7	MG	A	601	1/1	0.98	0.06	-	48,48,48,48	0

6.5 Other polymers [i](#)

There are no such residues in this entry.