W O R L D W I D E

wwPDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:47 PM GMT

PDB ID	:	4Z1M
Title	:	Bovine F1-ATPase inhibited by three copies of the inhibitor protein IF1 crystallised in the presence of thiophosphate.
Authors	:	Bason, J.V.; Montgomery, M.G.; Leslie, A.G.W.; Walker, J.E.
Deposited on	:	2015-03-27
Resolution	:	3.30 Å(reported)

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 (i)

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

The reported resolution of this entry is 3.30 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.
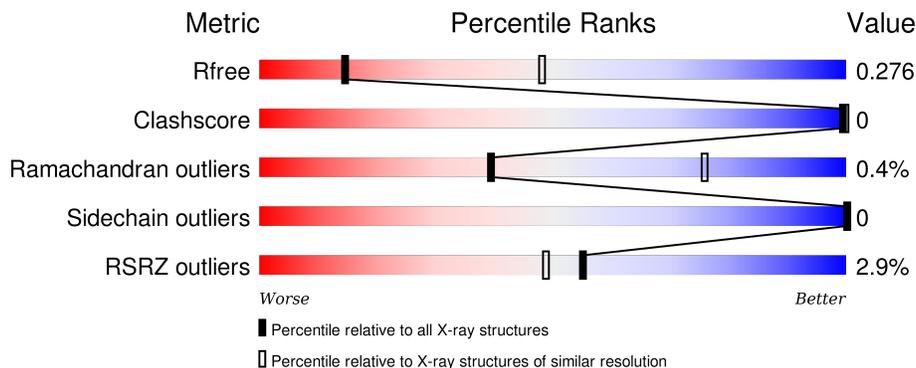
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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 <=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	94% • 5%
1	B	510	94% • 5%
1	C	510	% 94% • 5%
2	D	482	2% 96% • •
2	E	482	2% 96% • •

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Mol	Chain	Length	Quality of chain
2	F	482	96%
3	G	273	14% 67% 32%
4	H	66	5% 62% 38%
4	I	66	11% 42% 58%
4	J	66	20% 32% 67%

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
8	CL	F	503	-	-	-	X
8	CL	G	301	-	-	-	X
8	CL	G	302	-	-	-	X

2 Entry composition (i)

There are 10 unique types of molecules in this entry. The entry contains 24201 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	487	Total 3723	C 2349	N 656	O 706	S 12	0	1	0
1	B	487	Total 3706	C 2333	N 655	O 706	S 12	0	0	0
1	C	483	Total 3684	C 2323	N 651	O 698	S 12	0	0	0

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	469	Total 3558	C 2254	N 605	O 688	S 11	0	0	0
2	E	470	Total 3563	C 2257	N 606	O 689	S 11	0	0	0
2	F	469	Total 3558	C 2254	N 605	O 688	S 11	0	0	0

- Molecule 3 is a protein called ATP synthase subunit gamma, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	187	Total 1467	C 919	N 267	O 274	S 7	0	0	0

- Molecule 4 is a protein called ATPase inhibitor, mitochondrial.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
4	H	41	Total 317	C 192	N 65	O 60	0	0	0
4	I	28	Total 236	C 144	N 49	O 43	0	0	0
4	J	22	Total 189	C 117	N 38	O 34	0	0	0

There are 21 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	39	ALA	LYS	engineered mutation	UNP P01096
H	61	HIS	-	expression tag	UNP P01096
H	62	HIS	-	expression tag	UNP P01096
H	63	HIS	-	expression tag	UNP P01096
H	64	HIS	-	expression tag	UNP P01096
H	65	HIS	-	expression tag	UNP P01096
H	66	HIS	-	expression tag	UNP P01096
I	39	ALA	LYS	engineered mutation	UNP P01096
I	61	HIS	-	expression tag	UNP P01096
I	62	HIS	-	expression tag	UNP P01096
I	63	HIS	-	expression tag	UNP P01096
I	64	HIS	-	expression tag	UNP P01096
I	65	HIS	-	expression tag	UNP P01096
I	66	HIS	-	expression tag	UNP P01096
J	39	ALA	LYS	engineered mutation	UNP P01096
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 5 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).
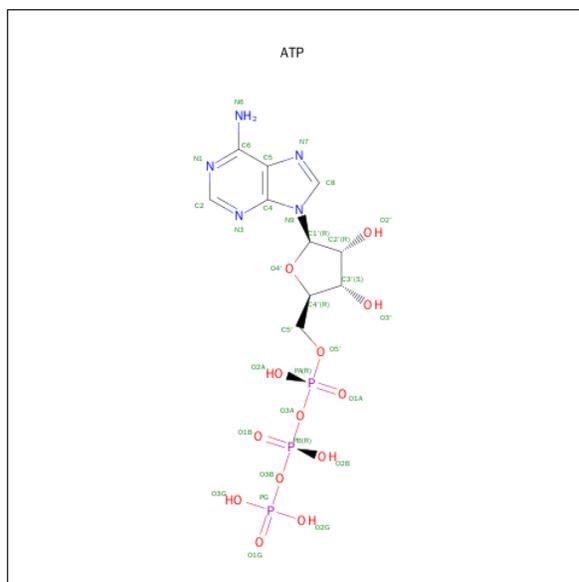
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	B	1	Total	C	N	O	P	0	0
			31	10	5	13	3		
5	C	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).
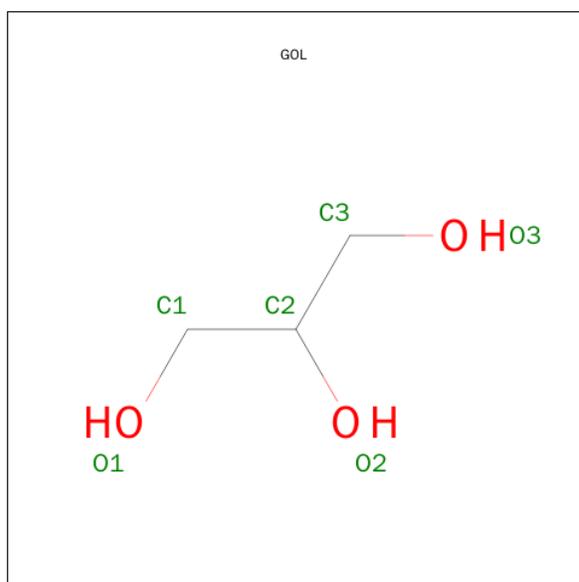
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total 6	C 3	O 3	0	0
7	B	1	Total 6	C 3	O 3	0	0

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	G	2	Total 2	Cl 2	0	0
8	B	1	Total 1	Cl 1	0	0
8	C	2	Total 2	Cl 2	0	0
8	F	2	Total 2	Cl 2	0	0
8	E	4	Total 4	Cl 4	0	0

- Molecule 9 is A D E N O S I N E - 5'- D I P H O S P H A T E (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).

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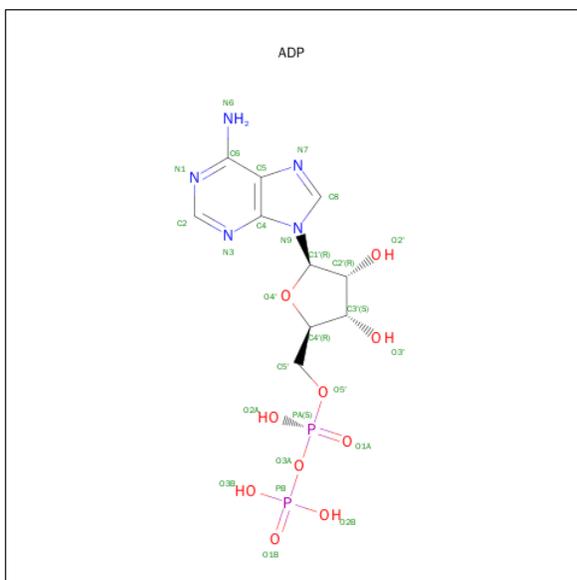
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
9	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
9	F	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

• Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	A	4	Total	O	0	0
			4	4		
10	B	4	Total	O	0	0
			4	4		
10	C	5	Total	O	0	0
			5	5		
10	D	5	Total	O	0	0
			5	5		
10	E	3	Total	O	0	0
			3	3		
10	F	4	Total	O	0	0
			4	4		

3 Residue-property plots ⓘ

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
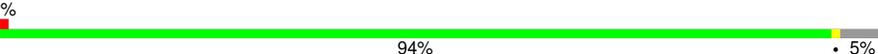
- Molecule 2: ATP synthase subunit beta, mitochondrial

Chain F:

ALA ALA GLN ALA SER PRO SER PRO LYS ALA GLY ALA T9 I13 Q73 I108 K111 G161 K162 T163 I166 F243 D352 H477 SER
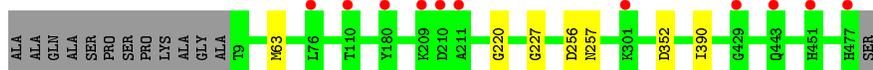
• Molecule 3: ATP synthase subunit gamma, mitochondrial

Chain G:

A1 T2 I16 L38 R42 V43 Y44 GLY VAL GLY SER LEU ALA LEU TYR GLU LYS ALA ASP ILE LYS THR PRO GLU ASP LYS LYS HIS LEU ILE GLY VAL SER S73 S84 S91 GLU ALA ALA ASN LEU ALA ALA GLY LYS GLU VAL LYS ILE ILE GLY V108

G109 I112 T119 H120 Q123 V126 T127 P136 T137 F138 G139 D140 A141 S142 L146 E147 L148 L149 N150 S151 G152 Y153 GLU PHE ASP GLU GLY SER ILE ILE PHE ASN R164 F165 R166 S167 T173 GLU GLU LYS PRO ILE PHE SER LEU ASP THR ILE SER ALA GLU SER

MET SER ILE TYR ASP ASP ILE ASP ALA ASP VAL LEU ARG ASN TYR Q205 E206 Y207 S208 L209 A210 N211 I212 I213 Y214 Y215 S216 E219 L272 ASP

• Molecule 4: ATPase inhibitor, mitochondrial

Chain H:

GLY SER GLU GLY ASP VAL ASN ARG S10 A44 K47 H48 H49 E50 ASN GLU ILE SER HIS HIS ALA LYS GLU ILE HIS HIS HIS HIS HIS

• Molecule 4: ATPase inhibitor, mitochondrial

Chain I:

GLY SER GLU GLY ASP ASN VAL ARG SER ALA GLY ALA VAL ARG ASP ALA GLY ALA PHE G23 K24 R25 E26 A43 A44 L45 K46 K47 H48 H49 E50 ASN GLU ILE SER HIS HIS ALA LYS GLU ILE HIS HIS HIS HIS HIS

• Molecule 4: ATPase inhibitor, mitochondrial

Chain J:

GLY SER GLU GLY ASP ASN VAL ARG SER SER ALA GLY ALA VAL ARG ASP ALA GLY ALA PHE GLY LYS ARG GLU GLN ALA E29 E30 F34 R35 A36 R37 A38 A39 L42 A43 A44 L45 K46 K47 H48 H49 E50 ASN GLU ILE SER HIS HIS ALA LYS GLU ILE HIS HIS HIS

HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	108.77Å 155.29Å 271.02Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.31 – 3.30 46.31 – 3.30	Depositor EDS
% Data completeness (in resolution range)	95.7 (46.31-3.30) 95.8 (46.31-3.30)	Depositor EDS
R_{merge}	0.23	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.77 (at 3.32Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.239 , 0.275 0.239 , 0.276	Depositor DCC
R_{free} test set	3346 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	74.2	Xtriage
Anisotropy	0.052	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 21.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< |L| > = 0.44, < L^2 > = 0.27$	Xtriage
Outliers	0 of 66849 reflections	Xtriage
F_o,F_c correlation	0.89	EDS
Total number of atoms	24201	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.64% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1] Intensities estimated from amplitudes.
[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, MG, ATP, ADP, 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	0.28	0/3778	0.46	0/5096
1	B	0.28	0/3754	0.46	0/5064
1	C	0.29	0/3733	0.45	0/5035
2	D	0.29	0/3616	0.45	0/4906
2	E	0.28	0/3621	0.46	0/4913
2	F	0.28	0/3616	0.46	0/4906
3	G	0.30	0/1480	0.45	0/1978
4	H	0.29	0/321	0.37	0/425
4	I	0.32	0/239	0.41	0/315
4	J	0.30	0/192	0.42	0/254
All	All	0.29	0/24350	0.46	0/32892

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	3723	0	3823	3	0
1	B	3706	0	3814	4	0
1	C	3684	0	3793	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	3558	0	3605	6	0
2	E	3563	0	3611	4	0
2	F	3558	0	3605	2	0
3	G	1467	0	1536	1	0
4	H	317	0	303	0	0
4	I	236	0	229	0	0
4	J	189	0	181	0	0
5	A	31	0	12	0	0
5	B	31	0	12	0	0
5	C	31	0	12	0	0
6	A	1	0	0	0	0
6	B	1	0	0	0	0
6	C	1	0	0	0	0
6	D	1	0	0	0	0
6	F	1	0	0	0	0
7	A	6	0	8	0	0
7	B	6	0	8	0	0
8	B	1	0	0	0	0
8	C	2	0	0	0	0
8	E	4	0	0	0	0
8	F	2	0	0	0	0
8	G	2	0	0	0	0
9	D	27	0	12	0	0
9	F	27	0	12	0	0
10	A	4	0	0	0	0
10	B	4	0	0	0	0
10	C	5	0	0	1	0
10	D	5	0	0	0	0
10	E	3	0	0	0	0
10	F	4	0	0	0	0
All	All	24201	0	24576	21	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 0.

All (21) 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:D:63:MET:CE	2:D:227:GLY:O	2.11	0.98
2:D:63:MET:HE1	2:D:227:GLY:O	1.69	0.92
1:B:179:ALA:HB1	1:B:267:ILE:HD13	1.69	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:63:MET:CE	2:D:227:GLY:C	2.74	0.56
2:E:97:VAL:HG13	2:E:98:ILE:HG23	1.91	0.52
1:B:34:ILE:HD13	1:B:39:ALA:HB2	1.93	0.51
1:A:179:ALA:HB1	1:A:267:ILE:HD13	1.93	0.51
1:B:383:MET:HG3	1:B:438:ILE:HD11	1.92	0.50
2:F:13:ILE:HD12	2:F:73:GLN:HB3	1.97	0.47
2:E:170:ILE:HG21	2:E:215:VAL:HG22	1.95	0.47
1:A:265:LEU:HD11	1:A:324:LEU:HD13	1.96	0.46
2:D:256:ASP:HA	2:D:257:ASN:HA	1.78	0.46
1:B:286:ARG:HA	2:E:275:ILE:HD12	1.99	0.45
1:A:327:ILE:HD11	1:A:342:VAL:HG21	1.97	0.45
1:C:327:ILE:HD11	1:C:342:VAL:HG21	1.98	0.45
2:D:390:ILE:HD11	3:G:16:ILE:HG23	1.99	0.45
2:D:63:MET:HE2	2:D:227:GLY:C	2.37	0.44
1:C:423:ARG:HD2	1:C:461:ILE:HD11	2.00	0.43
2:F:163:THR:HA	2:F:166:ILE:HG22	2.02	0.42
1:C:172:GLN:NE2	10:C:701:HOH:O	2.52	0.41
2:E:256:ASP:HA	2:E:257:ASN:HA	1.80	0.41

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	486/510 (95%)	467 (96%)	17 (4%)	2 (0%)	39	76
1	B	483/510 (95%)	462 (96%)	21 (4%)	0	100	100
1	C	479/510 (94%)	460 (96%)	18 (4%)	1 (0%)	52	85
2	D	467/482 (97%)	432 (92%)	33 (7%)	2 (0%)	39	76
2	E	468/482 (97%)	439 (94%)	29 (6%)	0	100	100
2	F	467/482 (97%)	437 (94%)	28 (6%)	2 (0%)	39	76

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	G	177/273 (65%)	165 (93%)	9 (5%)	3 (2%)	11	47
4	H	39/66 (59%)	39 (100%)	0	0	100	100
4	I	26/66 (39%)	26 (100%)	0	0	100	100
4	J	20/66 (30%)	18 (90%)	1 (5%)	1 (5%)	3	19
All	All	3112/3447 (90%)	2945 (95%)	156 (5%)	11 (0%)	39	76

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	401	ALA
3	G	2	THR
2	D	220	GLY
3	G	126	VAL
4	J	30	GLU
3	G	127	THR
1	A	408	SER
2	D	352	ASP
2	F	352	ASP
1	C	376	SER
2	F	161	GLY

5.3.2 Protein sidechains (i)

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	394/412 (96%)	394 (100%)	0	100	100
1	B	393/412 (95%)	393 (100%)	0	100	100
1	C	390/412 (95%)	390 (100%)	0	100	100
2	D	379/386 (98%)	379 (100%)	0	100	100
2	E	379/386 (98%)	379 (100%)	0	100	100
2	F	379/386 (98%)	379 (100%)	0	100	100
3	G	160/231 (69%)	160 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	H	27/49 (55%)	27 (100%)	0	100	100
4	I	21/49 (43%)	21 (100%)	0	100	100
4	J	17/49 (35%)	17 (100%)	0	100	100
All	All	2539/2772 (92%)	2539 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	405	GLN
1	B	432	GLN
3	G	225	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 23 ligands modelled in this entry, 16 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
5	ATP	A	601	6	24,33,33	1.02	1 (4%)	31,52,52	1.90	5 (16%)
7	GOL	A	603	-	5,5,5	0.19	0	5,5,5	0.22	0
5	ATP	B	601	6	24,33,33	1.04	1 (4%)	31,52,52	1.94	4 (12%)
7	GOL	B	604	-	5,5,5	0.22	0	5,5,5	0.34	0
5	ATP	C	601	6	24,33,33	1.02	1 (4%)	31,52,52	1.95	5 (16%)
9	ADP	D	600	6	22,29,29	1.05	1 (4%)	27,45,45	1.92	4 (14%)
9	ADP	F	501	6	22,29,29	1.07	1 (4%)	27,45,45	1.93	4 (14%)

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
5	ATP	A	601	6	-	0/18/38/38	0/3/3/3
7	GOL	A	603	-	-	0/4/4/4	0/0/0/0
5	ATP	B	601	6	-	0/18/38/38	0/3/3/3
7	GOL	B	604	-	-	0/4/4/4	0/0/0/0
5	ATP	C	601	6	-	0/18/38/38	0/3/3/3
9	ADP	D	600	6	-	0/12/32/32	0/3/3/3
9	ADP	F	501	6	-	0/12/32/32	0/3/3/3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	601	ATP	C5-C4	3.20	1.47	1.40
9	D	600	ADP	C5-C4	3.20	1.47	1.40
9	F	501	ADP	C5-C4	3.24	1.47	1.40
5	C	601	ATP	C5-C4	3.27	1.47	1.40
5	B	601	ATP	C5-C4	3.29	1.47	1.40

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	601	ATP	N3-C2-N1	-7.56	123.10	128.89
5	B	601	ATP	N3-C2-N1	-7.35	123.27	128.89
9	F	501	ADP	N3-C2-N1	-7.28	123.32	128.89
5	A	601	ATP	N3-C2-N1	-7.26	123.33	128.89
9	D	600	ADP	N3-C2-N1	-7.15	123.42	128.89
5	B	601	ATP	PA-O3A-PB	-4.06	121.32	132.73
5	C	601	ATP	PA-O3A-PB	-3.55	122.76	132.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	F	501	ADP	C2'-C1'-N9	-3.38	109.13	114.29
5	A	601	ATP	PA-O3A-PB	-3.37	123.25	132.73
5	B	601	ATP	C4-C5-N7	-3.26	106.48	109.48
5	A	601	ATP	PB-O3B-PG	-3.20	121.92	132.67
5	A	601	ATP	C4-C5-N7	-3.20	106.53	109.48
9	D	600	ADP	C4-C5-N7	-3.13	106.60	109.48
5	B	601	ATP	PB-O3B-PG	-3.04	122.49	132.67
9	D	600	ADP	PA-O3A-PB	-2.98	122.67	132.67
9	F	501	ADP	C4-C5-N7	-2.92	106.79	109.48
9	F	501	ADP	PA-O3A-PB	-2.90	122.95	132.67
5	C	601	ATP	C4-C5-N7	-2.88	106.83	109.48
5	C	601	ATP	C2'-C1'-N9	-2.75	110.09	114.29
9	D	600	ADP	C2'-C1'-N9	-2.75	110.09	114.29
5	C	601	ATP	PB-O3B-PG	-2.62	123.88	132.67
5	A	601	ATP	C2'-C1'-N9	-2.32	110.75	114.29

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 (i)

6.1 Protein, DNA and RNA chains (i)

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%)	-0.18	2 (0%)	93	92	47, 63, 95, 140	0
1	B	487/510 (95%)	-0.23	2 (0%)	93	92	41, 60, 92, 122	0
1	C	483/510 (94%)	0.04	5 (1%)	84	80	54, 83, 109, 142	0
2	D	469/482 (97%)	0.07	11 (2%)	64	57	56, 81, 112, 123	0
2	E	470/482 (97%)	-0.05	8 (1%)	73	67	40, 62, 109, 152	0
2	F	469/482 (97%)	0.03	4 (0%)	85	82	50, 79, 108, 134	0
3	G	187/273 (68%)	1.09	37 (19%)	1	1	56, 120, 160, 180	0
4	H	41/66 (62%)	0.29	3 (7%)	18	15	66, 90, 124, 138	0
4	I	28/66 (42%)	1.55	7 (25%)	1	1	110, 128, 146, 158	0
4	J	22/66 (33%)	2.30	13 (59%)	0	0	123, 134, 141, 144	0
All	All	3143/3447 (91%)	0.05	92 (2%)	55	49	40, 75, 124, 180	0

All (92) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	G	211	ASN	5.7
3	G	138	PHE	5.6
3	G	149	LEU	5.1
4	I	48	HIS	5.0
3	G	213	ILE	5.0
3	G	207	TYR	4.8
2	E	393	MET	4.7
1	C	404	ALA	4.6
4	J	43	ALA	4.5
3	G	215	TYR	4.5
3	G	136	PRO	4.3
2	E	394	ASP	4.2
3	G	205	GLN	4.1

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Mol	Chain	Res	Type	RSRZ
2	E	391	LEU	4.1
3	G	151	SER	4.0
3	G	209	LEU	4.0
2	D	209	LYS	3.9
3	G	166	ARG	3.8
3	G	142	SER	3.8
3	G	212	ILE	3.7
3	G	43	VAL	3.6
4	J	47	LYS	3.6
2	D	477	HIS	3.6
3	G	126	VAL	3.6
3	G	210	ALA	3.5
4	J	42	LEU	3.5
4	J	37	ARG	3.5
2	F	477	HIS	3.4
3	G	206	GLU	3.3
2	E	477	HIS	3.3
2	E	387	ILE	3.2
3	G	42	ARG	3.1
1	C	24	ASP	2.9
4	J	30	GLU	2.9
4	J	49	HIS	2.9
4	I	46	LYS	2.9
2	E	396	LEU	2.9
2	F	108	ILE	2.8
4	H	49	HIS	2.8
2	D	429	GLY	2.8
4	I	25	ARG	2.8
3	G	148	LEU	2.8
4	J	48	HIS	2.7
3	G	120	HIS	2.7
4	I	26	GLU	2.7
4	J	34	PHE	2.7
3	G	123	GLN	2.7
4	I	44	ALA	2.7
3	G	165	PHE	2.6
3	G	214	TYR	2.6
4	H	47	LYS	2.6
2	E	395	GLU	2.6
2	F	111	LYS	2.6
4	J	29	GLU	2.6
4	J	38	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
3	G	216	SER	2.5
3	G	137	THR	2.5
4	J	45	LEU	2.5
2	D	110	THR	2.4
2	D	451	HIS	2.4
3	G	146	LEU	2.4
4	I	43	ALA	2.4
2	D	210	ASP	2.3
3	G	139	GLY	2.3
2	D	180	TYR	2.3
3	G	140	ASP	2.3
3	G	119	THR	2.3
4	I	49	HIS	2.2
1	A	510	ALA	2.2
2	D	76	LEU	2.2
2	E	455	GLN	2.2
2	D	211	ALA	2.2
3	G	109	GLY	2.2
1	C	124	LYS	2.2
2	D	443	GLN	2.2
1	B	16	ILE	2.1
1	A	403	PHE	2.1
3	G	150	ASN	2.1
2	F	243	PHE	2.1
3	G	38	LEU	2.1
3	G	167	SER	2.1
1	B	398	ARG	2.1
2	D	301	LYS	2.1
3	G	84	SER	2.1
4	J	36	ALA	2.1
1	C	489	ILE	2.0
3	G	208	SER	2.0
3	G	112	ILE	2.0
4	H	44	ALA	2.0
4	J	39	ALA	2.0
3	G	219	GLU	2.0
1	C	485	THR	2.0

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

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
8	CL	F	503	1/1	0.84	0.48	8.33	60,60,60,60	0
8	CL	G	302	1/1	0.87	0.38	4.66	86,86,86,86	0
8	CL	G	301	1/1	0.88	0.24	3.38	70,70,70,70	0
8	CL	E	502	1/1	0.87	0.23	1.99	52,52,52,52	0
7	GOL	A	603	6/6	0.92	0.25	1.38	47,48,48,49	0
7	GOL	B	604	6/6	0.92	0.23	1.11	51,51,51,51	0
8	CL	B	603	1/1	0.89	0.21	0.81	52,52,52,52	0
9	ADP	F	501	27/27	0.94	0.24	0.64	63,70,76,76	0
9	ADP	D	600	27/27	0.91	0.24	0.34	88,93,96,98	0
5	ATP	C	601	31/31	0.92	0.20	0.09	72,81,90,91	4
8	CL	F	504	1/1	0.89	0.17	-0.05	51,51,51,51	0
5	ATP	B	601	31/31	0.96	0.18	-0.26	53,62,71,72	0
6	MG	F	502	1/1	0.82	0.20	-0.46	67,67,67,67	0
5	ATP	A	601	31/31	0.94	0.18	-0.50	59,61,64,65	4
6	MG	D	601	1/1	0.86	0.20	-1.38	85,85,85,85	0
8	CL	E	501	1/1	0.98	0.09	-3.87	44,44,44,44	0
8	CL	E	504	1/1	0.90	0.18	-	69,69,69,69	0
8	CL	C	604	1/1	0.74	0.24	-	52,52,52,52	0
6	MG	B	602	1/1	0.97	0.24	-	50,50,50,50	0
6	MG	A	602	1/1	0.92	0.15	-	60,60,60,60	0
6	MG	C	602	1/1	0.87	0.18	-	72,72,72,72	0
8	CL	C	603	1/1	0.90	0.22	-	85,85,85,85	0
8	CL	E	503	1/1	0.92	0.17	-	54,54,54,54	0

6.5 Other polymers (i)

There are no such residues in this entry.