Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 11:25 am BST

PDB ID	:	2CLY
Title	:	Subcomplex of the stator of bovine mitochondrial ATP synthase
Authors	:	Kane Dickson, V.; Silvester, J.A.; Fearnley, I.M.; Leslie, A.G.W.; Walker, J.E.
Deposited on	:	2006-05-03
Resolution	:	2.80 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
https://www.wwpdb.org/validation/2017/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:

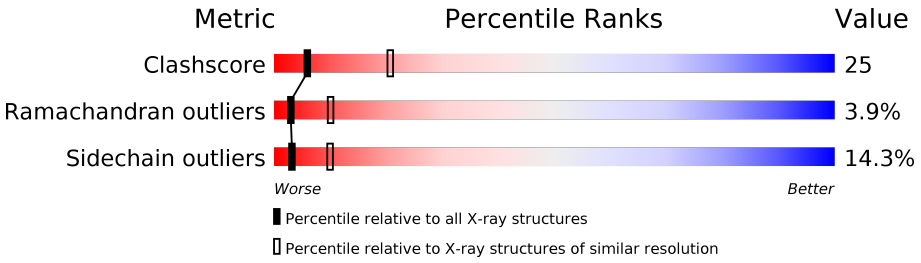
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.80 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	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)

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 respectively. 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%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	214	26% 18% 5% 51%
1	D	214	25% 20% 5% 51%
2	B	160	39% 28% 6% • 25%
2	E	160	42% 24% 9% • 24%
3	C	77	51% 30% 5% 14%
3	F	77	48% 32% 5% 14%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 4845 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 B CHAIN, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	105	Total	C	N	O	S	0	0	0
			894	556	169	164	5			
1	D	105	Total	C	N	O	S	0	0	0
			894	556	169	164	5			

- Molecule 2 is a protein called ATP SYNTHASE D CHAIN, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	120	Total	C	N	O	S	0	0	0
			969	620	161	186	2			
2	E	121	Total	C	N	O	S	0	0	0
			980	626	165	187	2			

- Molecule 3 is a protein called ATP SYNTHASE COUPLING FACTOR 6, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	66	Total	C	N	O	S	0	0	0
			551	352	92	105	2			
3	F	66	Total	C	N	O	S	0	0	0
			551	352	92	105	2			

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	1	Total	O	0	0
			1	1		
4	B	1	Total	O	0	0
			1	1		
4	C	1	Total	O	0	0
			1	1		
4	D	1	Total	O	0	0
			1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	2	Total O 2 2	0	0

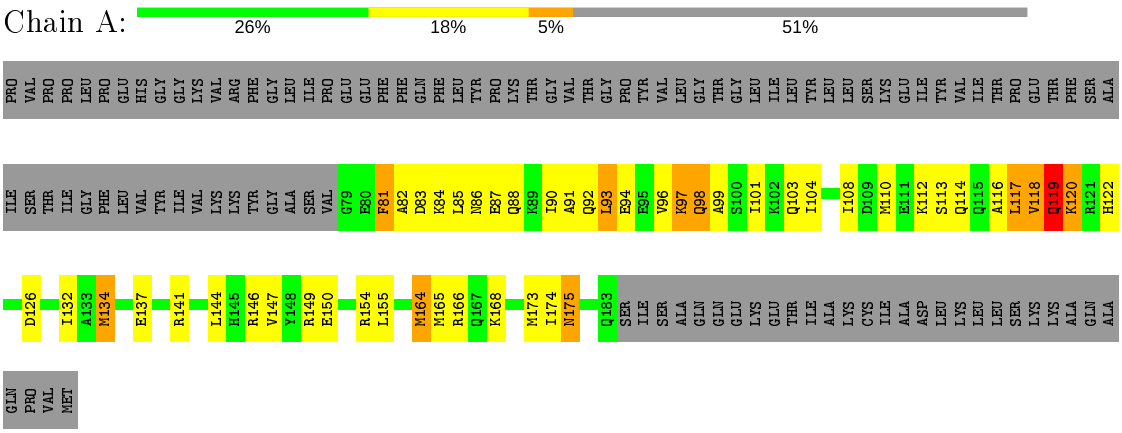
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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. 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.

Note EDS was not executed.

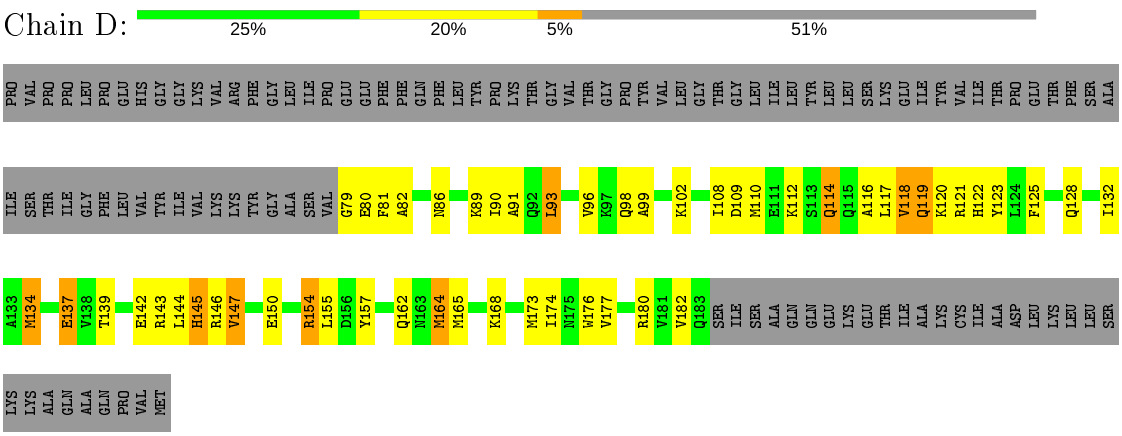
- Molecule 1: ATP SYNTHASE B CHAIN, MITOCHONDRIAL

Chain A:



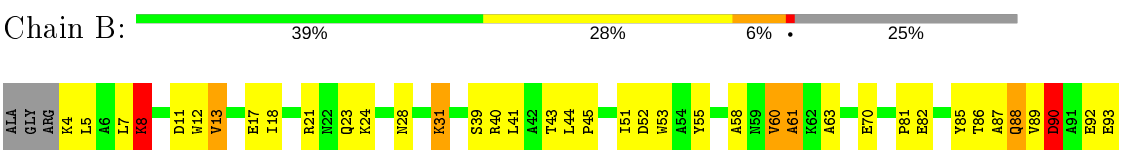
- Molecule 1: ATP SYNTHASE B CHAIN, MITOCHONDRIAL

Chain D:



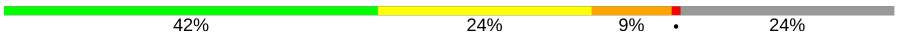
- Molecule 2: ATP SYNTHASE D CHAIN, MITOCHONDRIAL

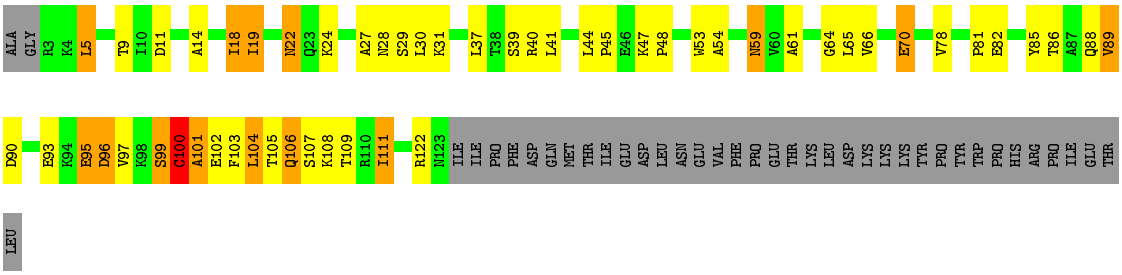
Chain B:



• Molecule 2: ATP SYNTHASE D CHAIN, MITOCHONDRIAL

Chain E:



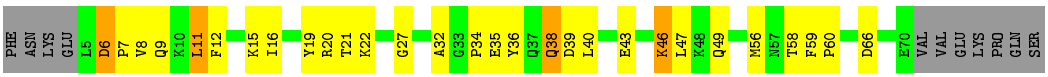


• Molecule 3: ATP SYNTHASE COUPLING FACTOR 6, MITOCHONDRIAL

Chain C:

• Molecule 3: ATP SYNTHASE COUPLING FACTOR 6, MITOCHONDRIAL

Chain F:



4 Data and refinement statistics (i)

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	50.50Å 79.35Å 115.67Å 90.00° 93.08° 90.00°	Depositor
Resolution (Å)	115.47 – 2.80	Depositor
% Data completeness (in resolution range)	93.3 (115.47-2.80)	Depositor
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.231 , 0.295	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	4845	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

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	0.56	0/905	0.68	0/1210
1	D	0.80	5/905 (0.6%)	0.88	4/1210 (0.3%)
2	B	0.61	0/988	0.76	1/1335 (0.1%)
2	E	0.56	0/999	0.75	0/1349
3	C	0.57	0/564	0.70	0/757
3	F	0.62	0/564	0.74	0/757
All	All	0.63	5/4925 (0.1%)	0.76	5/6618 (0.1%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	146	ARG	C-N	9.60	1.56	1.34
1	D	142	GLU	C-O	6.98	1.36	1.23
1	D	146	ARG	C-O	6.79	1.36	1.23
1	D	147	VAL	N-CA	5.75	1.57	1.46
1	D	145	HIS	N-CA	-5.63	1.35	1.46

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	146	ARG	O-C-N	-9.03	108.26	122.70
1	D	146	ARG	NE-CZ-NH1	-8.63	115.98	120.30
1	D	146	ARG	CA-C-O	7.54	135.93	120.10
2	B	90	ASP	CB-CG-OD1	6.32	123.98	118.30
1	D	145	HIS	N-CA-CB	5.65	120.77	110.60

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	894	0	900	67	0
1	D	894	0	900	68	0
2	B	969	0	980	54	0
2	E	980	0	993	56	0
3	C	551	0	534	27	0
3	F	551	0	534	22	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
4	C	1	0	0	0	0
4	D	1	0	0	1	0
4	E	2	0	0	0	0
All	All	4845	0	4841	242	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 25.

All (242) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ALA:O	1:A:120:LYS:HB2	1.27	1.25
1:D:116:ALA:HB1	1:D:120:LYS:HD3	1.17	1.15
1:A:116:ALA:HB1	1:A:120:LYS:NZ	1.64	1.11
1:A:173:MET:HG3	3:C:22:LYS:HE2	1.14	1.11
1:D:177:VAL:HG11	3:F:19:TYR:HE2	1.23	1.03
1:A:120:LYS:HD3	2:B:18:ILE:HG22	1.38	1.00
1:D:121:ARG:HD2	2:E:95:GLU:OE2	1.59	0.99
1:D:120:LYS:HD2	2:E:18:ILE:HG21	1.44	0.99
1:A:116:ALA:HB1	1:A:120:LYS:CE	1.92	0.99
1:D:168:LYS:HE3	3:F:39:ASP:HB2	1.45	0.96
1:A:116:ALA:HB1	1:A:120:LYS:HD2	1.46	0.96
1:A:134:MET:HG3	2:B:41:LEU:HD11	1.47	0.95
1:A:116:ALA:HB1	1:A:120:LYS:HZ2	1.31	0.94
1:A:116:ALA:HB1	1:A:120:LYS:CD	1.98	0.93
1:D:162:GLN:HE22	2:E:61:ALA:H	0.97	0.93
1:D:120:LYS:HD2	2:E:18:ILE:CG2	1.99	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ALA:CB	1:A:120:LYS:NZ	2.32	0.91
1:D:162:GLN:NE2	2:E:61:ALA:H	1.69	0.90
1:A:173:MET:HG3	3:C:22:LYS:CE	2.02	0.90
1:D:144:LEU:O	1:D:147:VAL:HG22	1.71	0.89
1:D:177:VAL:HG11	3:F:19:TYR:CE2	2.09	0.87
1:D:116:ALA:HB1	1:D:120:LYS:CD	2.03	0.87
1:A:118:VAL:O	1:A:119:GLN:C	2.13	0.86
3:C:61:ASN:HB3	2:E:90:ASP:OD1	1.75	0.86
1:A:134:MET:CG	2:B:41:LEU:HD11	2.06	0.84
1:A:117:LEU:H	1:A:117:LEU:HD23	1.41	0.84
1:D:116:ALA:CB	1:D:120:LYS:HD3	2.05	0.84
1:D:110:MET:HG3	2:E:107:SER:OG	1.79	0.82
1:D:117:LEU:HD23	1:D:120:LYS:HE2	1.61	0.82
2:E:108:LYS:O	2:E:111:ILE:HG22	1.80	0.81
1:A:134:MET:HG3	2:B:41:LEU:CD1	2.12	0.80
2:B:60:VAL:HG22	2:B:61:ALA:H	1.46	0.80
1:A:116:ALA:O	1:A:120:LYS:CB	2.22	0.79
1:D:120:LYS:HG3	2:E:18:ILE:HD13	1.64	0.78
2:B:82:GLU:OE2	2:E:81:PRO:HA	1.85	0.77
1:D:173:MET:HG3	3:F:22:LYS:HG2	1.68	0.75
1:A:134:MET:CG	2:B:41:LEU:CD1	2.65	0.75
2:B:13:VAL:O	2:B:17:GLU:HG2	1.89	0.73
1:A:116:ALA:CB	1:A:120:LYS:HZ2	1.98	0.72
2:B:82:GLU:HG3	2:E:82:GLU:HG3	1.72	0.72
1:A:122:HIS:HD2	1:A:126:ASP:OD2	1.72	0.72
1:A:120:LYS:HD3	2:B:18:ILE:CG2	2.18	0.71
1:D:176:TRP:O	1:D:180:ARG:HG2	1.91	0.71
1:A:117:LEU:N	1:A:117:LEU:HD23	2.05	0.70
1:D:162:GLN:HE22	2:E:61:ALA:N	1.82	0.70
2:E:95:GLU:O	2:E:95:GLU:HG3	1.88	0.69
2:E:53:TRP:CD2	2:E:70:GLU:HG3	2.28	0.69
2:B:116:LYS:O	2:B:119:GLU:HB3	1.93	0.68
1:D:114:GLN:HE22	2:E:108:LYS:HG3	1.59	0.67
1:D:144:LEU:O	1:D:147:VAL:CG2	2.40	0.67
1:A:144:LEU:O	1:A:147:VAL:HG22	1.95	0.66
1:D:116:ALA:O	1:D:120:LYS:HG2	1.95	0.66
1:A:119:GLN:CG	1:A:120:LYS:H	2.09	0.66
1:A:122:HIS:CD2	1:A:126:ASP:OD2	2.49	0.66
1:A:116:ALA:CB	1:A:120:LYS:HD2	2.23	0.65
3:C:61:ASN:HB3	2:E:90:ASP:CG	2.17	0.65
1:A:173:MET:CG	3:C:22:LYS:HE2	2.09	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:6:ASP:N	3:C:7:PRO:HD2	2.12	0.65
1:A:119:GLN:HG3	1:A:120:LYS:H	1.63	0.64
1:D:144:LEU:HD23	2:E:78:VAL:HG21	1.80	0.63
1:A:98:GLN:O	1:A:101:ILE:HG13	1.97	0.63
1:A:90:ILE:HG23	1:A:91:ALA:N	2.14	0.63
1:D:82:ALA:HB1	1:D:86:ASN:HD21	1.64	0.62
2:B:96:ASP:O	2:B:100:CYS:HB3	1.99	0.62
1:A:164:MET:HE2	1:A:165:MET:N	2.14	0.62
1:A:132:ILE:HD12	2:B:85:TYR:HB2	1.81	0.62
2:E:100:CYS:O	2:E:101:ALA:C	2.36	0.61
2:B:86:THR:HA	2:B:88:GLN:NE2	2.16	0.61
2:E:95:GLU:O	2:E:99:SER:HB2	2.00	0.60
1:A:93:LEU:HA	1:A:96:VAL:HB	1.83	0.60
3:F:16:ILE:O	3:F:20:ARG:HG3	2.01	0.59
2:E:122:ARG:HG2	2:E:122:ARG:O	2.02	0.59
2:E:100:CYS:O	2:E:103:PHE:N	2.35	0.59
3:F:6:ASP:C	3:F:8:VAL:H	2.06	0.59
2:E:59:ASN:OD1	2:E:59:ASN:N	2.36	0.59
2:B:12:TRP:CZ3	2:B:31:LYS:HG2	2.38	0.58
1:A:116:ALA:CB	1:A:120:LYS:HZ1	2.14	0.58
1:D:128:GLN:HB3	2:E:88:GLN:NE2	2.19	0.58
2:E:96:ASP:N	2:E:96:ASP:OD1	2.36	0.58
1:D:137:GLU:OE1	1:D:137:GLU:HA	2.04	0.58
3:F:15:LYS:HB3	3:F:19:TYR:OH	2.03	0.58
2:E:102:GLU:O	2:E:106:GLN:HB2	2.04	0.58
2:B:88:GLN:O	2:B:89:VAL:C	2.41	0.58
3:C:65:GLU:HG2	3:C:68:LYS:CE	2.34	0.58
2:B:108:LYS:HA	2:B:111:ILE:HG22	1.87	0.57
2:B:24:LYS:HE2	2:B:28:ASN:HD21	1.69	0.57
1:A:114:GLN:O	1:A:118:VAL:HG23	2.05	0.57
1:A:118:VAL:HG12	1:A:119:GLN:H	1.69	0.57
3:F:35:GLU:HA	3:F:38:GLN:OE1	2.05	0.57
2:B:99:SER:O	2:B:100:CYS:O	2.23	0.56
2:E:53:TRP:CG	2:E:70:GLU:HG3	2.40	0.56
3:C:20:ARG:O	3:C:23:ARG:HG3	2.06	0.56
2:E:86:THR:HG22	2:E:89:VAL:HB	1.88	0.56
1:A:110:MET:HG3	2:B:107:SER:OG	2.05	0.56
3:C:46:LYS:HG3	3:C:47:LEU:N	2.22	0.55
2:B:111:ILE:O	2:B:115:GLU:HG3	2.06	0.55
1:D:154:ARG:HD3	4:D:2001:HOH:O	2.05	0.55
1:A:134:MET:HG2	2:B:41:LEU:CD1	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:43:THR:O	2:B:45:PRO:HD3	2.06	0.55
3:C:65:GLU:HG2	3:C:68:LYS:HE3	1.89	0.55
3:C:35:GLU:HA	3:C:38:GLN:OE1	2.08	0.54
3:F:15:LYS:HB3	3:F:19:TYR:CZ	2.43	0.54
1:D:168:LYS:HE3	3:F:39:ASP:CB	2.30	0.54
1:A:98:GLN:HG3	1:A:99:ALA:N	2.23	0.54
3:F:6:ASP:HA	3:F:9:GLN:OE1	2.07	0.54
2:B:60:VAL:HG22	2:B:61:ALA:N	2.19	0.54
1:D:81:PHE:CD1	1:D:82:ALA:N	2.76	0.54
2:B:106:GLN:O	2:B:109:THR:HG22	2.08	0.53
2:B:87:ALA:HA	2:B:90:ASP:OD1	2.09	0.53
3:F:6:ASP:H	3:F:7:PRO:HD2	1.73	0.53
1:A:90:ILE:CG2	1:A:91:ALA:N	2.71	0.53
1:D:150:GLU:O	1:D:154:ARG:HG2	2.09	0.53
1:D:164:MET:HE2	1:D:165:MET:N	2.24	0.53
1:A:85:LEU:O	1:A:88:GLN:HB3	2.08	0.53
1:D:110:MET:HG3	2:E:107:SER:HG	1.72	0.53
1:D:154:ARG:O	1:D:157:TYR:HB3	2.09	0.52
2:B:88:GLN:H	2:B:88:GLN:CD	2.13	0.52
1:D:157:TYR:CE2	3:F:56:MET:HG3	2.44	0.52
1:A:81:PHE:CG	1:A:82:ALA:N	2.78	0.52
1:A:110:MET:SD	2:B:110:ARG:NH1	2.82	0.52
1:D:120:LYS:CD	2:E:18:ILE:HG21	2.29	0.52
1:A:117:LEU:N	1:A:117:LEU:CD2	2.72	0.52
3:C:22:LYS:HD2	3:C:30:VAL:HG21	1.92	0.52
3:F:46:LYS:O	3:F:49:GLN:HB2	2.10	0.51
1:D:168:LYS:HG2	3:F:36:TYR:CE1	2.45	0.51
1:A:118:VAL:O	1:A:119:GLN:O	2.27	0.51
1:A:119:GLN:O	1:A:120:LYS:C	2.48	0.51
2:E:47:LYS:HB3	2:E:48:PRO:HD2	1.93	0.51
1:D:117:LEU:HD23	1:D:120:LYS:CE	2.35	0.51
2:E:88:GLN:O	2:E:90:ASP:N	2.44	0.51
1:A:108:ILE:HG23	1:A:112:LYS:HE3	1.92	0.50
1:D:157:TYR:CD2	3:F:56:MET:HG3	2.46	0.50
1:A:137:GLU:HG3	2:B:5:LEU:HD11	1.92	0.50
3:C:65:GLU:HG2	3:C:68:LYS:NZ	2.26	0.50
1:D:118:VAL:HG12	1:D:119:GLN:N	2.26	0.50
2:E:19:ILE:HG21	2:E:27:ALA:HB2	1.93	0.50
2:B:99:SER:O	2:B:100:CYS:C	2.50	0.50
3:C:61:ASN:N	3:C:61:ASN:OD1	2.44	0.50
1:A:116:ALA:CB	1:A:120:LYS:CE	2.78	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:86:THR:O	2:B:86:THR:HG22	2.11	0.50
1:A:141:ARG:NH1	2:B:41:LEU:HD23	2.27	0.49
1:D:108:ILE:HG23	1:D:112:LYS:NZ	2.27	0.49
2:B:81:PRO:HA	2:E:82:GLU:OE2	2.12	0.49
1:A:87:GLU:O	1:A:90:ILE:HG22	2.12	0.49
1:A:134:MET:HG2	2:B:41:LEU:HD11	1.90	0.49
1:D:93:LEU:HA	1:D:96:VAL:HB	1.94	0.49
1:D:86:ASN:HA	1:D:89:LYS:HB2	1.94	0.49
3:C:6:ASP:H	3:C:7:PRO:HD2	1.78	0.48
1:D:123:TYR:CE1	2:E:11:ASP:HB2	2.47	0.48
3:C:22:LYS:HD2	3:C:30:VAL:CG2	2.43	0.48
3:F:8:VAL:O	3:F:11:LEU:HB2	2.13	0.48
2:B:90:ASP:OD1	2:B:90:ASP:N	2.35	0.48
2:B:96:ASP:O	2:B:97:VAL:C	2.52	0.48
3:C:58:THR:HG22	3:C:59:PHE:O	2.13	0.48
2:E:86:THR:HG22	2:E:86:THR:O	2.14	0.48
2:B:21:ARG:C	2:B:23:GLN:H	2.17	0.48
1:D:134:MET:HG2	2:E:37:LEU:HB3	1.95	0.47
2:B:7:LEU:O	2:B:8:LYS:C	2.52	0.47
2:E:86:THR:CG2	2:E:89:VAL:HB	2.43	0.47
1:A:99:ALA:HB1	1:A:103:GLN:NE2	2.28	0.47
1:D:90:ILE:HG23	1:D:91:ALA:N	2.30	0.47
2:E:44:LEU:HA	2:E:45:PRO:HD2	1.74	0.47
2:E:88:GLN:HA	2:E:88:GLN:OE1	2.15	0.47
2:B:96:ASP:N	2:B:96:ASP:OD1	2.44	0.47
3:C:22:LYS:HZ3	3:C:30:VAL:HG22	1.80	0.46
1:D:116:ALA:O	1:D:117:LEU:C	2.54	0.46
2:B:40:ARG:CZ	2:B:44:LEU:HG	2.45	0.46
1:D:125:PHE:HA	2:E:88:GLN:HE21	1.81	0.46
1:D:134:MET:HG3	2:E:41:LEU:HD22	1.97	0.46
2:B:122:ARG:O	2:B:122:ARG:HG2	2.14	0.46
1:D:119:GLN:O	1:D:122:HIS:CD2	2.68	0.46
2:E:53:TRP:O	2:E:54:ALA:C	2.53	0.46
1:A:174:ILE:HG13	1:A:175:ASN:N	2.31	0.46
1:D:173:MET:CG	3:F:22:LYS:HG2	2.43	0.45
3:C:17:ARG:O	3:C:20:ARG:HB2	2.16	0.45
2:E:22:ASN:OD1	2:E:22:ASN:N	2.50	0.45
2:E:93:GLU:HA	2:E:96:ASP:OD2	2.15	0.45
1:D:164:MET:HE3	1:D:164:MET:C	2.37	0.45
1:A:146:ARG:HA	1:A:149:ARG:NH1	2.31	0.45
3:C:12:PHE:O	3:C:16:ILE:HG13	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:ILE:CG2	1:A:91:ALA:H	2.28	0.44
1:D:116:ALA:C	1:D:120:LYS:HG2	2.38	0.44
1:D:120:LYS:HD2	2:E:18:ILE:HG22	1.91	0.44
2:E:19:ILE:H	2:E:19:ILE:HG12	1.67	0.44
3:C:37:GLN:OE1	3:C:40:LEU:HD23	2.18	0.44
1:D:164:MET:CE	1:D:164:MET:C	2.86	0.44
1:A:88:GLN:O	1:A:92:GLN:HG2	2.18	0.44
1:A:119:GLN:CG	1:A:120:LYS:N	2.78	0.44
2:B:44:LEU:HD23	2:B:44:LEU:HA	1.91	0.44
2:E:14:ALA:O	2:E:18:ILE:HG23	2.16	0.44
2:B:55:TYR:O	2:B:58:ALA:HB3	2.18	0.43
1:D:145:HIS:HE1	2:E:48:PRO:HA	1.83	0.43
2:E:100:CYS:O	2:E:104:LEU:N	2.50	0.43
2:E:96:ASP:C	2:E:100:CYS:HG	2.19	0.43
1:D:137:GLU:HG3	2:E:5:LEU:HD13	2.01	0.43
1:A:116:ALA:C	1:A:120:LYS:HD2	2.38	0.43
2:B:51:ILE:O	2:B:53:TRP:N	2.51	0.43
2:E:88:GLN:C	2:E:90:ASP:N	2.71	0.43
2:B:100:CYS:SG	2:B:101:ALA:N	2.92	0.43
2:B:7:LEU:HD23	2:B:7:LEU:HA	1.76	0.43
3:C:6:ASP:N	3:C:7:PRO:CD	2.81	0.43
1:A:150:GLU:O	1:A:154:ARG:HG2	2.19	0.43
2:B:86:THR:HG21	2:B:89:VAL:HG23	2.00	0.43
1:A:141:ARG:CZ	2:B:41:LEU:HD23	2.48	0.42
2:B:99:SER:OG	2:B:100:CYS:N	2.52	0.42
1:D:173:MET:HG3	3:F:22:LYS:CG	2.43	0.42
1:A:113:SER:O	1:A:116:ALA:HB3	2.20	0.42
3:C:55:ASP:OD1	3:C:57:ASN:HB2	2.18	0.42
3:F:46:LYS:HG3	3:F:47:LEU:N	2.34	0.42
3:C:6:ASP:OD2	3:C:9:GLN:NE2	2.52	0.42
1:D:114:GLN:O	1:D:118:VAL:HG23	2.20	0.42
1:D:164:MET:O	1:D:164:MET:HE3	2.19	0.42
1:D:82:ALA:HB1	1:D:86:ASN:ND2	2.33	0.42
2:E:24:LYS:HG2	2:E:28:ASN:HD21	1.84	0.42
2:B:87:ALA:HA	2:B:90:ASP:CG	2.40	0.42
3:C:17:ARG:HH11	3:C:20:ARG:NH1	2.17	0.42
1:A:164:MET:HE2	1:A:165:MET:CA	2.49	0.42
2:E:40:ARG:NH1	2:E:44:LEU:HG	2.35	0.42
2:B:86:THR:CG2	2:B:89:VAL:HG23	2.50	0.41
3:C:22:LYS:HZ2	3:C:30:VAL:HG13	1.83	0.41
1:D:128:GLN:O	1:D:132:ILE:HG12	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:53:TRP:CH2	2:B:70:GLU:HA	2.55	0.41
1:D:119:GLN:O	1:D:120:LYS:C	2.59	0.41
1:D:90:ILE:CG2	1:D:91:ALA:N	2.83	0.41
2:B:98:LYS:HA	2:B:98:LYS:HD3	1.79	0.41
1:D:118:VAL:O	1:D:119:GLN:C	2.58	0.41
1:D:139:THR:O	1:D:143:ARG:HG3	2.20	0.41
1:A:117:LEU:O	1:A:118:VAL:O	2.39	0.41
1:D:79:GLY:C	1:D:81:PHE:H	2.23	0.41
3:F:39:ASP:O	3:F:40:LEU:C	2.59	0.41
1:A:146:ARG:O	1:A:150:GLU:HG3	2.21	0.41
1:D:116:ALA:O	1:D:118:VAL:N	2.54	0.41
2:B:92:GLU:O	2:B:95:GLU:N	2.53	0.41
1:D:98:GLN:HE22	1:D:102:LYS:HG3	1.86	0.41
1:A:90:ILE:HG23	1:A:91:ALA:H	1.86	0.41
2:E:105:THR:O	2:E:108:LYS:N	2.54	0.41
1:A:91:ALA:O	1:A:94:GLU:HB3	2.21	0.40
1:A:93:LEU:HD23	1:A:97:LYS:HE3	2.03	0.40
3:C:20:ARG:HA	3:C:23:ARG:HG2	2.04	0.40
1:D:98:GLN:HG3	1:D:99:ALA:N	2.36	0.40
2:E:65:LEU:O	2:E:66:VAL:C	2.60	0.40
3:F:59:PHE:CG	3:F:60:PRO:HD2	2.56	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	103/214 (48%)	87 (84%)	12 (12%)	4 (4%)	3 10
1	D	103/214 (48%)	84 (82%)	17 (16%)	2 (2%)	8 26
2	B	118/160 (74%)	88 (75%)	24 (20%)	6 (5%)	2 6
2	E	119/160 (74%)	91 (76%)	24 (20%)	4 (3%)	3 13

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	C	64/77 (83%)	54 (84%)	8 (12%)	2 (3%)	4 14
3	F	64/77 (83%)	53 (83%)	7 (11%)	4 (6%)	1 3
All	All	571/902 (63%)	457 (80%)	92 (16%)	22 (4%)	3 10

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	118	VAL
1	A	119	GLN
1	A	120	LYS
2	B	63	ALA
2	B	100	CYS
3	C	32	ALA
1	D	118	VAL
2	E	100	CYS
3	F	32	ALA
1	A	81	PHE
2	B	61	ALA
2	E	89	VAL
2	E	101	ALA
1	D	114	GLN
2	E	64	GLY
2	B	52	ASP
3	F	34	PRO
2	B	8	LYS
3	F	27	GLY
2	B	60	VAL
3	F	6	ASP
3	C	27	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	97/190 (51%)	82 (84%)	15 (16%)	2 8

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	97/190 (51%)	86 (89%)	11 (11%)	6 18
2	B	104/142 (73%)	90 (86%)	14 (14%)	4 11
2	E	105/142 (74%)	84 (80%)	21 (20%)	1 4
3	C	60/71 (84%)	54 (90%)	6 (10%)	7 22
3	F	60/71 (84%)	52 (87%)	8 (13%)	4 12
All	All	523/806 (65%)	448 (86%)	75 (14%)	3 10

All (75) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ASP
1	A	84	LYS
1	A	86	ASN
1	A	93	LEU
1	A	97	LYS
1	A	98	GLN
1	A	104	ILE
1	A	117	LEU
1	A	119	GLN
1	A	134	MET
1	A	155	LEU
1	A	164	MET
1	A	166	ARG
1	A	168	LYS
1	A	175	ASN
2	B	4	LYS
2	B	8	LYS
2	B	11	ASP
2	B	13	VAL
2	B	31	LYS
2	B	39	SER
2	B	88	GLN
2	B	90	ASP
2	B	93	GLU
2	B	94	LYS
2	B	95	GLU
2	B	96	ASP
2	B	99	SER
2	B	111	ILE
3	C	8	VAL

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Mol	Chain	Res	Type
3	C	12	PHE
3	C	23	ARG
3	C	30	VAL
3	C	43	GLU
3	C	61	ASN
1	D	80	GLU
1	D	93	LEU
1	D	109	ASP
1	D	119	GLN
1	D	134	MET
1	D	137	GLU
1	D	154	ARG
1	D	155	LEU
1	D	164	MET
1	D	174	ILE
1	D	182	VAL
2	E	5	LEU
2	E	9	THR
2	E	18	ILE
2	E	19	ILE
2	E	22	ASN
2	E	29	SER
2	E	30	LEU
2	E	31	LYS
2	E	39	SER
2	E	59	ASN
2	E	70	GLU
2	E	85	TYR
2	E	95	GLU
2	E	96	ASP
2	E	97	VAL
2	E	99	SER
2	E	100	CYS
2	E	104	LEU
2	E	106	GLN
2	E	109	THR
2	E	111	ILE
3	F	11	LEU
3	F	12	PHE
3	F	21	THR
3	F	38	GLN
3	F	43	GLU

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Mol	Chain	Res	Type
3	F	46	LYS
3	F	58	THR
3	F	66	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	98	GLN
1	A	103	GLN
2	B	28	ASN
1	D	86	ASN
1	D	98	GLN
1	D	114	GLN
1	D	162	GLN
1	D	163	ASN
2	E	28	ASN

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

There are no ligands in this entry.

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

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.