



# Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:38 AM UTC

PDB ID : 2CLY / pdb\_00002cly  
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](mailto: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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4-5-2 with Phenix2.0  
Xtrriage (Phenix) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.49

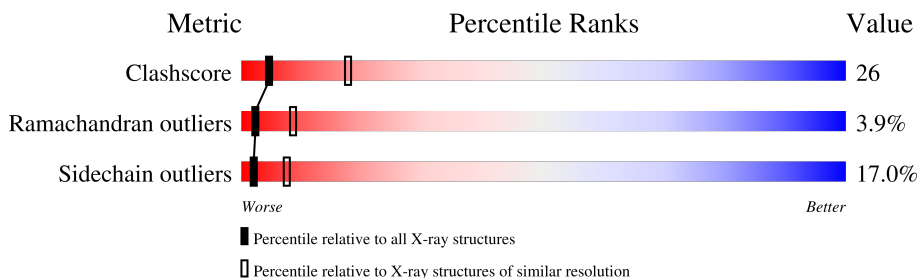
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (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 of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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  $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	214	25% (green), 18% (yellow), 6% (orange), 51% (grey)
1	D	214	22% (green), 20% (yellow), 7% (orange), 51% (grey)
2	B	160	38% (green), 29% (yellow), 8% (orange), 25% (grey)
2	E	160	40% (green), 25% (yellow), 9% (orange), 24% (grey)
3	C	77	48% (green), 30% (yellow), 6% (orange), 14% (grey)
3	F	77	45% (green), 32% (yellow), 8% (orange), 14% (grey)

## 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
			Total	C	N	O	S			
1	A	105	Total 894	C 556	N 169	O 164	S 5	0	0	0
1	D	105	Total 894	C 556	N 169	O 164	S 5	0	0	0

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

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

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

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

- Molecule 4 is water.

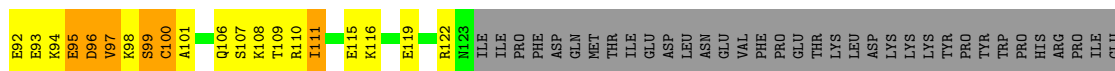
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total 1 O 1	0	0
4	B	1	Total 1 O 1	0	0
4	C	1	Total 1 O 1	0	0
4	D	1	Total 1 O 1	0	0

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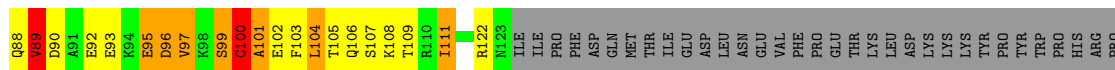
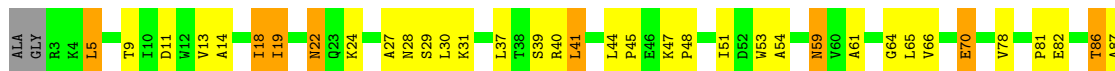
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	E	2	Total O 2 2	0	0





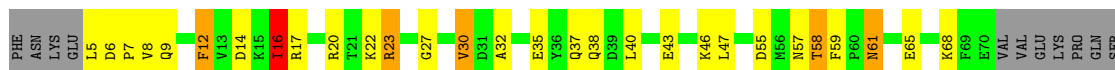
THR  
LEU

• Molecule 2: ATP SYNTHASE D CHAIN, MITOCHONDRIAL



I12  
GLU  
THR  
LEU

• Molecule 3: ATP SYNTHASE COUPLING FACTOR 6, MITOCHONDRIAL



• Molecule 3: ATP SYNTHASE COUPLING FACTOR 6, MITOCHONDRIAL



## 4 Data and refinement statistics

Xtrriage (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, $\alpha$ , $\beta$ , $\gamma$	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.	Xtrriage
Total number of atoms	4845	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	66.0	wwPDB-VP

## 5 Model quality i

### 5.1 Standard geometry i

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	0.74	0/905	0.97	2/1210 (0.2%)
1	D	1.18	6/905 (0.7%)	1.30	10/1210 (0.8%)
2	B	0.74	0/988	1.09	1/1335 (0.1%)
2	E	0.73	1/999 (0.1%)	1.04	2/1349 (0.1%)
3	C	0.63	0/564	1.04	2/757 (0.3%)
3	F	0.67	0/564	1.13	3/757 (0.4%)
All	All	0.82	7/4925 (0.1%)	1.10	20/6618 (0.3%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	146	ARG	C-N	18.43	1.56	1.33
1	D	142	GLU	C-O	10.01	1.36	1.24
1	D	146	ARG	C-O	9.54	1.36	1.24
1	D	145	HIS	N-CA	-9.49	1.35	1.46
1	D	147	VAL	N-CA	9.29	1.57	1.46
2	E	86	THR	CA-C	7.39	1.61	1.53
1	D	146	ARG	CA-C	5.36	1.60	1.52

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	146	ARG	CA-C-O	13.58	135.93	119.49
1	D	146	ARG	O-C-N	-10.87	108.26	122.39
2	B	97	VAL	N-CA-C	-10.43	99.41	110.36
1	D	144	LEU	CA-C-N	10.15	133.63	120.44
1	D	144	LEU	C-N-CA	10.15	133.63	120.44
1	D	147	VAL	N-CA-CB	7.80	120.00	110.64
1	D	145	HIS	N-CA-CB	7.42	120.77	110.01
1	A	107	ALA	N-CA-C	-6.86	103.03	111.33
1	D	147	VAL	N-CA-C	-6.45	104.87	110.74
2	E	86	THR	N-CA-C	6.38	119.54	109.39
1	D	107	ALA	N-CA-C	-6.38	104.24	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	87	ALA	N-CA-C	-6.35	105.36	113.23
1	A	121	ARG	N-CA-C	5.82	118.38	111.33
3	F	12	PHE	N-CA-C	-5.68	104.99	111.07
3	C	16	ILE	N-CA-CB	5.68	116.81	110.51
1	D	174	ILE	CB-CA-C	-5.65	104.75	111.81
1	D	146	ARG	NE-CZ-NH1	-5.51	115.98	121.50
3	C	16	ILE	CB-CA-C	-5.48	104.87	111.88
3	F	33	GLY	CA-C-N	5.42	126.62	119.84
3	F	33	GLY	C-N-CA	5.42	126.62	119.84

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	74	0
1	D	894	0	900	71	0
2	B	969	0	980	54	0
2	E	980	0	993	58	0
3	C	551	0	534	26	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	253	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 26.

All (253) 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
1:A:116:ALA:CB	1:A:120:LYS:NZ	2.32	0.91
1:A:118:VAL:O	1:A:119:GLN:C	2.13	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
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:D:164:MET:HE2	1:D:165:MET:N	2.03	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD23	1:A:117:LEU:N	2.05	0.70
1:D:162:GLN:HE22	2:E:61:ALA:N	1.82	0.70
3:C:61:ASN:HB3	2:E:90:ASP:CG	2.17	0.70
2:E:53:TRP:CD2	2:E:70:GLU:HG3	2.28	0.69
2:E:95:GLU:O	2:E:95:GLU:HG3	1.88	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
2:E:100:CYS:O	2:E:101:ALA:C	2.36	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
1:A:173:MET:CG	3:C:22:LYS:HE2	2.09	0.65
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
3:F:6:ASP:C	3:F:8:VAL:H	2.06	0.63
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:88:GLN:O	2:B:89:VAL:C	2.41	0.62
2:B:96:ASP:O	2:B:100:CYS:HB3	1.99	0.62
1:A:132:ILE:HD12	2:B:85:TYR:HB2	1.81	0.62
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:O	2:E:122:ARG:HG2	2.02	0.59
2:E:100:CYS:O	2:E:103:PHE:N	2.35	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:OD1	2:E:96:ASP:N	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:65:GLU:HG2	3:C:68:LYS:CE	2.34	0.58
1:A:164:MET:HE2	1:A:165:MET:N	2.20	0.57
2:B:24:LYS:HE2	2:B:28:ASN:HD21	1.69	0.57
2:B:108:LYS:HA	2:B:111:ILE:HG22	1.87	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
2:B:88:GLN:H	2:B:88:GLN:CD	2.13	0.57
3:F:35:GLU:HA	3:F:38:GLN:OE1	2.05	0.57
1:D:164:MET:HE2	1:D:164:MET:C	2.29	0.56
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:119:GLN:O	1:A:120:LYS:C	2.48	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
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
2:B:99:SER:O	2:B:100:CYS:C	2.50	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
1:A:116:ALA:C	1:A:120:LYS:HB2	2.24	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:87:ALA:HA	2:B:90:ASP:OD1	2.09	0.53
2:B:106:GLN:O	2:B:109:THR:HG22	2.08	0.53
3:C:22:LYS:HZ3	3:C:30:VAL:HG22	1.73	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
2:B:96:ASP:O	2:B:97:VAL:C	2.52	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:21:ARG:C	2:B:23:GLN:H	2.17	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:7:LEU:O	2:B:8:LYS:C	2.52	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:D:116:ALA:O	1:D:117:LEU:C	2.54	0.51
2:E:47:LYS:HB3	2:E:48:PRO:HD2	1.93	0.51
1:A:118:VAL:O	1:A:119:GLN:O	2.27	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:E:53:TRP:O	2:E:54:ALA:C	2.53	0.50
3:C:61:ASN:OD1	3:C:61:ASN:N	2.44	0.50
1:A:116:ALA:CB	1:A:120:LYS:CE	2.78	0.50
2:B:86:THR:HG22	2:B:86:THR:O	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:116:ALA:C	1:D:120:LYS:HG2	2.38	0.49
1:D:164:MET:C	1:D:164:MET:CE	2.86	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
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
1:A:116:ALA:C	1:A:120:LYS:HD2	2.38	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:88:GLN:C	2:E:90:ASP:N	2.71	0.48
1:D:134:MET:HG2	2:E:37:LEU:HB3	1.95	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:OE1	2:E:88:GLN:HA	2.15	0.47
2:B:96:ASP:OD1	2:B:96:ASP:N	2.44	0.47
2:B:87:ALA:HA	2:B:90:ASP:CG	2.40	0.47
1:D:79:GLY:C	1:D:81:PHE:H	2.23	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:118:VAL:O	1:D:119:GLN:C	2.58	0.46
1:D:119:GLN:O	1:D:122:HIS:CD2	2.68	0.46
1:A:174:ILE:HG13	1:A:175:ASN:N	2.31	0.46
3:F:39:ASP:O	3:F:40:LEU:C	2.59	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
2:E:65:LEU:O	2:E:66:VAL:C	2.60	0.45
1:A:146:ARG:HA	1:A:149:ARG:NH1	2.31	0.45
2:E:96:ASP:O	2:E:97:VAL:C	2.59	0.45
3:C:12:PHE:O	3:C:16:ILE:HG13	2.17	0.45
1:A:90:ILE:CG2	1:A:91:ALA:H	2.28	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:166:ARG:O	1:D:167:GLN:C	2.59	0.44
1:A:116:ALA:O	1:A:117:LEU:C	2.61	0.44
1:A:88:GLN:O	1:A:92:GLN:HG2	2.18	0.44
1:A:112:LYS:O	1:A:113:SER:C	2.60	0.44
2:B:44:LEU:HD23	2:B:44:LEU:HA	1.91	0.44
1:D:119:GLN:O	1:D:120:LYS:C	2.59	0.44
2:E:14:ALA:O	2:E:18:ILE:HG23	2.16	0.44
1:A:161:VAL:O	1:A:162:GLN:C	2.61	0.44
2:E:88:GLN:O	2:E:89:VAL:C	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:100:CYS:O	2:E:104:LEU:N	2.50	0.43
1:A:98:GLN:O	1:A:99:ALA:C	2.62	0.43
1:D:137:GLU:HG3	2:E:5:LEU:HD13	2.01	0.43
2:B:51:ILE:O	2:B:53:TRP:N	2.51	0.43
2:B:7:LEU:HD23	2:B:7:LEU:HA	1.76	0.43
2:B:100:CYS:SG	2:B:101:ALA:N	2.92	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:D:148:TYR:O	1:D:149:ARG:C	2.62	0.43
1:A:117:LEU:C	1:A:118:VAL:O	2.62	0.42
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:82:ALA:HB1	1:D:86:ASN:ND2	2.33	0.42
1:D:114:GLN:O	1:D:118:VAL:HG23	2.20	0.42
2:E:24:LYS:HG2	2:E:28:ASN:HD21	1.84	0.42
3:C:17:ARG:HH11	3:C:20:ARG:NH1	2.17	0.42
1:D:81:PHE:CD1	1:D:81:PHE:C	2.97	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
1:A:99:ALA:C	1:A:103:GLN:HE21	2.29	0.41
1:D:128:GLN:O	1:D:132:ILE:HG12	2.19	0.41
2:B:53:TRP:CH2	2:B:70:GLU:HA	2.55	0.41
2:B:98:LYS:HD3	2:B:98:LYS:HA	1.79	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:A:146:ARG:O	1:A:150:GLU:HG3	2.21	0.41
1:D:90:ILE:CG2	1:D:91:ALA:N	2.83	0.41
1:D:116:ALA:O	1:D:118:VAL:N	2.54	0.41
1:A:90:ILE:HG23	1:A:91:ALA:H	1.86	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:D:122:HIS:O	1:D:123:TYR:C	2.63	0.41
2:E:92:GLU:O	2:E:93:GLU:C	2.64	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:LEU:HD23	1:A:97:LYS:HE3	2.03	0.40
1:A:119:GLN:CG	1:A:120:LYS:N	2.78	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
3:F:59:PHE:CG	3:F:60:PRO:HD2	2.56	0.40
1:A:114:GLN:C	1:A:116:ALA:N	2.78	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%)	2	8
1	D	103/214 (48%)	84 (82%)	17 (16%)	2 (2%)	6	22
2	B	118/160 (74%)	88 (75%)	24 (20%)	6 (5%)	1	5
2	E	119/160 (74%)	91 (76%)	24 (20%)	4 (3%)	3	11
3	C	64/77 (83%)	54 (84%)	8 (12%)	2 (3%)	3	12
3	F	64/77 (83%)	53 (83%)	7 (11%)	4 (6%)	1	3
All	All	571/902 (63%)	457 (80%)	92 (16%)	22 (4%)	2	8

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

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Mol	Chain	Res	Type
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%)	81 (84%)	16 (16%)	2	8
1	D	97/190 (51%)	82 (84%)	15 (16%)	2	9
2	B	104/142 (73%)	89 (86%)	15 (14%)	3	11
2	E	105/142 (74%)	82 (78%)	23 (22%)	1	3
3	C	60/71 (84%)	50 (83%)	10 (17%)	2	8
3	F	60/71 (84%)	50 (83%)	10 (17%)	2	8
All	All	523/806 (65%)	434 (83%)	89 (17%)	2	7

All (89) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	83	ASP
1	A	86	ASN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	93	LEU
1	A	96	VAL
1	A	97	LYS
1	A	98	GLN
1	A	101	ILE
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	168	LYS
1	A	174	ILE
1	A	175	ASN
2	B	4	LYS
2	B	11	ASP
2	B	13	VAL
2	B	30	LEU
2	B	31	LYS
2	B	39	SER
2	B	46	GLU
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	5	LEU
3	C	8	VAL
3	C	12	PHE
3	C	14	ASP
3	C	16	ILE
3	C	23	ARG
3	C	30	VAL
3	C	43	GLU
3	C	58	THR
3	C	61	ASN
1	D	80	GLU
1	D	93	LEU
1	D	98	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	D	109	ASP
1	D	119	GLN
1	D	132	ILE
1	D	134	MET
1	D	137	GLU
1	D	154	ARG
1	D	155	LEU
1	D	164	MET
1	D	165	MET
1	D	174	ILE
1	D	181	VAL
1	D	182	VAL
2	E	5	LEU
2	E	9	THR
2	E	13	VAL
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	41	LEU
2	E	51	ILE
2	E	59	ASN
2	E	70	GLU
2	E	89	VAL
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	109	THR
2	E	111	ILE
3	F	8	VAL
3	F	11	LEU
3	F	12	PHE
3	F	21	THR
3	F	38	GLN
3	F	39	ASP
3	F	43	GLU

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Mol	Chain	Res	Type
3	F	44	LEU
3	F	58	THR
3	F	66	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	GLN
1	A	98	GLN
1	A	103	GLN
1	A	130	ASN
1	A	145	HIS
2	B	28	ASN
1	D	86	ASN
1	D	98	GLN
1	D	103	GLN
1	D	115	GLN
1	D	162	GLN
1	D	163	ASN
1	D	175	ASN
2	E	28	ASN
2	E	88	GLN
2	E	123	ASN

### 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 oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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

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.