



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 10:17 PM UTC

PDB ID : 2W6J / pdb_00002w6j
Title : Low resolution structures of bovine mitochondrial F1-ATPase during controlled dehydration: Hydration State 5.
Authors : Sanchez-Weatherby, J.; Felisaz, F.; Gobbo, A.; Huet, J.; Ravelli, R.B.G.; Bowler, M.W.; Cipriani, F.
Deposited on : 2008-12-18
Resolution : 3.84 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 types of validation reports are described at

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

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

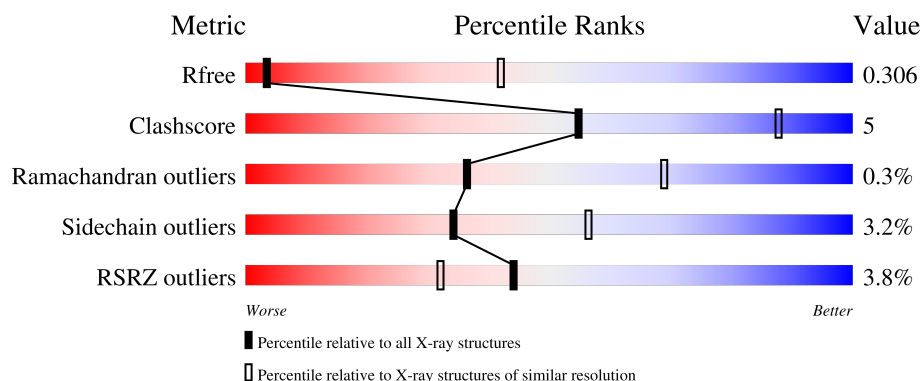
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.84 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}	180053	1169 (4.00-3.68)
Clashscore	190562	1211 (4.00-3.68)
Ramachandran outliers	187476	1156 (4.00-3.68)
Sidechain outliers	187428	1149 (4.00-3.68)
RSRZ outliers	180081	1168 (4.00-3.68)

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 ≥ 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 $\leq 5\%$. 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	553	4% 75% 11% • 12%
1	B	553	3% 81% 5% • 13%
1	C	553	5% 79% 9% • 11%
2	D	528	3% 78% 9% • 12%
2	E	528	4% 77% 9% • 13%

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Mol	Chain	Length	Quality of chain
2	F	528	 3% 80% 7% • 12%
3	G	298	 50% 10% • 39%
4	H	168	 1% 36% 10% • 51%
5	I	51	 39% 10% 51%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 23874 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	0	0
			3715	2341	656	706	12			
1	B	480	Total	C	N	O	S	0	0	0
			3663	2308	648	695	12			
1	C	490	Total	C	N	O	S	0	0	0
			3735	2353	659	711	12			

- 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	182	Total	C	N	O	S	0	0	1
			1397	881	250	260	6			

- Molecule 4 is a protein called F1-ATPASE DELTA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	83	Total	C	N	O	S	0	0	0
			620	391	102	126	1			

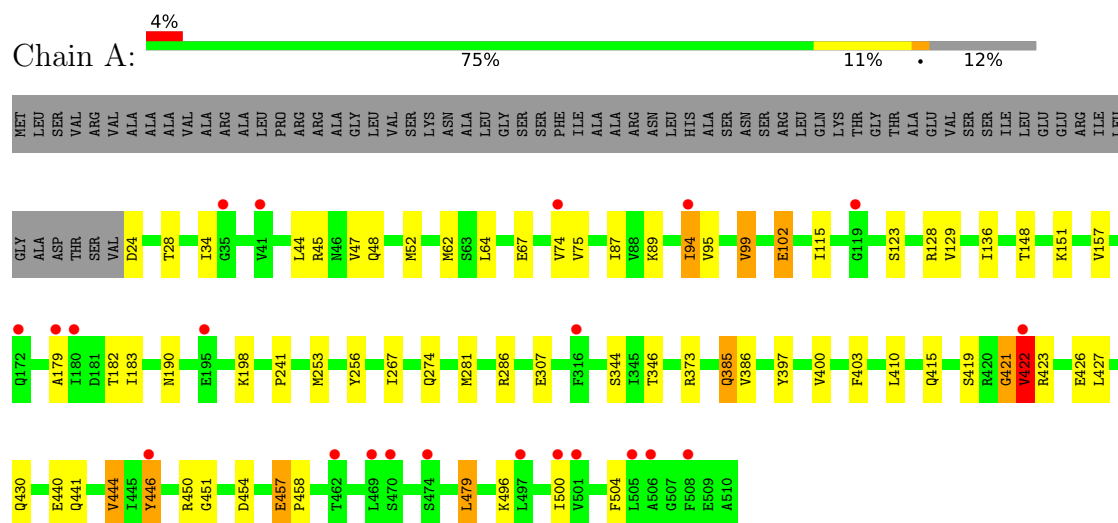
- Molecule 5 is a protein called ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	I	25	Total 203	C 130	N 38	O 34	S 1	0	0	0

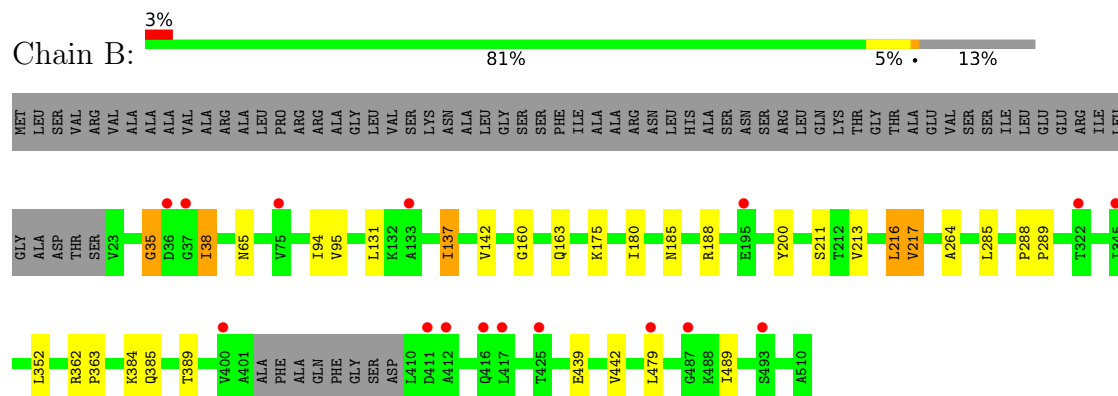
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

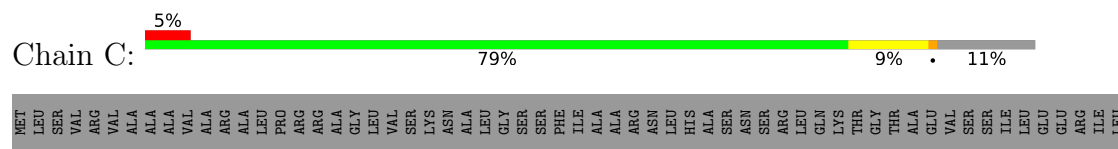
• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM, MITOCHONDRIAL

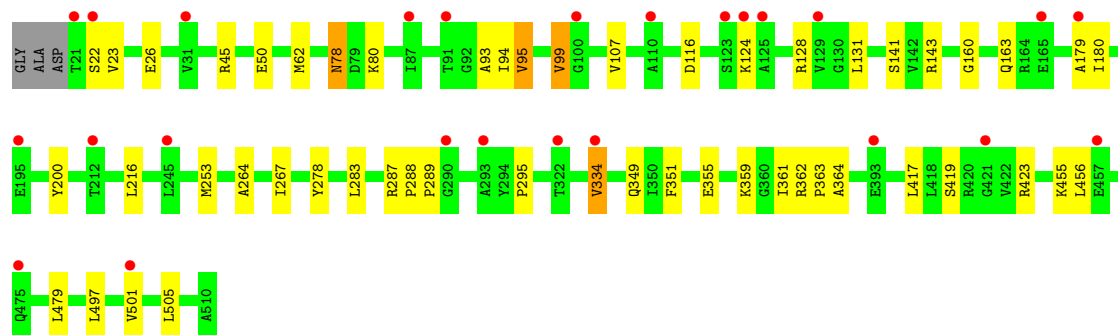


• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM, MITOCHONDRIAL

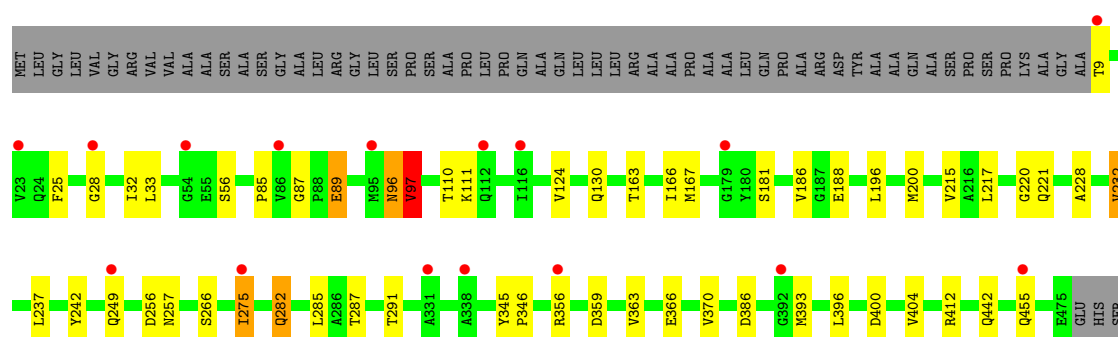
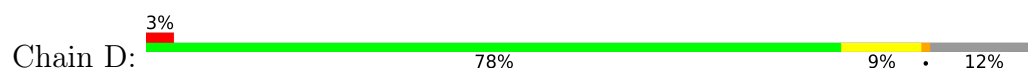


• Molecule 1: ATP SYNTHASE SUBUNIT ALPHA HEART ISOFORM, MITOCHONDRIAL

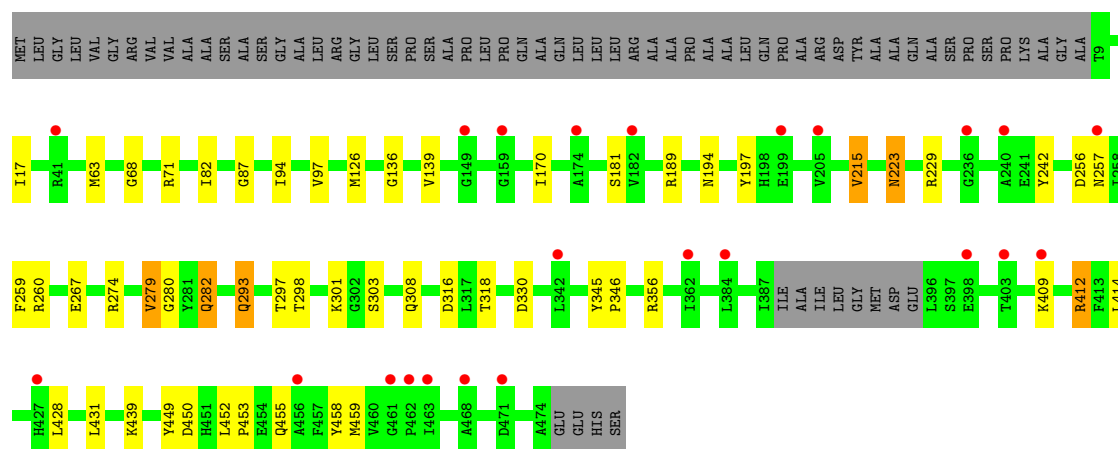
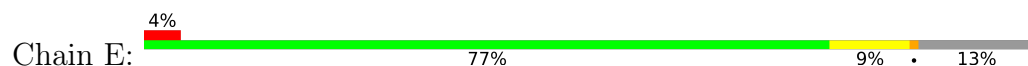




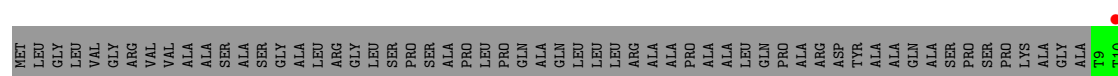
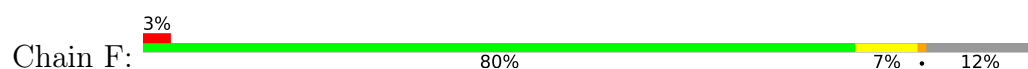
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL

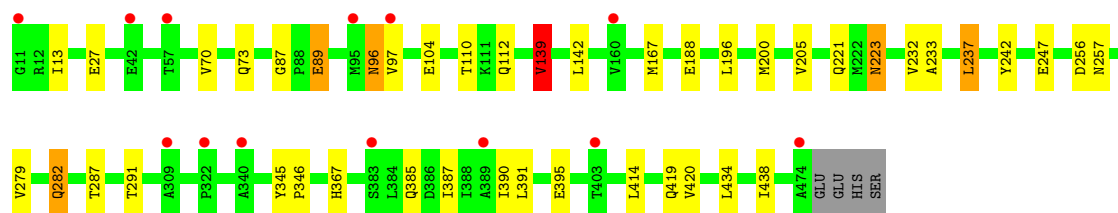


• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL



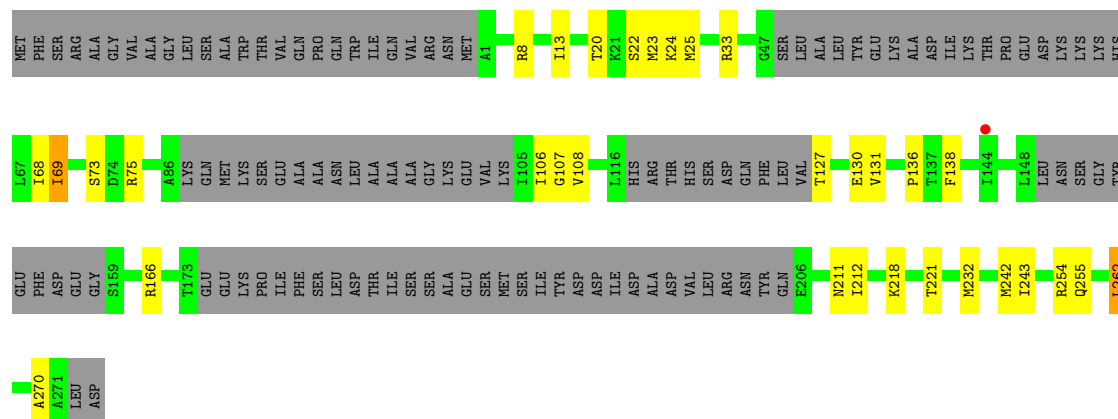
• Molecule 2: ATP SYNTHASE SUBUNIT BETA, MITOCHONDRIAL





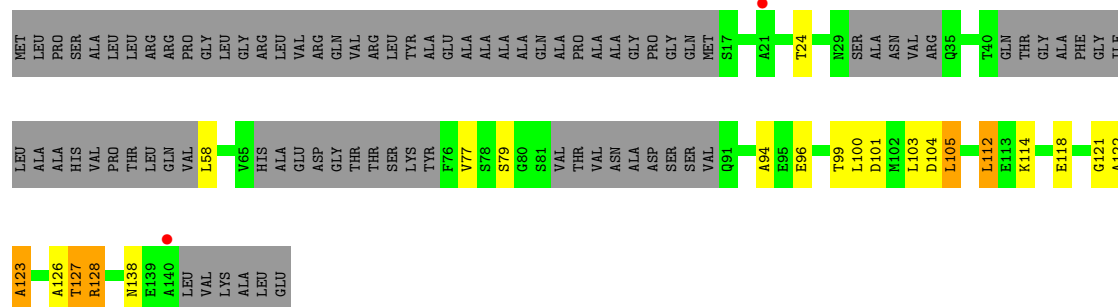
• Molecule 3: ATP SYNTHASE SUBUNIT GAMMA, MITOCHONDRIAL

Chain G: 50% 10% 39%



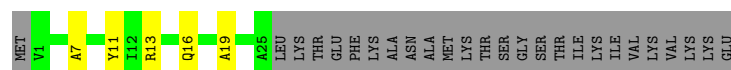
• Molecule 4: F1-ATPASE DELTA SUBUNIT

Chain H: 36% 10% 51%



• Molecule 5: ATP SYNTHASE SUBUNIT EPSILON, MITOCHONDRIAL

Chain I: 39% 10% 51%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	106.93Å 124.07Å 264.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	132.45 – 3.84 132.23 – 3.84	Depositor EDS
% Data completeness (in resolution range)	95.3 (132.45-3.84) 95.3 (132.23-3.84)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.52 (at 3.89Å)	Xtriage
Refinement program	REFMAC 5.5.0038	Depositor
R, R_{free}	0.305 , (Not available) 0.307 , 0.306	Depositor DCC
R_{free} test set	1665 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	73.4	Xtriage
Anisotropy	0.375	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 3.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.79	EDS
Total number of atoms	23874	wwPDB-VP
Average B, all atoms (Å ²)	20.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.09% 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, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.51	1/3766 (0.0%)	0.81	5/5080 (0.1%)
1	B	0.51	1/3711 (0.0%)	0.79	0/5005
1	C	0.48	0/3786	0.81	2/5108 (0.0%)
2	D	0.50	0/3596	0.77	3/4879 (0.1%)
2	E	0.48	0/3528	0.78	2/4786 (0.0%)
2	F	0.52	0/3587	0.79	1/4867 (0.0%)
3	G	0.52	1/1406 (0.1%)	0.84	0/1880
4	H	0.44	0/623	0.92	2/840 (0.2%)
5	I	0.50	0/207	0.83	0/279
All	All	0.50	3/24210 (0.0%)	0.80	15/32724 (0.0%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	422	VAL	CA-CB	8.65	1.66	1.54
3	G	270	ALA	C-N	-6.98	1.23	1.33
1	B	137	ILE	CA-CB	5.01	1.57	1.53

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	256	ASP	CA-C-N	6.62	133.62	121.70
2	E	256	ASP	C-N-CA	6.62	133.62	121.70
4	H	127	THR	CA-C-N	6.17	132.80	121.70
4	H	127	THR	C-N-CA	6.17	132.80	121.70
1	A	421	GLY	CA-C-N	-5.93	111.30	121.97
1	A	421	GLY	C-N-CA	-5.93	111.30	121.97
2	D	232	VAL	N-CA-C	5.84	119.23	111.17
1	C	93	ALA	N-CA-C	5.64	116.53	108.74
2	D	97	VAL	CB-CA-C	-5.52	104.69	112.14
2	D	232	VAL	N-CA-CB	-5.50	101.90	110.54
2	F	139	VAL	CB-CA-C	-5.50	104.71	112.14
1	C	23	VAL	N-CA-C	-5.37	108.05	113.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	75	VAL	N-CA-C	5.32	116.23	108.58
1	A	457	GLU	CA-C-N	5.17	126.30	119.84
1	A	457	GLU	C-N-CA	5.17	126.30	119.84

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3715	0	3813	43	1
1	B	3663	0	3773	17	0
1	C	3735	0	3834	22	0
2	D	3539	0	3593	44	1
2	E	3472	0	3526	43	0
2	F	3530	0	3587	29	0
3	G	1397	0	1481	21	0
4	H	620	0	614	29	0
5	I	203	0	205	4	0
All	All	23874	0	24426	230	1

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 5.

All (230) 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)
4:H:122:ALA:HA	4:H:123:ALA:CB	1.74	1.15
3:G:68:ILE:HB	3:G:69:ILE:HA	1.31	1.09
2:D:89:GLU:HG3	2:D:110:THR:HB	1.29	1.08
2:D:228:ALA:O	2:D:232:VAL:HG13	1.52	1.08
4:H:104:ASP:HA	4:H:105:LEU:HB2	1.31	1.06
2:E:316:ASP:OD2	3:G:254:ARG:NH2	1.91	1.03
4:H:121:GLY:HA3	4:H:122:ALA:HB3	1.40	1.02
4:H:122:ALA:HA	4:H:123:ALA:HB2	1.38	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:99:THR:HA	4:H:100:LEU:HB2	1.46	0.97
2:E:282:GLN:H	2:E:282:GLN:HE21	1.14	0.96
2:F:282:GLN:H	2:F:282:GLN:HE21	1.06	0.94
1:A:94:ILE:HD11	1:A:128:ARG:HG2	1.53	0.91
2:D:282:GLN:H	2:D:282:GLN:HE21	0.94	0.89
4:H:104:ASP:CA	4:H:105:LEU:HB2	2.01	0.89
4:H:122:ALA:HA	4:H:123:ALA:HB3	1.56	0.87
4:H:104:ASP:HA	4:H:105:LEU:CB	2.07	0.84
4:H:122:ALA:CA	4:H:123:ALA:HB2	2.10	0.80
2:D:282:GLN:H	2:D:282:GLN:NE2	1.78	0.79
2:E:293:GLN:HE22	2:E:308:GLN:HE22	1.32	0.78
2:F:97:VAL:HG12	2:F:232:VAL:HB	1.66	0.77
4:H:99:THR:CA	4:H:100:LEU:HB2	2.16	0.76
1:A:151:LYS:H	1:A:430:GLN:HE22	1.30	0.76
2:D:85:PRO:HB3	2:D:110:THR:HG21	1.69	0.74
2:D:282:GLN:HE21	2:D:282:GLN:N	1.79	0.74
2:F:223:ASN:HD22	2:F:223:ASN:H	1.36	0.73
1:A:52:MET:HG3	1:A:95:VAL:HG22	1.71	0.72
2:E:136:GLY:HA3	2:E:431:LEU:HD12	1.72	0.72
2:D:200:MET:HE1	2:D:217:LEU:HD21	1.69	0.72
2:F:196:LEU:HD11	2:F:200:MET:HE3	1.74	0.69
3:G:136:PRO:HD3	3:G:221:THR:HG21	1.74	0.69
1:A:62:MET:HE2	1:A:64:LEU:HD21	1.75	0.69
2:D:89:GLU:HG3	2:D:110:THR:CB	2.17	0.68
2:D:96:ASN:C	2:D:96:ASN:HD22	2.02	0.66
2:F:97:VAL:CG1	2:F:232:VAL:HB	2.25	0.66
3:G:68:ILE:CB	3:G:69:ILE:HA	2.12	0.66
2:F:282:GLN:HE21	2:F:282:GLN:N	1.88	0.66
2:D:181:SER:HB2	2:D:215:VAL:HG22	1.77	0.66
2:F:96:ASN:C	2:F:96:ASN:HD22	2.05	0.64
1:A:102:GLU:HG3	1:A:123:SER:HA	1.80	0.64
4:H:127:THR:N	4:H:128:ARG:HB2	2.12	0.64
2:F:167:MET:HE1	2:F:196:LEU:HD13	1.79	0.63
4:H:127:THR:H	4:H:128:ARG:HB2	1.64	0.63
1:A:419:SER:O	1:A:423:ARG:HD3	1.99	0.63
4:H:99:THR:HA	4:H:100:LEU:CB	2.26	0.62
1:C:160:GLY:H	1:C:163:GLN:NE2	1.98	0.62
2:D:196:LEU:HG	2:D:200:MET:HE2	1.81	0.61
2:D:89:GLU:CG	2:D:110:THR:HB	2.18	0.61
4:H:127:THR:H	4:H:128:ARG:CB	2.13	0.61
2:F:97:VAL:HG12	2:F:232:VAL:CB	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:128:ARG:HD2	1:C:131:LEU:HG	1.83	0.60
2:D:188:GLU:O	2:D:221:GLN:HB3	2.02	0.59
1:B:137:ILE:HG21	2:F:104:GLU:CD	2.28	0.59
4:H:99:THR:HB	4:H:101:ASP:H	1.68	0.59
3:G:23:MET:SD	3:G:232:MET:HE2	2.43	0.59
1:B:38:ILE:HD12	1:B:285:LEU:HD21	1.86	0.58
4:H:103:LEU:HB3	4:H:105:LEU:HD13	1.83	0.58
2:D:85:PRO:HB3	2:D:110:THR:CG2	2.32	0.58
2:E:257:ASN:OD1	2:E:260:ARG:HG3	2.03	0.58
2:E:412:ARG:HG2	2:E:458:TYR:HB2	1.86	0.57
1:A:190:ASN:HA	1:A:198:LYS:HG2	1.86	0.57
4:H:127:THR:CA	4:H:128:ARG:HB2	2.34	0.57
2:D:186:VAL:HG13	2:D:232:VAL:CG2	2.35	0.57
1:C:180:ILE:HD11	1:C:216:LEU:HD21	1.86	0.56
1:A:44:LEU:HB3	1:A:47:VAL:HG13	1.86	0.56
4:H:58:LEU:N	5:I:11:TYR:HH	2.02	0.56
2:E:345:TYR:HA	2:E:346:PRO:C	2.30	0.56
1:B:160:GLY:H	1:B:163:GLN:NE2	2.04	0.56
2:D:366:GLU:O	2:D:370:VAL:HG23	2.06	0.56
1:A:440:GLU:O	1:A:444:VAL:HG12	2.05	0.56
2:D:87:GLY:HA2	2:D:242:TYR:CE2	2.41	0.56
2:E:229:ARG:HH22	2:E:267:GLU:CD	2.13	0.56
1:A:44:LEU:O	1:A:47:VAL:HG22	2.07	0.55
1:B:385:GLN:HE22	1:B:489:ILE:HB	1.71	0.55
1:B:211:SER:HA	2:E:126:MET:HE2	1.88	0.55
1:B:160:GLY:H	1:B:163:GLN:HE21	1.55	0.54
2:E:223:ASN:HD22	2:E:223:ASN:H	1.56	0.54
4:H:127:THR:HB	4:H:128:ARG:HB2	1.88	0.54
2:F:223:ASN:HD22	2:F:223:ASN:N	2.02	0.54
1:A:45:ARG:HA	2:E:71:ARG:NH2	2.22	0.54
2:E:170:ILE:HG21	2:E:215:VAL:HG22	1.90	0.54
1:A:422:VAL:O	1:A:426:GLU:HG2	2.08	0.54
1:B:439:GLU:O	1:B:442:VAL:HG12	2.08	0.54
2:E:282:GLN:H	2:E:282:GLN:NE2	1.96	0.54
1:A:410:LEU:HD12	1:A:415:GLN:HG3	1.89	0.54
1:B:175:LYS:HG2	1:B:352:LEU:HD12	1.89	0.53
2:F:89:GLU:HG2	2:F:110:THR:HG22	1.89	0.53
1:A:179:ALA:HB1	1:A:267:ILE:HG12	1.89	0.53
1:A:427:LEU:HD22	1:A:444:VAL:HG23	1.91	0.53
1:B:180:ILE:HD11	1:B:216:LEU:HD21	1.91	0.52
1:C:497:LEU:O	1:C:501:VAL:HG22	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:188:GLU:O	2:F:221:GLN:HB3	2.09	0.52
1:A:136:ILE:HG23	2:E:194:ASN:HA	1.90	0.52
1:C:94:ILE:HG22	1:C:95:VAL:H	1.75	0.52
2:E:293:GLN:HA	2:E:293:GLN:HE21	1.74	0.52
2:E:345:TYR:HB2	2:E:459:MET:HE1	1.91	0.52
3:G:73:SER:HA	3:G:131:VAL:HG23	1.92	0.52
4:H:99:THR:HB	4:H:101:ASP:N	2.26	0.51
2:D:220:GLY:HA3	2:D:232:VAL:HG11	1.92	0.51
1:A:67:GLU:HG2	2:E:17:ILE:HD11	1.93	0.51
2:D:221:GLN:HE21	2:D:221:GLN:HA	1.76	0.51
1:A:183:ILE:HD11	1:A:267:ILE:HD13	1.93	0.51
1:A:74:VAL:HG21	1:A:281:MET:HE3	1.94	0.50
2:F:87:GLY:HA2	2:F:242:TYR:CE2	2.46	0.50
3:G:23:MET:HE3	3:G:75:ARG:NH2	2.26	0.50
4:H:126:ALA:HB2	5:I:7:ALA:O	2.11	0.50
1:C:362:ARG:HA	1:C:363:PRO:C	2.36	0.50
2:E:452:LEU:HB3	2:E:453:PRO:HD2	1.94	0.50
3:G:20:THR:HA	3:G:232:MET:HE3	1.93	0.50
2:E:136:GLY:HA3	2:E:431:LEU:CD1	2.40	0.50
1:A:48:GLN:HB3	2:E:68:GLY:HA2	1.92	0.49
1:C:355:GLU:HG2	1:C:359:LYS:HE2	1.93	0.49
1:A:148:THR:HA	1:A:182:THR:HG23	1.94	0.49
2:E:223:ASN:HD22	2:E:223:ASN:N	2.09	0.49
4:H:127:THR:CB	4:H:128:ARG:HB2	2.43	0.49
1:B:362:ARG:HA	1:B:363:PRO:C	2.37	0.49
1:C:50:GLU:HB3	1:C:62:MET:HE2	1.95	0.49
4:H:121:GLY:HA3	4:H:122:ALA:CB	2.18	0.49
1:B:185:ASN:OD1	1:B:188:ARG:NH1	2.37	0.49
1:A:74:VAL:HG22	1:A:241:PRO:HG3	1.93	0.48
1:C:278:TYR:CE2	1:C:295:PRO:HG2	2.48	0.48
1:B:35:GLY:O	2:E:274:ARG:NH2	2.46	0.48
2:D:386:ASP:OD2	3:G:8:ARG:NE	2.40	0.48
2:F:390:ILE:HD11	3:G:242:MET:SD	2.52	0.48
1:A:446:TYR:CE1	1:A:450:ARG:HD2	2.48	0.48
2:D:96:ASN:C	2:D:96:ASN:ND2	2.71	0.48
2:F:287:THR:O	2:F:291:THR:HG23	2.13	0.48
2:E:257:ASN:OD1	2:E:260:ARG:N	2.47	0.48
2:F:221:GLN:HE21	2:F:221:GLN:HA	1.79	0.48
2:E:449:TYR:HD2	2:E:452:LEU:HD12	1.78	0.48
1:A:115:ILE:O	2:D:124:VAL:HG13	2.14	0.48
1:C:26:GLU:HA	1:C:45:ARG:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:GLY:H	1:C:163:GLN:HE21	1.60	0.47
4:H:121:GLY:CA	4:H:122:ALA:HB3	2.29	0.47
5:I:13:ARG:HH11	5:I:16:GLN:NE2	2.11	0.47
1:A:457:GLU:HA	1:A:458:PRO:HD2	1.75	0.47
2:E:257:ASN:OD1	2:E:259:PHE:HB3	2.13	0.47
3:G:13:ILE:HG22	3:G:243:ILE:HG13	1.95	0.47
4:H:96:GLU:HG2	5:I:19:ALA:HB1	1.97	0.47
2:D:266:SER:HB3	2:D:282:GLN:HE22	1.80	0.47
1:A:397:TYR:CD1	1:A:421:GLY:HA3	2.50	0.47
1:A:286:ARG:NH1	2:D:275:ILE:HD11	2.30	0.47
2:E:94:ILE:HD11	2:E:197:TYR:CD1	2.50	0.47
2:E:330:ASP:HA	2:E:356:ARG:HD2	1.97	0.47
1:A:74:VAL:HG21	1:A:281:MET:HG2	1.96	0.47
1:A:44:LEU:HB3	1:A:47:VAL:CG1	2.45	0.46
1:A:385:GLN:HG3	1:A:386:VAL:HG13	1.97	0.46
2:E:87:GLY:HA2	2:E:242:TYR:CE2	2.50	0.46
3:G:22:SER:HA	3:G:25:MET:HE3	1.96	0.46
1:A:446:TYR:HE1	1:A:450:ARG:HD2	1.80	0.46
1:C:141:SER:HB2	1:C:143:ARG:HH21	1.79	0.46
2:E:412:ARG:HH11	2:E:455:GLN:HE22	1.64	0.46
1:B:211:SER:CA	2:E:126:MET:HE2	2.46	0.46
2:E:63:MET:HE3	2:E:97:VAL:CG1	2.46	0.46
1:B:213:VAL:O	1:B:217:VAL:HG12	2.15	0.46
1:A:344:SER:O	2:E:189:ARG:NH2	2.45	0.45
2:D:130:GLN:HE22	2:D:356:ARG:HD2	1.81	0.45
1:C:78:ASN:HD22	1:C:80:LYS:H	1.63	0.45
2:E:126:MET:HE1	2:E:297:THR:OG1	2.16	0.45
1:C:107:VAL:HB	1:C:116:ASP:HB3	1.99	0.45
3:G:69:ILE:HG23	3:G:107:GLY:H	1.81	0.45
2:D:287:THR:O	2:D:291:THR:HG23	2.16	0.45
2:E:280:GLY:HA2	3:G:262:LEU:HD21	1.99	0.45
4:H:122:ALA:N	4:H:123:ALA:HB2	2.31	0.45
1:A:400:VAL:HG13	1:A:403:PHE:CE1	2.52	0.44
2:D:386:ASP:CG	3:G:8:ARG:HE	2.24	0.44
2:E:181:SER:HB2	2:E:215:VAL:HG13	1.99	0.44
2:F:391:LEU:HB3	2:F:395:GLU:HG3	1.98	0.44
4:H:112:LEU:HG	4:H:138:ASN:HB3	1.99	0.44
2:D:25:PHE:O	2:D:56:SER:HB3	2.18	0.44
1:B:94:ILE:O	1:B:95:VAL:C	2.60	0.44
2:D:256:ASP:HA	2:D:257:ASN:HA	1.81	0.44
2:F:282:GLN:H	2:F:282:GLN:NE2	1.90	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:99:VAL:HG22	1:A:253:MET:HA	1.99	0.44
1:A:441:GLN:O	1:A:444:VAL:HG13	2.17	0.44
1:A:500:ILE:O	1:A:504:PHE:HB2	2.17	0.44
2:E:63:MET:HE1	2:E:97:VAL:HG21	1.99	0.44
2:F:96:ASN:C	2:F:96:ASN:ND2	2.74	0.44
3:G:68:ILE:HB	3:G:69:ILE:HD13	2.00	0.44
1:A:99:VAL:HG13	1:A:256:TYR:HB2	1.99	0.43
2:D:370:VAL:HG21	2:D:442:GLN:HG3	1.99	0.43
2:E:409:LYS:NZ	2:E:450:ASP:HA	2.33	0.43
3:G:20:THR:HG22	3:G:232:MET:CE	2.48	0.43
2:D:221:GLN:HA	2:D:221:GLN:NE2	2.33	0.43
1:C:179:ALA:HB1	1:C:267:ILE:HD13	2.00	0.43
2:F:139:VAL:HG13	2:F:414:LEU:HB3	2.00	0.43
2:D:9:THR:HG21	2:D:28:GLY:HA3	2.00	0.43
2:D:345:TYR:HA	2:D:346:PRO:C	2.44	0.43
2:D:97:VAL:HG22	2:D:232:VAL:HG12	2.01	0.43
3:G:69:ILE:HA	3:G:69:ILE:HD13	1.91	0.42
1:A:346:THR:O	1:A:373:ARG:NH2	2.51	0.42
2:F:223:ASN:H	2:F:223:ASN:ND2	2.12	0.42
2:D:359:ASP:O	2:D:363:VAL:HG22	2.20	0.42
2:D:396:LEU:HD22	2:D:400:ASP:HB3	2.02	0.42
2:E:139:VAL:HG12	2:E:414:LEU:HD22	2.01	0.42
2:F:345:TYR:HA	2:F:346:PRO:C	2.44	0.42
1:C:283:LEU:HD21	1:C:289:PRO:HB3	2.02	0.42
1:C:419:SER:O	1:C:423:ARG:HD2	2.20	0.42
1:A:28:THR:HG22	1:A:89:LYS:HG2	2.02	0.42
1:A:48:GLN:OE1	2:E:68:GLY:HA2	2.19	0.42
2:F:13:ILE:HD12	2:F:73:GLN:HB3	2.02	0.42
2:F:142:LEU:HD12	2:F:438:ILE:HD13	2.01	0.42
1:A:24:ASP:O	1:A:28:THR:OG1	2.37	0.41
1:C:334:VAL:HG13	1:C:351:PHE:CE1	2.55	0.41
2:D:393:MET:HE1	2:D:404:VAL:HG11	2.02	0.41
2:D:412:ARG:HE	2:D:455:GLN:NE2	2.18	0.41
4:H:79:SER:O	4:H:94:ALA:HA	2.20	0.41
2:D:386:ASP:OD1	3:G:8:ARG:NH2	2.53	0.41
2:F:70:VAL:H	2:F:73:GLN:HE21	1.68	0.41
2:E:318:THR:OG1	3:G:255:GLN:NE2	2.52	0.41
1:A:151:LYS:H	1:A:430:GLN:NE2	2.07	0.41
2:D:163:THR:O	2:D:166:ILE:HG22	2.20	0.41
2:D:285:LEU:C	2:D:285:LEU:HD23	2.44	0.41
2:D:32:ILE:O	2:D:33:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:166:ILE:CG2	2:D:167:MET:HE2	2.51	0.41
4:H:123:ALA:H	4:H:128:ARG:HD3	1.86	0.41
1:C:99:VAL:HG22	1:C:253:MET:HA	2.02	0.41
1:A:479:LEU:HG	1:A:496:LYS:HD3	2.03	0.41
1:B:200:TYR:O	1:B:264:ALA:HA	2.21	0.41
1:C:361:ILE:O	1:C:364:ALA:HA	2.20	0.41
2:E:63:MET:HE2	2:E:82:ILE:HD13	2.03	0.41
2:F:367:HIS:CE1	2:F:434:LEU:HD11	2.56	0.41
1:B:288:PRO:HA	1:B:289:PRO:HD3	1.92	0.41
1:C:200:TYR:O	1:C:264:ALA:HA	2.20	0.41
2:E:298:THR:HG23	2:E:303:SER:HB3	2.03	0.41
2:E:257:ASN:ND2	2:E:259:PHE:H	2.19	0.40
3:G:138:PHE:HE1	3:G:211:ASN:HD22	1.68	0.40
2:F:256:ASP:HA	2:F:257:ASN:HA	1.90	0.40
2:D:188:GLU:H	2:D:221:GLN:NE2	2.19	0.40
1:C:287:ARG:HA	1:C:288:PRO:HD3	1.96	0.40
2:F:233:ALA:O	2:F:237:LEU:HD13	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:GLN:CD	2:D:111:LYS:NZ[4_545]	2.17	0.03

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	485/553 (88%)	469 (97%)	15 (3%)	1 (0%)	43	74
1	B	476/553 (86%)	465 (98%)	10 (2%)	1 (0%)	43	74
1	C	488/553 (88%)	476 (98%)	12 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	465/528 (88%)	445 (96%)	20 (4%)	0	100	100
2	E	454/528 (86%)	444 (98%)	9 (2%)	1 (0%)	43	74
2	F	464/528 (88%)	450 (97%)	13 (3%)	1 (0%)	43	74
3	G	170/298 (57%)	161 (95%)	8 (5%)	1 (1%)	21	55
4	H	73/168 (44%)	64 (88%)	6 (8%)	3 (4%)	2	21
5	I	23/51 (45%)	22 (96%)	1 (4%)	0	100	100
All	All	3098/3760 (82%)	2996 (97%)	94 (3%)	8 (0%)	36	69

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	H	123	ALA
4	H	128	ARG
4	H	105	LEU
2	E	279	VAL
1	B	35	GLY
3	G	106	ILE
2	F	279	VAL
1	A	451	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	393/444 (88%)	378 (96%)	15 (4%)	29	53
1	B	389/444 (88%)	380 (98%)	9 (2%)	44	63
1	C	396/444 (89%)	384 (97%)	12 (3%)	36	57
2	D	377/417 (90%)	370 (98%)	7 (2%)	50	66
2	E	370/417 (89%)	361 (98%)	9 (2%)	43	63
2	F	376/417 (90%)	362 (96%)	14 (4%)	30	54
3	G	152/251 (61%)	142 (93%)	10 (7%)	15	42

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	H	66/128 (52%)	61 (92%)	5 (8%)	12	38
5	I	19/42 (45%)	19 (100%)	0	100	100
All	All	2538/3004 (84%)	2457 (97%)	81 (3%)	34	56

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	ILE
1	A	87	ILE
1	A	94	ILE
1	A	99	VAL
1	A	102	GLU
1	A	129	VAL
1	A	157	VAL
1	A	274	GLN
1	A	307	GLU
1	A	385	GLN
1	A	422	VAL
1	A	444	VAL
1	A	446	TYR
1	A	454	ASP
1	A	479	LEU
1	B	38	ILE
1	B	65	ASN
1	B	131	LEU
1	B	142	VAL
1	B	216	LEU
1	B	217	VAL
1	B	384	LYS
1	B	389	THR
1	B	479	LEU
1	C	22	SER
1	C	78	ASN
1	C	95	VAL
1	C	99	VAL
1	C	124	LYS
1	C	334	VAL
1	C	349	GLN
1	C	417	LEU
1	C	455	LYS
1	C	456	LEU

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Mol	Chain	Res	Type
1	C	479	LEU
1	C	505	LEU
2	D	89	GLU
2	D	96	ASN
2	D	97	VAL
2	D	237	LEU
2	D	249	GLN
2	D	275	ILE
2	D	282	GLN
2	E	215	VAL
2	E	223	ASN
2	E	279	VAL
2	E	282	GLN
2	E	293	GLN
2	E	301	LYS
2	E	412	ARG
2	E	428	LEU
2	E	439	LYS
2	F	27	GLU
2	F	89	GLU
2	F	96	ASN
2	F	112	GLN
2	F	139	VAL
2	F	205	VAL
2	F	223	ASN
2	F	237	LEU
2	F	247	GLU
2	F	282	GLN
2	F	385	GLN
2	F	387	ILE
2	F	419	GLN
2	F	420	VAL
3	G	24	LYS
3	G	33	ARG
3	G	69	ILE
3	G	108	VAL
3	G	127	THR
3	G	130	GLU
3	G	166	ARG
3	G	212	ILE
3	G	218	LYS
3	G	262	LEU

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Mol	Chain	Res	Type
4	H	24	THR
4	H	77	VAL
4	H	112	LEU
4	H	114	LYS
4	H	118	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (63) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	186	GLN
1	A	274	GLN
1	A	330	GLN
1	A	430	GLN
1	A	471	HIS
1	A	475	GLN
1	B	48	GLN
1	B	163	GLN
1	B	186	GLN
1	B	208	GLN
1	B	330	GLN
1	B	466	ASN
1	B	503	ASN
1	C	78	ASN
1	C	163	GLN
1	C	186	GLN
1	C	263	HIS
1	C	330	GLN
1	C	341	ASN
1	C	349	GLN
1	C	396	GLN
1	C	471	HIS
1	C	476	HIS
2	D	73	GLN
2	D	96	ASN
2	D	130	GLN
2	D	177	HIS
2	D	194	ASN
2	D	221	GLN
2	D	282	GLN
2	D	427	HIS
2	D	442	GLN
2	D	455	GLN

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Mol	Chain	Res	Type
2	E	171	ASN
2	E	172	ASN
2	E	177	HIS
2	E	223	ASN
2	E	249	GLN
2	E	282	GLN
2	E	293	GLN
2	E	367	HIS
2	E	375	GLN
2	E	419	GLN
2	E	427	HIS
2	E	442	GLN
2	E	451	HIS
2	E	455	GLN
2	F	51	GLN
2	F	73	GLN
2	F	96	ASN
2	F	112	GLN
2	F	194	ASN
2	F	221	GLN
2	F	223	ASN
2	F	282	GLN
2	F	419	GLN
2	F	427	HIS
2	F	443	GLN
3	G	211	ASN
3	G	225	GLN
3	G	255	GLN
4	H	138	ASN
5	I	16	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [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 ⓘ

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	487/553 (88%)	0.61	22 (4%)	38	28	10, 20, 20, 20	4 (0%)
1	B	480/553 (86%)	0.67	16 (3%)	49	34	15, 20, 20, 20	1 (0%)
1	C	490/553 (88%)	0.64	25 (5%)	33	26	20, 20, 20, 20	0
2	D	467/528 (88%)	0.59	16 (3%)	48	34	10, 20, 20, 20	2 (0%)
2	E	458/528 (86%)	0.68	23 (5%)	34	26	12, 20, 20, 20	2 (0%)
2	F	466/528 (88%)	0.64	14 (3%)	52	36	14, 20, 20, 20	3 (0%)
3	G	182/298 (61%)	0.50	1 (0%)	87	71	20, 20, 20, 20	0
4	H	83/168 (49%)	0.57	2 (2%)	59	42	20, 20, 20, 20	0
5	I	25/51 (49%)	0.38	0	100	100	20, 20, 20, 20	0
All	All	3138/3760 (83%)	0.63	119 (3%)	44	32	10, 20, 20, 20	12 (0%)

All (119) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	275	ILE	6.7
1	B	400	VAL	5.4
1	A	501	VAL	5.4
1	A	497	LEU	4.5
1	A	94	ILE	4.5
1	A	74	VAL	4.5
1	C	421	GLY	4.4
2	D	86	VAL	4.1
1	B	487	GLY	4.1
1	C	21	THR	3.9
1	A	500	ILE	3.8
2	E	462	PRO	3.7
2	D	249	GLN	3.7
4	H	140	ALA	3.7
2	E	384	LEU	3.6

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Mol	Chain	Res	Type	RSRZ
2	E	461	GLY	3.5
2	F	11	GLY	3.4
2	D	28	GLY	3.3
1	B	36	ASP	3.3
1	A	505	LEU	3.3
1	C	22	SER	3.2
1	C	475	GLN	3.1
1	A	446	TYR	3.0
1	C	195	GLU	3.0
1	C	165	GLU	3.0
1	A	35	GLY	3.0
1	C	393	GLU	2.9
1	B	493	SER	2.9
2	E	342	LEU	2.9
2	D	116	ILE	2.9
1	A	119	GLY	2.9
1	B	412	ALA	2.8
1	C	125	ALA	2.8
2	E	398	GLU	2.8
1	A	172	GLN	2.8
2	F	340	ALA	2.8
1	A	316	PHE	2.7
2	E	257	ASN	2.7
1	B	133	ALA	2.7
1	A	474	SER	2.6
2	D	54	GLY	2.6
2	E	149	GLY	2.6
2	E	199	GLU	2.6
2	F	95	MET	2.6
2	F	309	ALA	2.6
1	A	470	SER	2.5
2	F	383	SER	2.5
2	E	240	ALA	2.5
2	F	474	ALA	2.5
2	E	41	ARG	2.5
2	F	57	THR	2.5
2	F	97	VAL	2.5
1	B	322	THR	2.5
2	F	10	THR	2.5
2	E	468	ALA	2.5
2	E	159	GLY	2.5
1	B	425	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	C	91	THR	2.5
1	C	334	VAL	2.5
2	E	362	ILE	2.4
2	F	389	ALA	2.4
1	B	37	GLY	2.4
2	E	471	ASP	2.4
1	B	416	GLN	2.4
1	B	479	LEU	2.4
2	D	179	GLY	2.3
3	G	144	ILE	2.3
1	A	462	THR	2.3
1	C	322	THR	2.3
2	E	403	THR	2.3
2	F	403	THR	2.3
1	A	506	ALA	2.3
1	C	87	ILE	2.3
1	A	422	VAL	2.3
1	C	31	VAL	2.3
1	C	129	VAL	2.3
2	D	392	GLY	2.3
1	C	212	THR	2.2
2	D	331	ALA	2.2
2	D	112	GLN	2.2
1	A	180	ILE	2.2
1	C	110	ALA	2.2
1	A	195	GLU	2.2
1	B	195	GLU	2.2
2	F	322	PRO	2.2
2	D	9	THR	2.2
2	E	174	ALA	2.1
2	D	23	VAL	2.1
1	A	508	PHE	2.1
1	A	469	LEU	2.1
1	B	417	LEU	2.1
1	C	501	VAL	2.1
1	C	179	ALA	2.1
1	A	41	VAL	2.1
2	E	409	LYS	2.1
2	D	95	MET	2.1
2	D	455	GLN	2.1
1	C	290	GLY	2.1
1	A	179	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	463	ILE	2.1
1	C	245	LEU	2.1
2	F	42	GLU	2.1
2	D	356	ARG	2.1
1	C	123	SER	2.1
1	B	75	VAL	2.1
2	E	236	GLY	2.0
1	B	411	ASP	2.0
4	H	21	ALA	2.0
2	F	160	VAL	2.0
1	B	345	ILE	2.0
1	C	124	LYS	2.0
1	C	457	GLU	2.0
2	D	338	ALA	2.0
2	E	182	VAL	2.0
1	C	100	GLY	2.0
2	E	427	HIS	2.0
1	C	293	ALA	2.0
2	E	456	ALA	2.0
2	E	205	VAL	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.