W O R L D W I D E

wwPDB

P R O T E I N   D A T A   B A N K

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 27, 2014 – 01:24 PM GMT

PDB ID	:	2DPY
Title	:	Crystal structure of the flagellar type III ATPase FliI
Authors	:	Imada, K.; Namba, K.; Minamino, T.
Deposited on	:	2006-05-18
Resolution	:	2.40 Å(reported)

1 Overall quality at a glance ⓘ

The reported resolution of this entry is 2.40 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	Percentile Ranks	Value
Rfree		0.293
Clashscore		29
Ramachandran outliers		2.7%
Sidechain outliers		7.2%
RSRZ outliers		6.7%

Worse   *Better*

▌ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution
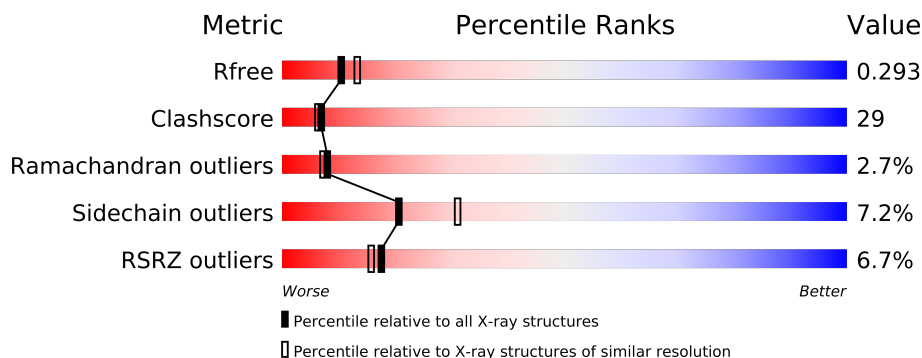
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	66092	2207 (2.40-2.40)
Clashscore	79885	2789 (2.40-2.40)
Ramachandran outliers	78287	2736 (2.40-2.40)
Sidechain outliers	78261	2737 (2.40-2.40)
RSRZ outliers	66119	2210 (2.40-2.40)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	438	
1	B	438	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

| Mol	Type	Chain	Res	Geometry	Electron density
2	ADP	B	600	-	X

2   Entry composition ⓘ

There are 3 unique types of molecules in this entry. The entry contains 6604 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Flagellum-specific ATP synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	422	Total	C	N	O	S	0	0	0
			3211	2032	575	594	10			
1	B	426	Total	C	N	O	S	0	0	0
			3233	2045	579	599	10			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).
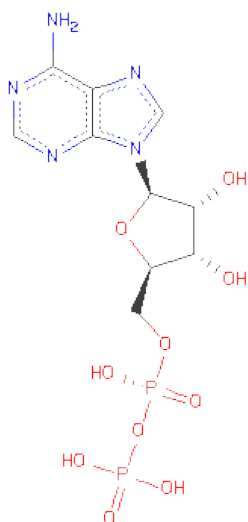
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	71	Total	O	0	0
			71	71		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	62	Total O 62 62		0	0

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: Flagellum-specific ATP synthase

Chain A:

- Molecule 1: Flagellum-specific ATP synthase

Chain B:

A386 R387 V388 R389 L390 F391 L394 N401 R402 D403 L404 V405 S406 V407 Y410 A411 K412 P416 M417 L418 D419 K420 A421 I422 T423 L424 W425 P426 Q427 Q434 W442 E443 L446 Q447 D450 L451 I452 F453 P454 T455 V456
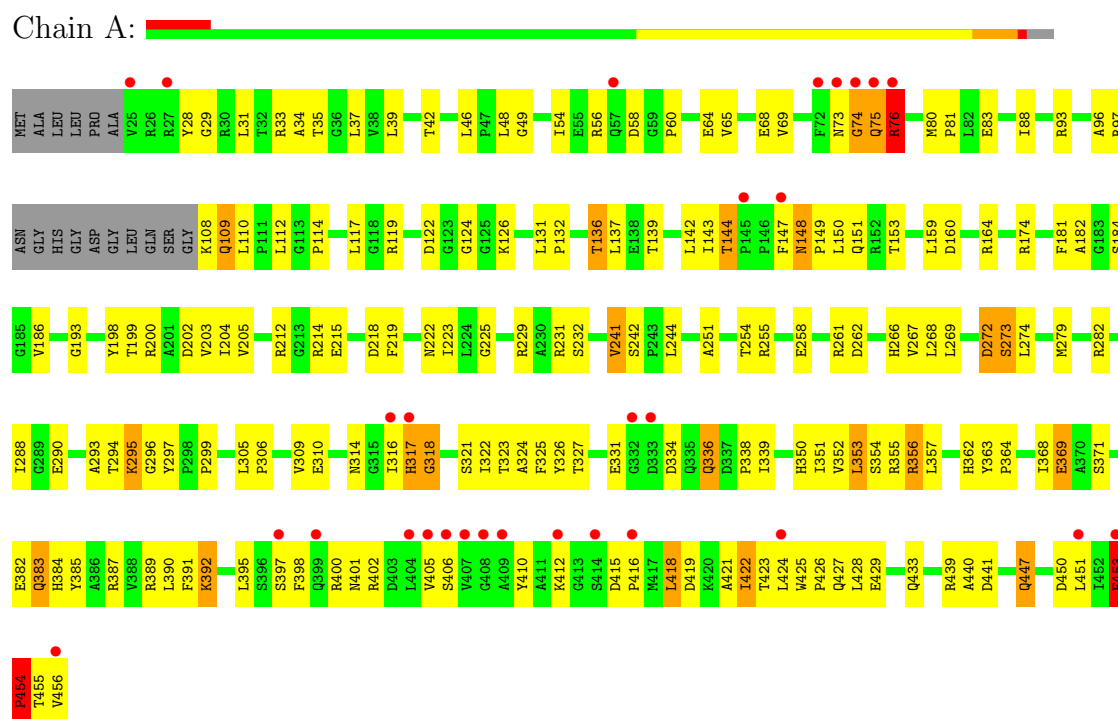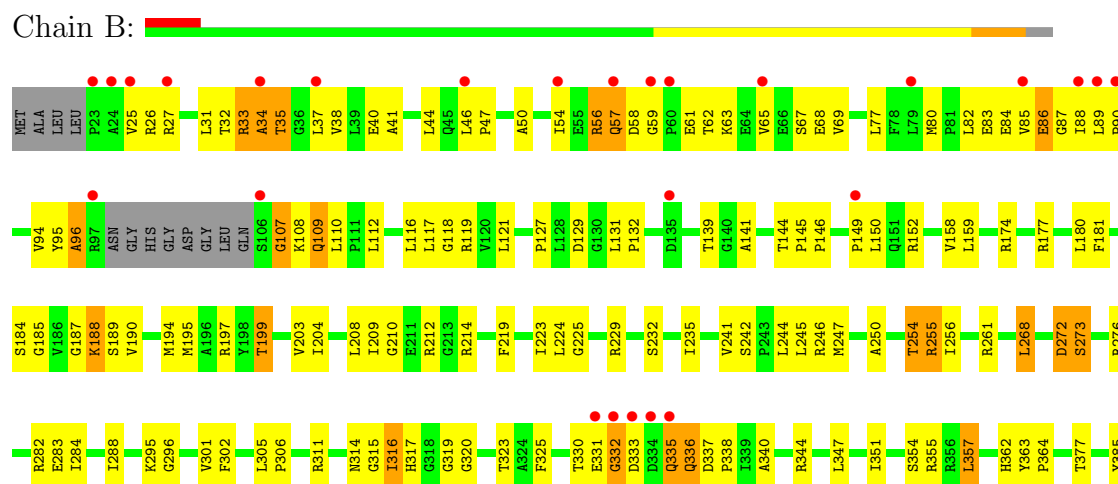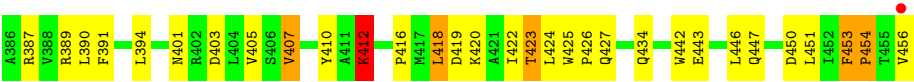
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	48.16Å　　72.75Å　　125.74Å 90.00°　　94.13°　　90.00°	Depositor
Resolution (Å)	45.98　–　2.40 45.98　–　2.40	Depositor EDS
% Data completeness (in resolution range)	99.4 (45.98-2.40) 99.6 (45.98-2.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	3.85 (at 2.39Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.244　,　0.295 0.243　,　0.293	Depositor DCC
R_{free} test set	1680 reflections (4.95%)	DCC
Wilson B-factor (Å^2)	43.1	Xtriage
Anisotropy	0.407	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 33.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$<|L|> = 0.49, <L^2> = 0.32$	Xtriage
Outliers	0 of 33946 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6604	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.88% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ADP

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	0.40	0/3268	0.71	3/4431 (0.1%)
1	B	0.39	0/3291	0.68	1/4462 (0.0%)
All	All	0.39	0/6559	0.69	4/8893 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2
1	B	0	2
All	All	0	4

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	273	SER	N-CA-CB	9.16	124.24	110.50
1	A	318	GLY	N-CA-C	-9.03	90.53	113.10
1	B	273	SER	N-CA-CB	7.54	121.81	110.50
1	A	29	GLY	N-CA-C	-5.93	98.28	113.10

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	272	ASP	Mainchain,Peptide
1	B	272	ASP	Mainchain,Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3211	0	3277	186	0
1	B	3233	0	3298	191	0
2	B	27	0	12	8	0
3	A	71	0	0	3	0
3	B	62	0	0	16	0
All	All	6604	0	6587	376	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 29.

All (376) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:412:LYS:HD3	1:B:412:LYS:H	1.30	0.97
1:B:450:ASP:HA	1:B:454:PRO:HG3	1.46	0.97
1:A:356:ARG:HD3	1:A:356:ARG:H	1.27	0.96
1:B:54:ILE:HG23	1:B:65:VAL:HB	1.50	0.92
1:A:148:ASN:ND2	1:A:151:GLN:HE21	1.67	0.91
1:A:261:ARG:HH11	1:A:261:ARG:HG2	1.35	0.90
1:B:38:VAL:HG21	1:B:288:ILE:HD11	1.57	0.87
1:A:148:ASN:HD21	1:A:151:GLN:HE21	1.22	0.86
1:B:109:GLN:HG3	1:B:139:THR:HG22	1.55	0.86
1:A:33:ARG:HH11	1:A:35:THR:HG21	1.45	0.82
1:A:142:LEU:HD21	1:A:251:ALA:HB1	1.59	0.82
1:B:450:ASP:HA	1:B:454:PRO:CG	2.10	0.81
1:A:425:TRP:CE3	1:A:428:LEU:HD11	2.16	0.81
1:B:158:VAL:HG12	3:B:656:HOH:O	1.80	0.79
1:B:209:ILE:HG22	1:B:276:ARG:HB3	1.64	0.79
1:B:295:LYS:HD3	1:B:338:PRO:CD	2.13	0.79
1:B:419:ASP:O	1:B:423:THR:HG23	1.83	0.79
1:A:387:ARG:HD2	1:A:454:PRO:HG3	1.66	0.78
1:B:107:GLY:HA2	3:B:628:HOH:O	1.85	0.77
1:A:153:THR:HG21	1:A:317:HIS:HB2	1.66	0.77
1:B:242:SER:OG	1:B:245:LEU:HD23	1.84	0.77
1:A:279:MET:HG2	1:A:282:ARG:HH22	1.49	0.76

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:336:GLN:NE2	1:B:336:GLN:H	1.83	0.76
1:B:27:ARG:HG3	3:B:640:HOH:O	1.86	0.75
1:B:204:ILE:HG23	1:B:268:LEU:HD12	1.69	0.75
1:A:136:THR:O	1:A:137:LEU:HB2	1.84	0.75
1:A:282:ARG:HG2	1:A:282:ARG:HH11	1.50	0.74
1:A:447:GLN:O	1:A:451:LEU:HG	1.86	0.74
1:A:453:PHE:HB3	1:A:454:PRO:HD3	1.68	0.74
1:A:33:ARG:HD3	1:A:35:THR:OG1	1.87	0.73
1:B:187:GLY:HA2	2:B:600:ADP:H5'1	1.71	0.73
1:B:412:LYS:CD	1:B:412:LYS:H	2.02	0.73
1:B:56:ARG:HD2	1:B:63:LYS:HD2	1.70	0.73
1:B:85:VAL:HG22	1:B:88:ILE:HD12	1.71	0.72
1:B:141:ALA:O	1:B:255:ARG:HD3	1.89	0.72
1:B:447:GLN:O	1:B:451:LEU:HG	1.90	0.72
1:B:412:LYS:N	1:B:412:LYS:HD3	2.04	0.71
1:B:453:PHE:HB2	1:B:454:PRO:CD	2.21	0.71
1:B:85:VAL:HG13	1:B:88:ILE:HD12	1.73	0.71
1:A:182:ALA:HB2	1:A:353:LEU:HB2	1.72	0.71
1:A:314:ASN:HD22	1:A:321:SER:HB2	1.56	0.70
1:A:305:LEU:HB2	1:A:306:PRO:HD3	1.74	0.69
1:A:428:LEU:HD12	1:A:429:GLU:N	2.07	0.69
1:A:136:THR:HG23	1:A:137:LEU:H	1.57	0.69
1:B:453:PHE:H	1:B:454:PRO:HD2	1.57	0.69
1:A:33:ARG:NH1	1:A:35:THR:HG21	2.07	0.69
1:A:415:ASP:OD2	1:A:418:LEU:HB2	1.92	0.69
1:A:109:GLN:HG3	1:A:139:THR:HB	1.75	0.69
1:B:174:ARG:HA	1:B:323:THR:OG1	1.93	0.68
1:B:295:LYS:HD3	1:B:338:PRO:HD3	1.74	0.67
1:B:302:PHE:HZ	1:B:338:PRO:HB3	1.60	0.67
1:A:279:MET:HG2	1:A:282:ARG:NH2	2.10	0.67
1:A:424:LEU:HD23	1:A:427:GLN:NE2	2.08	0.67
1:B:416:PRO:O	1:B:420:LYS:HG3	1.95	0.67
1:B:282:ARG:HH21	1:B:296:GLY:HA3	1.59	0.67
1:A:147:PHE:HE2	1:A:316:ILE:H	1.41	0.67
1:B:302:PHE:CZ	1:B:338:PRO:HB3	2.30	0.66
1:A:96:ALA:O	1:A:97:ARG:HB2	1.96	0.66
1:A:383:GLN:HB3	3:A:509:HOH:O	1.95	0.66
1:B:212:ARG:HD3	1:B:214:ARG:NH1	2.10	0.66
1:B:44:LEU:HG	1:B:46:LEU:HD23	1.79	0.65
1:B:316:ILE:HG13	1:B:317:HIS:H	1.60	0.65
1:B:57:GLN:HA	1:B:57:GLN:HE21	1.60	0.65
1:B:225:GLY:O	1:B:229:ARG:HG3	1.96	0.65

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:148:ASN:C	1:A:150:LEU:H	2.00	0.65
1:A:33:ARG:HH11	1:A:35:THR:CG2	2.09	0.65
1:A:200:ARG:HE	1:A:439:ARG:HH21	1.45	0.65
1:A:153:THR:CG2	1:A:317:HIS:HB2	2.27	0.65
1:B:58:ASP:HB2	1:B:63:LYS:HE2	1.78	0.65
1:B:187:GLY:HA2	2:B:600:ADP:H8	1.62	0.64
1:B:31:LEU:HD13	1:B:54:ILE:HD13	1.78	0.64
1:A:261:ARG:NH1	1:A:261:ARG:HG2	2.10	0.64
1:B:121:LEU:HD23	1:B:127:PRO:HA	1.80	0.64
1:B:190:VAL:HG12	1:B:194:MET:HE2	1.79	0.63
1:A:317:HIS:HD2	1:A:318:GLY:H	1.47	0.63
1:A:453:PHE:CB	1:A:454:PRO:HD3	2.29	0.63
1:A:108:LYS:HE2	1:A:110:LEU:HD21	1.80	0.63
1:B:47:PRO:O	1:B:69:VAL:HG11	1.99	0.63
1:A:148:ASN:HD21	1:A:151:GLN:NE2	1.95	0.62
1:B:25:VAL:HG22	1:B:26:ARG:H	1.63	0.62
1:B:119:ARG:NH1	1:B:119:ARG:HB3	2.15	0.62
1:B:82:LEU:HA	1:B:245:LEU:HD21	1.80	0.62
1:A:425:TRP:HA	1:A:428:LEU:HG	1.81	0.62
1:A:439:ARG:HG3	1:A:439:ARG:HH11	1.64	0.62
1:B:56:ARG:HD2	1:B:63:LYS:CD	2.30	0.62
1:A:200:ARG:HE	1:A:439:ARG:NH2	1.96	0.61
1:A:401:ASN:CG	1:A:418:LEU:HD11	2.21	0.61
1:A:114:PRO:O	1:A:117:LEU:HD23	2.01	0.61
1:A:73:ASN:O	1:A:75:GLN:N	2.34	0.61
1:A:288:ILE:HD12	1:A:290:GLU:H	1.65	0.61
1:A:159:LEU:HD22	1:A:323:THR:HG21	1.83	0.61
1:B:363:TYR:HA	1:B:364:PRO:C	2.21	0.60
1:B:56:ARG:HD3	1:B:57:GLN:N	2.16	0.60
1:B:84:GLU:HG3	3:B:611:HOH:O	2.00	0.60
1:A:387:ARG:HD2	1:A:454:PRO:CG	2.31	0.60
1:B:119:ARG:HH11	1:B:119:ARG:HB3	1.65	0.60
1:B:57:GLN:HA	1:B:61:GLU:O	2.02	0.60
1:B:184:SER:O	1:B:355:ARG:NH2	2.34	0.60
1:A:142:LEU:HD21	1:A:251:ALA:CB	2.30	0.60
1:B:194:MET:HE1	2:B:600:ADP:N6	2.16	0.60
1:B:50:ALA:H	1:B:69:VAL:CG1	2.14	0.60
1:B:250:ALA:O	1:B:254:THR:HG22	2.00	0.60
1:A:42:THR:OG1	1:A:76:ARG:NE	2.36	0.59
1:A:261:ARG:HH11	1:A:261:ARG:CG	2.13	0.59
1:A:148:ASN:O	1:A:150:LEU:N	2.34	0.59
1:A:200:ARG:NE	1:A:439:ARG:HH21	2.00	0.59

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:109:GLN:HE21	1:A:109:GLN:CA	2.16	0.58
1:B:235:ILE:N	1:B:235:ILE:HD12	2.18	0.58
1:B:390:LEU:HD13	1:B:453:PHE:CD2	2.38	0.58
1:B:456:VAL:OXT	1:B:456:VAL:HG12	2.04	0.58
1:A:383:GLN:HG2	1:A:387:ARG:NH1	2.19	0.58
1:A:109:GLN:HG3	1:A:139:THR:CB	2.34	0.58
1:A:31:LEU:HD11	1:A:39:LEU:HB3	1.84	0.58
1:A:261:ARG:NH1	1:A:262:ASP:OD1	2.35	0.57
1:B:57:GLN:NE2	1:B:61:GLU:O	2.36	0.57
1:A:405:VAL:HG22	1:A:410:TYR:HB2	1.85	0.57
1:B:424:LEU:O	1:B:427:GLN:HB2	2.05	0.57
1:A:174:ARG:HH11	1:A:317:HIS:HE1	1.51	0.57
1:B:208:LEU:C	1:B:209:ILE:HD12	2.25	0.57
1:B:241:VAL:HG12	1:B:245:LEU:HB2	1.87	0.56
1:A:356:ARG:N	1:A:356:ARG:HD3	2.10	0.56
1:A:164:ARG:HB2	1:A:440:ALA:CB	2.36	0.56
1:B:387:ARG:HD3	1:B:454:PRO:CG	2.35	0.56
1:A:336:GLN:NE2	1:A:336:GLN:N	2.54	0.56
1:A:385:TYR:O	1:A:389:ARG:HG3	2.05	0.56
1:B:336:GLN:HE21	1:B:336:GLN:H	1.54	0.56
1:A:122:ASP:OD2	1:A:126:LYS:HB2	2.06	0.55
1:B:442:TRP:CE2	1:B:446:LEU:HD11	2.41	0.55
1:B:340:ALA:O	1:B:344:ARG:HG3	2.05	0.55
1:A:297:TYR:OH	1:A:339:ILE:HD11	2.07	0.55
1:B:254:THR:HG23	1:B:311:ARG:NH2	2.21	0.55
1:B:185:GLY:HA2	3:B:633:HOH:O	2.07	0.55
1:B:385:TYR:HE2	1:B:389:ARG:HH21	1.54	0.55
1:B:387:ARG:HD3	1:B:454:PRO:HD3	1.89	0.55
1:B:110:LEU:O	1:B:139:THR:HG23	2.06	0.55
1:A:114:PRO:HA	1:A:117:LEU:HD23	1.89	0.55
1:A:164:ARG:NH2	1:A:433:GLN:O	2.40	0.55
1:B:25:VAL:HG22	1:B:26:ARG:N	2.22	0.55
1:A:306:PRO:O	1:A:310:GLU:HB2	2.05	0.55
1:A:64:GLU:OE1	1:A:97:ARG:NH2	2.40	0.55
1:B:96:ALA:N	3:B:640:HOH:O	2.40	0.54
1:A:119:ARG:NH2	1:A:132:PRO:O	2.40	0.54
1:A:317:HIS:CD2	1:A:318:GLY:H	2.24	0.54
1:A:416:PRO:HA	1:A:419:ASP:OD2	2.07	0.54
1:B:189:SER:HB2	2:B:600:ADP:O2A	2.07	0.54
1:B:453:PHE:HB2	1:B:454:PRO:HD3	1.89	0.54
1:B:197:ARG:HD3	1:B:224:LEU:O	2.08	0.54
1:B:210:GLY:HA3	1:B:276:ARG:CG	2.37	0.54

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:194:MET:SD	3:B:625:HOH:O	2.58	0.54
1:A:383:GLN:OE1	1:A:384:HIS:HB2	2.07	0.54
1:B:50:ALA:O	1:B:68:GLU:HA	2.08	0.54
1:A:412:LYS:NZ	1:A:419:ASP:HA	2.23	0.54
1:A:450:ASP:OD1	1:A:456:VAL:HG22	2.09	0.54
1:A:398:PHE:O	1:A:402:ARG:HB2	2.07	0.53
1:B:333:ASP:HB2	3:B:648:HOH:O	2.07	0.53
1:A:401:ASN:ND2	1:A:418:LEU:HD11	2.23	0.53
1:A:142:LEU:HD11	1:A:251:ALA:HB3	1.91	0.53
1:A:109:GLN:NE2	1:A:109:GLN:HA	2.24	0.53
1:B:301:VAL:O	1:B:305:LEU:HD13	2.08	0.53
1:B:131:LEU:HD12	1:B:131:LEU:N	2.22	0.53
1:B:442:TRP:NE1	1:B:446:LEU:HD11	2.23	0.53
1:B:235:ILE:HD11	1:B:256:ILE:HD12	1.90	0.53
1:A:297:TYR:CZ	1:A:339:ILE:HD11	2.44	0.53
1:B:41:ALA:HB1	1:B:94:VAL:HG21	1.91	0.53
1:B:152:ARG:HH12	1:B:177:ARG:HH12	1.55	0.53
1:A:453:PHE:HB3	1:A:454:PRO:CD	2.39	0.52
1:B:69:VAL:HG21	1:B:77:LEU:HD11	1.91	0.52
1:A:117:LEU:HD11	1:A:203:VAL:HG13	1.90	0.52
1:A:336:GLN:H	1:A:336:GLN:HE21	1.57	0.52
1:A:74:GLY:HA2	3:A:521:HOH:O	2.08	0.52
1:B:453:PHE:N	1:B:454:PRO:HD2	2.18	0.52
1:A:109:GLN:HE21	1:A:109:GLN:HA	1.75	0.52
1:B:129:ASP:HB2	3:B:612:HOH:O	2.09	0.52
1:A:295:LYS:HB2	1:A:338:PRO:HG3	1.91	0.52
1:A:164:ARG:HB2	1:A:440:ALA:HB1	1.91	0.52
1:B:195:MET:O	1:B:199:THR:HB	2.10	0.52
1:B:387:ARG:HD3	1:B:454:PRO:HG3	1.91	0.52
1:A:65:VAL:HG13	1:A:83:GLU:HB2	1.92	0.51
1:A:54:ILE:HG21	1:A:88:ILE:HD13	1.92	0.51
1:A:205:VAL:CG2	1:A:269:LEU:CD1	2.88	0.51
1:B:109:GLN:HE21	1:B:109:GLN:N	2.08	0.51
1:A:205:VAL:HG23	1:A:269:LEU:HD12	1.92	0.51
1:A:387:ARG:HG2	1:A:454:PRO:HD3	1.92	0.51
1:B:241:VAL:HG12	1:B:242:SER:N	2.25	0.51
1:B:443:GLU:HG2	1:B:447:GLN:HE21	1.76	0.51
1:B:59:GLY:C	1:B:61:GLU:H	2.13	0.51
1:B:377:THR:HG23	3:B:631:HOH:O	2.11	0.51
1:B:401:ASN:O	1:B:405:VAL:HG23	2.10	0.51
1:B:335:GLN:NE2	1:B:335:GLN:N	2.58	0.51
1:B:112:LEU:HA	1:B:116:LEU:CD2	2.41	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:407:VAL:O	1:B:407:VAL:HG13	2.10	0.51
1:B:85:VAL:HG22	1:B:88:ILE:CD1	2.40	0.51
1:A:391:PHE:CZ	1:A:428:LEU:HB2	2.45	0.51
1:B:204:ILE:O	1:B:232:SER:HA	2.11	0.50
1:B:335:GLN:O	1:B:337:ASP:N	2.44	0.50
1:A:450:ASP:CG	1:A:456:VAL:HG22	2.31	0.50
1:A:109:GLN:O	1:A:110:LEU:HD23	2.11	0.50
1:B:152:ARG:HH12	1:B:177:ARG:NH1	2.08	0.50
1:B:336:GLN:NE2	1:B:336:GLN:N	2.58	0.50
1:A:422:ILE:HG13	1:A:423:THR:N	2.26	0.50
1:A:331:GLU:HG3	1:A:331:GLU:O	2.11	0.50
1:A:225:GLY:O	1:A:229:ARG:HG3	2.11	0.50
1:B:110:LEU:C	1:B:139:THR:HG23	2.32	0.50
1:A:142:LEU:O	1:A:142:LEU:HD23	2.11	0.50
1:B:108:LYS:O	1:B:141:ALA:HA	2.11	0.50
1:A:46:LEU:HB2	1:A:69:VAL:HG21	1.92	0.50
1:A:357:LEU:HD13	1:A:362:HIS:CD2	2.47	0.50
1:A:397:SER:O	1:A:401:ASN:HB3	2.12	0.49
1:A:160:ASP:O	1:A:199:THR:HA	2.12	0.49
1:B:144:THR:HB	1:B:145:PRO:HD2	1.94	0.49
1:B:214:ARG:HG3	1:B:214:ARG:HH11	1.77	0.49
1:A:363:TYR:HA	1:A:364:PRO:C	2.32	0.49
1:B:54:ILE:HA	1:B:94:VAL:HG12	1.94	0.49
1:B:410:TYR:HH	1:B:419:ASP:CG	2.16	0.49
1:B:131:LEU:HB3	1:B:132:PRO:HD2	1.94	0.49
1:A:455:THR:HG23	1:A:455:THR:O	2.12	0.49
1:B:112:LEU:HA	1:B:116:LEU:HD22	1.94	0.49
1:A:218:ASP:OD1	1:A:222:ASN:ND2	2.36	0.49
1:A:354:SER:OG	1:A:356:ARG:NE	2.45	0.49
1:B:62:THR:HG21	3:B:613:HOH:O	2.12	0.49
1:A:193:GLY:HA3	1:A:223:ILE:HG22	1.95	0.49
1:A:28:TYR:HD2	1:A:93:ARG:HB3	1.78	0.49
1:B:295:LYS:HD3	1:B:338:PRO:HD2	1.91	0.49
1:B:241:VAL:CG1	1:B:245:LEU:HB2	2.42	0.48
1:B:118:GLY:HA2	1:B:229:ARG:O	2.12	0.48
1:A:352:VAL:H	1:A:371:SER:HB3	1.78	0.48
1:A:148:ASN:C	1:A:150:LEU:N	2.66	0.48
1:B:159:LEU:HD23	1:B:159:LEU:C	2.33	0.48
1:B:330:THR:C	1:B:332:GLY:H	2.16	0.48
1:B:67:SER:HB2	1:B:80:MET:O	2.14	0.48
1:B:325:PHE:HE2	1:B:351:ILE:HD12	1.79	0.48
1:A:148:ASN:ND2	1:A:151:GLN:HG3	2.28	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:203:VAL:HG12	1:B:204:ILE:N	2.28	0.48
1:A:451:LEU:N	1:A:451:LEU:HD23	2.27	0.48
1:B:158:VAL:HG21	1:B:442:TRP:CZ3	2.48	0.48
1:B:394:LEU:HD11	1:B:453:PHE:HE2	1.79	0.48
1:B:109:GLN:HG3	1:B:139:THR:CG2	2.37	0.48
1:A:204:ILE:HB	1:A:232:SER:HB3	1.96	0.48
1:A:368:ILE:HD12	1:A:368:ILE:N	2.29	0.48
1:B:419:ASP:O	1:B:423:THR:CG2	2.57	0.47
1:A:153:THR:HG22	1:A:314:ASN:HB3	1.97	0.47
1:A:136:THR:OG1	1:A:137:LEU:N	2.47	0.47
1:A:455:THR:O	1:A:456:VAL:C	2.53	0.47
1:A:204:ILE:HD11	1:A:231:ARG:NH1	2.29	0.47
1:A:119:ARG:NH2	1:A:131:LEU:HB2	2.30	0.47
1:A:148:ASN:ND2	1:A:151:GLN:NE2	2.50	0.47
1:B:357:LEU:HG	1:B:362:HIS:CD2	2.50	0.47
1:B:109:GLN:HE21	1:B:109:GLN:CA	2.26	0.47
1:A:205:VAL:CG2	1:A:269:LEU:HD12	2.44	0.47
1:A:425:TRP:N	1:A:426:PRO:HD2	2.30	0.47
1:B:194:MET:HE1	2:B:600:ADP:HN61	1.79	0.47
1:A:400:ARG:HH11	1:A:400:ARG:HG2	1.79	0.47
1:B:188:LYS:HE2	1:B:272:ASP:OD2	2.15	0.47
1:B:204:ILE:HG23	1:B:268:LEU:CD1	2.44	0.46
1:B:424:LEU:O	1:B:427:GLN:N	2.48	0.46
1:A:336:GLN:N	1:A:336:GLN:HE21	2.12	0.46
1:A:75:GLN:O	1:A:76:ARG:HB2	2.14	0.46
1:B:332:GLY:O	1:B:333:ASP:HB2	2.15	0.46
1:B:387:ARG:HD3	1:B:454:PRO:CD	2.45	0.46
1:A:274:LEU:HD22	1:A:305:LEU:CD2	2.45	0.46
1:A:269:LEU:HB3	1:A:324:ALA:HB2	1.95	0.46
1:A:204:ILE:O	1:A:232:SER:HB2	2.15	0.46
1:A:241:VAL:HG13	1:A:242:SER:N	2.30	0.46
1:A:33:ARG:HG2	1:A:34:ALA:N	2.30	0.46
1:A:122:ASP:OD1	1:A:124:GLY:N	2.45	0.46
1:B:219:PHE:O	1:B:223:ILE:HB	2.15	0.46
1:A:282:ARG:HG2	1:A:282:ARG:NH1	2.26	0.46
1:B:434:GLN:NE2	3:B:625:HOH:O	2.49	0.46
1:A:391:PHE:O	1:A:395:LEU:HB2	2.16	0.46
1:A:305:LEU:CB	1:A:306:PRO:HD3	2.45	0.46
1:A:68:GLU:OE1	1:A:244:LEU:HD22	2.15	0.46
1:B:109:GLN:CG	1:B:139:THR:HG22	2.38	0.46
1:A:282:ARG:CG	1:A:282:ARG:HH11	2.24	0.46
1:B:245:LEU:HD13	3:B:659:HOH:O	2.16	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:204:ILE:HD13	1:B:268:LEU:HB3	1.97	0.46
1:A:241:VAL:CG1	1:A:242:SER:N	2.78	0.46
1:B:149:PRO:HG2	3:B:662:HOH:O	2.14	0.46
1:B:56:ARG:HD3	1:B:57:GLN:C	2.36	0.45
1:A:200:ARG:NE	1:A:439:ARG:NH2	2.60	0.45
1:B:261:ARG:HD2	1:B:315:GLY:CA	2.45	0.45
1:A:212:ARG:HB2	1:A:215:GLU:HG3	1.98	0.45
1:B:305:LEU:N	1:B:305:LEU:HD12	2.32	0.45
1:A:294:THR:C	1:A:296:GLY:H	2.20	0.45
1:B:272:ASP:HA	1:B:273:SER:HA	1.69	0.45
1:B:89:LEU:HB3	1:B:90:PRO:HD2	1.99	0.45
1:B:288:ILE:O	1:B:288:ILE:HG23	2.16	0.45
1:B:159:LEU:HD13	1:B:323:THR:HG21	1.98	0.45
1:B:80:MET:SD	1:B:244:LEU:HG	2.56	0.45
1:A:117:LEU:N	1:A:117:LEU:HD22	2.31	0.45
1:A:336:GLN:NE2	1:A:336:GLN:H	2.13	0.45
1:B:95:TYR:O	1:B:96:ALA:O	2.35	0.45
1:B:131:LEU:CD1	1:B:131:LEU:N	2.79	0.45
1:B:32:THR:HG21	1:B:40:GLU:OE2	2.17	0.45
1:B:54:ILE:CG2	1:B:65:VAL:HB	2.35	0.44
1:B:209:ILE:N	1:B:209:ILE:HD12	2.32	0.44
1:B:261:ARG:HD2	1:B:315:GLY:HA3	1.99	0.44
1:A:149:PRO:O	1:A:150:LEU:HD23	2.15	0.44
1:A:96:ALA:O	1:A:97:ARG:CB	2.65	0.44
1:A:293:ALA:HB2	1:A:299:PRO:HG3	1.98	0.44
1:B:85:VAL:CG2	1:B:88:ILE:HD12	2.46	0.44
1:A:219:PHE:HA	1:A:223:ILE:CG1	2.47	0.44
1:B:418:LEU:O	1:B:422:ILE:HG12	2.17	0.44
1:B:210:GLY:HA3	1:B:276:ARG:HG2	1.99	0.44
1:A:453:PHE:CB	1:A:454:PRO:CD	2.92	0.44
1:B:246:ARG:HD2	3:B:634:HOH:O	2.17	0.44
1:B:247:MET:CE	1:B:284:ILE:HD12	2.48	0.44
1:B:145:PRO:HA	1:B:146:PRO:HD2	1.92	0.44
1:A:425:TRP:O	1:A:428:LEU:HG	2.18	0.44
1:B:188:LYS:HD2	2:B:600:ADP:O2B	2.17	0.44
1:B:214:ARG:HG3	1:B:214:ARG:NH1	2.33	0.43
1:A:288:ILE:HD12	1:A:288:ILE:C	2.38	0.43
1:A:182:ALA:HB1	1:A:186:VAL:CG2	2.48	0.43
1:B:330:THR:O	1:B:332:GLY:N	2.50	0.43
1:B:305:LEU:N	1:B:306:PRO:HD2	2.33	0.43
1:B:34:ALA:O	1:B:35:THR:C	2.55	0.43
1:A:56:ARG:HG3	1:A:56:ARG:O	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:267:VAL:HG12	1:A:268:LEU:N	2.33	0.43
1:A:184:SER:O	1:A:355:ARG:NH2	2.51	0.43
1:A:258:GLU:HA	1:A:322:ILE:HD11	1.98	0.43
1:B:58:ASP:O	1:B:61:GLU:HB3	2.18	0.43
1:A:398:PHE:CD1	1:A:422:ILE:HG22	2.54	0.43
1:B:261:ARG:HG3	1:B:320:GLY:C	2.39	0.43
1:A:119:ARG:CZ	1:A:131:LEU:HB2	2.49	0.43
1:A:294:THR:O	1:A:296:GLY:N	2.46	0.43
1:B:37:LEU:HD11	1:B:283:GLU:HG2	2.01	0.43
1:B:314:ASN:HA	1:B:314:ASN:HD22	1.68	0.43
1:A:148:ASN:HD22	1:A:151:GLN:HG3	1.84	0.43
1:A:261:ARG:HD3	1:A:322:ILE:HG13	2.01	0.43
1:A:418:LEU:O	1:A:421:ALA:HB3	2.19	0.43
1:A:142:LEU:CD2	1:A:251:ALA:HB1	2.40	0.42
1:B:241:VAL:CG1	1:B:242:SER:N	2.81	0.42
1:A:273:SER:HA	1:A:327:THR:OG1	2.19	0.42
1:B:181:PHE:N	1:B:181:PHE:CD2	2.87	0.42
1:B:32:THR:HG23	1:B:33:ARG:N	2.34	0.42
1:A:254:THR:O	1:A:258:GLU:HG3	2.19	0.42
1:B:288:ILE:O	1:B:288:ILE:CG2	2.68	0.42
1:B:187:GLY:CA	2:B:600:ADP:H8	2.30	0.42
1:B:119:ARG:NH1	1:B:129:ASP:OD1	2.53	0.42
1:B:330:THR:C	1:B:332:GLY:N	2.72	0.42
1:A:205:VAL:HG23	1:A:269:LEU:CD1	2.50	0.42
1:A:325:PHE:HE2	1:A:351:ILE:HD12	1.85	0.42
1:A:205:VAL:CG2	1:A:269:LEU:HD13	2.50	0.42
1:A:181:PHE:CD2	1:A:181:PHE:N	2.87	0.42
1:B:319:GLY:N	3:B:605:HOH:O	2.53	0.42
1:B:85:VAL:CG1	1:B:88:ILE:HD12	2.47	0.42
1:A:401:ASN:OD1	1:A:418:LEU:HD11	2.20	0.41
1:B:117:LEU:O	1:B:119:ARG:HG2	2.20	0.41
1:A:369:GLU:HG3	1:A:392:LYS:NZ	2.34	0.41
1:A:202:ASP:OD1	1:A:266:HIS:HB2	2.20	0.41
1:B:425:TRP:N	1:B:426:PRO:HD2	2.35	0.41
1:A:142:LEU:C	1:A:142:LEU:HD23	2.39	0.41
1:A:153:THR:CB	1:A:317:HIS:HB2	2.50	0.41
1:A:144:THR:HG21	1:A:255:ARG:HE	1.85	0.41
1:B:109:GLN:NE2	1:B:109:GLN:CA	2.84	0.41
1:B:247:MET:HE1	1:B:284:ILE:HD12	2.01	0.41
1:A:272:ASP:HA	1:A:273:SER:HA	1.66	0.41
1:A:350:HIS:O	1:A:371:SER:HB2	2.21	0.41
1:B:57:GLN:O	1:B:59:GLY:N	2.54	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:198:TYR:HB3	1:A:439:ARG:NH1	2.35	0.41
1:A:75:GLN:O	1:A:76:ARG:HD3	2.21	0.41
1:A:406:SER:HB2	3:A:510:HOH:O	2.19	0.41
1:A:425:TRP:CZ3	1:A:428:LEU:HD11	2.54	0.41
1:A:182:ALA:HB1	1:A:186:VAL:HG21	2.03	0.41
1:A:200:ARG:HH21	1:A:439:ARG:HH21	1.69	0.41
1:B:335:GLN:H	1:B:335:GLN:NE2	2.18	0.41
1:A:200:ARG:NH2	1:A:439:ARG:HH21	2.18	0.41
1:A:424:LEU:HD23	1:A:427:GLN:HE22	1.85	0.40
1:B:407:VAL:O	1:B:407:VAL:CG1	2.69	0.40
1:B:390:LEU:O	1:B:394:LEU:HG	2.20	0.40
1:B:188:LYS:HB3	2:B:600:ADP:O1B	2.21	0.40
1:A:80:MET:HA	1:A:81:PRO:HD3	1.83	0.40
1:A:137:LEU:CD2	1:B:26:ARG:HB3	2.52	0.40
1:A:274:LEU:HG	1:A:326:TYR:HB3	2.03	0.40
1:B:86:GLU:CD	1:B:86:GLU:N	2.75	0.40
1:B:209:ILE:CG2	1:B:210:GLY:N	2.85	0.40
1:B:86:GLU:OE1	1:B:87:GLY:N	2.46	0.40

There are no symmetry-related clashes.

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	418/438 (95%)	379 (91%)	28 (7%)	11 (3%)	8	8
1	B	422/438 (96%)	368 (87%)	42 (10%)	12 (3%)	8	6
All	All	840/876 (96%)	747 (89%)	70 (8%)	23 (3%)	8	7

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	74	GLY
1	A	136	THR

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Mol	Chain	Res	Type
1	A	144	THR
1	A	454	PRO
1	B	34	ALA
1	B	35	THR
1	B	96	ALA
1	B	316	ILE
1	B	336	GLN
1	B	412	LYS
1	B	453	PHE
1	A	453	PHE
1	B	454	PRO
1	B	331	GLU
1	B	332	GLY
1	A	76	ARG
1	A	295	LYS
1	A	60	PRO
1	A	75	GLN
1	B	83	GLU
1	B	107	GLY
1	A	49	GLY
1	A	143	ILE

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	332/342 (97%)	306 (92%)	26 (8%)	18	27
1	B	334/342 (98%)	312 (93%)	22 (7%)	24	35
All	All	666/684 (97%)	618 (93%)	48 (7%)	21	31

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	37	LEU
1	A	48	LEU
1	A	58	ASP
1	A	76	ARG

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Mol	Chain	Res	Type
1	A	109	GLN
1	A	112	LEU
1	A	148	ASN
1	A	214	ARG
1	A	241	VAL
1	A	309	VAL
1	A	317	HIS
1	A	334	ASP
1	A	336	GLN
1	A	353	LEU
1	A	356	ARG
1	A	369	GLU
1	A	382	GLU
1	A	383	GLN
1	A	390	LEU
1	A	392	LYS
1	A	418	LEU
1	A	422	ILE
1	A	441	ASP
1	A	447	GLN
1	A	453	PHE
1	A	454	PRO
1	B	33	ARG
1	B	56	ARG
1	B	57	GLN
1	B	86	GLU
1	B	109	GLN
1	B	150	LEU
1	B	180	LEU
1	B	188	LYS
1	B	199	THR
1	B	254	THR
1	B	255	ARG
1	B	268	LEU
1	B	335	GLN
1	B	347	LEU
1	B	354	SER
1	B	357	LEU
1	B	391	PHE
1	B	403	ASP
1	B	407	VAL
1	B	412	LYS

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Mol	Chain	Res	Type
1	B	418	LEU
1	B	423	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	73	ASN
1	A	109	GLN
1	A	148	ASN
1	A	281	GLN
1	A	314	ASN
1	A	317	HIS
1	A	335	GLN
1	A	336	GLN
1	A	399	GLN
1	A	427	GLN
1	B	57	GLN
1	B	109	GLN
1	B	248	GLN
1	B	314	ASN
1	B	317	HIS
1	B	335	GLN
1	B	336	GLN
1	B	393	GLN
1	B	433	GLN
1	B	447	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 (i)

1 ligand is modelled in this entry.

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	#$|Z| > 2$
2	ADP	B	600	-	29,29,29	2.14	10 (34%)	45,45,45	2.19	7 (15%)

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
2	ADP	B	600	-	-	0/16/32/32	0/1/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	600	ADP	PA-O2A	-4.25	1.36	1.55
2	B	600	ADP	PB-O3A	-4.21	1.52	1.60
2	B	600	ADP	O4'-C1'	4.19	1.47	1.41
2	B	600	ADP	C1'-N9	3.73	1.60	1.48
2	B	600	ADP	PB-O2B	3.36	1.67	1.54
2	B	600	ADP	C2-N3	3.03	1.38	1.32
2	B	600	ADP	C4-N9	-2.67	1.33	1.37
2	B	600	ADP	C8-N9	-2.58	1.32	1.36
2	B	600	ADP	C5-N7	-2.53	1.30	1.40
2	B	600	ADP	C2-N1	2.40	1.38	1.33

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	600	ADP	N3-C2-N1	-10.05	120.31	128.71
2	B	600	ADP	O4'-C1'-N9	5.56	113.61	108.44
2	B	600	ADP	N3-C4-N9	4.56	133.67	125.43
2	B	600	ADP	C5-C4-N3	-3.07	119.02	125.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	600	ADP	C4-C5-N7	-3.03	106.93	109.52
2	B	600	ADP	C2-N3-C4	2.57	121.33	114.01
2	B	600	ADP	O2A-PA-O3A	2.47	116.85	105.14

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7   Other polymers (i)

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 ⓘ

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	422/438 (96%)	0.25	29 (6%)	17	15	22, 47, 96, 111	0
1	B	426/438 (97%)	0.35	27 (6%)	19	18	23, 48, 93, 113	0
All	All	848/876 (96%)	0.30	56 (6%)	17	16	22, 48, 94, 113	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	85	VAL	10.4
1	B	25	VAL	10.0
1	B	60	PRO	7.4
1	A	407	VAL	7.3
1	B	59	GLY	5.6
1	B	24	ALA	5.4
1	B	456	VAL	5.3
1	B	23	PRO	5.1
1	A	408	GLY	4.8
1	A	404	LEU	4.7
1	A	332	GLY	4.6
1	B	333	ASP	4.5
1	B	334	ASP	4.2
1	A	406	SER	4.2
1	A	456	VAL	4.1
1	B	65	VAL	4.1
1	B	54	ILE	3.8
1	A	414	SER	3.7
1	A	316	ILE	3.7
1	A	73	ASN	3.6
1	B	89	LEU	3.5
1	B	90	PRO	3.5
1	A	409	ALA	3.5
1	A	416	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
1	B	34	ALA	3.3
1	A	76	ARG	3.2
1	B	149	PRO	3.2
1	B	331	GLU	3.2
1	B	332	GLY	3.1
1	A	147	PHE	3.1
1	A	74	GLY	3.1
1	B	97	ARG	3.0
1	B	46	LEU	3.0
1	A	405	VAL	3.0
1	A	397	SER	3.0
1	B	57	GLN	3.0
1	A	75	GLN	2.9
1	B	135	ASP	2.9
1	A	27	ARG	2.9
1	A	317	HIS	2.8
1	A	145	PRO	2.8
1	A	424	LEU	2.8
1	B	335	GLN	2.7
1	A	412	LYS	2.7
1	A	333	ASP	2.7
1	A	453	PHE	2.5
1	B	37	LEU	2.5
1	A	25	VAL	2.3
1	A	72	PHE	2.3
1	B	106	SER	2.3
1	A	399	GLN	2.2
1	B	88	ILE	2.2
1	A	57	GLN	2.2
1	A	451	LEU	2.1
1	B	27	ARG	2.1
1	B	79	LEU	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 ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

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	RSR	LLDF	B-factors(Å²)	Q<0.9
2	ADP	B	600	27/27	0.43	3.82	127,130,133,133	0

6.5 Other polymers ⓘ

There are no such residues in this entry.