



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:25 PM UTC

PDB ID : 1F59 / pdb_00001f59
Title : IMPORTIN-BETA-FXFG NUCLEOPORIN COMPLEX
Authors : Bayliss, R.; Littlewood, T.; Stewart, M.
Deposited on : 2000-06-13
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 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) : **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

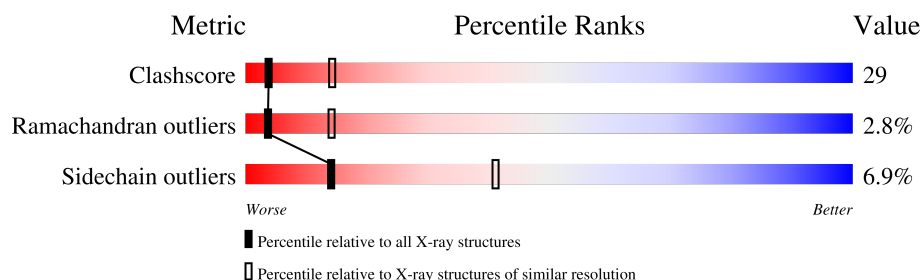
1 Overall quality at a glance

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 ≥ 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	442	54% 41% 5%
1	B	442	47% 47% 5%
2	C	28	32% 32% 14% 21%
2	D	28	46% 25% 29%

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7158 atoms, of which 0 are hydrogens and 0 are deuteriums.

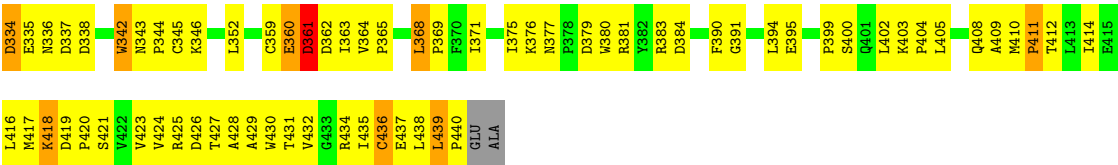
In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called IMPORTIN BETA-1.

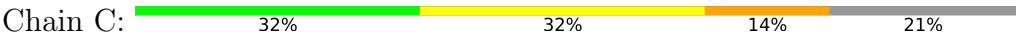
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	440	Total	C	N	O	S	0	0	0
			3440	2169	576	670	25			
1	B	440	Total	C	N	O	S	0	0	0
			3440	2169	576	670	25			

- Molecule 2 is a protein called FXFG NUCLEOPORIN REPEATS.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	22	Total	C	N	O	0	0	0
			148	96	23	29			
2	D	20	Total	C	N	O	0	0	0
			130	87	21	22			



• Molecule 2: FXFG NUCLEOPORIN REPEATS



• Molecule 2: FXFG NUCLEOPORIN REPEATS



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α , β , γ	67.25Å 211.79Å 125.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 2.80	Depositor
% Data completeness (in resolution range)	69.1 (40.00-2.80)	Depositor
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.225 , 0.262	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	7158	wwPDB-VP
Average B, all atoms (Å ²)	91.0	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	0.63	0/3504	1.06	14/4769 (0.3%)
1	B	0.51	0/3504	1.01	16/4769 (0.3%)
2	C	0.57	0/111	1.55	3/146 (2.1%)
2	D	0.48	0/93	0.88	0/121
All	All	0.58	0/7212	1.05	33/9805 (0.3%)

There are no bond length outliers.

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	338	ASP	N-CA-C	-12.09	95.40	110.88
1	A	337	ASP	N-CA-C	9.65	124.22	110.23
2	C	10	SER	N-CA-C	8.65	122.44	110.24
1	B	252	MET	N-CA-C	8.10	122.42	112.54
2	C	47	SER	N-CA-C	7.97	120.09	108.86
1	A	336	ASN	N-CA-C	-7.79	98.28	109.96
1	A	252	MET	N-CA-C	7.30	121.44	112.54
1	A	68	LYS	N-CA-C	-6.82	104.77	113.23
1	A	185	GLU	CA-C-N	6.69	128.21	119.84
1	A	185	GLU	C-N-CA	6.69	128.21	119.84
1	B	68	LYS	N-CA-C	-6.65	104.98	113.23
1	B	126	TRP	CA-C-N	6.62	126.31	119.82
1	B	126	TRP	C-N-CA	6.62	126.31	119.82
1	B	185	GLU	CA-C-N	6.27	127.68	119.84
1	B	185	GLU	C-N-CA	6.27	127.68	119.84
1	B	423	VAL	N-CA-C	-6.19	104.71	110.53
1	B	33	LEU	CA-C-N	-6.09	112.22	119.84
1	B	33	LEU	C-N-CA	-6.09	112.22	119.84
1	B	35	THR	N-CA-C	-6.02	104.63	111.07
1	A	105	ARG	CA-C-N	-6.00	112.34	119.84
1	A	105	ARG	C-N-CA	-6.00	112.34	119.84
1	A	126	TRP	CA-C-N	5.91	125.61	119.82
1	A	126	TRP	C-N-CA	5.91	125.61	119.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	105	ARG	CA-C-N	-5.86	112.52	119.84
1	B	105	ARG	C-N-CA	-5.86	112.52	119.84
1	A	89	ARG	N-CA-C	-5.72	105.41	112.90
1	B	125	GLN	N-CA-C	5.41	118.99	112.93
1	B	105	ARG	N-CA-C	5.34	119.51	112.35
1	B	439	LEU	N-CA-C	5.30	119.46	110.02
2	C	9	ASP	N-CA-C	-5.24	104.15	110.44
1	B	89	ARG	N-CA-C	-5.19	106.10	112.90
1	A	286	VAL	N-CA-C	-5.14	105.48	110.42
1	A	248	TYR	N-CA-C	5.03	116.48	110.44

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	3440	0	3431	190	0
1	B	3440	0	3431	217	0
2	C	148	0	102	15	0
2	D	130	0	95	6	0
All	All	7158	0	7059	408	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 29.

All (408) 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:181:MET:HE1	1:A:198:LEU:HD22	1.48	0.95
1:A:417:MET:HE1	1:B:414:ILE:HD11	1.46	0.95
1:B:181:MET:HE1	1:B:198:LEU:HD22	1.47	0.94
1:A:99:LEU:HB3	1:A:146:MET:HE1	1.57	0.86
1:A:417:MET:HE1	1:B:414:ILE:CD1	2.06	0.85
1:B:99:LEU:HB3	1:B:146:MET:HE1	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:333:GLN:HE22	1:B:384:ASP:HB3	1.42	0.83
1:B:73:LYS:O	1:B:77:GLN:HG3	1.77	0.82
1:A:73:LYS:O	1:A:77:GLN:HG3	1.80	0.82
1:A:410:MET:O	1:A:410:MET:HE3	1.81	0.80
1:A:413:LEU:HD22	1:A:432:VAL:HG23	1.65	0.79
1:B:410:MET:HE3	1:B:410:MET:O	1.82	0.79
1:A:46:ASN:HB3	1:A:49:ASN:ND2	1.97	0.78
1:B:201:SER:O	1:B:205:THR:HG23	1.84	0.78
1:B:1:MET:HB3	1:B:6:ILE:HD11	1.66	0.78
1:A:15:ARG:O	1:A:19:GLU:HG2	1.85	0.77
1:A:377:ASN:HD22	1:A:379:ASP:H	1.32	0.77
1:A:413:LEU:CD2	1:A:432:VAL:HG23	2.15	0.77
1:B:395:GLU:HB2	1:B:438:LEU:CD1	2.16	0.76
1:A:223:CYS:HB3	2:C:48:PHE:CZ	2.21	0.75
1:B:3:LEU:HD11	1:B:40:LEU:HD23	1.68	0.75
1:B:139:ASN:HD22	1:B:140:PRO:HD2	1.51	0.75
1:A:139:ASN:HD22	1:A:140:PRO:HD2	1.50	0.75
1:A:1:MET:HB3	1:A:6:ILE:HD11	1.66	0.75
1:A:201:SER:O	1:A:205:THR:HG23	1.88	0.74
1:B:377:ASN:HD22	1:B:379:ASP:H	1.34	0.73
1:B:245:MET:HE2	1:B:249:TYR:HD1	1.55	0.72
1:A:139:ASN:HD22	1:A:140:PRO:CD	2.02	0.72
1:A:333:GLN:HE22	1:A:384:ASP:HB3	1.53	0.72
1:A:377:ASN:ND2	1:A:379:ASP:H	1.87	0.72
1:B:99:LEU:HD22	1:B:149:SER:HB3	1.71	0.72
1:B:139:ASN:HD22	1:B:140:PRO:CD	2.03	0.72
1:B:98:THR:O	1:B:101:THR:HG23	1.90	0.71
1:A:99:LEU:HD22	1:A:149:SER:HB3	1.70	0.71
1:B:377:ASN:ND2	1:B:379:ASP:H	1.88	0.71
1:B:15:ARG:O	1:B:19:GLU:HG2	1.91	0.71
1:A:363:ILE:HG23	1:A:364:VAL:N	2.07	0.70
1:B:105:ARG:HH21	1:B:189:ASN:ND2	1.89	0.70
1:B:438:LEU:C	1:B:439:LEU:HD22	2.17	0.69
1:B:363:ILE:HG23	1:B:364:VAL:N	2.07	0.69
1:B:395:GLU:HB2	1:B:438:LEU:HD11	1.74	0.69
1:A:363:ILE:HG23	1:A:364:VAL:H	1.57	0.69
1:A:419:ASP:CG	1:A:420:PRO:HD2	2.18	0.69
1:B:334:ASP:C	1:B:336:ASN:H	1.99	0.68
1:B:223:CYS:HB3	2:D:48:PHE:CZ	2.29	0.68
1:B:214:GLU:O	1:B:218:ILE:HG13	1.93	0.68
1:B:376:LYS:HE3	1:B:412:THR:HG21	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:421:SER:O	1:B:425:ARG:HG3	1.92	0.68
1:A:245:MET:HE2	1:A:249:TYR:HD1	1.58	0.68
1:A:328:GLN:O	1:A:331:THR:HB	1.93	0.68
1:B:363:ILE:HG23	1:B:364:VAL:H	1.59	0.67
1:B:333:GLN:NE2	1:B:384:ASP:HB3	2.09	0.67
1:A:98:THR:O	1:A:101:THR:HG23	1.95	0.67
1:B:44:LEU:O	1:B:44:LEU:HG	1.93	0.66
1:B:328:GLN:O	1:B:331:THR:HB	1.94	0.66
1:B:268:MET:HE1	1:B:322:LEU:HD23	1.78	0.66
1:B:419:ASP:CG	1:B:420:PRO:HD2	2.21	0.65
1:B:428:ALA:O	1:B:432:VAL:HG23	1.96	0.65
1:B:368:LEU:HD11	1:B:405:LEU:HD22	1.78	0.65
1:B:126:TRP:CZ2	1:B:129:LEU:HD13	2.32	0.65
1:A:368:LEU:HD11	1:A:405:LEU:HD22	1.79	0.64
1:A:26:GLU:O	1:A:30:VAL:HG23	1.97	0.64
1:A:338:ASP:CG	1:A:341:ASP:HB3	2.23	0.64
1:A:268:MET:HE1	1:A:322:LEU:HD23	1.80	0.64
1:B:139:ASN:ND2	1:B:141:ASN:H	1.96	0.64
1:A:30:VAL:HG12	1:A:30:VAL:O	1.98	0.63
1:B:92:LYS:HD3	1:B:126:TRP:CD2	2.33	0.63
1:B:99:LEU:HB3	1:B:146:MET:CE	2.27	0.63
1:B:151:LEU:HD13	1:B:194:ALA:HB2	1.79	0.63
1:A:99:LEU:CD2	1:A:149:SER:HB3	2.29	0.63
1:B:99:LEU:CD2	1:B:149:SER:HB3	2.29	0.62
1:B:164:GLU:HA	1:B:167:GLN:HG3	1.80	0.62
1:A:99:LEU:HB3	1:A:146:MET:CE	2.27	0.62
1:A:46:ASN:HB3	1:A:49:ASN:HD22	1.63	0.62
1:A:250:GLN:HG3	1:A:309:HIS:CD2	2.34	0.62
1:B:226:THR:O	1:B:234:ARG:HG2	2.00	0.61
1:B:264:THR:HG21	1:B:282:PHE:CD2	2.35	0.61
1:B:146:MET:HE3	1:B:146:MET:HA	1.82	0.61
1:B:377:ASN:HD22	1:B:379:ASP:N	1.98	0.61
1:A:139:ASN:ND2	1:A:141:ASN:H	1.98	0.61
1:A:414:ILE:HA	1:A:417:MET:HG3	1.82	0.61
1:B:42:ARG:O	1:B:45:ALA:HB3	2.00	0.61
1:B:99:LEU:CB	1:B:146:MET:HE1	2.29	0.61
1:A:99:LEU:CB	1:A:146:MET:HE1	2.29	0.60
1:B:411:PRO:O	1:B:414:ILE:HG22	2.01	0.60
1:A:360:GLU:O	1:A:361:ASP:HB2	2.01	0.60
1:A:92:LYS:HD3	1:A:126:TRP:CD2	2.36	0.60
1:B:427:THR:O	1:B:430:TRP:HB3	2.00	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:LEU:HD13	1:A:194:ALA:HB2	1.84	0.60
1:B:431:THR:O	1:B:435:ILE:HG13	2.02	0.60
1:B:6:ILE:HD12	1:B:6:ILE:H	1.66	0.60
1:A:377:ASN:HD22	1:A:379:ASP:N	1.98	0.60
1:B:245:MET:HE2	1:B:249:TYR:CD1	2.37	0.59
1:A:250:GLN:HG3	1:A:309:HIS:HD2	1.67	0.59
1:A:146:MET:HA	1:A:146:MET:HE3	1.85	0.59
1:B:130:ILE:O	1:B:134:VAL:HG23	2.03	0.59
1:B:113:VAL:HG12	1:B:157:ILE:HD11	1.85	0.58
1:A:414:ILE:O	1:A:417:MET:HB2	2.03	0.58
1:A:105:ARG:HH21	1:A:189:ASN:ND2	2.01	0.58
1:A:411:PRO:O	1:A:414:ILE:HG22	2.03	0.58
2:C:47:SER:O	2:C:48:PHE:HD1	1.87	0.58
1:A:164:GLU:HA	1:A:167:GLN:HG3	1.84	0.57
1:A:182:ARG:HG2	2:C:11:LYS:NZ	2.20	0.57
1:A:245:MET:HE2	1:A:249:TYR:CD1	2.38	0.57
1:B:327:THR:HA	1:B:330:LEU:HD12	1.85	0.57
1:B:198:LEU:HG	1:B:240:ASN:ND2	2.20	0.57
1:B:333:GLN:OE1	1:B:381:ARG:HA	2.04	0.57
1:B:6:ILE:HD12	1:B:6:ILE:N	2.18	0.57
1:B:376:LYS:CE	1:B:412:THR:HG21	2.34	0.57
1:B:256:MET:HG2	1:B:314:TYR:CE1	2.39	0.57
1:A:6:ILE:N	1:A:6:ILE:HD12	2.20	0.57
1:A:139:ASN:HD22	1:A:140:PRO:N	2.02	0.57
1:A:335:GLU:CD	1:A:335:GLU:H	2.13	0.57
1:B:139:ASN:HD22	1:B:140:PRO:N	2.03	0.57
1:A:439:LEU:N	1:A:439:LEU:HD23	2.19	0.57
1:B:175:THR:HG23	2:D:14:PHE:O	2.04	0.57
1:B:83:ILE:HG22	1:B:84:ASP:N	2.20	0.57
1:B:360:GLU:O	1:B:361:ASP:HB2	2.04	0.57
1:B:277:LEU:HD22	1:B:342:TRP:HE1	1.70	0.57
1:B:92:LYS:HG2	1:B:126:TRP:CZ2	2.40	0.56
1:B:414:ILE:HA	1:B:417:MET:HG3	1.87	0.56
1:B:395:GLU:HB2	1:B:438:LEU:HD13	1.84	0.56
1:A:83:ILE:HG22	1:A:84:ASP:N	2.20	0.56
1:B:179:GLN:HE22	2:D:13:ALA:HA	1.69	0.56
1:A:65:LEU:HD13	1:A:116:ILE:HG12	1.87	0.56
1:B:105:ARG:NH2	1:B:189:ASN:ND2	2.54	0.56
1:B:343:ASN:HB2	1:B:344:PRO:CD	2.36	0.56
2:D:11:LYS:HD2	2:D:11:LYS:N	2.20	0.56
1:A:342:TRP:HE3	1:A:346:LYS:HD3	1.71	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:TRP:CE3	1:A:346:LYS:HD3	2.41	0.56
1:B:65:LEU:HD13	1:B:116:ILE:HG12	1.87	0.55
1:B:359:CYS:O	1:B:361:ASP:N	2.40	0.55
1:A:3:LEU:HD22	1:A:7:LEU:HG	1.87	0.55
1:B:121:ILE:N	1:B:122:PRO:HD2	2.21	0.55
1:B:47:PRO:C	1:B:49:ASN:H	2.13	0.55
1:B:256:MET:HG2	1:B:314:TYR:CD1	2.42	0.55
1:B:421:SER:HB3	1:B:424:VAL:HB	1.89	0.55
1:A:226:THR:O	1:A:234:ARG:HG2	2.07	0.55
1:A:438:LEU:C	1:A:439:LEU:HD23	2.32	0.54
1:B:182:ARG:HH11	1:B:183:LYS:H	1.56	0.54
1:B:3:LEU:HD22	1:B:7:LEU:HG	1.89	0.54
1:B:35:THR:O	1:B:39:GLU:HG3	2.07	0.54
1:A:264:THR:HG21	1:A:282:PHE:CD2	2.42	0.54
1:B:14:ASP:HB3	1:B:17:GLU:CG	2.38	0.54
1:B:333:GLN:O	1:B:381:ARG:NH2	2.41	0.54
1:A:92:LYS:HG2	1:A:126:TRP:CZ2	2.42	0.54
1:A:256:MET:HG2	1:A:314:TYR:CE1	2.43	0.54
1:A:359:CYS:O	1:A:361:ASP:N	2.41	0.54
1:A:126:TRP:CZ2	1:A:129:LEU:HD13	2.43	0.53
1:B:45:ALA:O	1:B:47:PRO:HD3	2.08	0.53
1:B:343:ASN:HB2	1:B:344:PRO:HD2	1.90	0.53
1:A:37:LEU:O	1:A:41:SER:HB3	2.08	0.53
1:A:130:ILE:O	1:A:134:VAL:HG23	2.09	0.53
1:B:1:MET:SD	1:B:5:THR:HG21	2.48	0.53
1:B:439:LEU:HD22	1:B:439:LEU:N	2.24	0.53
1:B:51:GLN:NE2	1:B:104:TYR:HB3	2.24	0.52
1:A:256:MET:HG2	1:A:314:TYR:CD1	2.45	0.52
1:B:383:ARG:NH1	1:B:419:ASP:OD1	2.43	0.52
1:A:223:CYS:HB3	2:C:48:PHE:CE1	2.44	0.52
1:A:431:THR:O	1:A:435:ILE:HG13	2.08	0.52
1:B:3:LEU:CD2	1:B:7:LEU:HG	2.40	0.52
1:A:387:VAL:CG1	1:A:427:THR:HG22	2.40	0.52
1:A:184:GLU:O	1:A:186:PRO:HD3	2.10	0.51
1:A:51:GLN:NE2	1:A:104:TYR:HB3	2.25	0.51
1:A:129:LEU:O	1:A:133:LEU:HG	2.10	0.51
1:A:410:MET:HE3	1:A:410:MET:C	2.34	0.51
1:B:410:MET:HE3	1:B:410:MET:C	2.36	0.51
1:A:327:THR:HA	1:A:330:LEU:HD12	1.93	0.51
1:B:65:LEU:HD13	1:B:116:ILE:CG1	2.41	0.51
1:B:129:LEU:O	1:B:133:LEU:HG	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ASN:HB3	2:C:16:PHE:O	2.10	0.51
1:A:287:CYS:O	1:A:288:ASP:C	2.53	0.51
1:A:360:GLU:O	1:A:361:ASP:CB	2.58	0.51
1:B:88:ARG:O	1:B:92:LYS:HB2	2.11	0.51
1:A:14:ASP:HB3	1:A:17:GLU:CG	2.40	0.50
1:A:198:LEU:HA	1:A:201:SER:OG	2.11	0.50
1:A:230:ASP:OD1	1:A:232:ARG:HB2	2.11	0.50
1:B:36:PHE:CE2	1:B:40:LEU:HD11	2.46	0.50
1:B:38:VAL:HG22	1:B:91:VAL:HG23	1.91	0.50
1:A:211:LYS:HG3	2:C:21:UNK:CB	2.40	0.50
1:B:24:PHE:CD1	1:B:24:PHE:C	2.89	0.50
1:A:182:ARG:CB	2:C:11:LYS:HZ2	2.24	0.50
1:A:413:LEU:HD21	1:A:432:VAL:HG23	1.93	0.50
1:A:139:ASN:HD22	1:A:139:ASN:C	2.19	0.50
1:B:184:GLU:O	1:B:186:PRO:HD3	2.11	0.50
1:B:287:CYS:O	1:B:288:ASP:C	2.55	0.50
1:A:80:TRP:O	1:A:88:ARG:HD3	2.12	0.50
1:A:16:LEU:O	1:A:17:GLU:C	2.55	0.50
1:A:33:LEU:HD12	1:A:37:LEU:HG	1.94	0.49
1:A:182:ARG:HH11	1:A:183:LYS:H	1.59	0.49
1:B:256:MET:HA	1:B:260:LEU:HB2	1.94	0.49
1:A:139:ASN:ND2	1:A:139:ASN:C	2.69	0.49
1:A:418:LYS:HB2	1:A:418:LYS:NZ	2.27	0.49
1:B:139:ASN:HD22	1:B:139:ASN:C	2.20	0.49
1:B:219:MET:HE2	1:B:252:MET:HE1	1.93	0.49
1:B:293:LEU:HD13	1:B:311:SER:HA	1.93	0.49
1:A:35:THR:O	1:A:39:GLU:HG3	2.11	0.49
1:A:363:ILE:CG2	1:A:364:VAL:N	2.76	0.49
1:B:137:VAL:HG11	1:B:176:ALA:O	2.12	0.49
1:B:216:HIS:HE1	1:B:254:THR:HG21	1.78	0.49
1:B:391:GLY:CA	1:B:431:THR:HG23	2.43	0.49
1:A:101:THR:O	1:A:101:THR:OG1	2.27	0.49
1:A:406:VAL:CG1	1:A:435:ILE:HG21	2.43	0.49
1:B:6:ILE:H	1:B:6:ILE:CD1	2.26	0.49
1:B:41:SER:O	1:B:94:TYR:HB3	2.13	0.49
1:B:126:TRP:CE2	1:B:129:LEU:HB2	2.48	0.49
1:B:414:ILE:O	1:B:417:MET:HB2	2.13	0.49
1:A:417:MET:CE	1:B:414:ILE:HD11	2.32	0.49
1:B:418:LYS:HB2	1:B:418:LYS:NZ	2.28	0.49
1:A:173:ILE:O	1:A:177:ILE:HG13	2.13	0.48
1:A:175:THR:HG23	2:C:14:PHE:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:ILE:CG2	1:A:364:VAL:H	2.25	0.48
1:B:3:LEU:CD1	1:B:40:LEU:HD23	2.41	0.48
1:A:29:ALA:O	1:A:33:LEU:HB2	2.13	0.48
1:B:242:VAL:HG11	1:B:281:GLU:CG	2.43	0.48
1:B:211:LYS:HG2	1:B:213:SER:HB3	1.95	0.48
1:B:360:GLU:O	1:B:361:ASP:CB	2.61	0.48
1:A:421:SER:O	1:A:425:ARG:HG3	2.13	0.48
1:B:265:ILE:HD13	1:B:268:MET:HE2	1.96	0.48
1:B:418:LYS:HB2	1:B:418:LYS:HZ3	1.79	0.48
1:A:68:LYS:O	1:A:70:PRO:HD3	2.14	0.48
1:B:173:ILE:O	1:B:177:ILE:HG13	2.14	0.48
1:A:198:LEU:HG	1:A:240:ASN:ND2	2.28	0.48
1:B:264:THR:HG21	1:B:282:PHE:CE2	2.49	0.48
1:A:113:VAL:HG12	1:A:157:ILE:HD11	1.96	0.48
1:A:211:LYS:HD3	1:A:214:GLU:HG3	1.96	0.48
1:B:181:MET:HE1	1:B:198:LEU:CD2	2.34	0.48
1:B:363:ILE:CG2	1:B:364:VAL:N	2.75	0.48
1:B:68:LYS:O	1:B:70:PRO:HD3	2.14	0.47
1:B:139:ASN:ND2	1:B:139:ASN:C	2.71	0.47
1:B:395:GLU:HB3	1:B:434:ARG:HH22	1.78	0.47
1:B:39:GLU:O	1:B:43:VAL:HG23	2.13	0.47
1:A:376:LYS:HE3	1:A:412:THR:HG21	1.95	0.47
1:B:184:GLU:H	1:B:184:GLU:CD	2.23	0.47
1:B:363:ILE:CG2	1:B:364:VAL:H	2.26	0.47
1:A:1:MET:HB3	1:A:6:ILE:CD1	2.40	0.47
1:A:69:ASP:C	1:A:69:ASP:OD1	2.58	0.47
1:A:376:LYS:CE	1:A:412:THR:HG21	2.45	0.47
1:A:192:LEU:HG	1:A:196:ASN:ND2	2.30	0.47
1:B:198:LEU:HA	1:B:201:SER:OG	2.15	0.47
1:B:215:ARG:O	1:B:217:PHE:N	2.48	0.47
1:B:32:ASN:HD22	1:B:32:ASN:HA	1.60	0.47
1:A:126:TRP:CE2	1:A:129:LEU:HB2	2.50	0.46
1:B:69:ASP:OD1	1:B:69:ASP:C	2.59	0.46
1:A:364:VAL:N	1:A:365:PRO:HD2	2.30	0.46
1:A:418:LYS:HB2	1:A:418:LYS:HZ3	1.80	0.46
1:B:33:LEU:O	1:B:33:LEU:HG	2.14	0.46
1:A:121:ILE:N	1:A:122:PRO:HD2	2.31	0.46
1:A:387:VAL:HG12	1:A:427:THR:HG22	1.98	0.46
1:B:128:GLU:O	1:B:131:PRO:HG2	2.15	0.46
1:B:201:SER:O	1:B:205:THR:CG2	2.60	0.46
1:A:435:ILE:O	1:A:435:ILE:HG22	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:6:ILE:HG23	1:B:21:ALA:HA	1.98	0.46
1:B:134:VAL:HG13	1:B:176:ALA:HB2	1.97	0.46
1:B:1:MET:HE3	1:B:6:ILE:CD1	2.45	0.46
1:B:47:PRO:C	1:B:49:ASN:N	2.74	0.46
1:B:195:THR:HG22	1:B:236:ALA:HB1	1.97	0.46
1:B:93:ASN:O	1:B:94:TYR:C	2.57	0.46
1:A:39:GLU:O	1:A:42:ARG:HB2	2.16	0.46
1:A:88:ARG:O	1:A:92:LYS:HB2	2.16	0.46
1:B:148:GLU:CD	1:B:189:ASN:HB3	2.41	0.46
1:A:34:PRO:O	1:A:38:VAL:HG23	2.16	0.46
1:B:6:ILE:O	1:B:7:LEU:C	2.58	0.46
1:B:336:ASN:C	1:B:338:ASP:N	2.71	0.46
1:A:409:ALA:C	1:A:411:PRO:HD2	2.41	0.45
1:A:242:VAL:HG11	1:A:281:GLU:HG3	1.98	0.45
1:B:438:LEU:C	1:B:440:PRO:HD3	2.41	0.45
1:A:184:GLU:CD	1:A:184:GLU:H	2.23	0.45
1:B:250:GLN:HG3	1:B:309:HIS:CD2	2.51	0.45
1:A:413:LEU:C	1:A:413:LEU:HD23	2.41	0.45
1:B:65:LEU:HB3	1:B:115:GLY:O	2.17	0.45
1:B:286:VAL:O	1:B:290:GLU:HG3	2.16	0.45
1:A:438:LEU:CB	1:A:439:LEU:HD23	2.46	0.45
1:B:334:ASP:C	1:B:336:ASN:N	2.68	0.45
1:B:130:ILE:N	1:B:131:PRO:HD2	2.31	0.45
1:B:417:MET:HB3	1:B:417:MET:HE2	1.67	0.45
1:A:6:ILE:O	1:A:7:LEU:C	2.59	0.45
1:B:105:ARG:HH11	1:B:105:ARG:HG2	1.81	0.45
1:B:174:LEU:HD23	1:B:178:ILE:HG12	1.99	0.45
1:B:217:PHE:O	1:B:221:VAL:HG23	2.16	0.45
1:B:371:ILE:CD1	1:B:390:PHE:HA	2.46	0.45
2:C:11:LYS:HG2	2:C:12:PRO:N	2.31	0.45
1:B:180:GLY:O	1:B:191:LYS:HA	2.17	0.45
1:A:105:ARG:NH2	1:A:189:ASN:ND2	2.65	0.45
1:B:171:ASN:HB3	2:D:16:PHE:O	2.17	0.44
1:A:182:ARG:CG	2:C:11:LYS:NZ	2.80	0.44
1:B:371:ILE:HD13	1:B:390:PHE:HB2	1.99	0.44
1:A:263:ILE:HD11	2:C:48:PHE:HZ	1.82	0.44
1:A:6:ILE:HD12	1:A:6:ILE:H	1.82	0.44
1:A:39:GLU:O	1:A:42:ARG:N	2.47	0.44
1:A:170:SER:O	1:A:171:ASN:C	2.60	0.44
1:A:242:VAL:HG11	1:A:281:GLU:CG	2.47	0.44
1:A:242:VAL:HG22	1:A:282:PHE:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:12:PRO:O	2:C:13:ALA:HB2	2.17	0.44
1:A:130:ILE:N	1:A:131:PRO:HD2	2.32	0.44
1:A:182:ARG:CB	2:C:11:LYS:NZ	2.80	0.44
1:B:16:LEU:O	1:B:17:GLU:C	2.60	0.44
1:A:371:ILE:HD13	1:A:390:PHE:HB2	1.99	0.44
1:B:146:MET:HE2	1:B:150:THR:OG1	2.18	0.44
1:B:198:LEU:HG	1:B:240:ASN:HD21	1.81	0.44
1:B:38:VAL:O	1:B:39:GLU:C	2.61	0.44
1:A:19:GLU:O	1:A:20:ALA:C	2.61	0.44
1:A:212:GLU:O	1:A:216:HIS:HB2	2.18	0.44
1:A:371:ILE:CD1	1:A:390:PHE:HA	2.48	0.44
1:B:126:TRP:N	1:B:127:PRO:CD	2.81	0.44
1:B:230:ASP:OD1	1:B:232:ARG:HB2	2.18	0.44
1:A:264:THR:HG21	1:A:282:PHE:CE2	2.52	0.43
1:A:265:ILE:HD13	1:A:268:MET:HE2	2.01	0.43
1:A:338:ASP:O	1:A:339:ASP:C	2.60	0.43
1:B:65:LEU:CD1	1:B:116:ILE:HG12	2.48	0.43
1:B:403:LYS:N	1:B:404:PRO:HD2	2.34	0.43
1:A:141:ASN:HD22	1:A:141:ASN:HA	1.64	0.43
1:A:120:GLU:OE1	1:A:126:TRP:HB2	2.18	0.43
1:B:96:LEU:HA	1:B:96:LEU:HD12	1.81	0.43
1:B:265:ILE:HD13	1:B:268:MET:CE	2.48	0.43
1:B:364:VAL:N	1:B:365:PRO:HD2	2.33	0.43
1:A:265:ILE:HD13	1:A:268:MET:CE	2.49	0.43
1:A:169:LYS:HA	1:A:172:GLU:OE1	2.19	0.43
1:B:30:VAL:HG12	1:B:30:VAL:O	2.18	0.43
1:B:136:ASN:OD1	1:B:136:ASN:N	2.50	0.43
1:A:213:SER:HB2	2:C:20:UNK:O	2.19	0.43
1:A:293:LEU:HD13	1:A:311:SER:HA	2.01	0.43
1:B:242:VAL:HG11	1:B:281:GLU:HG2	2.01	0.43
1:B:245:MET:HE3	1:B:245:MET:HA	2.01	0.43
1:B:380:TRP:CZ2	1:B:381:ARG:NH1	2.87	0.43
1:B:399:PRO:HG2	1:B:400:SER:H	1.83	0.43
1:A:170:SER:OG	1:A:171:ASN:N	2.51	0.43
1:A:245:MET:CE	1:A:249:TYR:HA	2.48	0.43
1:A:136:ASN:N	1:A:136:ASN:OD1	2.50	0.43
1:A:330:LEU:HA	1:A:345:CYS:SG	2.59	0.43
1:A:380:TRP:CZ2	1:A:381:ARG:NH1	2.87	0.43
1:A:395:GLU:HB2	1:A:438:LEU:HD11	2.01	0.43
1:B:80:TRP:O	1:B:88:ARG:HD3	2.19	0.43
1:B:215:ARG:C	1:B:217:PHE:H	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:LEU:HD13	1:A:60:GLN:NE2	2.34	0.43
1:A:215:ARG:HD2	1:A:255:TYR:OH	2.19	0.42
1:A:230:ASP:O	1:A:231:THR:C	2.62	0.42
1:B:215:ARG:C	1:B:217:PHE:N	2.77	0.42
1:B:215:ARG:HD3	1:B:251:TYR:HB3	2.00	0.42
1:B:25:LEU:HD22	1:B:36:PHE:CE1	2.54	0.42
1:B:101:THR:O	1:B:101:THR:OG1	2.29	0.42
1:B:402:LEU:HD12	1:B:439:LEU:HD11	2.01	0.42
1:B:375:ILE:HD11	1:B:416:LEU:HD11	2.00	0.42
1:B:435:ILE:O	1:B:439:LEU:HB2	2.19	0.42
1:A:20:ALA:O	1:A:21:ALA:C	2.62	0.42
1:A:368:LEU:N	1:A:369:PRO:HD2	2.33	0.42
1:B:418:LYS:O	1:B:418:LYS:HG3	2.18	0.42
1:A:345:CYS:O	1:A:346:LYS:C	2.61	0.42
1:A:95:VAL:HG12	1:A:96:LEU:N	2.35	0.42
1:A:105:ARG:HG2	1:A:105:ARG:HH11	1.84	0.42
1:A:417:MET:HB3	1:A:417:MET:HE2	1.59	0.42
1:B:230:ASP:O	1:B:231:THR:C	2.62	0.42
1:A:65:LEU:HD13	1:A:116:ILE:CG1	2.48	0.42
1:A:256:MET:HA	1:A:260:LEU:HB2	2.02	0.42
1:A:268:MET:HE1	1:A:322:LEU:CD2	2.48	0.42
1:A:126:TRP:N	1:A:127:PRO:CD	2.82	0.42
1:A:6:ILE:HG23	1:A:21:ALA:HA	2.01	0.42
1:A:93:ASN:O	1:A:94:TYR:C	2.60	0.42
1:A:410:MET:N	1:A:411:PRO:CD	2.82	0.42
1:B:414:ILE:HA	1:B:414:ILE:HD12	1.87	0.42
1:A:146:MET:HE2	1:A:150:THR:OG1	2.20	0.42
1:B:92:LYS:HG2	1:B:126:TRP:CH2	2.55	0.41
1:B:245:MET:CE	1:B:249:TYR:HA	2.49	0.41
1:B:417:MET:HE3	1:B:429:ALA:HB2	2.01	0.41
1:A:65:LEU:CD1	1:A:116:ILE:HG12	2.49	0.41
1:A:245:MET:HE3	1:A:245:MET:HA	2.02	0.41
1:B:218:ILE:HG13	1:B:218:ILE:H	1.72	0.41
1:A:92:LYS:HG2	1:A:126:TRP:CH2	2.56	0.41
1:B:3:LEU:HD11	1:B:40:LEU:CD2	2.46	0.41
1:B:14:ASP:HB3	1:B:17:GLU:HG2	2.02	0.41
1:A:418:LYS:HG3	1:A:418:LYS:O	2.20	0.41
1:A:438:LEU:HB3	1:A:439:LEU:HD23	2.02	0.41
1:B:206:LYS:HG2	1:B:210:ASP:OD2	2.21	0.41
1:B:223:CYS:HB3	2:D:48:PHE:CE1	2.55	0.41
1:A:174:LEU:HD23	1:A:178:ILE:HG12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:PRO:HG2	1:A:400:SER:H	1.86	0.41
1:A:403:LYS:N	1:A:404:PRO:HD2	2.36	0.41
1:B:178:ILE:HG21	1:B:217:PHE:HE2	1.85	0.41
1:B:257:GLY:N	1:B:258:PRO:HD2	2.36	0.41
1:B:345:CYS:O	1:B:346:LYS:C	2.64	0.41
1:A:11:VAL:O	1:A:12:SER:C	2.62	0.41
1:B:43:VAL:C	1:B:45:ALA:N	2.79	0.41
1:B:410:MET:N	1:B:411:PRO:CD	2.84	0.41
1:A:83:ILE:CG2	1:A:84:ASP:N	2.83	0.41
1:A:183:LYS:HD2	1:A:183:LYS:HA	1.94	0.41
1:B:43:VAL:C	1:B:45:ALA:H	2.28	0.41
1:B:409:ALA:C	1:B:411:PRO:HD2	2.46	0.41
1:B:426:ASP:O	1:B:427:THR:C	2.62	0.41
1:A:88:ARG:O	1:A:92:LYS:HE3	2.21	0.41
1:A:263:ILE:HD11	2:C:48:PHE:CZ	2.56	0.41
1:B:88:ARG:O	1:B:92:LYS:HE3	2.21	0.41
1:B:98:THR:C	1:B:101:THR:HG23	2.45	0.41
1:B:192:LEU:HG	1:B:196:ASN:ND2	2.36	0.41
1:B:277:LEU:CD2	1:B:342:TRP:NE1	2.84	0.41
1:A:134:VAL:HG13	1:A:176:ALA:HB2	2.02	0.40
1:B:4:ILE:HD12	1:B:43:VAL:HG13	2.03	0.40
1:B:107:SER:HB3	1:B:152:GLU:OE1	2.21	0.40
1:B:151:LEU:HD23	1:B:151:LEU:HA	1.94	0.40
1:B:329:THR:C	1:B:331:THR:H	2.28	0.40
1:B:436:CYS:O	1:B:437:GLU:C	2.64	0.40
1:B:352:LEU:HD23	1:B:352:LEU:HA	1.94	0.40
1:B:394:LEU:CD1	1:B:435:ILE:HG12	2.51	0.40
1:A:84:ASP:OD2	1:A:86:ASN:N	2.55	0.40
1:A:406:VAL:HG13	1:A:435:ILE:HD13	2.03	0.40
1:A:42:ARG:HG2	1:A:94:TYR:CE2	2.57	0.40
1:A:14:ASP:HB3	1:A:17:GLU:HG2	2.04	0.40
1:B:14:ASP:OD1	1:B:16:LEU:N	2.53	0.40
1:B:368:LEU:N	1:B:369:PRO:HD2	2.36	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	438/442 (99%)	381 (87%)	49 (11%)	8 (2%)	6	23
1	B	438/442 (99%)	370 (84%)	58 (13%)	10 (2%)	5	18
2	C	12/28 (43%)	7 (58%)	0	5 (42%)	0	0
2	D	10/28 (36%)	4 (40%)	4 (40%)	2 (20%)	0	0
All	All	898/940 (96%)	762 (85%)	111 (12%)	25 (3%)	4	14

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	339	ASP
1	A	360	GLU
1	A	361	ASP
1	B	360	GLU
1	B	361	ASP
2	C	45	ALA
1	A	186	PRO
1	A	411	PRO
1	B	31	GLU
1	B	186	PRO
1	B	216	HIS
2	C	12	PRO
1	A	31	GLU
1	B	213	SER
1	B	411	PRO
2	C	13	ALA
2	D	12	PRO
1	A	259	ALA
1	B	32	ASN
1	B	259	ALA
2	C	11	LYS
1	A	437	GLU

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Mol	Chain	Res	Type
1	B	342	TRP
2	D	17	GLY
2	C	17	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	381/382 (100%)	355 (93%)	26 (7%)	14	42
1	B	381/382 (100%)	353 (93%)	28 (7%)	13	38
2	C	11/11 (100%)	11 (100%)	0	100	100
2	D	8/11 (73%)	8 (100%)	0	100	100
All	All	781/786 (99%)	727 (93%)	54 (7%)	14	41

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	LEU
1	A	22	GLN
1	A	32	ASN
1	A	41	SER
1	A	51	GLN
1	A	101	THR
1	A	103	THR
1	A	108	SER
1	A	118	CYS
1	A	139	ASN
1	A	143	THR
1	A	161	ILE
1	A	174	LEU
1	A	266	GLU
1	A	270	SER
1	A	331	THR
1	A	333	GLN
1	A	335	GLU

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Mol	Chain	Res	Type
1	A	341	ASP
1	A	361	ASP
1	A	362	ASP
1	A	368	LEU
1	A	408	GLN
1	A	418	LYS
1	A	432	VAL
1	A	439	LEU
1	B	3	LEU
1	B	15	ARG
1	B	22	GLN
1	B	32	ASN
1	B	33	LEU
1	B	51	GLN
1	B	101	THR
1	B	103	THR
1	B	108	SER
1	B	118	CYS
1	B	139	ASN
1	B	143	THR
1	B	161	ILE
1	B	174	LEU
1	B	212	GLU
1	B	266	GLU
1	B	270	SER
1	B	331	THR
1	B	333	GLN
1	B	334	ASP
1	B	335	GLU
1	B	337	ASP
1	B	361	ASP
1	B	362	ASP
1	B	368	LEU
1	B	408	GLN
1	B	418	LYS
1	B	436	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (33) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	49	ASN

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Mol	Chain	Res	Type
1	A	51	GLN
1	A	125	GLN
1	A	139	ASN
1	A	141	ASN
1	A	165	GLN
1	A	171	ASN
1	A	179	GLN
1	A	189	ASN
1	A	196	ASN
1	A	208	ASN
1	A	240	ASN
1	A	309	HIS
1	A	333	GLN
1	A	377	ASN
1	A	401	GLN
1	B	32	ASN
1	B	51	GLN
1	B	125	GLN
1	B	139	ASN
1	B	141	ASN
1	B	165	GLN
1	B	171	ASN
1	B	179	GLN
1	B	189	ASN
1	B	220	GLN
1	B	250	GLN
1	B	309	HIS
1	B	328	GLN
1	B	336	ASN
1	B	377	ASN
1	B	401	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 ⓘ

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.