



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 04:26 AM UTC

PDB ID : 1O6P / pdb_00001o6p
Title : Importin Beta bound to a GLFG Nucleoporin peptide
Authors : Bayliss, R.; Stewart, M.
Deposited on : 2002-10-10
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

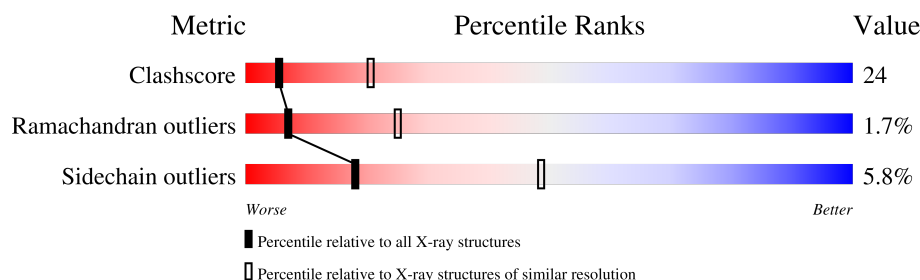
1 Overall quality at a glance

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	
1	B	442	
2	C	9	
2	D	9	
2	E	9	
2	F	9	

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 7022 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 SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	441	Total	C	N	O	S	0	0	1
			3441	2169	577	670	25			
1	B	441	Total	C	N	O	S	0	0	1
			3441	2169	577	670	25			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	97	HIS	GLN	conflict	UNP Q14974
B	97	HIS	GLN	conflict	UNP Q14974

- Molecule 2 is a protein called SYNTHETIC GLFG PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	C	5	Total	C	N	O	0	0	1
			28	19	5	4			
2	D	5	Total	C	N	O	0	0	1
			28	19	5	4			
2	E	4	Total	C	N	O	0	0	1
			24	17	4	3			
2	F	4	Total	C	N	O	0	0	1
			24	17	4	3			

- Molecule 3 is water.

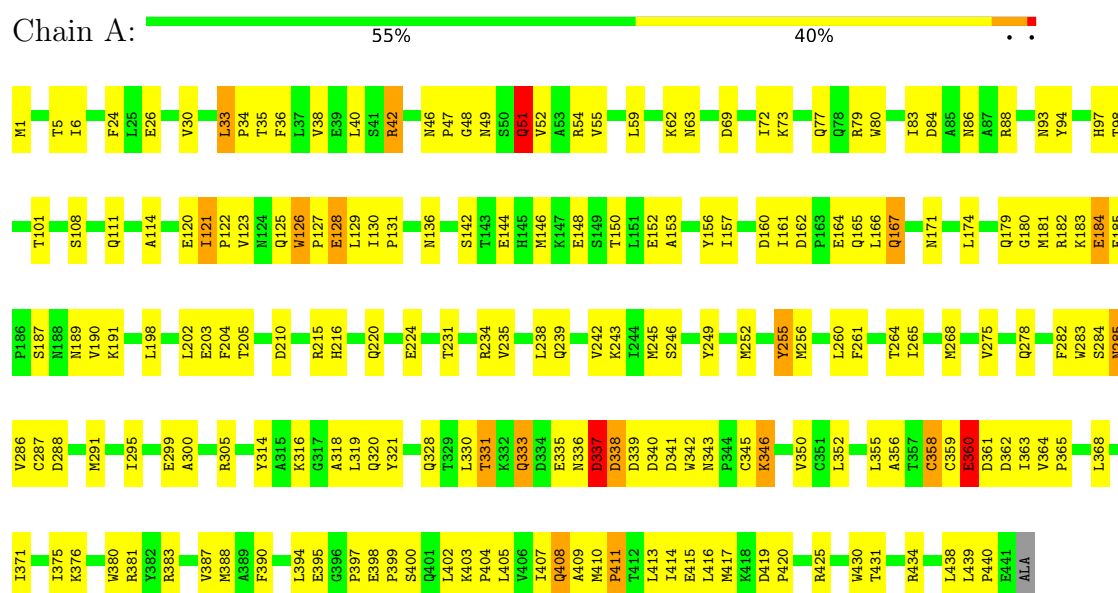
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	20	Total	O	0	0
			20	20		
3	B	16	Total	O	0	0
			16	16		

3 Residue-property plots

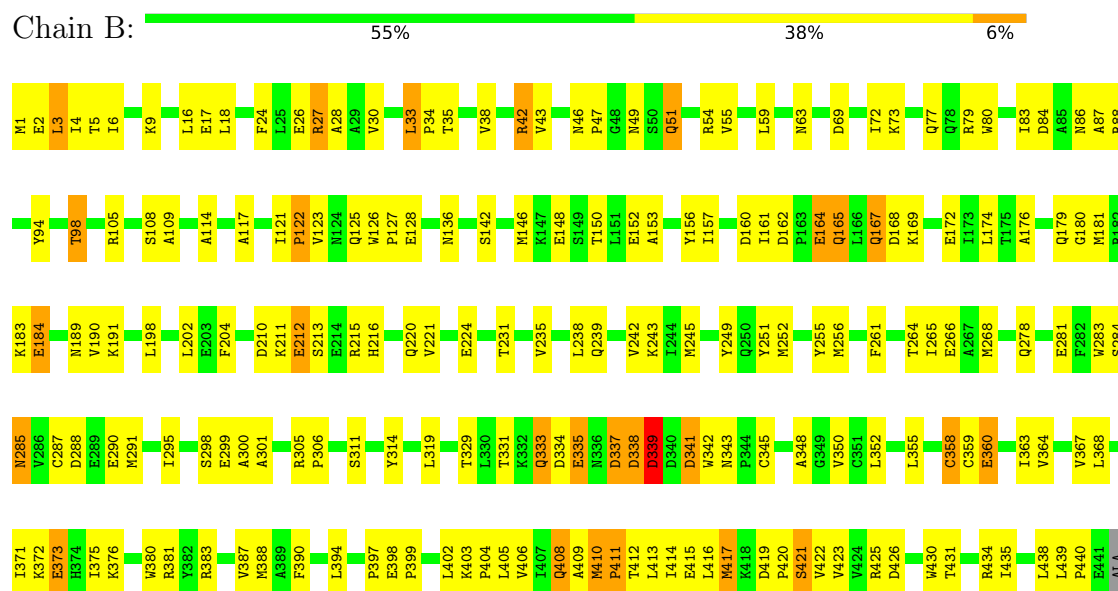
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

Note EDS was not executed.

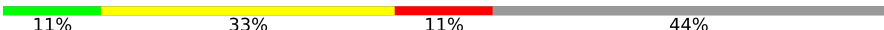
• Molecule 1: IMPORTIN BETA-1 SUBUNIT

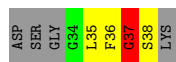


• Molecule 1: IMPORTIN BETA-1 SUBUNIT

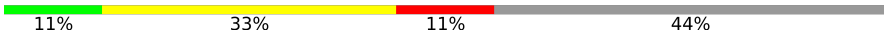


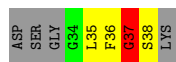
- Molecule 2: SYNTHETIC GLFG PEPTIDE

Chain C:  11% 33% 11% 44%



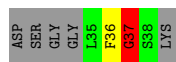
- Molecule 2: SYNTHETIC GLFG PEPTIDE

Chain D:  11% 33% 11% 44%



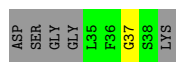
- Molecule 2: SYNTHETIC GLFG PEPTIDE

Chain E:  22% 11% 11% 56%



- Molecule 2: SYNTHETIC GLFG PEPTIDE

Chain F:  33% 11% 56%



4 Data and refinement statistics

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

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	125.82Å 67.03Å 129.26Å 90.00° 98.99° 90.00°	Depositor
Resolution (Å)	20.00 – 2.80	Depositor
% Data completeness (in resolution range)	91.8 (20.00-2.80)	Depositor
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.238 , 0.267	Depositor
Estimated twinning fraction	No twinning to report.	Xtrriage
Total number of atoms	7022	wwPDB-VP
Average B, all atoms (Å ²)	56.0	wwPDB-VP

5 Model quality [i](#)

5.1 Standard geometry [i](#)

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.67	1/3505 (0.0%)	1.07	14/4771 (0.3%)
1	B	0.68	2/3505 (0.1%)	1.13	18/4771 (0.4%)
2	C	1.23	1/28 (3.6%)	0.65	0/36
2	D	1.18	1/28 (3.6%)	0.60	0/36
2	E	1.31	1/24 (4.2%)	0.59	0/31
2	F	1.30	1/24 (4.2%)	0.76	0/31
All	All	0.68	7/7114 (0.1%)	1.10	32/9676 (0.3%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	440	PRO	C-N	-5.30	1.25	1.33
2	C	37	GLY	C-N	-5.27	1.25	1.33
2	D	37	GLY	C-N	-5.27	1.25	1.33
2	F	37	GLY	C-N	-5.27	1.25	1.33
2	E	37	GLY	C-N	-5.26	1.25	1.33
1	B	417	MET	SD-CE	5.24	1.92	1.79
1	B	440	PRO	C-N	-5.06	1.26	1.33

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	337	ASP	N-CA-C	16.07	124.18	108.75
1	A	337	ASP	N-CA-C	14.08	130.22	109.95
1	B	284	SER	N-CA-C	-9.47	102.23	113.88
1	B	339	ASP	N-CA-C	-9.44	101.89	113.97
1	B	337	ASP	CA-C-O	9.08	124.05	118.33
1	B	421	SER	N-CA-C	8.98	124.36	109.46
1	B	98	THR	N-CA-C	-8.39	101.38	111.69
1	B	16	LEU	N-CA-C	-8.15	99.09	111.56
1	A	339	ASP	N-CA-C	-7.82	103.84	113.15
1	A	126	TRP	CA-C-N	7.26	126.97	119.56
1	A	126	TRP	C-N-CA	7.26	126.97	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	105	ARG	N-CA-C	-7.20	101.03	110.39
1	A	284	SER	N-CA-C	-7.15	102.90	111.69
1	A	190	VAL	N-CA-C	-6.92	104.03	110.53
1	A	336	ASN	N-CA-C	6.84	122.17	113.55
1	B	160	ASP	N-CA-C	6.70	121.62	113.38
1	A	51	GLN	N-CA-C	-6.50	104.19	111.28
1	A	160	ASP	N-CA-C	6.46	121.33	113.38
1	B	87	ALA	N-CA-C	-6.22	104.42	111.14
1	B	51	GLN	N-CA-C	-5.99	104.87	111.82
1	B	341	ASP	N-CA-C	5.90	118.60	110.35
1	A	121	ILE	CB-CA-C	-5.84	108.16	114.35
1	B	190	VAL	N-CA-C	-5.82	105.06	110.53
1	B	33	LEU	N-CA-C	5.80	120.79	113.25
1	B	43	VAL	N-CA-C	-5.80	104.67	110.30
1	A	33	LEU	N-CA-C	5.72	120.69	113.25
1	B	335	GLU	N-CA-C	5.58	117.81	111.11
1	B	252	MET	N-CA-C	5.26	119.56	113.20
1	A	187	SER	N-CA-C	5.13	117.92	109.76
1	A	185	GLU	CA-C-N	5.09	124.27	118.97
1	A	185	GLU	C-N-CA	5.09	124.27	118.97
1	B	165	GLN	N-CA-C	5.08	118.97	112.26

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	3441	0	3431	167	0
1	B	3441	0	3431	160	0
2	C	28	0	25	3	0
2	D	28	0	25	3	0
2	E	24	0	22	2	0
2	F	24	0	22	0	0
3	A	20	0	0	1	0
3	B	16	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7022	0	6956	331	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 24.

All (331) 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:335:GLU:HG3	1:A:381:ARG:HH22	1.21	1.03
1:B:338:ASP:OD2	1:B:341:ASP:HB3	1.58	1.02
1:B:337:ASP:CG	1:B:338:ASP:H	1.61	0.98
1:A:338:ASP:CG	1:A:341:ASP:HB2	1.89	0.96
1:B:338:ASP:HB2	1:B:341:ASP:HB2	1.51	0.92
1:A:335:GLU:HG2	1:A:380:TRP:HZ2	1.34	0.89
1:A:181:MET:HE1	1:A:198:LEU:HD22	1.55	0.89
1:B:338:ASP:HB2	1:B:341:ASP:CB	2.04	0.88
1:B:409:ALA:C	1:B:411:PRO:HD2	1.99	0.88
1:B:337:ASP:CG	1:B:338:ASP:N	2.33	0.87
1:A:215:ARG:HD2	1:A:255:TYR:OH	1.81	0.81
1:B:337:ASP:OD1	1:B:338:ASP:N	2.12	0.81
1:B:181:MET:HE1	1:B:198:LEU:HD22	1.64	0.80
1:B:411:PRO:HG2	1:B:412:THR:H	1.46	0.79
1:B:335:GLU:HG3	1:B:381:ARG:NH2	1.99	0.77
1:A:136:ASN:HB3	1:A:146:MET:HE2	1.66	0.77
1:A:335:GLU:HG2	1:A:380:TRP:CZ2	2.18	0.76
1:A:330:LEU:HD22	1:A:388:MET:HE3	1.68	0.75
1:A:335:GLU:HG3	1:A:381:ARG:NH2	2.00	0.75
1:B:422:VAL:HG12	1:B:426:ASP:OD2	1.87	0.75
1:A:402:LEU:C	1:A:404:PRO:HD2	2.12	0.74
1:B:136:ASN:HB3	1:B:146:MET:HE2	1.71	0.73
1:A:410:MET:HE1	1:A:414:ILE:HD11	1.71	0.72
1:B:212:GLU:HB2	1:B:215:ARG:HH12	1.54	0.72
1:B:410:MET:O	1:B:414:ILE:HG12	1.91	0.71
1:B:338:ASP:CG	1:B:341:ASP:HB3	2.15	0.71
1:B:265:ILE:HA	1:B:268:MET:HE3	1.71	0.71
1:A:265:ILE:HA	1:A:268:MET:HE3	1.73	0.70
1:A:335:GLU:CG	1:A:381:ARG:HH22	2.03	0.70
1:B:368:LEU:HD21	1:B:405:LEU:HD11	1.73	0.69
1:B:335:GLU:CG	1:B:381:ARG:NH2	2.56	0.69
1:A:157:ILE:O	1:A:161:ILE:HG22	1.93	0.68
1:A:404:PRO:HA	1:A:407:ILE:HG12	1.76	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:216:HIS:ND1	1:B:255:TYR:OH	2.26	0.67
1:B:123:VAL:HG12	1:B:123:VAL:O	1.95	0.67
1:B:338:ASP:CB	1:B:341:ASP:CB	2.72	0.67
1:B:136:ASN:CG	1:B:146:MET:HE2	2.19	0.67
1:A:368:LEU:HD21	1:A:405:LEU:HD11	1.77	0.67
1:B:383:ARG:O	1:B:387:VAL:HG23	1.94	0.67
1:A:136:ASN:CG	1:A:146:MET:HE2	2.20	0.66
1:B:245:MET:HE2	1:B:249:TYR:CD2	2.29	0.66
1:A:130:ILE:HB	1:A:131:PRO:HD3	1.77	0.66
1:A:136:ASN:CB	1:A:146:MET:HE2	2.26	0.66
1:A:69:ASP:OD2	1:A:72:ILE:HG12	1.96	0.66
1:B:335:GLU:HG3	1:B:381:ARG:HH22	1.60	0.66
1:B:338:ASP:CB	1:B:341:ASP:HB2	2.24	0.66
1:B:266:GLU:OE1	1:B:266:GLU:HA	1.94	0.66
1:A:409:ALA:C	1:A:411:PRO:HD2	2.21	0.65
1:B:167:GLN:HG3	1:B:204:PHE:HB2	1.79	0.64
1:A:47:PRO:HA	1:A:54:ARG:NH1	2.12	0.64
1:B:406:VAL:O	1:B:410:MET:HE3	1.98	0.64
1:B:333:GLN:C	1:B:381:ARG:HH12	2.06	0.64
1:B:403:LYS:HG2	1:B:439:LEU:HD22	1.80	0.64
1:B:69:ASP:OD2	1:B:72:ILE:HG12	1.97	0.64
1:B:27:ARG:HD2	1:B:28:ALA:N	2.11	0.64
1:A:410:MET:O	1:A:414:ILE:HG12	1.98	0.63
1:A:238:LEU:O	1:A:242:VAL:HG23	1.98	0.63
1:A:93:ASN:OD1	1:A:97:HIS:CD2	2.52	0.63
1:B:334:ASP:OD2	1:B:338:ASP:OD1	2.16	0.63
1:A:246:SER:HB3	1:A:285:ASN:OD1	1.99	0.62
1:B:136:ASN:CB	1:B:146:MET:HE2	2.29	0.62
2:C:36:PHE:O	2:C:37:GLY:C	2.43	0.62
1:B:202:LEU:HD12	1:B:243:LYS:HD3	1.81	0.61
1:B:373:GLU:HG2	1:B:373:GLU:O	2.00	0.61
1:B:388:MET:CE	1:B:430:TRP:CZ3	2.83	0.61
1:B:153:ALA:O	1:B:157:ILE:HG13	2.00	0.61
2:D:36:PHE:O	2:D:37:GLY:C	2.44	0.61
1:A:342:TRP:HH2	1:A:350:VAL:HG21	1.66	0.60
1:A:93:ASN:O	1:A:97:HIS:CD2	2.54	0.60
1:A:88:ARG:HH12	1:A:125:GLN:HG2	1.67	0.60
1:B:435:ILE:O	1:B:438:LEU:N	2.35	0.60
1:A:174:LEU:HD13	1:A:205:THR:HG21	1.83	0.60
1:B:419:ASP:CG	1:B:420:PRO:HD2	2.27	0.59
1:A:93:ASN:CG	1:A:97:HIS:NE2	2.60	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:338:ASP:CB	1:B:341:ASP:HB3	2.32	0.59
1:B:46:ASN:HB3	1:B:49:ASN:ND2	2.17	0.59
1:B:264:THR:OG1	1:B:283:TRP:NE1	2.30	0.59
1:A:245:MET:HE2	1:A:249:TYR:CD2	2.37	0.59
1:B:18:LEU:C	1:B:18:LEU:HD23	2.27	0.58
1:B:238:LEU:O	1:B:242:VAL:HG23	2.03	0.58
1:A:123:VAL:HG12	1:A:123:VAL:O	2.02	0.58
1:A:128:GLU:O	1:A:131:PRO:HD2	2.03	0.58
1:A:338:ASP:C	1:A:340:ASP:H	2.10	0.58
1:A:184:GLU:N	1:A:184:GLU:OE1	2.36	0.58
1:A:403:LYS:HG3	1:A:439:LEU:HD13	1.86	0.58
1:A:360:GLU:O	1:A:397:PRO:HG3	2.04	0.58
1:B:388:MET:HE3	1:B:430:TRP:HZ3	1.69	0.58
1:A:287:CYS:O	1:A:291:MET:HG3	2.04	0.57
1:B:421:SER:O	1:B:425:ARG:N	2.24	0.57
1:B:342:TRP:HH2	1:B:350:VAL:HG21	1.67	0.57
1:A:93:ASN:ND2	1:A:97:HIS:NE2	2.53	0.57
1:B:338:ASP:HB2	1:B:341:ASP:HB3	1.85	0.57
1:A:383:ARG:O	1:A:387:VAL:HG23	2.05	0.57
1:A:265:ILE:HD13	1:A:268:MET:CE	2.34	0.57
1:A:59:LEU:CD1	1:A:62:LYS:HE3	2.34	0.56
1:A:216:HIS:HD2	1:A:255:TYR:OH	1.88	0.56
1:B:404:PRO:O	1:B:408:GLN:HG2	2.05	0.56
1:A:410:MET:N	1:A:411:PRO:HD2	2.21	0.56
1:A:343:ASN:ND2	1:A:345:CYS:HB3	2.20	0.56
1:A:404:PRO:O	1:A:407:ILE:HB	2.05	0.56
1:B:265:ILE:HD13	1:B:268:MET:CE	2.36	0.56
1:A:234:ARG:NH1	3:A:2017:HOH:O	2.39	0.56
1:A:333:GLN:HE22	1:A:388:MET:HE1	1.71	0.56
1:B:183:LYS:HD2	1:B:224:GLU:HB3	1.86	0.56
1:A:46:ASN:HB3	1:A:49:ASN:ND2	2.21	0.55
1:A:153:ALA:O	1:A:157:ILE:HG13	2.07	0.55
1:A:333:GLN:NE2	1:A:388:MET:HE1	2.22	0.55
1:A:387:VAL:CG2	1:A:416:LEU:HD13	2.36	0.55
1:B:42:ARG:HD3	1:B:94:TYR:CZ	2.43	0.54
1:B:169:LYS:HA	1:B:172:GLU:OE1	2.08	0.54
1:B:419:ASP:OD1	1:B:420:PRO:HD2	2.07	0.54
1:A:335:GLU:OE2	1:A:381:ARG:NH1	2.40	0.54
2:C:36:PHE:O	2:C:38:SER:N	2.41	0.54
1:B:295:ILE:HG22	1:B:299:GLU:OE2	2.08	0.53
1:B:88:ARG:HH12	1:B:125:GLN:HG2	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:414:ILE:CD1	1:A:417:MET:HE2	2.39	0.53
1:B:220:GLN:O	1:B:224:GLU:HG3	2.08	0.53
1:A:126:TRP:HD1	1:A:128:GLU:HG3	1.73	0.53
1:B:388:MET:HE3	1:B:430:TRP:CZ3	2.42	0.53
1:A:295:ILE:HG22	1:A:299:GLU:OE2	2.08	0.53
1:B:245:MET:HE2	1:B:249:TYR:HD2	1.74	0.53
1:B:339:ASP:OD1	1:B:339:ASP:C	2.52	0.53
1:B:388:MET:HE1	1:B:430:TRP:CZ3	2.42	0.53
1:A:26:GLU:O	1:A:30:VAL:HG23	2.09	0.53
1:B:430:TRP:CZ2	1:B:434:ARG:HD2	2.45	0.52
1:B:98:THR:HG21	1:B:109:ALA:HB2	1.91	0.52
1:B:380:TRP:HZ3	1:B:423:VAL:HG11	1.74	0.52
1:A:202:LEU:HD12	1:A:243:LYS:HD3	1.91	0.52
1:A:1:MET:HA	1:A:5:THR:HG21	1.92	0.52
1:A:51:GLN:HG3	1:A:52:VAL:N	2.25	0.52
1:B:430:TRP:CE2	1:B:434:ARG:HD2	2.44	0.52
1:B:184:GLU:N	1:B:184:GLU:OE1	2.43	0.52
2:D:36:PHE:O	2:D:38:SER:N	2.43	0.52
1:A:93:ASN:OD1	1:A:97:HIS:NE2	2.43	0.52
1:A:383:ARG:HH11	1:A:419:ASP:CG	2.18	0.52
1:B:265:ILE:HD13	1:B:268:MET:HE1	1.91	0.52
1:B:410:MET:N	1:B:411:PRO:HD2	2.23	0.52
1:A:203:GLU:OE2	1:A:243:LYS:HE2	2.10	0.52
1:B:80:TRP:O	1:B:88:ARG:HD3	2.10	0.52
1:B:122:PRO:HA	1:B:165:GLN:NE2	2.24	0.52
1:B:290:GLU:HG2	1:B:311:SER:OG	2.10	0.52
1:B:406:VAL:HG12	1:B:410:MET:CE	2.40	0.52
1:A:183:LYS:HD2	1:A:224:GLU:HB3	1.92	0.51
1:A:265:ILE:HA	1:A:268:MET:CE	2.40	0.51
1:A:265:ILE:HD13	1:A:268:MET:HE1	1.91	0.51
1:B:84:ASP:OD2	1:B:86:ASN:HB2	2.11	0.51
1:A:343:ASN:HD21	1:A:345:CYS:HB3	1.75	0.51
1:B:235:VAL:O	1:B:239:GLN:HG3	2.10	0.51
1:A:73:LYS:O	1:A:77:GLN:HG3	2.10	0.51
1:A:403:LYS:O	1:A:407:ILE:HG12	2.09	0.51
1:A:59:LEU:HD12	1:A:62:LYS:HE3	1.93	0.51
1:B:343:ASN:ND2	1:B:345:CYS:HB3	2.26	0.51
1:B:335:GLU:HG2	1:B:380:TRP:HZ2	1.76	0.51
1:A:36:PHE:CZ	1:A:40:LEU:HD11	2.46	0.51
1:B:179:GLN:NE2	1:B:179:GLN:HA	2.26	0.51
1:A:338:ASP:OD2	1:A:341:ASP:HB2	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ILE:N	1:A:122:PRO:HD2	2.26	0.51
1:B:157:ILE:O	1:B:161:ILE:HG22	2.11	0.50
1:A:235:VAL:O	1:A:239:GLN:HG3	2.10	0.50
1:A:430:TRP:CE2	1:A:434:ARG:HD2	2.46	0.50
1:A:182:ARG:NE	1:A:184:GLU:OE2	2.44	0.50
1:B:411:PRO:HG2	1:B:412:THR:N	2.23	0.50
1:A:333:GLN:HE22	1:A:388:MET:CE	2.24	0.50
1:A:403:LYS:N	1:A:404:PRO:HD2	2.25	0.50
1:A:59:LEU:HG	1:A:63:ASN:HD21	1.77	0.50
1:A:42:ARG:HD3	1:A:94:TYR:CZ	2.46	0.50
1:B:51:GLN:O	1:B:55:VAL:HG23	2.11	0.50
1:A:59:LEU:O	1:A:63:ASN:ND2	2.44	0.50
1:B:117:ALA:HB1	1:B:121:ILE:HD12	1.94	0.50
1:A:398:GLU:HG2	1:A:400:SER:OG	2.12	0.50
1:A:256:MET:HG2	1:A:314:TYR:CD1	2.48	0.49
1:A:33:LEU:HB3	1:A:34:PRO:HD3	1.93	0.49
1:A:80:TRP:O	1:A:88:ARG:HD3	2.12	0.49
1:B:47:PRO:HA	1:B:54:ARG:NH1	2.26	0.49
1:A:430:TRP:CZ2	1:A:434:ARG:HD2	2.47	0.49
1:A:171:ASN:HD22	2:E:36:PHE:C	2.20	0.49
1:A:179:GLN:HA	1:A:179:GLN:NE2	2.26	0.49
1:A:239:GLN:HG2	1:A:278:GLN:NE2	2.28	0.49
1:B:406:VAL:HG12	1:B:410:MET:HE1	1.94	0.49
1:A:316:LYS:HA	1:A:359:CYS:SG	2.53	0.49
1:B:383:ARG:HH11	1:B:419:ASP:CG	2.21	0.49
1:A:390:PHE:O	1:A:394:LEU:HG	2.13	0.49
1:A:399:PRO:HA	1:A:439:LEU:HD21	1.95	0.49
1:B:73:LYS:O	1:B:77:GLN:HG3	2.13	0.48
1:A:148:GLU:OE2	1:A:189:ASN:HB3	2.13	0.48
1:A:404:PRO:HA	1:A:407:ILE:CG1	2.43	0.48
1:B:26:GLU:O	1:B:30:VAL:HG23	2.13	0.48
1:B:417:MET:O	1:B:425:ARG:HG2	2.13	0.48
1:B:383:ARG:NH1	1:B:419:ASP:OD1	2.46	0.48
1:B:287:CYS:O	1:B:291:MET:HG3	2.13	0.48
1:A:33:LEU:HD23	1:A:83:ILE:HD11	1.95	0.48
1:B:148:GLU:OE2	1:B:189:ASN:HB3	2.13	0.48
1:A:300:ALA:HB1	1:A:305:ARG:O	2.14	0.48
1:A:337:ASP:HB3	1:A:338:ASP:OD1	2.13	0.48
1:B:122:PRO:CB	1:B:165:GLN:HE22	2.27	0.48
1:B:265:ILE:HA	1:B:268:MET:CE	2.41	0.48
1:A:404:PRO:CA	1:A:407:ILE:HG12	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:121:ILE:N	1:B:122:PRO:HD2	2.29	0.48
1:A:338:ASP:OD1	1:A:341:ASP:HB2	2.12	0.48
1:A:387:VAL:HG21	1:A:416:LEU:HD13	1.96	0.47
1:A:408:GLN:H	1:A:408:GLN:HG2	1.42	0.47
1:A:364:VAL:HB	1:A:365:PRO:CD	2.45	0.47
1:A:126:TRP:CD1	1:A:128:GLU:HG3	2.49	0.47
1:B:114:ALA:CB	1:B:156:TYR:HB3	2.44	0.47
1:A:383:ARG:NH1	1:A:419:ASP:OD1	2.48	0.47
1:B:413:LEU:HD11	1:B:431:THR:HG21	1.95	0.47
1:B:121:ILE:C	1:B:123:VAL:H	2.22	0.47
1:B:211:LYS:HE2	1:B:213:SER:HB3	1.96	0.47
1:B:403:LYS:N	1:B:404:PRO:HD2	2.29	0.46
1:A:414:ILE:HD12	1:A:417:MET:HE2	1.98	0.46
1:A:231:THR:O	1:A:235:VAL:HG23	2.15	0.46
1:A:220:GLN:O	1:A:224:GLU:HG3	2.16	0.46
1:B:1:MET:HA	1:B:5:THR:HG21	1.98	0.46
1:B:162:ASP:C	1:B:164:GLU:N	2.72	0.46
1:A:171:ASN:ND2	2:E:37:GLY:HA2	2.31	0.46
1:B:33:LEU:HD22	1:B:79:ARG:HD2	1.97	0.46
1:B:363:ILE:HG23	1:B:364:VAL:N	2.31	0.46
1:B:402:LEU:O	1:B:406:VAL:HG23	2.16	0.46
1:A:121:ILE:C	1:A:123:VAL:H	2.24	0.46
1:A:371:ILE:HD13	1:A:390:PHE:HB2	1.96	0.46
1:B:300:ALA:HB1	1:B:305:ARG:O	2.16	0.46
1:B:343:ASN:HD21	1:B:345:CYS:HB3	1.79	0.46
1:B:390:PHE:O	1:B:394:LEU:HG	2.16	0.46
1:A:333:GLN:O	1:A:381:ARG:NH2	2.45	0.45
1:A:361:ASP:C	1:A:363:ILE:H	2.25	0.45
1:B:422:VAL:HA	1:B:425:ARG:HB2	1.98	0.45
1:A:84:ASP:OD2	1:A:86:ASN:HB2	2.16	0.45
1:B:6:ILE:HG21	1:B:24:PHE:CD2	2.51	0.45
1:A:362:ASP:N	1:A:362:ASP:OD1	2.49	0.45
1:B:358:CYS:C	1:B:360:GLU:H	2.24	0.45
1:B:387:VAL:CG2	1:B:416:LEU:HD13	2.46	0.45
1:A:395:GLU:HB2	1:A:434:ARG:HH22	1.82	0.45
1:A:34:PRO:O	1:A:38:VAL:HG23	2.16	0.45
1:B:422:VAL:O	1:B:426:ASP:N	2.35	0.45
1:B:285:ASN:HD22	1:B:285:ASN:HA	1.54	0.44
1:B:414:ILE:HD13	1:B:417:MET:HE2	1.99	0.44
1:B:117:ALA:HB1	1:B:121:ILE:CD1	2.47	0.44
1:B:329:THR:HG21	1:B:348:ALA:HB2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:179:GLN:HA	1:A:179:GLN:HE21	1.82	0.44
1:A:114:ALA:CB	1:A:156:TYR:HB3	2.48	0.44
1:B:355:LEU:HD23	1:B:355:LEU:HA	1.87	0.44
1:B:419:ASP:CG	1:B:420:PRO:CD	2.90	0.44
1:A:144:GLU:CD	1:A:144:GLU:H	2.25	0.44
1:A:261:PHE:HZ	1:A:321:TYR:CD1	2.36	0.44
1:A:167:GLN:HG3	1:A:204:PHE:HB2	2.00	0.44
1:A:338:ASP:C	1:A:340:ASP:N	2.72	0.44
1:B:79:ARG:O	1:B:83:ILE:HG13	2.18	0.44
1:B:411:PRO:CG	1:B:412:THR:H	2.22	0.43
1:A:282:PHE:O	1:A:286:VAL:HG23	2.18	0.43
1:B:35:THR:HG23	2:C:35:LEU:HD21	2.00	0.43
1:A:46:ASN:C	1:A:48:GLY:H	2.26	0.43
1:A:234:ARG:NH2	1:A:275:VAL:HG11	2.33	0.43
1:A:413:LEU:HD11	1:A:431:THR:HG21	2.01	0.43
1:A:33:LEU:HD22	1:A:79:ARG:HD2	2.01	0.43
1:A:256:MET:HE1	1:A:283:TRP:CZ2	2.53	0.43
1:B:319:LEU:HD13	1:B:359:CYS:SG	2.59	0.43
1:B:333:GLN:CB	1:B:381:ARG:NH1	2.81	0.43
1:A:260:LEU:O	1:A:261:PHE:C	2.62	0.43
1:A:358:CYS:C	1:A:360:GLU:H	2.25	0.43
1:B:176:ALA:O	1:B:179:GLN:HB3	2.18	0.43
1:B:412:THR:O	1:B:416:LEU:HG	2.18	0.43
1:B:179:GLN:HA	1:B:179:GLN:HE21	1.82	0.43
1:B:256:MET:HG2	1:B:314:TYR:CD1	2.53	0.43
1:B:414:ILE:CD1	1:B:417:MET:HE2	2.48	0.43
1:A:342:TRP:CZ3	1:A:346:LYS:HB3	2.54	0.43
1:A:375:ILE:HG23	1:A:376:LYS:HG3	2.01	0.43
1:B:181:MET:HB3	1:B:221:VAL:CG1	2.49	0.43
1:B:215:ARG:NH2	1:B:251:TYR:CD1	2.87	0.43
1:A:380:TRP:CZ2	1:A:381:ARG:NH1	2.87	0.42
1:B:409:ALA:C	1:B:411:PRO:CD	2.84	0.42
1:B:261:PHE:O	1:B:265:ILE:HG12	2.18	0.42
1:A:162:ASP:C	1:A:164:GLU:N	2.76	0.42
1:A:387:VAL:HG22	1:A:416:LEU:HD13	2.00	0.42
1:B:373:GLU:O	1:B:373:GLU:CG	2.67	0.42
1:B:414:ILE:O	1:B:415:GLU:C	2.62	0.42
1:A:245:MET:CE	1:A:252:MET:HG3	2.50	0.42
1:A:328:GLN:O	1:A:331:THR:HB	2.20	0.42
1:B:126:TRP:N	1:B:127:PRO:CD	2.81	0.42
1:A:261:PHE:O	1:A:265:ILE:HG12	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:168:ASP:OD1	1:B:168:ASP:N	2.42	0.42
1:B:180:GLY:O	1:B:191:LYS:HA	2.19	0.42
1:A:42:ARG:HG2	1:A:94:TYR:CE2	2.54	0.42
1:B:305:ARG:HB2	1:B:306:PRO:HD2	2.00	0.42
1:A:146:MET:HE3	1:A:150:THR:OG1	2.20	0.42
1:A:419:ASP:O	1:A:425:ARG:CD	2.67	0.42
1:B:333:GLN:O	1:B:381:ARG:NH1	2.39	0.42
1:A:88:ARG:HH12	1:A:125:GLN:CG	2.32	0.42
1:A:355:LEU:HD23	1:A:355:LEU:HA	1.91	0.42
1:A:414:ILE:O	1:A:415:GLU:C	2.63	0.42
1:B:46:ASN:HB3	1:B:49:ASN:HD21	1.83	0.42
1:A:6:ILE:HG21	1:A:24:PHE:CD2	2.55	0.42
1:A:165:GLN:O	1:A:166:LEU:HG	2.19	0.42
1:A:335:GLU:CD	1:A:381:ARG:HH12	2.28	0.42
1:B:3:LEU:O	1:B:4:ILE:C	2.61	0.42
1:B:59:LEU:HG	1:B:63:ASN:HD21	1.85	0.42
1:A:356:ALA:O	1:A:360:GLU:HA	2.19	0.41
1:A:419:ASP:CG	1:A:420:PRO:HD2	2.44	0.41
1:B:9:LYS:HD3	1:B:17:GLU:CG	2.49	0.41
1:B:152:GLU:O	1:B:156:TYR:CD2	2.73	0.41
1:B:298:SER:O	1:B:301:ALA:HB3	2.19	0.41
1:A:35:THR:HG23	2:D:35:LEU:HD21	2.01	0.41
1:A:79:ARG:O	1:A:83:ILE:HG13	2.20	0.41
1:B:33:LEU:HD23	1:B:83:ILE:HD11	2.02	0.41
1:B:98:THR:CG2	1:B:109:ALA:HB2	2.49	0.41
1:B:122:PRO:HB3	1:B:165:GLN:HE22	1.85	0.41
1:A:414:ILE:HD13	1:A:417:MET:HE2	2.01	0.41
1:A:416:LEU:HA	1:A:419:ASP:HB2	2.03	0.41
1:B:34:PRO:O	1:B:38:VAL:HG23	2.21	0.41
1:B:367:VAL:HG12	1:B:371:ILE:HD11	2.02	0.41
1:B:438:LEU:O	1:B:439:LEU:C	2.60	0.41
1:A:98:THR:O	1:A:101:THR:HG23	2.21	0.41
1:A:363:ILE:HG23	1:A:364:VAL:N	2.35	0.41
1:B:256:MET:HE2	1:B:283:TRP:CH2	2.56	0.41
1:A:264:THR:HG21	1:A:282:PHE:CD2	2.55	0.41
1:A:346:LYS:O	1:A:350:VAL:HG23	2.21	0.41
1:B:359:CYS:O	1:B:360:GLU:C	2.64	0.41
1:B:360:GLU:O	1:B:397:PRO:HG3	2.19	0.41
1:A:180:GLY:O	1:A:191:LYS:HA	2.21	0.41
1:A:318:ALA:C	1:A:320:GLN:N	2.79	0.41
1:B:231:THR:O	1:B:235:VAL:HG23	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:375:ILE:HG23	1:B:376:LYS:HG3	2.03	0.41
1:B:398:GLU:HA	1:B:399:PRO:HD3	1.94	0.41
1:A:51:GLN:O	1:A:55:VAL:HG23	2.22	0.40
1:A:120:GLU:HB3	1:A:125:GLN:HB3	2.03	0.40
1:A:264:THR:HG21	1:A:282:PHE:CE2	2.56	0.40
1:A:403:LYS:HE2	1:A:439:LEU:HB3	2.03	0.40
1:B:146:MET:HE3	1:B:150:THR:OG1	2.21	0.40
1:A:398:GLU:HG3	1:A:399:PRO:HD2	2.02	0.40
1:A:398:GLU:HA	1:A:399:PRO:HD3	1.89	0.40
1:B:338:ASP:OD1	1:B:338:ASP:O	2.39	0.40
1:A:148:GLU:O	1:A:152:GLU:HG3	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	439/442 (99%)	398 (91%)	35 (8%)	6 (1%)	9	30
1	B	439/442 (99%)	400 (91%)	33 (8%)	6 (1%)	9	30
2	C	3/9 (33%)	2 (67%)	0	1 (33%)	0	0
2	D	3/9 (33%)	2 (67%)	0	1 (33%)	0	0
2	E	2/9 (22%)	1 (50%)	0	1 (50%)	0	0
2	F	2/9 (22%)	2 (100%)	0	0	100	100
All	All	888/920 (96%)	805 (91%)	68 (8%)	15 (2%)	7	25

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	360	GLU

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Mol	Chain	Res	Type
1	A	438	LEU
1	B	360	GLU
2	C	37	GLY
2	D	37	GLY
1	A	129	LEU
1	A	338	ASP
1	B	338	ASP
1	B	373	GLU
1	B	411	PRO
2	E	37	GLY
1	B	372	LYS
1	A	319	LEU
1	A	411	PRO
1	B	122	PRO

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%)	360 (94%)	21 (6%)	19	51
1	B	381/382 (100%)	357 (94%)	24 (6%)	16	45
2	C	2/6 (33%)	2 (100%)	0	100	100
2	D	2/6 (33%)	2 (100%)	0	100	100
2	E	2/6 (33%)	2 (100%)	0	100	100
2	F	2/6 (33%)	2 (100%)	0	100	100
All	All	770/788 (98%)	725 (94%)	45 (6%)	18	49

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	ARG
1	A	51	GLN
1	A	108	SER
1	A	111	GLN

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Mol	Chain	Res	Type
1	A	127	PRO
1	A	128	GLU
1	A	142	SER
1	A	167	GLN
1	A	184	GLU
1	A	210	ASP
1	A	255	TYR
1	A	285	ASN
1	A	288	ASP
1	A	331	THR
1	A	333	GLN
1	A	337	ASP
1	A	346	LYS
1	A	352	LEU
1	A	358	CYS
1	A	360	GLU
1	A	408	GLN
1	B	2	GLU
1	B	3	LEU
1	B	27	ARG
1	B	42	ARG
1	B	108	SER
1	B	128	GLU
1	B	142	SER
1	B	164	GLU
1	B	167	GLN
1	B	174	LEU
1	B	184	GLU
1	B	210	ASP
1	B	212	GLU
1	B	278	GLN
1	B	281	GLU
1	B	285	ASN
1	B	288	ASP
1	B	331	THR
1	B	333	GLN
1	B	339	ASP
1	B	352	LEU
1	B	358	CYS
1	B	408	GLN
1	B	410	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	32	ASN
1	A	60	GLN
1	A	63	ASN
1	A	75	GLN
1	A	111	GLN
1	A	141	ASN
1	A	171	ASN
1	A	179	GLN
1	A	208	ASN
1	A	216	HIS
1	A	278	GLN
1	A	333	GLN
1	A	401	GLN
1	B	32	ASN
1	B	63	ASN
1	B	97	HIS
1	B	141	ASN
1	B	165	GLN
1	B	171	ASN
1	B	208	ASN
1	B	285	ASN
1	B	333	GLN
1	B	374	HIS
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 ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates

EDS was not executed - this section is therefore empty.

6.4 Ligands

EDS was not executed - this section is therefore empty.

6.5 Other polymers

EDS was not executed - this section is therefore empty.