



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:14 AM GMT

PDB ID : 2Q06
Title : Crystal structure of Influenza A Virus H5N1 Nucleoprotein
Authors : Ng, A.K.L.; Zhang, H.; Tan, K.; Wang, J.; Shaw, P.C.
Deposited on : 2007-05-21
Resolution : 3.30 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

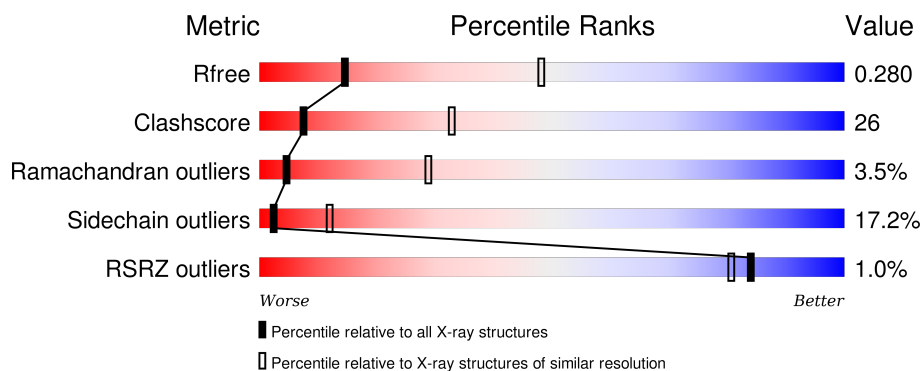
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.30 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}	91344	2060 (3.40-3.20)
Clashscore	102246	1058 (3.38-3.22)
Ramachandran outliers	100387	1038 (3.38-3.22)
Sidechain outliers	100360	1037 (3.38-3.22)
RSRZ outliers	91569	2070 (3.40-3.20)

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. 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	504	 48% 35% 9% • 7%
1	B	504	 47% 36% 9% • 8%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 7343 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 Nucleoprotein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	467	Total	C	N	O	S	0	0	0
			3678	2269	696	686	27			
1	B	465	Total	C	N	O	S	0	0	0
			3665	2260	695	683	27			

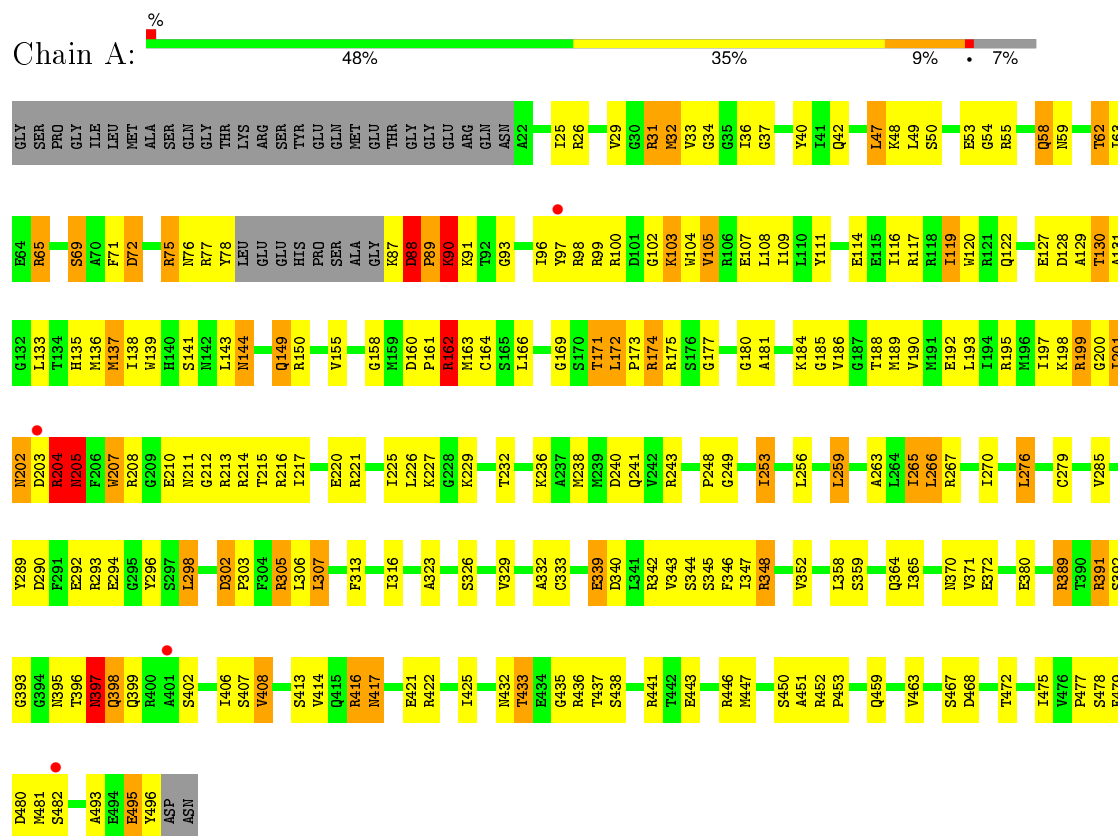
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	GLY	-	EXPRESSION TAG	UNP Q9PX50
A	-4	SER	-	EXPRESSION TAG	UNP Q9PX50
A	-3	PRO	-	EXPRESSION TAG	UNP Q9PX50
A	-2	GLY	-	EXPRESSION TAG	UNP Q9PX50
A	-1	ILE	-	EXPRESSION TAG	UNP Q9PX50
A	0	LEU	-	EXPRESSION TAG	UNP Q9PX50
B	-5	GLY	-	EXPRESSION TAG	UNP Q9PX50
B	-4	SER	-	EXPRESSION TAG	UNP Q9PX50
B	-3	PRO	-	EXPRESSION TAG	UNP Q9PX50
B	-2	GLY	-	EXPRESSION TAG	UNP Q9PX50
B	-1	ILE	-	EXPRESSION TAG	UNP Q9PX50
B	0	LEU	-	EXPRESSION TAG	UNP Q9PX50

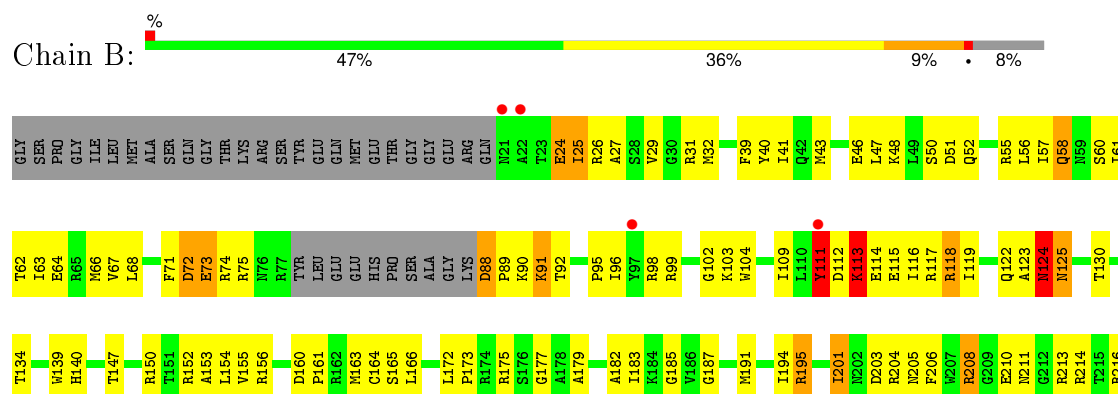
3 Residue-property plots

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: Nucleoprotein



• Molecule 1: Nucleoprotein





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 3	Depositor
Cell constants a, b, c, α , β , γ	153.58Å 153.58Å 153.58Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.32 – 3.30 46.31 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.32-3.30) 99.7 (46.31-3.30)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 3.32Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.202 , 0.279 0.203 , 0.280	Depositor DCC
R_{free} test set	945 reflections (5.42%)	DCC
Wilson B-factor (Å ²)	83.9	Xtriage
Anisotropy	0.000	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 76.0	EDS
Estimated twinning fraction	0.041 for l,-k,h	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	1 of 18379 reflections (0.005%)	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	7343	wwPDB-VP
Average B, all atoms (Å ²)	93.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.32% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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	0.45	0/3737	0.64	0/5024
1	B	0.46	0/3723	0.62	0/5003
All	All	0.45	0/7460	0.63	0/10027

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

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	31	ARG	Sidechain
1	A	479	PHE	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3678	0	3639	180	0
1	B	3665	0	3639	197	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	7343	0	7278	373	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 26.

All (373) 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:204:ARG:HA	1:A:204:ARG:HE	1.20	1.06
1:A:90:LYS:HD3	1:A:90:LYS:H	1.18	1.02
1:A:103:LYS:HD2	1:A:103:LYS:H	1.24	0.99
1:B:152:ARG:O	1:B:156:ARG:HG2	1.69	0.92
1:B:62:THR:HG22	1:B:66:MET:HE3	1.51	0.91
1:B:39:PHE:CZ	1:B:67:VAL:CG2	2.54	0.91
1:B:399:GLN:HE21	1:B:401:ALA:HB2	1.36	0.90
1:B:91:LYS:HB3	1:B:112:ASP:HA	1.54	0.90
1:B:39:PHE:CZ	1:B:67:VAL:HG21	2.08	0.89
1:B:88:ASP:HB2	1:B:89:PRO:HD3	1.54	0.89
1:A:433:THR:HG23	1:A:435:GLY:H	1.34	0.89
1:B:494:GLU:O	1:B:495:GLU:HG3	1.73	0.88
1:B:232:THR:OG1	1:B:235:GLN:HB2	1.74	0.86
1:B:124:ASN:H	1:B:124:ASN:HD22	1.19	0.85
1:B:317:ARG:HB3	1:B:318:PRO:HD2	1.57	0.84
1:A:340:ASP:OD1	1:A:342:ARG:HG3	1.76	0.84
1:B:124:ASN:N	1:B:124:ASN:HD22	1.76	0.83
1:B:314:SER:HB3	1:B:379:LEU:HD21	1.59	0.83
1:A:72:ASP:HB2	1:A:75:ARG:O	1.78	0.82
1:B:160:ASP:H	1:B:163:MET:HE2	1.45	0.80
1:A:207:TRP:HA	1:A:212:GLY:HA2	1.63	0.79
1:B:39:PHE:CE2	1:B:67:VAL:HG21	2.18	0.79
1:B:43:MET:HA	1:B:46:GLU:OE1	1.83	0.79
1:A:189:MET:O	1:A:193:LEU:HD12	1.84	0.78
1:B:90:LYS:O	1:B:113:LYS:HD2	1.84	0.77
1:A:298:LEU:HD22	1:A:298:LEU:H	1.47	0.77
1:A:213:ARG:O	1:A:217:ILE:HG12	1.86	0.76
1:A:65:ARG:O	1:A:69:SER:HB2	1.86	0.76
1:B:62:THR:HG22	1:B:66:MET:CE	2.17	0.74
1:A:221:ARG:O	1:A:225:ILE:HG12	1.89	0.73
1:B:399:GLN:NE2	1:B:401:ALA:HB2	2.04	0.72
1:B:74:ARG:O	1:B:75:ARG:NH1	2.23	0.72
1:B:346:PHE:HE2	1:B:463:VAL:HG21	1.55	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:ARG:NH1	1:B:214:ARG:HB3	2.05	0.72
1:B:55:ARG:HH11	1:B:283:LEU:HD22	1.53	0.71
1:B:150:ARG:HD2	1:B:153:ALA:H	1.53	0.71
1:A:208:ARG:HB3	1:A:208:ARG:HH11	1.52	0.71
1:B:465:GLU:OE2	1:B:466:LEU:N	2.23	0.71
1:A:163:MET:HB3	1:A:166:LEU:HD12	1.73	0.71
1:B:154:LEU:HD13	1:B:161:PRO:HA	1.72	0.70
1:A:201:ILE:HG12	1:A:249:GLY:HA2	1.73	0.70
1:B:55:ARG:NH2	1:B:311:GLN:HB3	2.06	0.70
1:A:185:GLY:HA2	1:A:270:ILE:HG21	1.73	0.70
1:A:62:THR:HG21	1:A:96:ILE:HG13	1.72	0.70
1:B:96:ILE:HD12	1:B:109:ILE:HG12	1.74	0.70
1:B:172:LEU:HD23	1:B:173:PRO:HD2	1.73	0.69
1:B:483:ASN:HB2	1:B:485:GLY:O	1.92	0.69
1:A:47:LEU:O	1:A:98:ARG:NH2	2.26	0.69
1:A:340:ASP:HB3	1:A:343:VAL:HG13	1.76	0.68
1:A:437:THR:O	1:A:441:ARG:HG3	1.94	0.68
1:A:103:LYS:H	1:A:103:LYS:CD	2.02	0.68
1:A:221:ARG:HB3	1:A:221:ARG:HH11	1.57	0.68
1:B:398:GLN:HB3	1:B:447:MET:CE	2.23	0.68
1:A:232:THR:O	1:A:236:LYS:HG3	1.94	0.68
1:B:203:ASP:CG	1:B:204:ARG:N	2.47	0.67
1:B:90:LYS:C	1:B:91:LYS:HG2	2.14	0.66
1:A:208:ARG:HB3	1:A:208:ARG:NH1	2.09	0.66
1:B:88:ASP:HB2	1:B:89:PRO:CD	2.22	0.66
1:A:204:ARG:NE	1:A:204:ARG:HA	2.01	0.66
1:B:71:PHE:CE2	1:B:117:ARG:HG3	2.31	0.66
1:A:348:ARG:NH2	1:A:380:GLU:O	2.28	0.66
1:B:203:ASP:CG	1:B:204:ARG:H	1.98	0.65
1:B:294:GLU:CD	1:B:294:GLU:H	1.99	0.65
1:A:137:MET:HG2	1:A:137:MET:O	1.95	0.65
1:B:246:ARG:HA	1:B:246:ARG:HH11	1.62	0.65
1:B:39:PHE:HZ	1:B:67:VAL:CG2	2.06	0.65
1:A:143:LEU:HA	1:A:332:ALA:HB1	1.79	0.65
1:B:245:SER:HB2	1:B:436:ARG:HH12	1.61	0.65
1:A:90:LYS:N	1:A:90:LYS:HD3	2.03	0.64
1:A:42:GLN:HE22	1:B:319:ASN:HB2	1.61	0.64
1:B:75:ARG:CZ	1:B:75:ARG:HA	2.27	0.64
1:B:495:GLU:OE1	1:B:495:GLU:C	2.35	0.64
1:B:440:MET:O	1:B:444:ILE:HG12	1.98	0.64
1:A:103:LYS:HD2	1:A:103:LYS:N	2.04	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:31:ARG:NH2	1:A:127:GLU:OE1	2.31	0.64
1:A:129:ALA:O	1:A:131:ALA:N	2.31	0.64
1:B:399:GLN:O	1:B:400:ARG:HB3	1.98	0.63
1:B:361:ARG:HG3	1:B:361:ARG:O	1.98	0.63
1:B:386:TRP:NE1	1:B:464:PHE:HB2	2.14	0.62
1:B:72:ASP:O	1:B:73:GLU:HB3	1.99	0.62
1:B:154:LEU:CD1	1:B:161:PRO:HA	2.29	0.62
1:B:91:LYS:HA	1:B:113:LYS:H	1.62	0.62
1:A:26:ARG:NH2	1:A:302:ASP:OD1	2.33	0.62
1:B:399:GLN:HG3	1:B:401:ALA:H	1.64	0.62
1:B:115:GLU:O	1:B:119:ILE:HG13	2.00	0.62
1:B:217:ILE:HG13	1:B:218:ALA:N	2.15	0.62
1:A:93:GLY:HA3	1:A:109:ILE:O	2.00	0.61
1:A:207:TRP:CZ2	1:A:248:PRO:HD2	2.35	0.61
1:B:90:LYS:O	1:B:91:LYS:HG2	2.00	0.61
1:B:88:ASP:CB	1:B:89:PRO:HD3	2.28	0.61
1:B:281:TYR:O	1:B:285:VAL:HG23	2.01	0.61
1:A:197:ILE:HG21	1:A:253:ILE:HG22	1.82	0.61
1:A:29:VAL:HG12	1:A:296:TYR:HB3	1.84	0.60
1:A:406:ILE:HG21	1:A:425:ILE:HD11	1.84	0.60
1:A:204:ARG:CA	1:A:204:ARG:HE	2.04	0.60
1:A:99:ARG:NH1	1:A:102:GLY:O	2.34	0.60
1:A:395:ASN:O	1:A:396:THR:HG23	2.01	0.60
1:B:124:ASN:N	1:B:124:ASN:ND2	2.47	0.59
1:A:155:VAL:O	1:A:158:GLY:N	2.34	0.59
1:A:370:ASN:ND2	1:A:372:GLU:HB3	2.17	0.59
1:A:175:ARG:O	1:A:175:ARG:HG3	2.02	0.59
1:B:276:LEU:N	1:B:276:LEU:HD12	2.18	0.59
1:A:290:ASP:O	1:A:294:GLU:HG2	2.02	0.59
1:B:353:ILE:HD11	1:B:358:LEU:HD12	1.84	0.59
1:B:346:PHE:CZ	1:B:477:PRO:HB3	2.38	0.58
1:A:205:ASN:HB2	1:A:208:ARG:HD2	1.85	0.58
1:B:213:ARG:O	1:B:216:ARG:HB3	2.03	0.58
1:B:429:PHE:HA	1:B:432:ASN:HD21	1.68	0.58
1:B:26:ARG:NH1	1:B:294:GLU:O	2.37	0.58
1:A:177:GLY:O	1:A:180:GLY:N	2.35	0.58
1:B:39:PHE:CZ	1:B:67:VAL:HG22	2.39	0.58
1:A:210:GLU:HG3	1:A:211:ASN:H	1.69	0.58
1:B:124:ASN:ND2	1:B:124:ASN:H	1.96	0.58
1:B:398:GLN:HB3	1:B:447:MET:HE3	1.85	0.58
1:B:494:GLU:HG3	1:B:495:GLU:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:89:PRO:HB2	1:A:90:LYS:HD3	1.85	0.58
1:B:346:PHE:CE1	1:B:477:PRO:HB3	2.39	0.58
1:B:492:ASN:O	1:B:493:ALA:HB2	2.03	0.57
1:A:421:GLU:O	1:A:425:ILE:HG12	2.04	0.57
1:B:214:ARG:CB	1:B:214:ARG:HH11	2.18	0.57
1:B:495:GLU:OE1	1:B:495:GLU:O	2.22	0.57
1:B:26:ARG:HG3	1:B:295:GLY:HA3	1.86	0.57
1:A:238:MET:O	1:A:238:MET:HG3	2.05	0.57
1:A:190:VAL:HG13	1:A:256:LEU:HB3	1.86	0.57
1:B:316:ILE:HG23	1:B:320:GLU:HB2	1.86	0.57
1:B:62:THR:HG23	1:B:95:PRO:HD2	1.86	0.57
1:B:41:ILE:HD13	1:B:286:ALA:HB2	1.86	0.56
1:B:60:SER:O	1:B:64:GLU:HG3	2.05	0.56
1:B:214:ARG:CB	1:B:214:ARG:NH1	2.68	0.56
1:B:185:GLY:HA2	1:B:270:ILE:HD12	1.87	0.56
1:A:216:ARG:HE	1:A:220:GLU:CG	2.18	0.56
1:A:160:ASP:CG	1:A:162:ARG:HB2	2.26	0.56
1:A:414:VAL:O	1:A:416:ARG:HG3	2.05	0.56
1:B:371:VAL:HA	1:B:374:MET:HG3	1.87	0.56
1:A:199:ARG:HA	1:A:199:ARG:HH11	1.70	0.56
1:B:139:TRP:CD1	1:B:140:HIS:HD2	2.23	0.56
1:B:104:TRP:O	1:B:371:VAL:HG22	2.06	0.55
1:B:430:LYS:HB3	1:B:445:ILE:HG21	1.88	0.55
1:B:24:GLU:OE1	1:B:25:ILE:HG22	2.07	0.55
1:A:276:LEU:HD22	1:A:307:LEU:HD21	1.87	0.55
1:A:371:VAL:HG12	1:A:371:VAL:O	2.06	0.55
1:B:57:ILE:O	1:B:61:ILE:HG12	2.06	0.55
1:B:466:LEU:C	1:B:468:ASP:H	2.11	0.55
1:A:172:LEU:HD12	1:A:173:PRO:HD2	1.88	0.55
1:B:317:ARG:HB2	1:B:320:GLU:OE2	2.06	0.55
1:B:396:THR:HG22	1:B:396:THR:O	2.06	0.55
1:A:181:ALA:HA	1:A:184:LYS:HD2	1.89	0.54
1:B:147:THR:HG22	1:B:328:LEU:HD21	1.89	0.54
1:A:76:ASN:O	1:A:173:PRO:HG3	2.07	0.54
1:A:184:LYS:O	1:A:229:LYS:NZ	2.31	0.54
1:B:57:ILE:HG23	1:B:58:GLN:N	2.22	0.54
1:A:292:GLU:HB2	1:B:368:ASN:CG	2.28	0.54
1:B:139:TRP:CZ2	1:B:277:PRO:HG3	2.43	0.54
1:A:406:ILE:CG2	1:A:406:ILE:O	2.55	0.54
1:B:483:ASN:C	1:B:485:GLY:H	2.11	0.53
1:B:194:ILE:HG12	1:B:253:ILE:HG23	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:GLY:HA3	1:B:442:THR:HA	1.90	0.53
1:B:238:MET:HB2	1:B:440:MET:CG	2.39	0.53
1:A:144:ASN:OD1	1:A:150:ARG:NH2	2.41	0.53
1:B:348:ARG:NH2	1:B:380:GLU:O	2.42	0.53
1:B:41:ILE:CD1	1:B:286:ALA:HB2	2.39	0.53
1:B:246:ARG:HH11	1:B:246:ARG:CA	2.22	0.53
1:A:365:ILE:HD12	1:A:365:ILE:N	2.24	0.53
1:B:398:GLN:HB3	1:B:447:MET:HE2	1.91	0.52
1:B:321:ASN:ND2	1:B:323:ALA:H	2.07	0.52
1:B:294:GLU:CD	1:B:294:GLU:N	2.63	0.52
1:B:470:LYS:O	1:B:472:THR:N	2.38	0.52
1:B:118:ARG:O	1:B:122:GLN:HG2	2.10	0.52
1:B:450:SER:HA	1:B:452:ARG:HH12	1.74	0.52
1:A:346:PHE:CE2	1:A:477:PRO:HB3	2.45	0.52
1:A:265:ILE:O	1:A:267:ARG:N	2.42	0.52
1:A:197:ILE:HG21	1:A:253:ILE:CG2	2.40	0.52
1:A:40:TYR:OH	1:A:54:GLY:O	2.20	0.52
1:B:283:LEU:O	1:B:287:SER:HB2	2.09	0.52
1:A:292:GLU:HB2	1:B:368:ASN:OD1	2.09	0.52
1:A:143:LEU:HA	1:A:332:ALA:CB	2.39	0.52
1:A:114:GLU:HB3	1:A:117:ARG:HH11	1.73	0.52
1:B:111:TYR:O	1:B:112:ASP:HB3	2.10	0.52
1:A:289:TYR:CE1	1:A:294:GLU:HG3	2.45	0.51
1:B:437:THR:O	1:B:441:ARG:HG3	2.10	0.51
1:A:144:ASN:OD1	1:A:171:THR:HG21	2.09	0.51
1:A:266:LEU:HA	1:A:396:THR:CG2	2.40	0.51
1:B:317:ARG:HD3	1:B:369:GLU:OE1	2.10	0.51
1:B:51:ASP:O	1:B:55:ARG:HD3	2.11	0.51
1:B:345:SER:HA	1:B:352:VAL:HG23	1.92	0.51
1:B:314:SER:HB2	1:B:379:LEU:HD11	1.93	0.51
1:B:433:THR:HG23	1:B:435:GLY:H	1.75	0.51
1:B:62:THR:O	1:B:66:MET:HB2	2.10	0.51
1:B:366:ALA:N	1:B:369:GLU:OE2	2.41	0.51
1:A:76:ASN:O	1:A:173:PRO:CB	2.59	0.51
1:B:191:MET:CE	1:B:195:ARG:HH12	2.24	0.51
1:B:134:THR:HG21	1:B:177:GLY:H	1.76	0.51
1:B:91:LYS:CB	1:B:112:ASP:HA	2.35	0.50
1:B:399:GLN:HE21	1:B:401:ALA:CB	2.16	0.50
1:B:214:ARG:HB3	1:B:214:ARG:CZ	2.41	0.50
1:A:72:ASP:CB	1:A:75:ARG:O	2.56	0.50
1:A:59:ASN:O	1:A:63:ILE:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:72:ASP:OD2	1:B:74:ARG:HB2	2.12	0.50
1:A:433:THR:HG22	1:A:438:SER:HB2	1.94	0.50
1:A:128:ASP:O	1:A:129:ALA:C	2.50	0.50
1:B:317:ARG:HB3	1:B:318:PRO:CD	2.34	0.50
1:A:75:ARG:NH1	1:A:175:ARG:HG2	2.27	0.50
1:A:298:LEU:HD22	1:A:298:LEU:N	2.22	0.49
1:B:172:LEU:CD2	1:B:173:PRO:HD2	2.42	0.49
1:A:116:ILE:HD13	1:A:116:ILE:N	2.26	0.49
1:A:40:TYR:CE2	1:A:279:CYS:HA	2.47	0.49
1:A:130:THR:HG22	1:A:133:LEU:HD12	1.95	0.49
1:B:270:ILE:O	1:B:391:ARG:HA	2.13	0.49
1:B:72:ASP:OD2	1:B:175:ARG:NH1	2.45	0.49
1:B:43:MET:HG2	1:B:63:ILE:HD12	1.95	0.49
1:B:56:LEU:HD21	1:B:315:LEU:HG	1.95	0.48
1:B:152:ARG:HA	1:B:155:VAL:HG22	1.95	0.48
1:B:55:ARG:NH1	1:B:283:LEU:HD13	2.28	0.48
1:A:201:ILE:CG1	1:A:249:GLY:HA2	2.43	0.48
1:A:344:SER:O	1:A:348:ARG:HB2	2.14	0.48
1:B:95:PRO:O	1:B:96:ILE:HG13	2.14	0.48
1:B:464:PHE:CE2	1:B:471:ALA:HB1	2.49	0.48
1:A:76:ASN:O	1:A:173:PRO:HB3	2.14	0.48
1:B:56:LEU:HG	1:B:58:GLN:HG2	1.95	0.48
1:A:463:VAL:HG22	1:A:475:ILE:HB	1.95	0.48
1:A:107:GLU:O	1:A:108:LEU:C	2.52	0.48
1:A:406:ILE:CG2	1:A:425:ILE:HD11	2.43	0.48
1:B:429:PHE:HA	1:B:432:ASN:ND2	2.29	0.48
1:A:451:ALA:O	1:A:452:ARG:HD3	2.14	0.48
1:B:317:ARG:HB2	1:B:320:GLU:CD	2.35	0.47
1:A:302:ASP:HA	1:A:305:ARG:NH1	2.29	0.47
1:A:77:ARG:O	1:A:78:TYR:C	2.52	0.47
1:A:240:ASP:OD2	1:A:243:ARG:NH2	2.46	0.47
1:B:238:MET:HB2	1:B:440:MET:HG2	1.97	0.47
1:B:353:ILE:HD11	1:B:358:LEU:CD1	2.43	0.47
1:A:238:MET:HE3	1:A:259:LEU:HD13	1.96	0.47
1:A:71:PHE:CZ	1:A:117:ARG:HG2	2.49	0.47
1:B:386:TRP:NE1	1:B:464:PHE:CB	2.77	0.47
1:A:259:LEU:HA	1:A:259:LEU:HD12	1.76	0.47
1:B:27:ALA:O	1:B:31:ARG:N	2.48	0.47
1:A:50:SER:HB3	1:A:53:GLU:CG	2.45	0.47
1:A:407:SER:OG	1:A:408:VAL:N	2.47	0.47
1:B:371:VAL:O	1:B:372:GLU:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:90:LYS:CD	1:A:90:LYS:H	2.01	0.47
1:A:216:ARG:HE	1:A:220:GLU:HG3	1.79	0.47
1:B:62:THR:HG21	1:B:95:PRO:O	2.15	0.47
1:A:26:ARG:NH1	1:A:294:GLU:O	2.47	0.47
1:A:450:SER:O	1:A:452:ARG:NH1	2.47	0.47
1:B:302:ASP:HB2	1:B:303:PRO:HD3	1.95	0.47
1:B:41:ILE:C	1:B:43:MET:H	2.17	0.47
1:B:386:TRP:CE2	1:B:464:PHE:HB2	2.50	0.47
1:A:266:LEU:HA	1:A:396:THR:HG21	1.95	0.47
1:A:199:ARG:O	1:A:203:ASP:HB3	2.14	0.47
1:A:89:PRO:C	1:A:91:LYS:H	2.17	0.46
1:A:226:LEU:HD23	1:A:226:LEU:O	2.14	0.46
1:A:329:VAL:O	1:A:333:CYS:SG	2.72	0.46
1:A:186:VAL:O	1:A:190:VAL:HG23	2.16	0.46
1:B:47:LEU:O	1:B:98:ARG:NH2	2.39	0.46
1:A:339:GLU:OE1	1:A:340:ASP:N	2.49	0.46
1:B:88:ASP:CB	1:B:89:PRO:CD	2.90	0.45
1:A:104:TRP:HB2	1:A:371:VAL:HG12	1.97	0.45
1:B:118:ARG:NH2	1:B:122:GLN:HG3	2.31	0.45
1:B:46:GLU:H	1:B:46:GLU:CD	2.19	0.45
1:B:203:ASP:OD2	1:B:206:PHE:N	2.48	0.45
1:A:29:VAL:O	1:A:32:MET:HG3	2.17	0.45
1:A:276:LEU:N	1:A:276:LEU:HD23	2.32	0.45
1:A:391:ARG:HB3	1:A:391:ARG:HE	1.58	0.45
1:A:323:ALA:O	1:A:326:SER:HB2	2.17	0.45
1:B:221:ARG:O	1:B:225:ILE:HG12	2.16	0.45
1:B:329:VAL:HG12	1:B:333:CYS:SG	2.56	0.45
1:A:406:ILE:HG23	1:A:421:GLU:HB2	1.99	0.45
1:B:315:LEU:HD13	1:B:374:MET:CE	2.47	0.45
1:A:467:SER:HA	1:B:156:ARG:HH22	1.81	0.45
1:A:175:ARG:CG	1:A:175:ARG:O	2.65	0.45
1:B:214:ARG:HB2	1:B:214:ARG:HH11	1.81	0.45
1:B:438:SER:O	1:B:441:ARG:HB2	2.17	0.45
1:B:406:ILE:HG23	1:B:425:ILE:HD11	1.99	0.45
1:B:55:ARG:HH21	1:B:311:GLN:HE21	1.65	0.44
1:A:161:PRO:C	1:A:163:MET:H	2.21	0.44
1:B:73:GLU:CG	1:B:73:GLU:O	2.66	0.44
1:A:392:SER:OG	1:A:393:GLY:N	2.50	0.44
1:A:397:ASN:HB2	1:A:398:GLN:H	1.55	0.44
1:B:114:GLU:HB2	1:B:117:ARG:NH1	2.32	0.44
1:A:263:ALA:HA	1:A:266:LEU:O	2.16	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:40:TYR:CE2	1:B:279:CYS:HA	2.53	0.44
1:A:495:GLU:O	1:A:496:TYR:HB2	2.17	0.44
1:A:221:ARG:CB	1:A:221:ARG:HH11	2.28	0.44
1:A:47:LEU:HB2	1:A:49:LEU:HG	1.99	0.44
1:A:289:TYR:CZ	1:A:294:GLU:HG3	2.53	0.44
1:A:211:ASN:HA	1:A:214:ARG:HB2	1.99	0.44
1:B:116:ILE:HA	1:B:119:ILE:HD12	1.99	0.44
1:A:62:THR:HG21	1:A:96:ILE:CG1	2.45	0.44
1:A:169:GLY:O	1:A:172:LEU:HB2	2.16	0.44
1:A:298:LEU:CD2	1:A:298:LEU:H	2.26	0.44
1:A:433:THR:HG22	1:A:438:SER:CA	2.48	0.44
1:A:75:ARG:HB2	1:A:174:ARG:O	2.18	0.44
1:B:317:ARG:CB	1:B:318:PRO:CD	2.93	0.44
1:B:216:ARG:NH1	1:B:246:ARG:NH1	2.66	0.44
1:A:129:ALA:C	1:A:131:ALA:H	2.21	0.44
1:B:75:ARG:NH2	1:B:90:LYS:NZ	2.66	0.43
1:B:61:ILE:HA	1:B:64:GLU:OE1	2.18	0.43
1:A:397:ASN:HA	1:A:447:MET:CE	2.48	0.43
1:A:55:ARG:HD2	1:A:313:PHE:CE1	2.53	0.43
1:B:123:ALA:O	1:B:125:ASN:N	2.51	0.43
1:B:315:LEU:HD13	1:B:374:MET:HE1	2.00	0.43
1:B:166:LEU:HB3	1:B:187:GLY:H	1.84	0.43
1:B:205:ASN:HA	1:B:208:ARG:HG2	1.99	0.43
1:A:37:GLY:HA3	1:A:285:VAL:HG21	1.99	0.43
1:B:339:GLU:OE1	1:B:340:ASP:N	2.50	0.43
1:B:317:ARG:O	1:B:318:PRO:C	2.56	0.43
1:A:172:LEU:HA	1:A:172:LEU:HD12	1.64	0.43
1:A:192:GLU:O	1:A:195:ARG:HB3	2.19	0.43
1:B:55:ARG:HG2	1:B:283:LEU:HD11	1.99	0.43
1:B:483:ASN:C	1:B:485:GLY:N	2.71	0.43
1:B:339:GLU:CD	1:B:343:VAL:HG11	2.39	0.43
1:A:119:ILE:O	1:A:120:TRP:C	2.56	0.43
1:B:68:LEU:HD23	1:B:68:LEU:HA	1.87	0.43
1:A:135:HIS:O	1:A:138:ILE:HB	2.18	0.43
1:A:76:ASN:HB3	1:A:77:ARG:H	1.58	0.43
1:B:254:GLU:HA	1:B:254:GLU:OE2	2.19	0.43
1:B:73:GLU:HG2	1:B:73:GLU:O	2.18	0.43
1:B:492:ASN:O	1:B:493:ALA:CB	2.65	0.43
1:A:188:THR:HG22	1:A:189:MET:N	2.33	0.43
1:B:308:GLN:HA	1:B:382:ARG:HG2	2.01	0.43
1:A:221:ARG:CB	1:A:221:ARG:NH1	2.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:238:MET:O	1:B:242:VAL:HG23	2.19	0.43
1:A:149:GLN:HA	1:A:149:GLN:HE21	1.84	0.43
1:A:345:SER:HA	1:A:352:VAL:HG23	2.01	0.43
1:B:66:MET:HG2	1:B:116:ILE:HD13	2.01	0.42
1:A:58:GLN:HE21	1:A:58:GLN:HB3	1.62	0.42
1:A:433:THR:HG23	1:A:435:GLY:N	2.17	0.42
1:B:160:ASP:OD1	1:B:161:PRO:HD2	2.20	0.42
1:A:87:LYS:O	1:A:88:ASP:CB	2.67	0.42
1:A:422:ARG:HG2	1:A:422:ARG:HH11	1.84	0.42
1:A:298:LEU:HD13	1:A:298:LEU:N	2.34	0.42
1:B:210:GLU:O	1:B:213:ARG:HB2	2.19	0.42
1:A:141:SER:HB2	1:A:172:LEU:HD13	2.00	0.42
1:A:97:TYR:HA	1:A:105:VAL:O	2.19	0.42
1:B:75:ARG:HA	1:B:75:ARG:NE	2.34	0.42
1:B:58:GLN:HG2	1:B:58:GLN:H	1.49	0.42
1:A:36:ILE:HG12	1:A:36:ILE:H	1.63	0.42
1:A:443:GLU:OE1	1:A:446:ARG:NH1	2.53	0.42
1:A:406:ILE:HG22	1:A:406:ILE:O	2.20	0.42
1:B:57:ILE:CG2	1:B:58:GLN:N	2.81	0.42
1:B:267:ARG:HG3	1:B:393:GLY:O	2.19	0.42
1:A:433:THR:HG22	1:A:438:SER:HA	2.01	0.42
1:A:417:ASN:H	1:A:417:ASN:HD22	1.66	0.42
1:B:341:LEU:HD22	1:B:352:VAL:O	2.20	0.42
1:B:112:ASP:O	1:B:114:GLU:N	2.53	0.42
1:B:51:ASP:O	1:B:55:ARG:CD	2.68	0.42
1:B:319:ASN:HD22	1:B:319:ASN:HA	1.54	0.42
1:A:143:LEU:HD12	1:A:143:LEU:O	2.20	0.41
1:B:99:ARG:HG2	1:B:102:GLY:O	2.20	0.41
1:A:198:LYS:C	1:A:200:GLY:N	2.73	0.41
1:A:75:ARG:HH11	1:A:175:ARG:HG2	1.85	0.41
1:B:390:THR:HB	1:B:392:SER:H	1.84	0.41
1:A:141:SER:OG	1:A:169:GLY:HA2	2.20	0.41
1:A:33:VAL:HG12	1:A:34:GLY:N	2.35	0.41
1:A:197:ILE:H	1:A:197:ILE:HG12	1.69	0.41
1:A:229:LYS:HD3	1:A:270:ILE:HG22	2.03	0.41
1:A:227:LYS:O	1:A:236:LYS:HE3	2.20	0.41
1:A:397:ASN:O	1:A:398:GLN:HB2	2.20	0.41
1:A:303:PRO:HG2	1:A:389:ARG:NH2	2.35	0.41
1:B:347:ILE:HA	1:B:385:TYR:HB2	2.02	0.41
1:A:432:ASN:N	1:A:432:ASN:HD22	2.19	0.41
1:A:399:GLN:HE21	1:A:399:GLN:HB2	1.59	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ARG:NH1	1:A:107:GLU:OE2	2.54	0.40
1:B:267:ARG:HG2	1:B:267:ARG:H	1.71	0.40
1:B:226:LEU:HD22	1:B:230:PHE:CE1	2.56	0.40
1:B:179:ALA:O	1:B:182:ALA:HB3	2.22	0.40
1:A:119:ILE:H	1:A:119:ILE:HG12	1.52	0.40
1:B:201:ILE:HD11	1:B:249:GLY:HA2	2.04	0.40
1:A:463:VAL:CG2	1:A:475:ILE:HB	2.51	0.40
1:A:195:ARG:HA	1:A:195:ARG:HD3	2.00	0.40
1:A:87:LYS:O	1:A:88:ASP:HB3	2.21	0.40
1:A:207:TRP:CZ2	1:A:248:PRO:CD	3.05	0.40
1:A:226:LEU:HD23	1:A:226:LEU:C	2.42	0.40
1:A:202:ASN:HD22	1:A:202:ASN:HA	1.54	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	463/504 (92%)	389 (84%)	58 (12%)	16 (4%)	4	29
1	B	461/504 (92%)	389 (84%)	56 (12%)	16 (4%)	4	29
All	All	924/1008 (92%)	778 (84%)	114 (12%)	32 (4%)	4	29

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	398	GLN
1	A	493	ALA
1	B	372	GLU
1	A	88	ASP
1	A	89	PRO
1	A	130	THR

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Mol	Chain	Res	Type
1	A	162	ARG
1	A	204	ARG
1	A	205	ASN
1	A	266	LEU
1	A	468	ASP
1	B	467	SER
1	B	471	ALA
1	A	48	LYS
1	A	90	LYS
1	A	397	ASN
1	B	111	TYR
1	B	124	ASN
1	B	125	ASN
1	B	245	SER
1	B	486	SER
1	B	493	ALA
1	B	295	GLY
1	B	318	PRO
1	B	483	ASN
1	B	195	ARG
1	B	402	SER
1	B	423	ALA
1	A	453	PRO
1	B	113	LYS
1	A	201	ILE
1	A	265	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	387/420 (92%)	321 (83%)	66 (17%)	2	12
1	B	387/420 (92%)	320 (83%)	67 (17%)	2	11
All	All	774/840 (92%)	641 (83%)	133 (17%)	2	12

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	25	ILE
1	A	32	MET
1	A	47	LEU
1	A	58	GLN
1	A	62	THR
1	A	65	ARG
1	A	69	SER
1	A	72	ASP
1	A	75	ARG
1	A	88	ASP
1	A	90	LYS
1	A	103	LYS
1	A	105	VAL
1	A	111	TYR
1	A	119	ILE
1	A	122	GLN
1	A	136	MET
1	A	137	MET
1	A	139	TRP
1	A	144	ASN
1	A	149	GLN
1	A	162	ARG
1	A	164	CYS
1	A	171	THR
1	A	172	LEU
1	A	174	ARG
1	A	199	ARG
1	A	202	ASN
1	A	204	ARG
1	A	205	ASN
1	A	207	TRP
1	A	215	THR
1	A	241	GLN
1	A	253	ILE
1	A	259	LEU
1	A	276	LEU
1	A	293	ARG
1	A	298	LEU
1	A	302	ASP
1	A	305	ARG
1	A	306	LEU
1	A	307	LEU
1	A	316	ILE

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Mol	Chain	Res	Type
1	A	339	GLU
1	A	347	ILE
1	A	348	ARG
1	A	358	LEU
1	A	359	SER
1	A	364	GLN
1	A	389	ARG
1	A	391	ARG
1	A	397	ASN
1	A	402	SER
1	A	408	VAL
1	A	413	SER
1	A	416	ARG
1	A	417	ASN
1	A	433	THR
1	A	436	ARG
1	A	459	GLN
1	A	472	THR
1	A	478	SER
1	A	480	ASP
1	A	481	MET
1	A	482	SER
1	A	495	GLU
1	B	24	GLU
1	B	25	ILE
1	B	29	VAL
1	B	32	MET
1	B	48	LYS
1	B	50	SER
1	B	52	GLN
1	B	58	GLN
1	B	72	ASP
1	B	73	GLU
1	B	88	ASP
1	B	91	LYS
1	B	92	THR
1	B	103	LYS
1	B	111	TYR
1	B	113	LYS
1	B	118	ARG
1	B	124	ASN
1	B	130	THR

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Mol	Chain	Res	Type
1	B	164	CYS
1	B	165	SER
1	B	183	ILE
1	B	201	ILE
1	B	208	ARG
1	B	211	ASN
1	B	226	LEU
1	B	236	LYS
1	B	246	ARG
1	B	252	GLU
1	B	267	ARG
1	B	294	GLU
1	B	302	ASP
1	B	306	LEU
1	B	316	ILE
1	B	319	ASN
1	B	339	GLU
1	B	343	VAL
1	B	348	ARG
1	B	353	ILE
1	B	358	LEU
1	B	361	ARG
1	B	364	GLN
1	B	368	ASN
1	B	369	GLU
1	B	371	VAL
1	B	383	SER
1	B	384	ARG
1	B	388	ILE
1	B	389	ARG
1	B	397	ASN
1	B	398	GLN
1	B	406	ILE
1	B	416	ARG
1	B	424	THR
1	B	433	THR
1	B	436	ARG
1	B	439	ASP
1	B	440	MET
1	B	445	ILE
1	B	454	GLU
1	B	459	GLN

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Mol	Chain	Res	Type
1	B	465	GLU
1	B	467	SER
1	B	472	THR
1	B	481	MET
1	B	486	SER
1	B	495	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	122	GLN
1	A	149	GLN
1	A	202	ASN
1	A	272	HIS
1	A	334	HIS
1	A	368	ASN
1	A	405	GLN
1	A	409	GLN
1	A	417	ASN
1	A	432	ASN
1	B	52	GLN
1	B	124	ASN
1	B	140	HIS
1	B	144	ASN
1	B	149	GLN
1	B	211	ASN
1	B	235	GLN
1	B	308	GLN
1	B	311	GLN
1	B	319	ASN
1	B	321	ASN
1	B	324	HIS
1	B	334	HIS
1	B	398	GLN
1	B	399	GLN
1	B	409	GLN
1	B	415	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates 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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	467/504 (92%)	-0.10	4 (0%) 85 82	31, 93, 109, 119	0
1	B	465/504 (92%)	-0.07	5 (1%) 82 78	73, 92, 106, 116	0
All	All	932/1008 (92%)	-0.09	9 (0%) 84 80	31, 93, 109, 119	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	21	ASN	10.5
1	B	97	TYR	2.5
1	A	401	ALA	2.4
1	B	22	ALA	2.3
1	A	482	SER	2.3
1	A	203	ASP	2.2
1	B	111	TYR	2.2
1	A	97	TYR	2.2
1	B	311	GLN	2.1

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 carbohydrates 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.