



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 03:36 AM GMT

PDB ID : 2GW1  
Title : Crystal Structure of the Yeast Tom70  
Authors : Wu, Y.; Sha, B.  
Deposited on : 2006-05-03  
Resolution : 3.00 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

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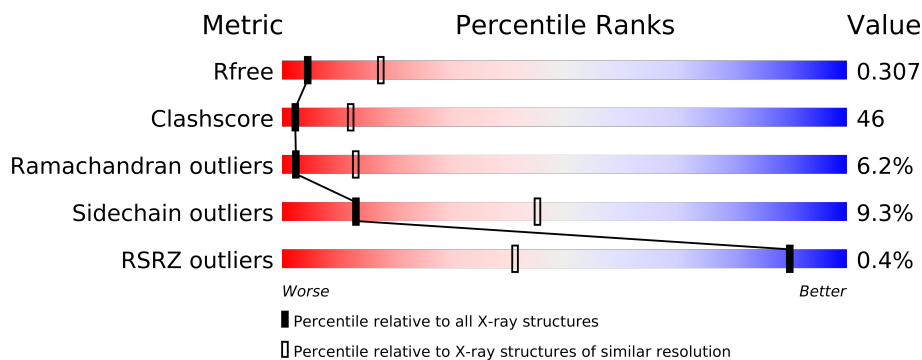
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 3.00 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))
$R_{free}$	66092	1216 (3.00-3.00)
Clashscore	79885	1594 (3.00-3.00)
Ramachandran outliers	78287	1537 (3.00-3.00)
Sidechain outliers	78261	1540 (3.00-3.00)
RSRZ outliers	66119	1217 (3.00-3.00)

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  $\geq 3$ , 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	514	
1	B	514	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 7984 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 Mitochondrial precursor proteins import receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	487	Total	C	N	O	S	0	0	0
			3929	2500	642	773	14			
1	B	487	Total	C	N	O	S	0	0	0
			3929	2500	642	773	14			

- Molecule 2 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	65	Total	O	0	0
			65	65		
2	B	61	Total	O	0	0
			61	61		



E577	K511	K446	Y382	L311
K578	L514	F447	Y383	L316
L579	L515	D448	N384	
Q580	T516	D449	Y385	
	R517	C450	F386	D322
A585	N518		D387	E323
E586	P519	L453		K324
A587	T520	F454	L390	
	V521		K391	E327
Q591	E522	K458	L392	K328
	N523		D393	L329
L594	P524	F461	S394	A330
R595	I525	P462	N395	I331
S596	E526	E463	N396	S332
D597	A527	A464		L333
P598	T528	P465	V399	E334
V599	N529	E466	Y400	H335
L600	L530	V467	Y401	T336
A601	L531	P468	H402	C337
	E532	N469	K403	T338
	K533	F470	G404	F339
	A534		Q405	K340
	S535	E473	M406	F341
	K536	I474	N407	L342
	L537	L475	F408	K343
	D538	T476	I409	I344
	P539	D477	L410	D345
	R540	K478	Q411	L347
	S541	N479	N412	
		D480	Y413	G348
		F481	D414	A349
	K545	D482		
	I546	K483	G417	D352
	G547	A484	K418	T353
	L548	L485	D419	K354
	A549	K486	F420	K355
	Q550	Q487	D421	A356
	M551	Y488	K422	T357
	K552	D489	A423	
	L553	L490	K424	F360
	Q554	A491	E425	P361
	E555	I492	L426	R362
	E556	E493	D427	V363
	D557	L494		I364
	I558	E495	M430	
	D559	N496	I431	T367
	E560	K497	F432	Y368
		L498	P433	K369
	T563	D499	Y434	A370
	L564	G500	I435	L371
	F565	I501	Q436	I372
	E566	Y502	L437	K373
	E567	V503	A374	A374
	S568	Q504	C439	D375
		I505	L440	R376
		A506	A441	I377
	L571	P507	Y442	B378
	A572	L508	R443	S379
		V509	E444	T380
	M575			E381
	E576			

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	44.88Å 168.60Å 82.99Å 90.00° 102.59° 90.00°	Depositor
Resolution (Å)	46.17 – 3.00 46.17 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.0 (46.17-3.00) 94.8 (46.17-2.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 2.91Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.259 , 0.316 0.254 , 0.307	Depositor DCC
$R_{free}$ test set	1128 reflections (4.83%)	DCC
Wilson B-factor (Å <sup>2</sup> )	83.2	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 47.4	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	2 of 25246 reflections (0.008%)	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	7984	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	79.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.25% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

## 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	0.29	0/3999	0.53	1/5379 (0.0%)
1	B	0.29	0/3999	0.51	0/5379
All	All	0.29	0/7998	0.52	1/10758 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	275	GLU	N-CA-C	-5.31	96.66	111.00

There are no chirality outliers.

There are no planarity outliers.

### 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	3929	0	3885	383	0
1	B	3929	0	3885	357	0
2	A	65	0	0	22	0
2	B	61	0	0	25	0
All	All	7984	0	7770	726	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 46.

All (726) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:439:CYS:SG	1:B:442:TYR:HB2	2.02	0.99
1:A:478:LYS:HE3	1:A:478:LYS:HA	1.45	0.98
1:B:148:LEU:HB3	1:B:179:LEU:HD11	1.46	0.96
1:B:255:THR:HG22	2:B:660:HOH:O	1.66	0.93
1:B:344:ASN:O	1:B:345:ASP:HB3	1.66	0.93
1:B:431:ILE:HD11	1:B:467:VAL:HG23	1.50	0.92
1:B:558:ILE:HG12	1:B:559:ASP:H	1.35	0.91
1:A:469:ASN:HD22	1:A:507:PRO:HG3	1.35	0.91
1:A:283:LEU:HD11	1:A:331:ILE:HD11	1.52	0.91
1:A:506:ALA:HB3	1:A:507:PRO:HD3	1.54	0.90
1:A:369:MET:SD	1:A:372:ILE:HD11	2.12	0.90
1:A:455:SER:HA	1:A:458:LYS:HB2	1.53	0.89
1:A:606:GLU:HG2	2:A:636:HOH:O	1.71	0.89
1:B:376:ARG:HH21	1:B:377:ASN:HB3	1.39	0.88
1:A:269:THR:HG23	1:A:270:PHE:H	1.38	0.88
1:A:439:CYS:SG	1:A:442:TYR:HB2	2.16	0.86
1:B:478:LYS:HE3	1:B:478:LYS:HA	1.56	0.86
1:B:376:ARG:HE	1:B:377:ASN:H	1.23	0.85
1:A:274:ASP:HA	1:A:280:ASP:HB3	1.59	0.84
1:B:468:PRO:HB2	1:B:491:ALA:HB2	1.58	0.84
1:A:293:ARG:HD2	1:A:501:ILE:HG22	1.60	0.82
1:A:341:PHE:HD2	1:A:372:ILE:HG22	1.43	0.82
1:A:435:ILE:HG21	1:A:470:PHE:HD2	1.45	0.82
1:A:331:ILE:HG22	1:A:362:ARG:HE	1.44	0.82
1:B:435:ILE:HG21	1:B:470:PHE:HD2	1.45	0.82
1:A:499:ASP:HA	2:A:611:HOH:O	1.79	0.81
1:B:488:TYR:O	1:B:492:ILE:HG13	1.79	0.81
1:B:105:LYS:HA	1:B:108:GLN:HE21	1.41	0.81
1:A:522:GLU:O	1:A:525:ILE:HG22	1.80	0.81
1:A:291:TYR:O	1:A:292:LYS:HG2	1.81	0.80
1:A:349:ALA:O	1:A:353:ILE:HG23	1.81	0.80
1:A:390:LEU:HD21	1:A:399:VAL:HG21	1.64	0.80
1:B:458:LYS:HE2	1:B:468:PRO:HG3	1.64	0.79
1:A:331:ILE:HG22	1:A:362:ARG:NE	1.99	0.78
1:A:521:VAL:HG23	1:A:522:GLU:HG3	1.66	0.77
1:A:344:ASN:CG	1:A:345:ASP:H	1.88	0.77
1:B:587:ALA:O	1:B:590:VAL:HG12	1.85	0.77
1:A:98:TYR:O	1:A:102:LEU:HG	1.85	0.76
1:B:558:ILE:HG12	1:B:559:ASP:N	1.99	0.76
1:A:222:LYS:HB2	2:A:651:HOH:O	1.84	0.76
1:B:551:MET:HE3	2:B:662:HOH:O	1.85	0.76
1:A:341:PHE:CD2	1:A:372:ILE:HG22	2.21	0.75

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:273:TYR:CE2	1:A:274:ASP:HB3	2.21	0.75
1:B:367:ILE:HD11	1:B:399:VAL:HG12	1.67	0.75
1:B:467:VAL:HB	1:B:468:PRO:HD3	1.68	0.74
1:A:473:GLU:O	1:A:476:THR:HG22	1.87	0.74
1:B:329:LEU:HD22	1:B:333:LEU:HG	1.68	0.74
1:B:506:ALA:HB3	1:B:507:PRO:HD3	1.68	0.74
1:B:293:ARG:HH21	1:B:502:TYR:HA	1.53	0.73
1:A:427:ASP:OD2	1:A:430:ASN:HB2	1.87	0.73
1:A:139:SER:O	1:A:143:VAL:HG23	1.89	0.73
1:B:253:SER:HB2	2:B:660:HOH:O	1.87	0.73
1:A:420:PHE:CZ	1:A:436:GLN:HG2	2.24	0.73
1:B:437:LEU:HD23	1:B:440:LEU:HD23	1.69	0.73
1:B:251:LEU:HD12	2:B:628:HOH:O	1.89	0.73
1:A:396:ASN:O	1:A:399:VAL:HG22	1.89	0.72
1:B:439:CYS:SG	1:B:474:ILE:HD13	2.30	0.72
1:A:390:LEU:CD2	1:A:399:VAL:HG21	2.19	0.71
1:A:274:ASP:HA	1:A:280:ASP:CB	2.20	0.71
1:B:331:ILE:HG22	1:B:362:ARG:HE	1.54	0.71
1:B:278:GLU:HG3	1:B:311:LEU:HD13	1.71	0.71
1:A:594:ILE:HG22	1:A:604:ILE:HD11	1.72	0.71
1:A:119:ILE:HG22	1:A:123:ASN:ND2	2.06	0.71
1:B:217:SER:O	1:B:220:LYS:HG2	1.90	0.71
1:A:360:PHE:HD2	1:A:361:PRO:HD2	1.56	0.70
1:A:269:THR:HA	2:A:630:HOH:O	1.91	0.70
1:A:312:PHE:HB3	1:A:329:LEU:HB2	1.74	0.70
1:A:505:ILE:HG23	1:A:534:ALA:HB1	1.72	0.70
1:A:503:VAL:HG12	1:A:507:PRO:HD3	1.74	0.70
1:A:505:ILE:HG12	1:A:538:ASP:HB2	1.72	0.70
1:B:399:VAL:HG23	1:B:400:TYR:H	1.57	0.70
1:A:98:TYR:HA	1:A:101:ALA:HB3	1.74	0.70
1:B:463:GLU:HA	1:B:494:LEU:HD22	1.73	0.70
1:A:214:GLN:HG3	1:B:586:GLU:HG2	1.72	0.70
1:A:379:SER:C	1:A:381:GLU:H	1.96	0.69
1:A:273:TYR:CE2	1:A:284:MET:HG3	2.27	0.69
1:A:363:VAL:HG11	1:A:396:ASN:ND2	2.06	0.69
1:B:418:LYS:HE2	2:B:610:HOH:O	1.91	0.69
1:A:467:VAL:HB	1:A:468:PRO:HD3	1.75	0.69
1:B:520:THR:HG22	1:B:522:GLU:H	1.57	0.69
1:A:207:LEU:HD13	1:B:204:GLU:CD	2.14	0.68
1:A:169:LEU:HD23	1:A:192:LEU:HD13	1.73	0.68
1:B:598:PRO:HA	1:B:601:ALA:HB3	1.74	0.68
1:B:522:GLU:O	1:B:525:ILE:HG22	1.92	0.68

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:409:ILE:HD12	1:B:410:LEU:N	2.08	0.68
1:A:361:PRO:O	1:A:362:ARG:HB3	1.91	0.68
1:B:431:ILE:HG12	1:B:435:ILE:HD11	1.75	0.68
1:B:331:ILE:HG22	1:B:362:ARG:NE	2.08	0.67
1:B:353:ILE:O	1:B:357:ILE:HG13	1.95	0.67
1:B:349:ALA:O	1:B:353:ILE:HG23	1.94	0.67
1:B:525:ILE:HD12	1:B:528:THR:HG21	1.76	0.67
1:A:455:SER:HA	1:A:458:LYS:CB	2.25	0.67
1:B:302:ASP:HB2	1:B:339:PHE:CE2	2.29	0.67
1:A:322:ASP:O	1:A:326:LYS:HG3	1.94	0.67
1:B:427:ASP:OD2	1:B:430:ASN:HB2	1.95	0.67
1:A:488:TYR:O	1:A:492:ILE:HG13	1.95	0.67
1:B:151:VAL:O	1:B:155:SER:HB2	1.94	0.67
1:A:449:ASP:O	1:A:453:LEU:HB2	1.94	0.66
1:B:420:PHE:CZ	1:B:436:GLN:HG2	2.29	0.66
1:A:105:LYS:HD3	1:A:121:TYR:HE2	1.60	0.66
1:A:579:LEU:O	1:A:583:THR:HG23	1.95	0.66
1:A:285:ASN:HD21	1:A:300:LYS:NZ	1.94	0.66
1:A:558:ILE:HD13	1:A:559:ASP:H	1.61	0.66
1:B:503:VAL:HG12	1:B:507:PRO:HD3	1.77	0.66
1:A:151:VAL:O	1:A:155:SER:HB2	1.96	0.66
1:B:431:ILE:HD13	1:B:466:GLU:HB2	1.77	0.66
1:A:275:GLU:C	1:A:277:ASN:H	1.99	0.66
1:B:376:ARG:HE	1:B:377:ASN:N	1.93	0.66
1:A:386:PHE:HB2	2:A:631:HOH:O	1.94	0.66
1:B:182:PHE:CE2	1:B:213:LYS:HD3	2.31	0.66
1:A:441:ALA:HA	2:A:656:HOH:O	1.95	0.65
1:B:511:LYS:O	1:B:515:LEU:HB2	1.95	0.65
1:B:119:ILE:HG23	1:B:138:LEU:HD21	1.78	0.65
1:B:293:ARG:HB3	1:B:501:ILE:HG22	1.78	0.65
1:A:293:ARG:CD	1:A:501:ILE:HG22	2.25	0.65
1:A:522:GLU:HB2	2:A:635:HOH:O	1.95	0.65
1:A:399:VAL:HG23	1:A:400:TYR:N	2.12	0.65
1:A:219:LEU:HD12	1:B:579:LEU:HD23	1.79	0.65
1:A:318:LYS:HD3	1:A:318:LYS:O	1.96	0.65
1:B:263:ILE:HD12	1:B:263:ILE:N	2.11	0.65
1:B:596:SER:O	1:B:597:ASP:C	2.35	0.65
1:B:353:ILE:O	1:B:353:ILE:HD12	1.97	0.64
1:A:397:SER:HB2	1:A:426:LEU:CB	2.28	0.64
1:B:558:ILE:HD13	1:B:558:ILE:H	1.62	0.64
1:B:276:SER:O	1:B:281:LYS:HE2	1.97	0.64
1:B:505:ILE:CD1	1:B:538:ASP:HB2	2.27	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:119:ILE:HG22	1:A:123:ASN:HD21	1.61	0.64
1:B:329:LEU:CD2	1:B:333:LEU:HG	2.27	0.64
1:B:369:MET:O	1:B:372:ILE:HG13	1.97	0.64
1:B:532:GLU:HG3	2:B:646:HOH:O	1.98	0.64
1:B:114:LYS:HB3	1:B:117:ASP:HB2	1.79	0.64
1:B:558:ILE:CG1	1:B:559:ASP:H	2.09	0.64
1:B:316:LEU:HD12	1:B:329:LEU:HD12	1.80	0.64
1:B:142:TYR:CD1	1:B:150:LYS:HB3	2.33	0.64
1:B:556:GLU:HA	2:B:637:HOH:O	1.98	0.64
1:A:431:ILE:HD13	1:A:466:GLU:HB2	1.80	0.64
1:A:459:ARG:O	1:A:462:PRO:HD3	1.98	0.63
1:A:182:PHE:CE1	1:A:213:LYS:HB3	2.32	0.63
1:A:353:ILE:HD11	1:A:369:MET:HB2	1.80	0.63
1:B:372:ILE:HD12	1:B:373:MET:N	2.14	0.63
1:B:341:PHE:CD2	1:B:372:ILE:HG22	2.33	0.63
1:A:251:LEU:HD23	1:A:257:MET:HE3	1.80	0.63
1:A:520:THR:HB	1:A:523:ASN:CB	2.28	0.63
1:B:178:GLY:O	1:B:517:ARG:HD2	1.99	0.63
1:B:289:ASN:HB3	1:B:297:SER:O	1.99	0.63
1:B:327:GLU:O	1:B:331:ILE:HG23	1.98	0.63
1:A:520:THR:HB	1:A:523:ASN:HB3	1.81	0.63
1:B:192:LEU:HD11	1:B:198:PHE:CD1	2.34	0.63
1:A:576:GLU:HG2	1:A:577:GLU:OE2	1.99	0.62
1:B:473:GLU:O	1:B:476:THR:HG22	1.98	0.62
1:A:251:LEU:HD23	1:A:257:MET:CE	2.29	0.62
1:B:160:GLU:HA	2:B:613:HOH:O	1.98	0.62
1:A:397:SER:HB2	1:A:426:LEU:HB2	1.81	0.62
1:B:192:LEU:HD11	1:B:198:PHE:HD1	1.64	0.62
1:B:505:ILE:HG22	1:B:509:VAL:HG23	1.81	0.62
1:B:277:ASN:HD21	1:B:279:ALA:HB3	1.65	0.62
1:A:458:LYS:HA	1:A:467:VAL:HG11	1.80	0.62
1:B:411:GLN:HB2	2:B:632:HOH:O	2.00	0.62
1:A:103:LYS:HB2	1:A:134:PHE:HE1	1.65	0.62
1:A:505:ILE:HD12	1:A:505:ILE:N	2.15	0.61
1:B:406:MET:O	1:B:409:ILE:HG13	1.99	0.61
1:B:505:ILE:HD12	1:B:505:ILE:N	2.15	0.61
1:B:387:ASP:HA	1:B:390:LEU:HD12	1.83	0.61
1:A:147:ASP:O	1:A:151:VAL:HG23	2.00	0.61
1:B:204:GLU:HG2	1:B:208:GLU:OE2	2.01	0.61
1:A:204:GLU:N	1:A:205:PRO:HD2	2.16	0.61
1:B:105:LYS:HD3	1:B:121:TYR:CE2	2.36	0.61
1:A:287:LEU:O	1:A:287:LEU:HD23	1.99	0.61

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:502:TYR:CD1	1:A:502:TYR:N	2.67	0.61
1:B:555:GLN:CA	1:B:555:GLN:HE21	2.14	0.61
1:A:431:ILE:HG12	1:A:435:ILE:HD11	1.83	0.61
1:B:105:LYS:HA	1:B:108:GLN:NE2	2.14	0.60
1:A:525:ILE:HA	1:A:528:THR:HG22	1.83	0.60
1:B:489:ASP:HA	1:B:492:ILE:HD12	1.83	0.60
1:A:446:LYS:HA	1:A:446:LYS:HE2	1.82	0.60
1:B:182:PHE:HE2	1:B:213:LYS:HD3	1.67	0.60
1:B:119:ILE:HG22	1:B:123:ASN:HD22	1.67	0.60
1:B:449:ASP:O	1:B:453:LEU:HB2	2.00	0.60
1:B:558:ILE:N	1:B:558:ILE:HD13	2.17	0.60
1:B:454:PHE:O	1:B:458:LYS:HB2	2.01	0.60
1:B:268:LEU:HD12	1:B:268:LEU:N	2.16	0.60
1:B:212:ASN:HD22	1:B:212:ASN:C	2.04	0.60
1:A:468:PRO:HG2	1:A:494:LEU:HD12	1.84	0.59
1:A:422:LYS:O	1:A:426:LEU:HD13	2.02	0.59
1:B:386:PHE:O	1:B:390:LEU:HG	2.03	0.59
1:B:197:ASP:HA	2:B:615:HOH:O	2.01	0.59
1:B:221:GLU:HG3	1:B:222:LYS:HD2	1.84	0.59
1:A:353:ILE:HD12	1:A:353:ILE:O	2.03	0.59
1:A:426:LEU:O	1:A:427:ASP:HB2	2.01	0.59
1:A:334:GLU:O	1:A:338:ILE:HG12	2.01	0.59
1:A:594:ILE:CG2	1:A:604:ILE:HD11	2.33	0.59
1:B:260:PHE:HE1	1:B:338:ILE:CD1	2.16	0.59
1:B:336:THR:O	1:B:340:LYS:HG2	2.02	0.59
1:A:396:ASN:O	1:A:398:SER:N	2.36	0.59
1:A:500:GLY:HA3	1:A:502:TYR:HE1	1.68	0.58
1:A:334:GLU:HG3	1:A:365:SER:OG	2.02	0.58
1:A:431:ILE:CD1	1:A:466:GLU:HB2	2.32	0.58
1:B:324:LYS:O	1:B:328:LYS:HD3	2.03	0.58
1:A:454:PHE:CD2	1:A:471:PHE:HB2	2.38	0.58
1:B:374:ALA:HB1	1:B:406:MET:HE1	1.85	0.58
1:A:488:TYR:CE2	1:A:510:GLY:HA3	2.38	0.58
1:B:422:LYS:O	1:B:426:LEU:HD13	2.03	0.58
1:A:505:ILE:CD1	1:A:538:ASP:HB2	2.34	0.58
1:A:379:SER:O	1:A:381:GLU:N	2.36	0.58
1:A:440:LEU:HD23	2:A:656:HOH:O	2.04	0.58
1:B:367:ILE:HD11	1:B:399:VAL:CG1	2.34	0.58
1:B:558:ILE:H	1:B:558:ILE:CD1	2.16	0.58
1:A:439:CYS:HB2	1:A:454:PHE:CE1	2.38	0.58
1:A:293:ARG:HB3	1:A:501:ILE:HB	1.85	0.58
1:B:130:GLU:HB3	2:B:630:HOH:O	2.03	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:511:LYS:HD3	1:A:530:LEU:HD11	1.86	0.57
1:A:435:ILE:HG21	1:A:470:PHE:CD2	2.33	0.57
1:A:455:SER:CA	1:A:458:LYS:HB2	2.29	0.57
1:A:263:ILE:N	1:A:263:ILE:HD12	2.19	0.57
1:B:263:ILE:HG13	1:B:432:PHE:CD1	2.39	0.57
1:B:435:ILE:HG21	1:B:470:PHE:CD2	2.35	0.57
1:B:552:LYS:NZ	1:B:560:GLU:HB3	2.20	0.57
1:A:542:GLU:OE2	1:A:572:ALA:HB2	2.04	0.57
1:A:468:PRO:HB2	1:A:491:ALA:HB2	1.85	0.57
1:B:145:VAL:O	1:B:145:VAL:HG12	2.03	0.57
1:B:575:MET:HA	1:B:578:LYS:HG3	1.86	0.57
1:A:470:PHE:O	1:A:473:GLU:HG2	2.05	0.57
1:B:107:ASN:O	1:B:111:ARG:HG3	2.05	0.57
1:A:505:ILE:H	1:A:505:ILE:HD12	1.70	0.57
1:B:119:ILE:HG22	1:B:123:ASN:ND2	2.20	0.57
1:A:435:ILE:O	1:A:438:ALA:HB3	2.05	0.56
1:B:252:PRO:HG2	1:B:257:MET:HG3	1.88	0.56
1:A:491:ALA:O	1:A:495:GLU:HB2	2.05	0.56
1:A:334:GLU:OE2	1:A:364:ASN:HB2	2.06	0.56
1:B:331:ILE:CG2	1:B:362:ARG:HE	2.18	0.56
1:B:601:ALA:HA	1:B:604:ILE:HD12	1.88	0.56
1:B:422:LYS:HD3	1:B:422:LYS:O	2.05	0.56
1:B:273:TYR:CE2	1:B:274:ASP:HB2	2.39	0.56
1:A:367:ILE:HD11	1:A:399:VAL:HG12	1.87	0.56
1:A:211:LEU:HD22	1:B:208:GLU:OE1	2.06	0.56
1:A:344:ASN:CG	1:A:345:ASP:N	2.57	0.56
1:A:525:ILE:HA	1:A:528:THR:CG2	2.36	0.56
1:B:525:ILE:O	1:B:528:THR:HG22	2.06	0.56
1:A:354:LYS:O	1:A:358:GLU:HG3	2.06	0.56
1:A:295:PRO:C	1:A:297:SER:H	2.09	0.56
1:A:524:PHE:O	1:A:528:THR:HG22	2.05	0.56
1:A:310:ARG:O	1:A:314:GLU:HG3	2.05	0.56
1:B:148:LEU:HB3	1:B:179:LEU:CD1	2.29	0.56
1:A:540:ARG:HB3	1:A:540:ARG:HH11	1.70	0.56
1:B:600:LEU:O	1:B:604:ILE:HG13	2.06	0.56
1:B:295:PRO:C	1:B:297:SER:H	2.09	0.56
1:A:505:ILE:CG1	1:A:538:ASP:HB2	2.36	0.55
1:B:221:GLU:C	1:B:222:LYS:HD2	2.26	0.55
1:B:95:LYS:HD3	1:B:128:LEU:HD22	1.88	0.55
1:A:575:MET:HB3	1:B:576:GLU:HG2	1.86	0.55
1:B:260:PHE:CE1	1:B:338:ILE:HD11	2.42	0.55
1:A:563:THR:O	1:A:567:GLU:HG3	2.06	0.55

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:435:ILE:O	1:B:438:ALA:HB3	2.06	0.55
1:A:363:VAL:HG21	1:A:393:ASP:HB2	1.87	0.55
1:B:545:LYS:HG3	1:B:571:LEU:HD12	1.88	0.55
1:B:461:PHE:N	1:B:462:PRO:CD	2.70	0.55
1:A:393:ASP:CB	1:A:396:ASN:HB2	2.37	0.55
1:B:410:LEU:C	1:B:412:ASN:H	2.10	0.55
1:A:481:PHE:HE2	1:A:517:ARG:HG2	1.71	0.55
1:A:265:LYS:HG3	1:A:265:LYS:O	2.06	0.55
1:A:382:TYR:HA	1:A:385:TYR:CD1	2.42	0.55
1:B:418:LYS:HD3	1:B:418:LYS:O	2.06	0.55
1:A:286:GLY:HA2	1:A:301:ALA:HA	1.88	0.55
1:B:520:THR:HB	1:B:523:ASN:HB2	1.89	0.55
1:B:119:ILE:HD13	1:B:142:TYR:CE2	2.42	0.55
1:A:200:ASP:C	1:A:202:SER:H	2.11	0.55
1:B:439:CYS:C	1:B:441:ALA:H	2.11	0.54
1:B:342:LEU:C	1:B:344:ASN:N	2.58	0.54
1:B:431:ILE:CD1	1:B:466:GLU:HB2	2.37	0.54
1:B:203:ILE:HD12	1:B:204:GLU:N	2.21	0.54
1:A:279:ALA:HA	1:A:311:LEU:HD12	1.89	0.54
1:A:360:PHE:CD2	1:A:361:PRO:HD2	2.40	0.54
1:B:342:LEU:C	1:B:344:ASN:H	2.11	0.54
1:B:468:PRO:HA	1:B:487:GLN:OE1	2.08	0.54
1:A:288:SER:O	1:A:292:LYS:HD2	2.07	0.54
1:A:334:GLU:OE2	1:A:362:ARG:HD3	2.07	0.54
1:B:373:MET:O	1:B:376:ARG:HG3	2.07	0.54
1:A:277:ASN:O	1:A:281:LYS:HG3	2.07	0.54
1:A:469:ASN:O	1:A:472:ALA:HB3	2.07	0.54
1:A:109:PHE:HB3	1:A:117:ASP:HB2	1.90	0.54
1:B:338:ILE:HD13	1:B:338:ILE:O	2.08	0.54
1:A:410:LEU:C	1:A:412:ASN:H	2.10	0.54
1:A:309:ALA:O	1:A:313:GLU:HB2	2.07	0.54
1:B:268:LEU:HD12	1:B:268:LEU:H	1.73	0.54
1:A:546:ILE:HG23	1:A:568:SER:HB3	1.90	0.54
1:A:347:LEU:HG	1:B:376:ARG:HB3	1.90	0.53
1:A:393:ASP:HB3	1:A:396:ASN:HB2	1.89	0.53
1:B:563:THR:O	1:B:567:GLU:HG3	2.08	0.53
1:A:134:PHE:O	1:A:138:LEU:HG	2.07	0.53
1:A:204:GLU:O	1:A:208:GLU:HG3	2.07	0.53
1:A:578:LYS:O	1:A:582:ILE:HG13	2.08	0.53
1:B:514:LEU:HD23	1:B:515:LEU:N	2.24	0.53
1:A:496:ASN:HA	2:A:669:HOH:O	2.09	0.53
1:B:446:LYS:HD2	1:B:449:ASP:OD1	2.08	0.53

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:110:PHE:HD2	1:B:141:CYS:HG	1.55	0.53
1:A:382:TYR:C	1:A:384:ASN:H	2.12	0.53
1:A:94:GLU:O	1:A:97:LYS:HB3	2.08	0.53
1:B:334:GLU:OE1	1:B:364:ASN:HB3	2.09	0.53
1:A:431:ILE:O	1:A:435:ILE:HG13	2.09	0.53
1:A:100:LEU:HD13	1:A:100:LEU:C	2.29	0.53
1:A:530:LEU:HG	2:A:654:HOH:O	2.09	0.53
1:B:525:ILE:C	1:B:528:THR:HG22	2.30	0.52
1:A:200:ASP:O	1:A:202:SER:N	2.42	0.52
1:A:399:VAL:HG23	1:A:400:TYR:H	1.73	0.52
1:B:363:VAL:HG23	1:B:392:LEU:HB2	1.89	0.52
1:A:345:ASP:OD1	1:B:376:ARG:HB2	2.10	0.52
1:B:431:ILE:CD1	1:B:467:VAL:HG23	2.31	0.52
1:B:575:MET:HA	1:B:578:LYS:CG	2.40	0.52
1:B:439:CYS:C	1:B:441:ALA:N	2.63	0.52
1:A:499:ASP:HB3	2:A:618:HOH:O	2.10	0.52
1:B:291:TYR:O	1:B:292:LYS:HB3	2.09	0.52
1:B:361:PRO:O	1:B:362:ARG:CB	2.57	0.52
1:B:277:ASN:ND2	1:B:279:ALA:HB3	2.24	0.52
1:A:386:PHE:CE1	1:A:403:ARG:HA	2.45	0.52
1:A:381:GLU:O	1:A:384:ASN:HB3	2.09	0.52
1:B:270:PHE:CE2	1:B:328:LYS:HE2	2.45	0.52
1:B:219:LEU:O	1:B:219:LEU:HD13	2.09	0.51
1:A:537:LEU:HD12	1:A:537:LEU:N	2.25	0.51
1:A:319:ASN:HB3	1:A:322:ASP:HB2	1.93	0.51
1:A:147:ASP:OD1	1:A:150:LYS:HB2	2.09	0.51
1:A:96:ASP:HA	1:A:99:ALA:HB3	1.91	0.51
1:B:107:ASN:HA	1:B:122:TYR:OH	2.10	0.51
1:B:421:ASP:O	1:B:425:GLU:HG3	2.10	0.51
1:B:148:LEU:HD21	1:B:518:ASN:HD22	1.75	0.51
1:B:556:GLU:HG2	2:B:637:HOH:O	2.10	0.51
1:A:546:ILE:HG13	1:A:547:GLY:N	2.25	0.51
1:B:439:CYS:SG	1:B:442:TYR:CB	2.89	0.51
1:B:458:LYS:NZ	1:B:490:LEU:HD11	2.25	0.51
1:A:285:ASN:HD22	1:A:304:SER:HB3	1.76	0.51
1:B:469:ASN:ND2	1:B:507:PRO:HG3	2.25	0.51
1:B:579:LEU:HD13	1:B:579:LEU:O	2.10	0.51
1:B:552:LYS:HZ2	1:B:560:GLU:HB3	1.76	0.51
1:A:195:ASN:OD1	1:A:196:GLY:N	2.42	0.51
1:B:219:LEU:C	1:B:219:LEU:HD13	2.31	0.51
1:A:379:SER:C	1:A:381:GLU:N	2.64	0.51
1:A:326:LYS:HD2	1:A:359:LEU:HD23	1.92	0.51

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:431:ILE:HG23	1:B:432:PHE:N	2.26	0.51
1:B:554:GLN:C	1:B:556:GLU:H	2.13	0.51
1:B:546:ILE:HG23	1:B:568:SER:HB3	1.93	0.51
1:A:472:ALA:HB1	1:A:488:TYR:CD1	2.46	0.51
1:B:409:ILE:C	1:B:411:GLN:H	2.15	0.51
1:A:446:LYS:HD3	1:A:449:ASP:OD2	2.10	0.51
1:A:574:THR:HB	1:A:577:GLU:OE2	2.11	0.51
1:B:322:ASP:OD1	1:B:324:LYS:HB2	2.11	0.51
1:B:167:LYS:HE2	1:B:171:ARG:NH2	2.26	0.51
1:B:255:THR:N	2:B:660:HOH:O	2.33	0.50
1:A:514:LEU:HD12	1:A:515:LEU:N	2.26	0.50
1:B:501:ILE:O	1:B:501:ILE:HD13	2.11	0.50
1:B:270:PHE:HE2	1:B:328:LYS:HE2	1.76	0.50
1:B:408:PHE:CD1	1:B:440:LEU:HD13	2.45	0.50
1:B:597:ASP:O	1:B:599:VAL:N	2.44	0.50
1:A:575:MET:CB	1:B:576:GLU:HG2	2.41	0.50
1:A:605:GLN:HE21	1:A:605:GLN:CA	2.23	0.50
1:B:363:VAL:CG2	1:B:392:LEU:HB2	2.41	0.50
1:A:355:LYS:NZ	1:A:355:LYS:HB2	2.27	0.50
1:B:344:ASN:O	1:B:345:ASP:CB	2.49	0.50
1:A:295:PRO:O	1:A:297:SER:N	2.44	0.50
1:A:602:LYS:O	2:A:636:HOH:O	2.19	0.50
1:B:260:PHE:HE1	1:B:338:ILE:HD11	1.77	0.50
1:B:546:ILE:HG23	1:B:568:SER:CB	2.42	0.50
1:B:594:ILE:C	1:B:596:SER:H	2.15	0.50
1:A:493:GLU:O	1:A:496:ASN:ND2	2.45	0.50
1:B:263:ILE:HD13	2:B:616:HOH:O	2.12	0.50
1:A:302:ASP:O	1:A:306:THR:HG23	2.11	0.50
1:A:275:GLU:C	1:A:277:ASN:N	2.65	0.50
1:B:572:ALA:O	1:B:578:LYS:HE2	2.11	0.50
1:A:283:LEU:CD1	1:A:331:ILE:HD11	2.32	0.50
1:B:372:ILE:C	1:B:372:ILE:HD12	2.31	0.50
1:B:505:ILE:HD13	1:B:538:ASP:HB2	1.94	0.50
1:A:431:ILE:HD12	1:A:464:ALA:HB1	1.92	0.50
1:A:506:ALA:HB3	1:A:507:PRO:CD	2.36	0.50
1:B:501:ILE:HG23	1:B:502:TYR:N	2.26	0.50
1:A:415:GLN:HA	1:A:415:GLN:HE21	1.75	0.50
1:B:108:GLN:HG2	1:B:111:ARG:NH2	2.27	0.49
1:A:515:LEU:HB3	1:A:523:ASN:OD1	2.12	0.49
1:B:126:LEU:HD21	1:B:134:PHE:HB2	1.94	0.49
1:B:221:GLU:HG3	1:B:222:LYS:CD	2.42	0.49
1:B:167:LYS:HE2	1:B:171:ARG:HH22	1.77	0.49

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:532:GLU:HA	1:A:548:LEU:HD11	1.93	0.49
1:A:270:PHE:HE1	1:A:284:MET:HG2	1.77	0.49
1:B:532:GLU:O	1:B:536:LYS:HG2	2.12	0.49
1:B:131:ASP:HB3	1:B:134:PHE:CD2	2.46	0.49
1:B:266:PRO:HA	1:B:291:TYR:CE1	2.47	0.49
1:A:274:ASP:CA	1:A:280:ASP:HB3	2.38	0.49
1:A:504:GLY:O	1:A:507:PRO:HD2	2.12	0.49
1:A:345:ASP:CG	1:A:347:LEU:HB2	2.32	0.49
1:A:440:LEU:HA	2:A:670:HOH:O	2.12	0.49
1:B:163:PRO:HG3	2:B:613:HOH:O	2.13	0.49
1:A:267:GLU:C	1:A:287:LEU:HD21	2.33	0.49
1:B:444:GLU:O	1:B:446:LYS:N	2.35	0.49
1:A:566:GLU:O	1:A:569:ALA:HB3	2.13	0.49
1:B:424:LYS:HD2	1:B:434:TYR:CZ	2.48	0.49
1:A:396:ASN:HD22	1:A:399:VAL:HG13	1.77	0.49
1:A:415:GLN:NE2	1:A:415:GLN:HA	2.28	0.49
1:A:505:ILE:H	1:A:505:ILE:CD1	2.24	0.49
1:A:369:MET:O	1:A:372:ILE:HG12	2.13	0.48
1:A:347:LEU:HG	1:B:376:ARG:CB	2.43	0.48
1:A:446:LYS:HA	1:A:446:LYS:CE	2.43	0.48
1:A:585:ALA:O	1:A:589:LYS:HG3	2.12	0.48
1:A:189:LEU:HD22	1:A:203:ILE:HG13	1.94	0.48
1:A:594:ILE:HD13	1:B:187:PHE:CE2	2.47	0.48
1:A:269:THR:CG2	1:A:270:PHE:H	2.17	0.48
1:A:397:SER:HB2	1:A:426:LEU:HB3	1.95	0.48
1:A:385:TYR:HD2	1:A:388:LYS:HD2	1.77	0.48
1:B:548:LEU:HB3	1:B:564:LEU:HD13	1.95	0.48
1:B:516:THR:C	1:B:518:ASN:H	2.17	0.48
1:A:338:ILE:HD13	1:A:338:ILE:N	2.27	0.48
1:B:499:ASP:OD2	1:B:500:GLY:N	2.47	0.48
1:B:469:ASN:HD21	1:B:507:PRO:HA	1.78	0.48
1:B:598:PRO:C	1:B:600:LEU:N	2.65	0.48
1:A:454:PHE:O	1:A:458:LYS:N	2.46	0.48
1:B:251:LEU:CD2	1:B:252:PRO:HD2	2.44	0.48
1:B:598:PRO:C	1:B:600:LEU:H	2.14	0.48
1:B:505:ILE:CD1	1:B:505:ILE:N	2.77	0.48
1:A:114:LYS:HB3	1:A:114:LYS:NZ	2.28	0.48
1:B:251:LEU:HD21	1:B:339:PHE:CD2	2.48	0.48
1:B:411:GLN:O	1:B:413:TYR:N	2.39	0.48
1:A:442:TYR:C	1:A:444:GLU:H	2.17	0.48
1:B:501:ILE:CG2	1:B:502:TYR:N	2.77	0.48
1:A:251:LEU:HB3	1:A:257:MET:HE1	1.96	0.48

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:214:GLN:HE21	1:B:218:LYS:HG2	1.78	0.48
1:B:293:ARG:NH2	1:B:502:TYR:HA	2.24	0.48
1:B:430:ASN:O	1:B:433:PRO:HD2	2.14	0.48
1:A:289:ASN:ND2	1:A:300:LYS:HD2	2.29	0.47
1:A:417:GLY:HA2	1:A:420:PHE:CD1	2.49	0.47
1:B:204:GLU:N	1:B:205:PRO:HD2	2.29	0.47
1:B:114:LYS:HB3	1:B:117:ASP:CB	2.44	0.47
1:B:212:ASN:ND2	1:B:212:ASN:C	2.67	0.47
1:B:332:SER:O	1:B:336:THR:HG23	2.14	0.47
1:B:485:LEU:HD23	1:B:485:LEU:O	2.13	0.47
1:B:399:VAL:HG23	1:B:400:TYR:HD1	1.79	0.47
1:B:203:ILE:C	1:B:203:ILE:HD12	2.34	0.47
1:A:263:ILE:HG21	1:A:401:TYR:CD1	2.49	0.47
1:A:174:SER:HA	2:A:644:HOH:O	2.14	0.47
1:B:490:LEU:O	1:B:493:GLU:HB3	2.14	0.47
1:A:431:ILE:HD12	1:A:464:ALA:CB	2.44	0.47
1:A:475:LEU:HB2	1:A:484:ALA:HB2	1.96	0.47
1:A:382:TYR:C	1:A:384:ASN:N	2.66	0.47
1:B:475:LEU:HB2	1:B:484:ALA:HB2	1.96	0.47
1:B:465:PRO:C	1:B:468:PRO:HD2	2.34	0.47
1:A:417:GLY:HA2	1:A:420:PHE:HD1	1.80	0.47
1:A:505:ILE:CG2	1:A:534:ALA:HB1	2.43	0.47
1:A:384:ASN:O	1:A:387:ASP:HB3	2.13	0.47
1:B:409:ILE:CD1	1:B:410:LEU:HG	2.44	0.47
1:A:124:TRP:HA	1:A:127:GLU:HG2	1.96	0.47
1:A:549:ALA:HB2	1:A:564:LEU:CB	2.45	0.47
1:A:506:ALA:CB	1:A:507:PRO:HD3	2.36	0.47
1:A:263:ILE:HG22	1:A:263:ILE:O	2.15	0.47
1:A:512:ALA:O	1:A:516:THR:HG23	2.14	0.47
1:B:511:LYS:HA	1:B:514:LEU:HD22	1.96	0.47
1:B:190:SER:O	1:B:193:SER:HB3	2.15	0.47
1:A:289:ASN:HB3	1:A:297:SER:O	2.15	0.47
1:A:468:PRO:O	1:A:472:ALA:HB2	2.14	0.47
1:B:525:ILE:HA	1:B:528:THR:CG2	2.45	0.47
1:A:496:ASN:ND2	1:A:496:ASN:N	2.62	0.47
1:A:477:ASP:C	1:A:479:ASN:H	2.17	0.47
1:A:294:SER:OG	1:A:297:SER:HB2	2.15	0.47
1:A:393:ASP:HB3	2:A:622:HOH:O	2.15	0.47
1:A:387:ASP:O	1:A:391:LYS:HG3	2.15	0.47
1:A:195:ASN:CG	1:A:196:GLY:H	2.17	0.47
1:A:549:ALA:HA	1:A:564:LEU:HD12	1.96	0.47
1:A:416:ALA:C	1:A:418:LYS:H	2.18	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:468:PRO:CB	1:B:491:ALA:HB2	2.39	0.47
1:A:266:PRO:HA	1:A:291:TYR:CE1	2.50	0.47
1:A:292:LYS:HG3	1:A:292:LYS:O	2.15	0.47
1:B:209:ARG:HD2	1:B:213:LYS:HZ3	1.80	0.47
1:A:549:ALA:HB2	1:A:564:LEU:HB3	1.96	0.47
1:A:207:LEU:HD13	1:B:204:GLU:OE1	2.15	0.47
1:B:555:GLN:O	1:B:556:GLU:HB2	2.15	0.47
1:A:201:ALA:HA	1:A:204:GLU:CG	2.45	0.46
1:A:285:ASN:HD21	1:A:300:LYS:HZ3	1.61	0.46
1:B:525:ILE:HA	1:B:528:THR:HG22	1.97	0.46
1:A:187:PHE:O	1:A:191:VAL:HG23	2.15	0.46
1:A:292:LYS:O	1:A:293:ARG:C	2.53	0.46
1:A:289:ASN:HA	1:A:292:LYS:HD3	1.98	0.46
1:B:369:MET:SD	1:B:372:ILE:HD11	2.56	0.46
1:B:511:LYS:CE	1:B:530:LEU:HD11	2.46	0.46
1:A:266:PRO:HB3	1:A:291:TYR:CG	2.50	0.46
1:A:367:ILE:HD11	1:A:399:VAL:CG1	2.46	0.46
1:A:496:ASN:HD22	1:A:496:ASN:N	2.12	0.46
1:A:399:VAL:HG23	1:A:400:TYR:CD1	2.51	0.46
1:B:103:LYS:HB2	1:B:134:PHE:HE1	1.80	0.46
1:A:410:LEU:C	1:A:412:ASN:N	2.69	0.46
1:A:183:ALA:HB3	2:A:632:HOH:O	2.14	0.46
1:B:525:ILE:O	1:B:529:ASN:ND2	2.49	0.46
1:A:458:LYS:HG2	1:A:467:VAL:CG1	2.45	0.46
1:A:327:GLU:O	1:A:331:ILE:HG23	2.15	0.46
1:A:360:PHE:HD2	1:A:361:PRO:CD	2.26	0.46
1:A:540:ARG:CB	1:A:540:ARG:HH11	2.28	0.46
1:B:186:MET:SD	1:B:211:LEU:HA	2.55	0.46
1:A:214:GLN:HE21	1:A:218:LYS:HG2	1.80	0.46
1:B:529:ASN:HA	2:B:646:HOH:O	2.15	0.46
1:A:469:ASN:CB	1:A:503:VAL:HG11	2.46	0.46
1:A:338:ILE:HD12	1:A:368:TYR:CG	2.51	0.46
1:A:273:TYR:O	1:A:274:ASP:O	2.33	0.46
1:A:439:CYS:HB2	1:A:454:PHE:HE1	1.80	0.45
1:A:503:VAL:O	1:A:503:VAL:HG12	2.16	0.45
1:A:430:ASN:O	1:A:433:PRO:HD2	2.16	0.45
1:B:186:MET:CE	1:B:211:LEU:HA	2.46	0.45
1:A:373:MET:C	1:A:375:ASP:N	2.68	0.45
1:B:175:ALA:O	1:B:179:LEU:HD12	2.16	0.45
1:B:447:PHE:O	1:B:450:CYS:N	2.48	0.45
1:A:432:PHE:HA	1:A:435:ILE:HG13	1.98	0.45
1:A:520:THR:HB	1:A:523:ASN:HB2	1.99	0.45

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:558:ILE:O	1:A:562:ILE:HG13	2.16	0.45
1:B:212:ASN:HD21	1:B:580:GLN:HG3	1.81	0.45
1:B:98:TYR:HB3	1:B:128:LEU:CD1	2.47	0.45
1:B:402:HIS:O	1:B:405:GLN:HB2	2.15	0.45
1:A:485:LEU:O	1:A:485:LEU:HD23	2.16	0.45
1:B:157:LYS:HE3	2:B:626:HOH:O	2.16	0.45
1:B:597:ASP:OD1	1:B:597:ASP:O	2.34	0.45
1:A:605:GLN:HE21	1:A:605:GLN:HA	1.81	0.45
1:B:491:ALA:O	1:B:495:GLU:HB2	2.17	0.45
1:A:399:VAL:CG2	1:A:400:TYR:N	2.79	0.45
1:A:108:GLN:C	1:A:110:PHE:N	2.70	0.45
1:A:289:ASN:HA	1:A:292:LYS:CD	2.47	0.45
1:A:495:GLU:OE2	1:A:502:TYR:O	2.35	0.45
1:A:520:THR:HG22	1:A:522:GLU:H	1.81	0.45
1:B:594:ILE:HG22	1:B:604:ILE:HD11	1.99	0.45
1:A:558:ILE:HG12	1:A:559:ASP:N	2.30	0.45
1:B:131:ASP:OD1	1:B:133:VAL:N	2.50	0.45
1:A:469:ASN:HB2	1:A:503:VAL:HG11	1.99	0.45
1:A:461:PHE:C	2:A:671:HOH:O	2.55	0.45
1:B:393:ASP:O	1:B:396:ASN:N	2.50	0.45
1:A:596:SER:O	1:A:597:ASP:O	2.35	0.45
1:A:273:TYR:CD2	1:A:274:ASP:N	2.85	0.45
1:B:119:ILE:HG23	1:B:138:LEU:CD2	2.45	0.45
1:B:575:MET:HA	1:B:578:LYS:HB2	1.99	0.45
1:B:263:ILE:O	1:B:263:ILE:HG22	2.17	0.44
1:A:454:PHE:CE2	1:A:471:PHE:HB2	2.51	0.44
1:A:277:ASN:HD21	1:A:279:ALA:HB3	1.82	0.44
1:A:406:MET:O	1:A:410:LEU:HG	2.17	0.44
1:B:432:PHE:CD2	1:B:435:ILE:HD12	2.52	0.44
1:B:528:THR:N	2:B:657:HOH:O	2.49	0.44
1:B:96:ASP:OD2	1:B:129:LYS:HD2	2.17	0.44
1:B:438:ALA:O	1:B:450:CYS:HA	2.18	0.44
1:A:119:ILE:HG12	1:A:141:CYS:SG	2.57	0.44
1:B:533:LYS:O	1:B:536:LYS:HB2	2.18	0.44
1:A:481:PHE:HD1	1:A:481:PHE:H	1.64	0.44
1:A:465:PRO:C	1:A:468:PRO:HD2	2.37	0.44
1:B:440:LEU:O	1:B:440:LEU:HD12	2.16	0.44
1:B:443:ARG:NH2	2:B:635:HOH:O	2.49	0.44
1:A:361:PRO:CB	1:A:392:LEU:HD11	2.47	0.44
1:B:382:TYR:HA	1:B:385:TYR:CD1	2.53	0.44
1:A:500:GLY:HA3	1:A:502:TYR:CE1	2.50	0.44
1:A:520:THR:O	1:A:521:VAL:C	2.56	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:399:VAL:HG23	1:B:400:TYR:CD1	2.53	0.44
1:B:331:ILE:CG2	1:B:362:ARG:NE	2.80	0.44
1:A:590:VAL:O	1:A:594:ILE:HG12	2.18	0.44
1:A:263:ILE:HD12	1:A:263:ILE:H	1.83	0.44
1:A:407:ASN:O	1:A:412:ASN:HB3	2.18	0.44
1:A:582:ILE:HD12	1:B:219:LEU:HB2	1.99	0.44
1:B:378:ASP:HB2	2:B:667:HOH:O	2.17	0.44
1:B:379:SER:C	1:B:381:GLU:H	2.20	0.44
1:A:475:LEU:CB	1:A:484:ALA:HB2	2.48	0.44
1:A:283:LEU:HD11	1:A:331:ILE:CD1	2.35	0.44
1:B:353:ILE:HD11	1:B:369:MET:HB2	1.99	0.44
1:A:521:VAL:HG23	1:A:522:GLU:N	2.33	0.44
1:B:293:ARG:O	1:B:294:SER:O	2.35	0.44
1:A:119:ILE:CG2	1:A:123:ASN:HD21	2.30	0.44
1:A:99:ALA:HA	1:A:128:LEU:HD12	2.00	0.44
1:B:177:GLU:HB2	1:B:210:ASN:OD1	2.17	0.44
1:A:269:THR:HG23	1:A:270:PHE:N	2.19	0.44
1:B:104:ASP:O	1:B:108:GLN:HG3	2.18	0.44
1:B:399:VAL:HG23	1:B:400:TYR:N	2.27	0.44
1:A:404:GLY:O	1:A:408:PHE:HB2	2.18	0.44
1:A:469:ASN:HD22	1:A:507:PRO:CG	2.19	0.44
1:A:439:CYS:SG	1:A:474:ILE:HD13	2.58	0.43
1:A:583:THR:HG22	1:B:215:ALA:CB	2.47	0.43
1:A:267:GLU:O	1:A:268:LEU:HG	2.17	0.43
1:B:201:ALA:HA	2:B:621:HOH:O	2.18	0.43
1:A:524:PHE:HA	1:A:524:PHE:HD2	1.73	0.43
1:B:410:LEU:C	1:B:412:ASN:N	2.71	0.43
1:A:114:LYS:HB3	1:A:117:ASP:OD1	2.17	0.43
1:A:312:PHE:CE1	1:A:328:LYS:HB3	2.53	0.43
1:A:279:ALA:HB3	1:A:315:GLN:HE22	1.84	0.43
1:A:496:ASN:HD22	1:A:497:LYS:N	2.16	0.43
1:A:170:LEU:O	1:A:170:LEU:HD23	2.19	0.43
1:B:504:GLY:O	1:B:507:PRO:HD2	2.18	0.43
1:A:186:MET:SD	1:A:211:LEU:HA	2.58	0.43
1:B:548:LEU:CB	1:B:564:LEU:HD13	2.47	0.43
1:A:406:MET:O	1:A:409:ILE:HG12	2.18	0.43
1:B:496:ASN:C	1:B:498:LEU:H	2.20	0.43
1:A:279:ALA:HB2	1:A:311:LEU:HB3	2.00	0.43
1:B:505:ILE:CG2	1:B:509:VAL:HG23	2.48	0.43
1:B:445:ASN:ND2	2:B:668:HOH:O	2.52	0.43
1:A:111:ARG:HH11	1:A:111:ARG:HG3	1.83	0.43
1:A:113:LYS:HD2	1:A:113:LYS:N	2.34	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:558:ILE:N	1:B:558:ILE:CD1	2.80	0.43
1:A:605:GLN:NE2	1:A:605:GLN:HA	2.33	0.43
1:A:461:PHE:N	2:A:671:HOH:O	2.47	0.43
1:B:537:LEU:O	1:B:539:PRO:HD3	2.17	0.43
1:B:591:GLN:OE1	1:B:591:GLN:HA	2.17	0.43
1:A:501:ILE:O	1:A:502:TYR:C	2.56	0.43
1:B:515:LEU:HB3	1:B:527:ALA:HB2	2.01	0.43
1:A:600:LEU:HD11	1:B:194:LEU:HD12	2.00	0.43
1:A:525:ILE:CA	1:A:528:THR:HG22	2.47	0.43
1:A:558:ILE:CG1	1:A:559:ASP:N	2.82	0.43
1:B:475:LEU:CB	1:B:484:ALA:HB2	2.49	0.43
1:B:453:LEU:HD12	1:B:453:LEU:HA	1.92	0.43
1:A:404:GLY:HA3	1:A:420:PHE:CE2	2.54	0.43
1:B:520:THR:HG22	1:B:521:VAL:N	2.34	0.43
1:A:105:LYS:HD3	1:A:121:TYR:CE2	2.46	0.43
1:B:572:ALA:HB1	1:B:577:GLU:HB2	2.01	0.43
1:A:108:GLN:C	1:A:110:PHE:H	2.21	0.43
1:A:600:LEU:HD13	1:A:600:LEU:O	2.19	0.43
1:B:342:LEU:HA	1:B:342:LEU:HD23	1.88	0.43
1:B:505:ILE:HG22	1:B:505:ILE:O	2.18	0.43
1:A:285:ASN:HD21	1:A:300:LYS:HZ2	1.66	0.42
1:A:503:VAL:HG12	1:A:507:PRO:CD	2.47	0.42
1:A:390:LEU:HD21	1:A:399:VAL:CG2	2.42	0.42
1:B:437:LEU:CD2	1:B:440:LEU:HD23	2.42	0.42
1:B:295:PRO:O	1:B:297:SER:N	2.49	0.42
1:A:411:GLN:HA	1:A:413:TYR:CE2	2.54	0.42
1:B:179:LEU:HD12	1:B:179:LEU:N	2.34	0.42
1:B:345:ASP:OD1	1:B:347:LEU:HB2	2.19	0.42
1:B:516:THR:C	1:B:518:ASN:N	2.72	0.42
1:B:552:LYS:HG3	1:B:564:LEU:CD1	2.50	0.42
1:B:100:LEU:HD13	1:B:100:LEU:C	2.38	0.42
1:B:442:TYR:C	1:B:444:GLU:N	2.73	0.42
1:A:484:ALA:O	1:A:488:TYR:HD1	2.01	0.42
1:B:404:GLY:O	1:B:408:PHE:HB2	2.19	0.42
1:B:537:LEU:C	1:B:539:PRO:HD3	2.40	0.42
1:A:329:LEU:HD22	1:A:329:LEU:O	2.19	0.42
1:B:520:THR:H	1:B:523:ASN:HB2	1.84	0.42
1:A:410:LEU:O	1:A:412:ASN:N	2.52	0.42
1:B:362:ARG:HG2	1:B:362:ARG:HH11	1.84	0.42
1:B:552:LYS:HG3	1:B:564:LEU:HD12	2.02	0.42
1:A:263:ILE:HG12	1:A:401:TYR:CE1	2.54	0.42
1:B:565:PHE:HB3	1:B:585:ALA:HB2	2.00	0.42

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:139:SER:O	1:B:143:VAL:HG23	2.20	0.42
1:B:442:TYR:C	1:B:444:GLU:H	2.21	0.42
1:A:488:TYR:HE2	1:A:510:GLY:HA3	1.85	0.42
1:B:515:LEU:HD12	1:B:523:ASN:O	2.20	0.42
1:B:260:PHE:HE1	1:B:338:ILE:HD12	1.85	0.42
1:B:431:ILE:HG12	1:B:435:ILE:CD1	2.46	0.42
1:B:376:ARG:NH2	1:B:377:ASN:HB3	2.20	0.42
1:A:446:LYS:CA	1:A:446:LYS:HE2	2.49	0.42
1:B:554:GLN:C	1:B:556:GLU:N	2.73	0.42
1:B:555:GLN:HA	1:B:555:GLN:HE21	1.84	0.42
1:A:511:LYS:HD3	1:A:530:LEU:CD1	2.50	0.42
1:B:432:PHE:HD2	1:B:435:ILE:HD12	1.85	0.42
1:A:294:SER:HA	1:A:295:PRO:HD3	1.91	0.42
1:B:478:LYS:CE	1:B:478:LYS:HA	2.39	0.42
1:B:417:GLY:HA2	1:B:437:LEU:HD21	2.00	0.42
1:A:385:TYR:CD2	1:A:388:LYS:HD2	2.55	0.42
1:B:374:ALA:CB	1:B:406:MET:HE1	2.50	0.42
1:A:201:ALA:HA	1:A:204:GLU:HG2	2.02	0.42
1:A:199:ASN:O	1:A:200:ASP:HB2	2.20	0.42
1:B:550:GLN:NE2	2:B:645:HOH:O	2.52	0.42
1:A:364:ASN:HB3	1:A:368:TYR:CE2	2.54	0.41
1:A:396:ASN:ND2	1:A:398:SER:OG	2.53	0.41
1:B:360:PHE:O	1:B:361:PRO:C	2.58	0.41
1:A:326:LYS:O	1:A:330:ALA:N	2.52	0.41
1:A:574:THR:CB	1:A:577:GLU:OE2	2.68	0.41
1:A:122:TYR:O	1:A:126:LEU:HG	2.20	0.41
1:B:435:ILE:HG13	1:B:435:ILE:H	1.67	0.41
1:A:285:ASN:ND2	1:A:300:LYS:NZ	2.65	0.41
1:A:505:ILE:N	1:A:505:ILE:CD1	2.80	0.41
1:A:251:LEU:H	1:A:251:LEU:CD1	2.34	0.41
1:A:603:LYS:C	2:A:636:HOH:O	2.58	0.41
1:B:341:PHE:CE2	1:B:372:ILE:HA	2.54	0.41
1:A:386:PHE:O	1:A:390:LEU:HG	2.19	0.41
1:A:98:TYR:CD1	1:A:101:ALA:HB3	2.55	0.41
1:B:410:LEU:O	1:B:412:ASN:N	2.54	0.41
1:A:270:PHE:CD2	1:A:270:PHE:O	2.74	0.41
1:B:134:PHE:O	1:B:138:LEU:HB2	2.20	0.41
1:B:519:PRO:HB3	1:B:524:PHE:CZ	2.54	0.41
1:A:444:GLU:CD	2:A:656:HOH:O	2.58	0.41
1:A:603:LYS:HA	2:A:636:HOH:O	2.21	0.41
1:B:353:ILE:HD12	1:B:353:ILE:C	2.41	0.41
1:B:478:LYS:O	1:B:479:ASN:HB2	2.21	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:204:GLU:HB3	1:B:205:PRO:CD	2.51	0.41
1:B:370:ALA:HB1	1:B:386:PHE:CE1	2.55	0.41
1:A:531:LEU:HD13	1:A:547:GLY:HA3	2.02	0.41
1:B:465:PRO:O	1:B:468:PRO:HD2	2.19	0.41
1:B:525:ILE:CA	1:B:528:THR:HG22	2.51	0.41
1:B:131:ASP:HA	1:B:132:PRO:HD3	1.91	0.41
1:A:478:LYS:CE	1:A:478:LYS:HA	2.29	0.41
1:A:440:LEU:HD23	1:A:441:ALA:N	2.36	0.41
1:B:520:THR:HB	1:B:523:ASN:H	1.85	0.41
1:A:279:ALA:HB2	1:A:311:LEU:CB	2.50	0.41
1:A:277:ASN:HD21	1:A:315:GLN:HE22	1.68	0.41
1:A:421:ASP:O	1:A:425:GLU:HG2	2.20	0.41
1:B:493:GLU:HG3	2:B:652:HOH:O	2.19	0.41
1:A:442:TYR:C	1:A:444:GLU:N	2.74	0.41
1:A:431:ILE:HD11	1:A:467:VAL:HG23	2.02	0.41
1:A:492:ILE:HG12	1:A:507:PRO:HB2	2.03	0.41
1:B:333:LEU:HD11	1:B:355:LYS:HD2	2.03	0.41
1:B:503:VAL:HG12	1:B:507:PRO:CD	2.48	0.41
1:B:600:LEU:HD23	1:B:600:LEU:HA	1.88	0.41
1:A:565:PHE:CE1	1:A:584:PHE:HB3	2.55	0.41
1:B:253:SER:O	1:B:256:SER:OG	2.35	0.41
1:A:437:LEU:O	1:A:438:ALA:C	2.59	0.41
1:A:341:PHE:CD1	1:A:341:PHE:C	2.94	0.41
1:B:375:ASP:O	1:B:376:ARG:O	2.39	0.41
1:A:312:PHE:HB2	1:A:329:LEU:HD23	2.01	0.41
1:A:393:ASP:HB2	1:A:396:ASN:HB2	2.03	0.41
1:B:547:GLY:O	1:B:551:MET:HG2	2.21	0.41
1:B:500:GLY:HA3	1:B:502:TYR:HE1	1.86	0.41
1:B:502:TYR:O	1:B:504:GLY:N	2.53	0.41
1:A:420:PHE:CE1	1:A:436:GLN:HG2	2.55	0.41
1:B:109:PHE:CD1	1:B:117:ASP:HB3	2.56	0.41
1:A:529:ASN:HB3	2:A:654:HOH:O	2.21	0.41
1:B:424:LYS:HD2	1:B:434:TYR:CE2	2.55	0.41
1:A:434:TYR:O	1:A:438:ALA:HB2	2.20	0.41
1:A:503:VAL:O	1:A:504:GLY:O	2.39	0.41
1:B:341:PHE:CG	1:B:372:ILE:HG22	2.56	0.40
1:A:280:ASP:OD1	1:A:328:LYS:HD3	2.21	0.40
1:B:505:ILE:CG2	1:B:534:ALA:HB1	2.51	0.40
1:B:295:PRO:C	1:B:297:SER:N	2.75	0.40
1:B:486:LYS:HE3	2:B:614:HOH:O	2.19	0.40
1:B:549:ALA:O	1:B:553:LEU:HB2	2.20	0.40
1:B:263:ILE:H	1:B:263:ILE:HD12	1.84	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:464:ALA:HA	1:A:465:PRO:HD3	1.93	0.40
1:A:465:PRO:O	1:A:468:PRO:HD2	2.22	0.40
1:A:345:ASP:HA	1:A:346:PRO:HD3	1.85	0.40
1:A:204:GLU:N	1:A:205:PRO:CD	2.84	0.40
1:A:454:PHE:O	1:A:458:LYS:HB2	2.21	0.40
1:A:519:PRO:HB3	1:A:524:PHE:CZ	2.57	0.40
1:A:126:LEU:HD21	1:A:134:PHE:HB2	2.03	0.40
1:B:480:ASP:O	1:B:482:ASP:N	2.53	0.40
1:A:327:GLU:HG3	1:A:360:PHE:CD1	2.57	0.40
1:A:453:LEU:HD12	1:A:453:LEU:HA	1.94	0.40
1:B:381:GLU:OE1	1:B:384:ASN:HB3	2.20	0.40
1:B:162:LYS:HD3	1:B:165:TYR:CD2	2.56	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	483/514 (94%)	377 (78%)	81 (17%)	25 (5%)	3	18
1	B	483/514 (94%)	385 (80%)	63 (13%)	35 (7%)	2	8
All	All	966/1028 (94%)	762 (79%)	144 (15%)	60 (6%)	2	13

All (60) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	195	ASN
1	A	201	ALA
1	A	274	ASP
1	A	361	PRO
1	A	397	SER
1	A	504	GLY
1	A	597	ASP
1	B	95	LYS

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Mol	Chain	Res	Type
1	B	274	ASP
1	B	294	SER
1	B	345	ASP
1	B	361	PRO
1	B	376	ARG
1	B	598	PRO
1	A	380	THR
1	A	495	GLU
1	A	502	TYR
1	B	195	ASN
1	B	200	ASP
1	B	252	PRO
1	B	276	SER
1	B	412	ASN
1	B	445	ASN
1	B	446	LYS
1	B	503	VAL
1	B	595	ARG
1	A	199	ASN
1	A	270	PHE
1	A	293	ARG
1	A	294	SER
1	A	438	ALA
1	A	501	ILE
1	B	277	ASN
1	B	344	ASN
1	B	481	PHE
1	B	500	GLY
1	B	502	TYR
1	B	541	SER
1	A	343	LYS
1	A	345	ASP
1	A	411	GLN
1	A	427	ASP
1	A	462	PRO
1	B	113	LYS
1	B	378	ASP
1	B	413	TYR
1	B	414	ASP
1	A	268	LEU
1	A	291	TYR
1	A	296	GLU

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Mol	Chain	Res	Type
1	B	362	ARG
1	B	394	SER
1	B	555	GLN
1	B	597	ASP
1	B	266	PRO
1	B	411	GLN
1	B	504	GLY
1	B	462	PRO
1	B	558	ILE
1	A	521	VAL

### 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	425/448 (95%)	380 (89%)	45 (11%)	10	36
1	B	425/448 (95%)	391 (92%)	34 (8%)	17	53
All	All	850/896 (95%)	771 (91%)	79 (9%)	13	45

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	98	TYR
1	A	100	LEU
1	A	113	LYS
1	A	116	ASP
1	A	155	SER
1	A	165	TYR
1	A	198	PHE
1	A	219	LEU
1	A	270	PHE
1	A	274	ASP
1	A	283	LEU
1	A	290	LEU
1	A	334	GLU
1	A	347	LEU
1	A	352	ASP

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Mol	Chain	Res	Type
1	A	353	ILE
1	A	357	ILE
1	A	360	PHE
1	A	361	PRO
1	A	376	ARG
1	A	393	ASP
1	A	430	ASN
1	A	440	LEU
1	A	446	LYS
1	A	454	PHE
1	A	476	THR
1	A	478	LYS
1	A	490	LEU
1	A	495	GLU
1	A	496	ASN
1	A	499	ASP
1	A	501	ILE
1	A	502	TYR
1	A	524	PHE
1	A	532	GLU
1	A	536	LYS
1	A	540	ARG
1	A	543	GLN
1	A	555	GLN
1	A	558	ILE
1	A	566	GLU
1	A	573	ARG
1	A	574	THR
1	A	600	LEU
1	A	605	GLN
1	B	98	TYR
1	B	104	ASP
1	B	116	ASP
1	B	165	TYR
1	B	212	ASN
1	B	290	LEU
1	B	316	LEU
1	B	329	LEU
1	B	331	ILE
1	B	338	ILE
1	B	345	ASP
1	B	347	LEU

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Mol	Chain	Res	Type
1	B	352	ASP
1	B	353	ILE
1	B	361	PRO
1	B	393	ASP
1	B	396	ASN
1	B	430	ASN
1	B	439	CYS
1	B	453	LEU
1	B	454	PHE
1	B	478	LYS
1	B	488	TYR
1	B	490	LEU
1	B	495	GLU
1	B	501	ILE
1	B	514	LEU
1	B	515	LEU
1	B	538	ASP
1	B	550	GLN
1	B	553	LEU
1	B	555	GLN
1	B	558	ILE
1	B	566	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	107	ASN
1	A	123	ASN
1	A	137	ASN
1	A	212	ASN
1	A	277	ASN
1	A	285	ASN
1	A	289	ASN
1	A	315	GLN
1	A	384	ASN
1	A	396	ASN
1	A	415	GLN
1	A	430	ASN
1	A	469	ASN
1	A	479	ASN
1	A	496	ASN
1	A	543	GLN

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Mol	Chain	Res	Type
1	A	580	GLN
1	A	605	GLN
1	B	108	GLN
1	B	123	ASN
1	B	137	ASN
1	B	212	ASN
1	B	214	GLN
1	B	277	ASN
1	B	315	GLN
1	B	377	ASN
1	B	396	ASN
1	B	405	GLN
1	B	407	ASN
1	B	415	GLN
1	B	430	ASN
1	B	469	ASN
1	B	479	ASN
1	B	518	ASN
1	B	529	ASN
1	B	555	GLN
1	B	580	GLN
1	B	605	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 ⓘ

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 ⓘ

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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	487/514 (94%)	-0.08	4 (0%) 83 26	40, 76, 125, 154	0
1	B	487/514 (94%)	-0.13	0 100 100	36, 74, 123, 162	0
All	All	974/1028 (94%)	-0.11	4 (0%) 90 41	36, 75, 125, 162	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	98	TYR	2.9
1	A	439	CYS	2.5
1	A	121	TYR	2.3
1	A	438	ALA	2.1

### 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 ⓘ

There are no ligands in this entry.

### 6.5 Other polymers ⓘ

There are no such residues in this entry.