



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:01 PM UTC

PDB ID : 2GW1 / pdb_00002gw1
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 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)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

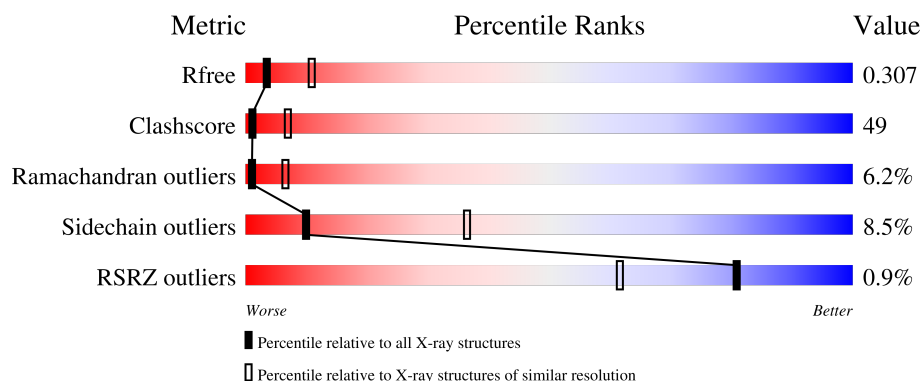
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

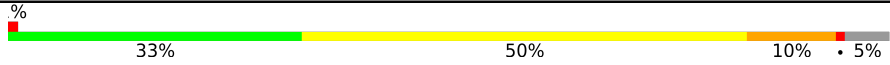
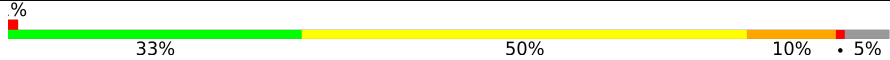
The reported resolution of this entry is 3.00 Å.

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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 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 $\leq 5\%$. 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	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 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 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			

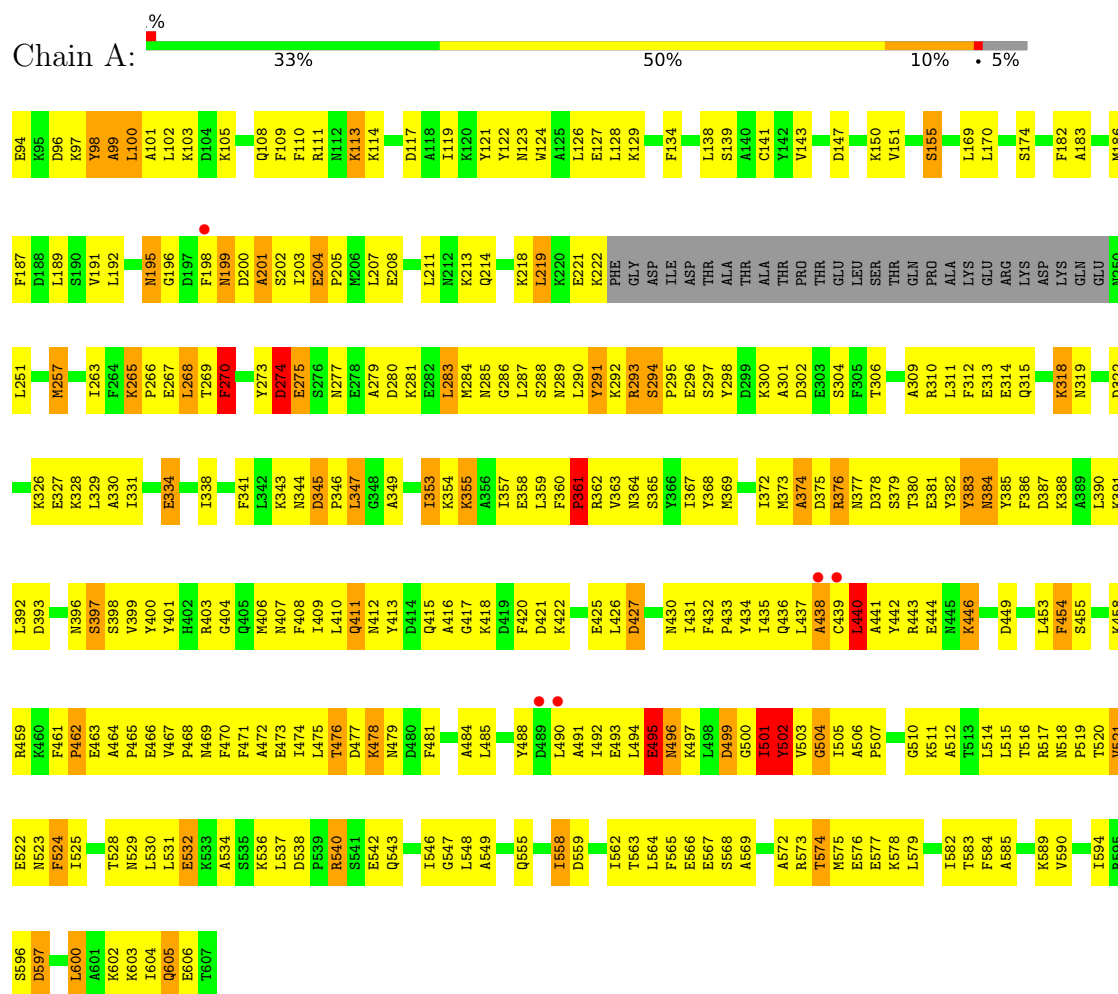
- Molecule 2 is water.

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

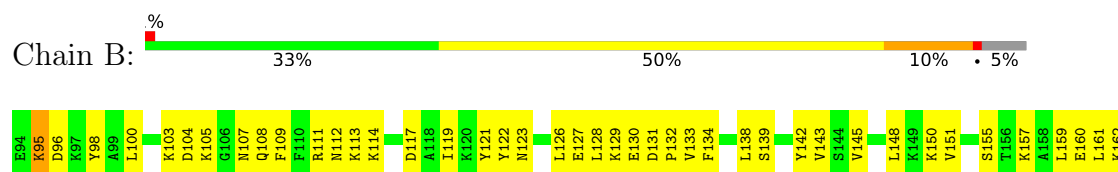
3 Residue-property plots

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 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: Mitochondrial precursor proteins import receptor



- Molecule 1: Mitochondrial precursor proteins import receptor



M575	E576	E577	K578	L579	Q580	A585	E586	A587	V590	Q591	T594	R595	S596	P597	P598	V599	L600	A601	I604	T607																																					
G510	K511	A512	T513	L514	L515	T516	R517	N518	P519	T520	V521	E522	N523	F524	E525	T526	N527	L528	L529	S530	E531	E532	K533	A534	S535	K536	L537	P538	P539	R540	S541	K545	I546	Q547	L548	A549	Q550	R551	K552	L553	Q554	E555	E556	P557	L558	D559	E560	T563	L564	F565	E566	E567	S568	L571	A572	V509	
F447	D448	D449	C450	L453	F454	K458	R459	K460	F461	P462	E463	A464	P465	E466	V467	P468	F470	F471	A472	E473	L474	L475	T476	D477	K478	N479	D480	F481	D482	K483	A484	Q485	K486	Q487	Y488	D489	L490	A491	L492	E493	L494	E495	N496	L497	L498	D499	G500	I501	Y502	V503	G504	A441	Y442	R443	E444	N445	K446
Y383	N384	Y385	F386	D387	L390	K391	L392	D393	S394	N395	N396	V399	Y400	Y401	H402	R403	G404	Q405	M406	N407	F408	T409	L410	Q411	N412	Y413	D414	Q417	R418	D419	F420	D421	K422	L423	K424	E425	L426	D427	N430	T431	F432	P433	Y434	T435	Q436	L437	A438	C439	L440	A441	Y442	R443	E444	N445	K446		
L311	L316	D322	E323	K324	E327	K328	L329	A330	I331	S332	L333	E334	H335	T336	G337	I338	F339	K340	F341	L342	K343	N344	D345	P346	L347	G348	A349	I353	E354	K355	A356	I357	F360	P361	R362	V363	N364	I367	Y368	M369	A370	L371	I372	K373	A374	D375	R376	N377	D378	S379	T380	Y382					
THR	PRO	THR	GLU	LEU	SER	THR	GLN	PRO	ALA	LYS	GLU	ARG	LYS	ASP	LYS	GLN	N250	L251	P252	S253	V254	T255	S256	M257	F260	P261	Q262	I263	P266	E267	L268	T269	F270	Y273	D274	E275	S276	N277	E278	A279	D280	K281	N289	L290	Y291	K292	R293	S294	P295	F296	S297	D302					
P163	D164	Y165	S166	K167	R171	A175	N176	E177	G178	L179	F182	M186	F187	S190	V191	L192	S193	L194	N195	G196	D197	F198	N199	D200	A201	S202	L203	E204	P205	E208	R209	N210	L211	N212	K213	Q214	A215	K216	S217	K218	L219	K220	E221	K222	PHE	GLY	ASP	ILE	ASP	THR	ALA	ALA					

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	44.88Å 168.60Å 82.99Å 90.00° 102.59° 90.00°	Depositor
Resolution (Å)	46.17 – 3.00 46.17 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.0 (46.17-3.00) 97.0 (46.17-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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	1221 reflections (4.84%)	wwPDB-VP
Wilson B-factor (Å ²)	83.2	Xtriage
Anisotropy	0.200	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 61.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	7984	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

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	0.33	0/3999	0.89	11/5379 (0.2%)
1	B	0.32	0/3999	0.88	14/5379 (0.3%)
All	All	0.32	0/7998	0.88	25/10758 (0.2%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	221	GLU	N-CA-C	-10.70	100.23	113.18
1	B	343	LYS	N-CA-C	-8.81	102.44	113.01
1	B	599	VAL	N-CA-C	-8.50	101.95	113.00
1	B	440	LEU	N-CA-C	-7.81	103.63	113.01
1	A	99	ALA	N-CA-C	-7.48	102.49	111.69
1	A	275	GLU	N-CA-C	-6.64	96.66	110.80
1	A	443	ARG	N-CA-C	-6.58	105.36	113.19
1	A	440	LEU	N-CA-C	-6.48	103.49	111.33
1	B	460	LYS	N-CA-C	-6.45	105.99	114.31
1	A	383	TYR	N-CA-C	-6.40	105.58	113.19
1	A	265	LYS	N-CA-C	-6.03	102.06	109.65
1	B	293	ARG	CB-CA-C	-5.86	109.81	116.54
1	B	538	ASP	CA-C-N	5.70	125.41	119.82
1	B	538	ASP	C-N-CA	5.70	125.41	119.82
1	A	318	LYS	N-CA-C	-5.54	106.36	113.23
1	B	383	TYR	N-CA-C	-5.53	106.21	113.12
1	B	471	PHE	N-CA-C	-5.47	104.84	112.45
1	B	273	TYR	N-CA-C	5.31	117.40	109.59
1	B	443	ARG	N-CA-C	-5.23	106.60	112.87
1	A	376	ARG	N-CA-C	5.17	117.53	109.52
1	B	127	GLU	N-CA-C	-5.13	107.15	113.41
1	B	597	ASP	CA-C-N	5.13	126.25	119.84
1	B	597	ASP	C-N-CA	5.13	126.25	119.84
1	A	374	ALA	N-CA-C	-5.02	106.25	112.38
1	A	384	ASN	N-CA-C	-5.00	107.56	113.97

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	3929	0	3885	405	0
1	B	3929	0	3885	380	0
2	A	65	0	0	25	0
2	B	61	0	0	25	0
All	All	7984	0	7770	771	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 49.

All (771) 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: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:A:469:ASN:HD22	1:A:507:PRO:HG3	1.35	0.91
1:B:558:ILE:HG12	1:B:559:ASP:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:468:PRO:HB2	1:B:491:ALA:HB2	1.58	0.84
1:A:251:LEU:HD23	1:A:257:MET:HE1	1.60	0.83
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:344:ASN:CG	1:A:345:ASP:H	1.88	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: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:A:222:LYS:HB2	2:A:651:HOH:O	1.84	0.76
1:B:558:ILE:HG12	1:B:559:ASP:N	1.99	0.76
1:A:273:TYR:CE2	1:A:274:ASP:HB3	2.21	0.75
1:A:341:PHE:CD2	1:A:372:ILE:HG22	2.21	0.75
1:B:367:ILE:HD11	1:B:399:VAL:HG12	1.67	0.75
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:467:VAL:HB	1:B:468:PRO:HD3	1.68	0.74
1:A:379:SER:C	1:A:381:GLU:H	1.96	0.74
1:B:506:ALA:HB3	1:B:507:PRO:HD3	1.68	0.74
1:B:382:TYR:CE2	1:B:406:MET:HE2	2.22	0.74
1:A:427:ASP:OD2	1:A:430:ASN:HB2	1.87	0.73
1:B:293:ARG:HH21	1:B:502:TYR:HA	1.53	0.73
1:A:139:SER:O	1:A:143:VAL:HG23	1.89	0.73
1:A:207:LEU:HD13	1:B:204:GLU:CD	2.14	0.73
1:A:420:PHE:CZ	1:A:436:GLN:HG2	2.24	0.73
1:B:253:SER:HB2	2:B:660:HOH:O	1.87	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:B:551:MET:HE3	2:B:662:HOH:O	1.86	0.73
1:A:396:ASN:O	1:A:399:VAL:HG22	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:119:ILE:HG22	1:A:123:ASN:ND2	2.06	0.71
1:A:594:ILE:HG22	1:A:604:ILE:HD11	1.72	0.71
1:B:217:SER:O	1:B:220:LYS:HG2	1.90	0.71
1:A:275:GLU:C	1:A:277:ASN:H	1.99	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:360:PHE:HD2	1:A:361:PRO:HD2	1.56	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:A:214:GLN:HG3	1:B:586:GLU:HG2	1.72	0.70
1:B:463:GLU:HA	1:B:494:LEU:HD22	1.73	0.70
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:B:596:SER:O	1:B:597:ASP:C	2.35	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: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
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:353:ILE:HD11	1:B:369:MET:HE2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:151:VAL:O	1:A:155:SER:HB2	1.96	0.66
1:B:503:VAL:HG12	1:B:507:PRO:HD3	1.77	0.66
1:B:431:ILE:HD13	1:B:466:GLU:HB2	1.77	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:B:376:ARG:HE	1:B:377:ASN:N	1.93	0.66
1:A:441:ALA:HA	2:A:656:HOH:O	1.95	0.65
1:B:119:ILE:HG23	1:B:138:LEU:HD21	1.78	0.65
1:B:511:LYS:O	1:B:515:LEU:HB2	1.95	0.65
1:B:212:ASN:C	1:B:212:ASN:HD22	2.04	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:219:LEU:HD12	1:B:579:LEU:HD23	1.79	0.65
1:A:399:VAL:HG23	1:A:400:TYR:N	2.12	0.65
1:A:318:LYS:O	1:A:318:LYS:HD3	1.96	0.65
1:B:382:TYR:HE2	1:B:406:MET:HE2	1.59	0.65
1:B:263:ILE:N	1:B:263:ILE:HD12	2.11	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
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:114:LYS:HB3	1:B:117:ASP:HB2	1.79	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:142:TYR:CD1	1:B:150:LYS:HB3	2.33	0.64
1:B:316:LEU:HD12	1:B:329:LEU:HD12	1.80	0.64
1:B:556:GLU:HA	2:B:637:HOH:O	1.98	0.64
1:B:558:ILE:CG1	1:B:559:ASP:H	2.09	0.64
1:A:431:ILE:HD13	1:A:466:GLU:HB2	1.80	0.64
1:A:182:PHE:CE1	1:A:213:LYS:HB3	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:459:ARG:O	1:A:462:PRO:HD3	1.98	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: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:A:353:ILE:HD11	1:A:369:MET:HE2	1.80	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:277:ASN:HD21	1:B:279:ALA:HB3	1.65	0.62
1:B:505:ILE:HG22	1:B:509:VAL:HG23	1.81	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:N	1:A:505:ILE:HD12	2.15	0.61
1:B:406:MET:O	1:B:409:ILE:HG13	1.99	0.61
1:B:387:ASP:HA	1:B:390:LEU:HD12	1.83	0.61
1:B:505:ILE:HD12	1:B:505:ILE:N	2.15	0.61
1:A:147:ASP:O	1:A:151:VAL:HG23	2.00	0.61
1:A:204:GLU:N	1:A:205:PRO:HD2	2.16	0.61
1:B:204:GLU:HG2	1:B:208:GLU:OE2	2.01	0.61
1:A:344:ASN:CG	1:A:345:ASP:N	2.57	0.61
1:A:287:LEU:HD23	1:A:287:LEU:O	1.99	0.61
1:B:105:LYS:HD3	1:B:121:TYR:CE2	2.36	0.61
1:A:502:TYR:CD1	1:A:502:TYR:N	2.67	0.61
1:B:555:GLN:HE21	1:B:555:GLN:CA	2.14	0.61
1:A:431:ILE:HG12	1:A:435:ILE:HD11	1.83	0.61
1:A:295:PRO:C	1:A:297:SER:H	2.09	0.60
1:B:221:GLU:C	1:B:222:LYS:HD2	2.26	0.60
1:A:525:ILE:HA	1:A:528:THR:HG22	1.83	0.60
1:B:105:LYS:HA	1:B:108:GLN:NE2	2.14	0.60
1:B:295:PRO:C	1:B:297:SER:H	2.09	0.60
1:B:489:ASP:HA	1:B:492:ILE:HD12	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:446:LYS:HE2	1:A:446:LYS:HA	1.82	0.60
1:B:119:ILE:HG22	1:B:123:ASN:HD22	1.67	0.60
1:B:182:PHE:HE2	1:B:213:LYS:HD3	1.67	0.60
1:B:449:ASP:O	1:B:453:LEU:HB2	2.00	0.60
1:B:558:ILE:HD13	1:B:558:ILE:N	2.17	0.60
1:B:268:LEU:N	1:B:268:LEU:HD12	2.16	0.60
1:B:410:LEU:C	1:B:412:ASN:H	2.10	0.60
1:B:454:PHE:O	1:B:458:LYS:HB2	2.01	0.60
1:A:422:LYS:O	1:A:426:LEU:HD13	2.02	0.59
1:A:468:PRO:HG2	1:A:494:LEU:HD12	1.84	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:200:ASP:C	1:A:202:SER:H	2.11	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:B:342:LEU:C	1:B:344:ASN:N	2.58	0.59
1:A:594:ILE:CG2	1:A:604:ILE:HD11	2.33	0.59
1:B:342:LEU:C	1:B:344:ASN:H	2.11	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:334:GLU:HG3	1:A:365:SER:OG	2.02	0.58
1:A:500:GLY:HA3	1:A:502:TYR:HE1	1.68	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:A:410:LEU:C	1:A:412:ASN:H	2.10	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:379:SER:O	1:A:381:GLU:N	2.36	0.58
1:A:505:ILE:CD1	1:A:538:ASP:HB2	2.34	0.58
1:A:100:LEU:C	1:A:100:LEU:HD13	2.29	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:293:ARG:HB3	1:A:501:ILE:HB	1.85	0.58
1:A:439:CYS:HB2	1:A:454:PHE:CE1	2.38	0.58
1:A:382:TYR:C	1:A:384:ASN:H	2.12	0.57
1:A:511:LYS:HD3	1:A:530:LEU:HD11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:130:GLU:HB3	2:B:630:HOH:O	2.03	0.57
1:A:263:ILE:HD12	1:A:263:ILE:N	2.19	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:542:GLU:OE2	1:A:572:ALA:HB2	2.04	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:439:CYS:C	1:B:441:ALA:H	2.11	0.57
1:B:552:LYS:NZ	1:B:560:GLU:HB3	2.20	0.57
1:A:468:PRO:HB2	1:A:491:ALA:HB2	1.85	0.57
1:B:145:VAL:HG12	1:B:145:VAL:O	2.03	0.57
1:B:525:ILE:C	1:B:528:THR:HG22	2.30	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:A:505:ILE:HD12	1:A:505:ILE:H	1.70	0.57
1:B:107:ASN:O	1:B:111:ARG:HG3	2.05	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:334:GLU:OE2	1:A:364:ASN:HB2	2.06	0.56
1:A:491:ALA:O	1:A:495:GLU:HB2	2.05	0.56
1:B:273:TYR:CE2	1:B:274:ASP:HB2	2.39	0.56
1:B:331:ILE:CG2	1:B:362:ARG:HE	2.18	0.56
1:B:422:LYS:O	1:B:422:LYS:HD3	2.05	0.56
1:B:601:ALA:HA	1:B:604:ILE:HD12	1.88	0.56
1:A:211:LEU:HD22	1:B:208:GLU:OE1	2.06	0.56
1:A:367:ILE:HD11	1:A:399:VAL:HG12	1.87	0.56
1:A:354:LYS:O	1:A:358:GLU:HG3	2.06	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:310:ARG:O	1:A:314:GLU:HG3	2.05	0.56
1:A:524:PHE:O	1:A:528:THR:HG22	2.05	0.56
1:A:540:ARG:HH11	1:A:540:ARG:HB3	1.70	0.56
1:B:148:LEU:HB3	1:B:179:LEU:CD1	2.29	0.56
1:B:219:LEU:C	1:B:219:LEU:HD13	2.31	0.56
1:B:600:LEU:O	1:B:604:ILE:HG13	2.06	0.56
1:A:505:ILE:CG1	1:A:538:ASP:HB2	2.36	0.55
1:A:575:MET:HB3	1:B:576:GLU:HG2	1.86	0.55
1:B:95:LYS:HD3	1:B:128:LEU:HD22	1.88	0.55
1:A:563:THR:O	1:A:567:GLU:HG3	2.06	0.55
1:B:260:PHE:CE1	1:B:338:ILE:HD11	2.42	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:VAL:HG21	1:A:393:ASP:HB2	1.87	0.55
1:B:435:ILE:O	1:B:438:ALA:HB3	2.06	0.55
1:B:461:PHE:N	1:B:462:PRO:CD	2.70	0.55
1:B:545:LYS:HG3	1:B:571:LEU:HD12	1.88	0.55
1:A:393:ASP:CB	1:A:396:ASN:HB2	2.37	0.55
1:B:554:GLN:C	1:B:556:GLU:H	2.13	0.55
1:A:265:LYS:HG3	1:A:265:LYS:O	2.06	0.55
1:A:481:PHE:HE2	1:A:517:ARG:HG2	1.71	0.55
1:A:382:TYR:HA	1:A:385:TYR:CD1	2.42	0.55
1:B:372:ILE:HD12	1:B:372:ILE:C	2.31	0.55
1:B:418:LYS:O	1:B:418:LYS:HD3	2.06	0.55
1:A:286:GLY:HA2	1:A:301:ALA:HA	1.88	0.55
1:B:594:ILE:C	1:B:596:SER:H	2.15	0.55
1:A:379:SER:C	1:A:381:GLU:N	2.64	0.55
1:B:119:ILE:HD13	1:B:142:TYR:CE2	2.42	0.55
1:B:520:THR:HB	1:B:523:ASN:HB2	1.89	0.55
1:A:279:ALA:HA	1:A:311:LEU:HD12	1.89	0.54
1:B:203:ILE:HD12	1:B:204:GLU:N	2.21	0.54
1:B:431:ILE:CD1	1:B:466:GLU:HB2	2.37	0.54
1:A:360:PHE:CD2	1:A:361:PRO:HD2	2.40	0.54
1:B:409:ILE:C	1:B:411:GLN:H	2.15	0.54
1:A:277:ASN:O	1:A:281:LYS:HG3	2.07	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:B:468:PRO:HA	1:B:487:GLN:OE1	2.08	0.54
1:A:109:PHE:HB3	1:A:117:ASP:HB2	1.90	0.54
1:A:469:ASN:O	1:A:472:ALA:HB3	2.07	0.54
1:A:345:ASP:CG	1:A:347:LEU:HB2	2.32	0.54
1:B:338:ILE:HD13	1:B:338:ILE:O	2.08	0.54
1:A:267:GLU:C	1:A:287:LEU:HD21	2.33	0.54
1:A:309:ALA:O	1:A:313:GLU:HB2	2.07	0.54
1:A:546:ILE:HG23	1:A:568:SER:HB3	1.90	0.54
1:B:268:LEU:HD12	1:B:268:LEU:H	1.73	0.54
1:B:439:CYS:C	1:B:441:ALA:N	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:496:ASN:HA	2:A:669:HOH:O	2.09	0.53
1:B:514:LEU:HD23	1:B:515:LEU:N	2.24	0.53
1:B:446:LYS:HD2	1:B:449:ASP:OD1	2.08	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:442:TYR:C	1:A:444:GLU:H	2.17	0.53
1:B:598:PRO:C	1:B:600:LEU:N	2.65	0.53
1:A:530:LEU:HG	2:A:654:HOH:O	2.09	0.53
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:B:552:LYS:HZ2	1:B:560:GLU:HB3	1.74	0.52
1:B:598:PRO:C	1:B:600:LEU:H	2.14	0.52
1:A:345:ASP:OD1	1:B:376:ARG:HB2	2.10	0.52
1:B:203:ILE:HD12	1:B:203:ILE:C	2.34	0.52
1:A:382:TYR:C	1:A:384:ASN:N	2.66	0.52
1:B:431:ILE:CD1	1:B:467:VAL:HG23	2.31	0.52
1:B:465:PRO:C	1:B:468:PRO:HD2	2.34	0.52
1:B:575:MET:HA	1:B:578:LYS:CG	2.40	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:516:THR:C	1:B:518:ASN:H	2.17	0.52
1:A:195:ASN:CG	1:A:196:GLY:H	2.17	0.52
1:B:277:ASN:ND2	1:B:279:ALA:HB3	2.24	0.52
1:B:361:PRO:O	1:B:362:ARG:CB	2.57	0.52
1:A:381:GLU:O	1:A:384:ASN:HB3	2.09	0.52
1:A:386:PHE:CE1	1:A:403:ARG:HA	2.45	0.52
1:A:477:ASP:C	1:A:479:ASN:H	2.17	0.52
1:B:270:PHE:CE2	1:B:328:LYS:HE2	2.45	0.52
1:A:537:LEU:N	1:A:537:LEU:HD12	2.25	0.51
1:B:219:LEU:HD13	1:B:219:LEU:O	2.09	0.51
1:A:96:ASP:HA	1:A:99:ALA:HB3	1.91	0.51
1:A:147:ASP:OD1	1:A:150:LYS:HB2	2.09	0.51
1:A:319:ASN:HB3	1:A:322:ASP:HB2	1.93	0.51
1:A:416:ALA:C	1:A:418:LYS:H	2.18	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:A:257:MET:HE3	1:A:298:TYR:HB3	1.93	0.51
1:A:546:ILE:HG13	1:A:547:GLY:N	2.25	0.51
1:B:148:LEU:HD21	1:B:518:ASN:HD22	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:556:GLU:HG2	2:B:637:HOH:O	2.10	0.51
1:A:195:ASN:OD1	1:A:196:GLY:N	2.42	0.51
1:A:285:ASN:HD22	1:A:304:SER:HB3	1.76	0.51
1:A:292:LYS:O	1:A:293:ARG:C	2.53	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: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:209:ARG:HD2	1:B:213:LYS:HZ3	1.76	0.51
1:A:326:LYS:HD2	1:A:359:LEU:HD23	1.92	0.51
1:B:431:ILE:HG23	1:B:432:PHE:N	2.26	0.51
1:B:546:ILE:HG23	1:B:568:SER:HB3	1.93	0.51
1:A:410:LEU:C	1:A:412:ASN:N	2.69	0.51
1:A:446:LYS:HD3	1:A:449:ASP:OD2	2.10	0.51
1:A:472:ALA:HB1	1:A:488:TYR:CD1	2.46	0.51
1:A:574:THR:HB	1:A:577:GLU:OE2	2.11	0.51
1:B:167:LYS:HE2	1:B:171:ARG:NH2	2.26	0.51
1:B:322:ASP:OD1	1:B:324:LYS:HB2	2.11	0.51
1:A:514:LEU:HD12	1:A:515:LEU:N	2.26	0.50
1:B:255:THR:N	2:B:660:HOH:O	2.33	0.50
1:B:270:PHE:HE2	1:B:328:LYS:HE2	1.76	0.50
1:B:501:ILE:HD13	1:B:501:ILE:O	2.11	0.50
1:A:575:MET:CB	1:B:576:GLU:HG2	2.41	0.50
1:A:605:GLN:CA	1:A:605:GLN:HE21	2.23	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:355:LYS:HB2	1:A:355:LYS:NZ	2.27	0.50
1:B:363:VAL:CG2	1:B:392:LEU:HB2	2.41	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:344:ASN:O	1:B:345:ASP:CB	2.49	0.50
1:B:546:ILE:HG23	1:B:568:SER:CB	2.42	0.50
1:A:373:MET:C	1:A:375:ASP:N	2.68	0.50
1:A:493:GLU:O	1:A:496:ASN:ND2	2.45	0.50
1:A:302:ASP:O	1:A:306:THR:HG23	2.11	0.50
1:B:263:ILE:HD13	2:B:616:HOH:O	2.12	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:505:ILE:HD13	1:B:538:ASP:HB2	1.94	0.50
1:A:415:GLN:HE21	1:A:415:GLN:HA	1.75	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:515:LEU:HB3	1:A:523:ASN:OD1	2.12	0.49
1:A:532:GLU:HA	1:A:548:LEU:HD11	1.93	0.49
1:B:108:GLN:HG2	1:B:111:ARG:NH2	2.27	0.49
1:B:126:LEU:HD21	1:B:134:PHE:HB2	1.94	0.49
1:B:167:LYS:HE2	1:B:171:ARG:HH22	1.77	0.49
1:B:221:GLU:HG3	1:B:222:LYS:CD	2.42	0.49
1:A:270:PHE:HE1	1:A:284:MET:HG2	1.77	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:B:532:GLU:O	1:B:536:LYS:HG2	2.12	0.49
1:A:274:ASP:CA	1:A:280:ASP:HB3	2.38	0.49
1:A:461:PHE:C	2:A:671:HOH:O	2.55	0.49
1:A:504:GLY:O	1:A:507:PRO:HD2	2.12	0.49
1:A:285:ASN:HD21	1:A:300:LYS:HZ3	1.58	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: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:B:444:GLU:O	1:B:446:LYS:N	2.35	0.49
1:A:396:ASN:HD22	1:A:399:VAL:HG13	1.77	0.49
1:A:415:GLN:HA	1:A:415:GLN:NE2	2.28	0.49
1:B:212:ASN:C	1:B:212:ASN:ND2	2.67	0.49
1:A:465:PRO:C	1:A:468:PRO:HD2	2.37	0.49
1:A:505:ILE:CD1	1:A:505:ILE:H	2.24	0.49
1:A:520:THR:O	1:A:521:VAL:C	2.56	0.49
1:A:189:LEU:HD22	1:A:203:ILE:HG13	1.94	0.48
1:A:347:LEU:HG	1:B:376:ARG:CB	2.43	0.48
1:A:369:MET:O	1:A:372:ILE:HG12	2.13	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:B:379:SER:C	1:B:381:GLU:H	2.20	0.48
1:A:594:ILE:HD13	1:B:187:PHE:CE2	2.47	0.48
1:B:496:ASN:C	1:B:498:LEU:H	2.20	0.48
1:A:269:THR:CG2	1:A:270:PHE:H	2.17	0.48
1:A:385:TYR:HD2	1:A:388:LYS:HD2	1.77	0.48
1:A:397:SER:HB2	1:A:426:LEU:HB3	1.95	0.48
1:B:548:LEU:HB3	1:B:564:LEU:HD13	1.95	0.48
1:A:338:ILE:HD13	1:A:338:ILE:N	2.27	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469:ASN:HD21	1:B:507:PRO:HA	1.78	0.48
1:B:499:ASP:OD2	1:B:500:GLY:N	2.47	0.48
1:A:114:LYS:NZ	1:A:114:LYS:HB3	2.28	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:505:ILE:CD1	1:B:505:ILE:N	2.77	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:B:214:GLN:HE21	1:B:218:LYS:HG2	1.78	0.48
1:B:501:ILE:CG2	1:B:502:TYR:N	2.77	0.48
1:B:516:THR:C	1:B:518:ASN:N	2.72	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:114:LYS:HB3	1:B:117:ASP:CB	2.44	0.47
1:B:204:GLU:N	1:B:205:PRO:HD2	2.29	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:A:174:SER:HA	2:A:644:HOH:O	2.14	0.47
1:A:263:ILE:HG21	1:A:401:TYR:CD1	2.49	0.47
1:A:275:GLU:C	1:A:277:ASN:N	2.65	0.47
1:B:399:VAL:HG23	1:B:400:TYR:HD1	1.79	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:B:475:LEU:HB2	1:B:484:ALA:HB2	1.96	0.47
1:B:490:LEU:O	1:B:493:GLU:HB3	2.14	0.47
1:A:124:TRP:HA	1:A:127:GLU:HG2	1.96	0.47
1:A:384:ASN:O	1:A:387:ASP:HB3	2.13	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:549:ALA:HB2	1:A:564:LEU:CB	2.45	0.47
1:B:409:ILE:CD1	1:B:410:LEU:HG	2.44	0.47
1:A:263:ILE:O	1:A:263:ILE:HG22	2.15	0.47
1:A:501:ILE:O	1:A:502:TYR:C	2.56	0.47
1:A:506:ALA:CB	1:A:507:PRO:HD3	2.36	0.47
1:A:512:ALA:O	1:A:516:THR:HG23	2.14	0.47
1:B:100:LEU:HD13	1:B:100:LEU:C	2.38	0.47
1:B:190:SER:O	1:B:193:SER:HB3	2.15	0.47
1:B:511:LYS:HA	1:B:514:LEU:HD22	1.96	0.47
1:A:289:ASN:HB3	1:A:297:SER:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:468:PRO:O	1:A:472:ALA:HB2	2.14	0.47
1:A:496:ASN:ND2	1:A:496:ASN:N	2.62	0.47
1:B:525:ILE:HA	1:B:528:THR:CG2	2.45	0.47
1:B:537:LEU:C	1:B:539:PRO:HD3	2.40	0.47
1:A:108:GLN:C	1:A:110:PHE:H	2.21	0.47
1:A:294:SER:OG	1:A:297:SER:HB2	2.15	0.47
1:A:387:ASP:O	1:A:391:LYS:HG3	2.15	0.47
1:A:393:ASP:HB3	2:A:622:HOH:O	2.15	0.47
1:A:549:ALA:HA	1:A:564:LEU:HD12	1.96	0.47
1:B:442:TYR:C	1:B:444:GLU:H	2.21	0.47
1:A:266:PRO:HA	1:A:291:TYR:CE1	2.50	0.47
1:A:549:ALA:HB2	1:A:564:LEU:HB3	1.96	0.47
1:B:411:GLN:C	1:B:413:TYR:H	2.22	0.47
1:B:468:PRO:CB	1:B:491:ALA:HB2	2.39	0.47
1:A:207:LEU:HD13	1:B:204:GLU:OE1	2.15	0.47
1:B:410:LEU:C	1:B:412:ASN:N	2.71	0.47
1:B:442:TYR:C	1:B:444:GLU:N	2.73	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:187:PHE:O	1:A:191:VAL:HG23	2.15	0.46
1:B:525:ILE:HA	1:B:528:THR:HG22	1.97	0.46
1:B:554:GLN:C	1:B:556:GLU:N	2.73	0.46
1:B:360:PHE:O	1:B:361:PRO:C	2.58	0.46
1:A:289:ASN:HA	1:A:292:LYS:HD3	1.98	0.46
1:A:292:LYS:O	1:A:292:LYS:HG3	2.15	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:444:GLU:CD	2:A:656:HOH:O	2.58	0.46
1:A:496:ASN:N	1:A:496:ASN:HD22	2.12	0.46
1:A:183:ALA:HB3	2:A:632:HOH:O	2.14	0.46
1:A:399:VAL:HG23	1:A:400:TYR:CD1	2.51	0.46
1:A:603:LYS:C	2:A:636:HOH:O	2.58	0.46
1:B:103:LYS:HB2	1:B:134:PHE:HE1	1.80	0.46
1:B:353:ILE:HD12	1:B:353:ILE:C	2.41	0.46
1:B:525:ILE:O	1:B:529:ASN:ND2	2.49	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:458:LYS:HG2	1:A:467:VAL:CG1	2.45	0.46
1:A:540:ARG:HH11	1:A:540:ARG:CB	2.28	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:444:GLU:C	1:B:446:LYS:H	2.23	0.46
1:B:529:ASN:HA	2:B:646:HOH:O	2.15	0.46
1:A:273:TYR:O	1:A:274:ASP:O	2.33	0.46
1:A:338:ILE:HD12	1:A:368:TYR:CG	2.51	0.46
1:A:469:ASN:CB	1:A:503:VAL:HG11	2.46	0.46
1:A:295:PRO:C	1:A:297:SER:N	2.74	0.45
1:A:430:ASN:O	1:A:433:PRO:HD2	2.16	0.45
1:A:439:CYS:HB2	1:A:454:PHE:HE1	1.80	0.45
1:A:503:VAL:HG12	1:A:503:VAL:O	2.16	0.45
1:B:186:MET:CE	1:B:211:LEU:HA	2.46	0.45
1:A:108:GLN:C	1:A:110:PHE:N	2.70	0.45
1:A:437:LEU:O	1:A:438:ALA:C	2.59	0.45
1:B:175:ALA:O	1:B:179:LEU:HD12	2.16	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
1:A:558:ILE:O	1:A:562:ILE:HG13	2.16	0.45
1:B:98:TYR:HB3	1:B:128:LEU:CD1	2.47	0.45
1:B:212:ASN:HD21	1:B:580:GLN:HG3	1.81	0.45
1:B:402:HIS:O	1:B:405:GLN:HB2	2.15	0.45
1:B:447:PHE:O	1:B:450:CYS:N	2.48	0.45
1:A:374:ALA:CB	1:A:406:MET:HE1	2.47	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:A:605:GLN:HE21	1:A:605:GLN:HA	1.81	0.45
1:B:295:PRO:C	1:B:297:SER:N	2.75	0.45
1:B:597:ASP:O	1:B:597:ASP:OD1	2.34	0.45
1:A:341:PHE:CD1	1:A:341:PHE:C	2.94	0.45
1:A:399:VAL:CG2	1:A:400:TYR:N	2.79	0.45
1:B:491:ALA:O	1:B:495:GLU:HB2	2.17	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: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:B:594:ILE:HG22	1:B:604:ILE:HD11	1.99	0.45
1:A:287:LEU:HD23	1:A:287:LEU:C	2.42	0.45
1:A:469:ASN:HB2	1:A:503:VAL:HG11	1.99	0.45
1:A:584:PHE:O	1:A:585:ALA:C	2.58	0.45
1:A:596:SER:O	1:A:597:ASP:O	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:ASP:O	1:B:396:ASN:N	2.50	0.45
1:A:273:TYR:CD2	1:A:274:ASP:N	2.85	0.45
1:A:516:THR:C	1:A:518:ASN:N	2.75	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:A:147:ASP:CG	1:A:150:LYS:HB2	2.42	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:A:442:TYR:C	1:A:444:GLU:N	2.74	0.44
1:A:454:PHE:CE2	1:A:471:PHE:HB2	2.51	0.44
1:B:263:ILE:HG22	1:B:263:ILE:O	2.17	0.44
1:B:501:ILE:HD13	1:B:501:ILE:C	2.41	0.44
1:B:96:ASP:OD2	1:B:129:LYS:HD2	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:A:119:ILE:HG12	1:A:141:CYS:SG	2.57	0.44
1:A:481:PHE:H	1:A:481:PHE:HD1	1.64	0.44
1:B:438:ALA:O	1:B:450:CYS:HA	2.18	0.44
1:B:533:LYS:O	1:B:536:LYS:HB2	2.18	0.44
1:B:440:LEU:HD12	1:B:440:LEU:O	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: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:500:GLY:HA3	1:A:502:TYR:CE1	2.50	0.44
1:A:582:ILE:HD12	1:B:219:LEU:HB2	1.99	0.44
1:A:590:VAL:O	1:A:594:ILE:HG12	2.18	0.44
1:B:331:ILE:CG2	1:B:362:ARG:NE	2.80	0.44
1:B:378:ASP:HB2	2:B:667:HOH:O	2.17	0.44
1:B:399:VAL:HG23	1:B:400:TYR:CD1	2.53	0.44
1:A:99:ALA:HA	1:A:128:LEU:HD12	2.00	0.44
1:A:119:ILE:CG2	1:A:123:ASN:HD21	2.30	0.44
1:A:283:LEU:HD11	1:A:331:ILE:CD1	2.35	0.44
1:A:475:LEU:CB	1:A:484:ALA:HB2	2.48	0.44
1:A:521:VAL:HG23	1:A:522:GLU:N	2.33	0.44
1:B:112:ASN:C	1:B:114:LYS:H	2.24	0.44
1:B:177:GLU:HB2	1:B:210:ASN:OD1	2.17	0.44
1:B:293:ARG:O	1:B:294:SER:O	2.35	0.44
1:B:353:ILE:HD11	1:B:369:MET:HB2	1.99	0.44
1:A:269:THR:HG23	1:A:270:PHE:N	2.19	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:404:GLY:O	1:A:408:PHE:HB2	2.18	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:469:ASN:HD22	1:A:507:PRO:CG	2.19	0.44
1:A:477:ASP:C	1:A:479:ASN:N	2.76	0.44
1:A:267:GLU:O	1:A:268:LEU:HG	2.17	0.43
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:B:201:ALA:HA	2:B:621:HOH:O	2.18	0.43
1:A:114:LYS:HB3	1:A:117:ASP:OD1	2.17	0.43
1:A:524:PHE:HD2	1:A:524:PHE:HA	1.73	0.43
1:A:170:LEU:HD23	1:A:170:LEU:O	2.19	0.43
1:A:279:ALA:HB3	1:A:315:GLN:HE22	1.84	0.43
1:A:312:PHE:CE1	1:A:328:LYS:HB3	2.53	0.43
1:A:496:ASN:HD22	1:A:497:LYS:N	2.16	0.43
1:A:186:MET:SD	1:A:211:LEU:HA	2.58	0.43
1:A:406:MET:O	1:A:409:ILE:HG12	2.18	0.43
1:B:504:GLY:O	1:B:507:PRO:HD2	2.18	0.43
1:B:548:LEU:CB	1:B:564:LEU:HD13	2.47	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
1:A:279:ALA:HB2	1:A:311:LEU:HB3	2.00	0.43
1:B:445:ASN:ND2	2:B:668:HOH:O	2.52	0.43
1:B:505:ILE:CG2	1:B:509:VAL:HG23	2.48	0.43
1:A:461:PHE:N	2:A:671:HOH:O	2.47	0.43
1:A:605:GLN:HA	1:A:605:GLN:NE2	2.33	0.43
1:B:396:ASN:C	1:B:396:ASN:HD22	2.27	0.43
1:B:537:LEU:O	1:B:539:PRO:HD3	2.17	0.43
1:B:558:ILE:N	1:B:558:ILE:CD1	2.80	0.43
1:B:591:GLN:OE1	1:B:591:GLN:HA	2.17	0.43
1:A:600:LEU:HD11	1:B:194:LEU:HD12	2.00	0.43
1:B:515:LEU:HB3	1:B:527:ALA:HB2	2.01	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:114:LYS:HB3	1:B:117:ASP:CG	2.44	0.43
1:B:475:LEU:CB	1:B:484:ALA:HB2	2.49	0.43
1:A:105:LYS:HD3	1:A:121:TYR:CE2	2.46	0.43
1:A:373:MET:C	1:A:375:ASP:H	2.24	0.43
1:A:404:GLY:HA3	1:A:420:PHE:CE2	2.54	0.43
1:A:600:LEU:HD13	1:A:600:LEU:O	2.19	0.43
1:B:453:LEU:HD12	1:B:453:LEU:HA	1.92	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:520:THR:HG22	1:B:521:VAL:N	2.34	0.43
1:B:572:ALA:HB1	1:B:577:GLU:HB2	2.01	0.43
1:A:363:VAL:HG11	1:A:396:ASN:CG	2.43	0.43
1:B:342:LEU:HD23	1:B:342:LEU:HA	1.88	0.43
1:B:505:ILE:HG22	1:B:505:ILE:O	2.18	0.43
1:A:390:LEU:HD21	1:A:399:VAL:CG2	2.42	0.42
1:A:411:GLN:HA	1:A:413:TYR:CE2	2.54	0.42
1:A:503:VAL:HG12	1:A:507:PRO:CD	2.47	0.42
1:B:295:PRO:O	1:B:297:SER:N	2.49	0.42
1:B:437:LEU:CD2	1:B:440:LEU:HD23	2.42	0.42
1:A:594:ILE:C	1:A:596:SER:H	2.27	0.42
1:B:159:LEU:C	1:B:161:LEU:H	2.27	0.42
1:B:179:LEU:HD12	1:B:179:LEU:N	2.34	0.42
1:B:195:ASN:CG	1:B:196:GLY:N	2.76	0.42
1:B:345:ASP:OD1	1:B:347:LEU:HB2	2.19	0.42
1:B:490:LEU:CD1	1:B:490:LEU:C	2.92	0.42
1:B:552:LYS:HG3	1:B:564:LEU:CD1	2.50	0.42
1:A:484:ALA:O	1:A:488:TYR:HD1	2.01	0.42
1:B:262:GLY:C	1:B:432:PHE:HE1	2.27	0.42
1:B:404:GLY:O	1:B:408:PHE:HB2	2.19	0.42
1:A:329:LEU:O	1:A:329:LEU:HD22	2.19	0.42
1:A:410:LEU:O	1:A:412:ASN:N	2.52	0.42
1:B:520:THR:H	1:B:523:ASN:HB2	1.84	0.42
1:B:362:ARG:HH11	1:B:362:ARG:HG2	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:139:SER:O	1:B:143:VAL:HG23	2.20	0.42
1:B:565:PHE:HB3	1:B:585:ALA:HB2	2.00	0.42
1:A:488:TYR:HE2	1:A:510:GLY:HA3	1.85	0.42
1:B:260:PHE:HE1	1:B:338:ILE:HD12	1.85	0.42
1:B:501:ILE:O	1:B:502:TYR:C	2.63	0.42
1:B:515:LEU:HD12	1:B:523:ASN:O	2.20	0.42
1:A:409:ILE:C	1:A:411:GLN:H	2.28	0.42
1:A:446:LYS:HE2	1:A:446:LYS:CA	2.49	0.42
1:A:458:LYS:C	2:A:671:HOH:O	2.63	0.42
1:A:470:PHE:O	1:A:471:PHE:C	2.62	0.42
1:A:511:LYS:HD3	1:A:530:LEU:CD1	2.50	0.42
1:B:376:ARG:NH2	1:B:377:ASN:HB3	2.20	0.42
1:B:431:ILE:HG12	1:B:435:ILE:CD1	2.46	0.42
1:B:480:ASP:C	1:B:482:ASP:H	2.28	0.42
1:B:513:THR:C	1:B:515:LEU:N	2.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:555:GLN:HE21	1:B:555:GLN:HA	1.84	0.42
1:A:199:ASN:O	1:A:200:ASP:HB2	2.20	0.42
1:A:201:ALA:HA	1:A:204:GLU:HG2	2.02	0.42
1:A:294:SER:HA	1:A:295:PRO:HD3	1.91	0.42
1:A:385:TYR:CD2	1:A:388:LYS:HD2	2.55	0.42
1:B:417:GLY:HA2	1:B:437:LEU:HD21	2.00	0.42
1:B:432:PHE:HD2	1:B:435:ILE:HD12	1.85	0.42
1:B:478:LYS:HA	1:B:478:LYS:CE	2.39	0.42
1:B:480:ASP:C	1:B:482:ASP:N	2.78	0.42
1:B:550:GLN:NE2	2:B:645:HOH:O	2.52	0.42
1:A:122:TYR:O	1:A:126:LEU:HG	2.20	0.41
1:A:326:LYS:O	1:A:330:ALA:N	2.52	0.41
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:A:574:THR:CB	1:A:577:GLU:OE2	2.68	0.41
1:B:418:LYS:HD3	1:B:418:LYS:C	2.45	0.41
1:A:251:LEU:H	1:A:251:LEU:CD1	2.34	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:B:435:ILE:H	1:B:435:ILE:HG13	1.67	0.41
1:A:98:TYR:CD1	1:A:101:ALA:HB3	2.55	0.41
1:A:386:PHE:O	1:A:390:LEU:HG	2.19	0.41
1:B:341:PHE:CE2	1:B:372:ILE:HA	2.54	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:A:377:ASN:CG	1:A:378:ASP:H	2.28	0.41
1:A:383:TYR:C	2:A:631:HOH:O	2.63	0.41
1:A:461:PHE:C	1:A:463:GLU:H	2.29	0.41
1:B:112:ASN:C	1:B:114:LYS:N	2.78	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:129:LYS:NZ	2:A:661:HOH:O	2.53	0.41
1:A:432:PHE:C	1:A:434:TYR:N	2.79	0.41
1:A:531:LEU:HD13	1:A:547:GLY:HA3	2.02	0.41
1:A:603:LYS:HA	2:A:636:HOH:O	2.21	0.41
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:B:458:LYS:HZ1	1:B:490:LEU:HD11	1.85	0.41
1:B:478:LYS:O	1:B:479:ASN:HB2	2.21	0.41
1:B:493:GLU:C	1:B:495:GLU:N	2.78	0.41
1:B:131:ASP:HA	1:B:132:PRO:HD3	1.91	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:393:ASP:O	1:B:394:SER:C	2.63	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:A:277:ASN:HD21	1:A:315:GLN:HE22	1.68	0.41
1:A:279:ALA:HB2	1:A:311:LEU:CB	2.50	0.41
1:A:421:ASP:O	1:A:425:GLU:HG2	2.20	0.41
1:A:440:LEU:HD23	1:A:441:ALA:N	2.36	0.41
1:A:478:LYS:HA	1:A:478:LYS:CE	2.29	0.41
1:B:520:THR:HB	1:B:523:ASN:H	1.85	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:A:565:PHE:CE1	1:A:584:PHE:HB3	2.55	0.41
1:B:333:LEU:HD11	1:B:355:LYS:HD2	2.03	0.41
1:B:409:ILE:HD12	1:B:409:ILE:C	2.46	0.41
1:B:493:GLU:HG3	2:B:652:HOH:O	2.19	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: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:A:420:PHE:CE1	1:A:436:GLN:HG2	2.55	0.41
1:A:529:ASN:HB3	2:A:654:HOH:O	2.21	0.41
1:B:109:PHE:CD1	1:B:117:ASP:HB3	2.56	0.41
1:B:276:SER:O	1:B:277:ASN:C	2.63	0.41
1:B:375:ASP:O	1:B:376:ARG:O	2.39	0.41
1:B:424:LYS:HD2	1:B:434:TYR:CE2	2.55	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:B:514:LEU:HD23	1:B:514:LEU:C	2.46	0.41
1:B:547:GLY:O	1:B:551:MET:HG2	2.21	0.41
1:B:597:ASP:C	1:B:599:VAL:H	2.28	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:A:274:ASP:CG	1:A:275:GLU:N	2.78	0.40
1:A:280:ASP:OD1	1:A:328:LYS:HD3	2.21	0.40
1:A:353:ILE:HD12	1:A:353:ILE:C	2.46	0.40
1:A:596:SER:O	1:A:597:ASP:CG	2.64	0.40
1:B:196:GLY:C	1:B:198:PHE:H	2.29	0.40
1:B:341:PHE:CG	1:B:372:ILE:HG22	2.56	0.40
1:B:486:LYS:HE3	2:B:614:HOH:O	2.19	0.40
1:B:505:ILE:CG2	1:B:534:ALA:HB1	2.51	0.40
1:B:549:ALA:O	1:B:553:LEU:HB2	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:GLU:N	1:A:205:PRO:CD	2.84	0.40
1:A:345:ASP:HA	1:A:346:PRO:HD3	1.85	0.40
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:B:263:ILE:HD12	1:B:263:ILE:H	1.84	0.40
1:A:466:GLU:O	1:A:467:VAL:C	2.65	0.40
1:A:126:LEU:HD21	1:A:134:PHE:HB2	2.03	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: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:162:LYS:HD3	1:B:165:TYR:CD2	2.56	0.40
1:B:381:GLU:OE1	1:B:384:ASN:HB3	2.20	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	483/514 (94%)	377 (78%)	81 (17%)	25 (5%)	1	9
1	B	483/514 (94%)	385 (80%)	63 (13%)	35 (7%)	1	4
All	All	966/1028 (94%)	762 (79%)	144 (15%)	60 (6%)	1	6

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

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Mol	Chain	Res	Type
1	A	397	SER
1	A	504	GLY
1	A	597	ASP
1	B	95	LYS
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

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Mol	Chain	Res	Type
1	B	414	ASP
1	A	268	LEU
1	A	291	TYR
1	A	296	GLU
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%)	384 (90%)	41 (10%)	8	31
1	B	425/448 (95%)	394 (93%)	31 (7%)	13	42
All	All	850/896 (95%)	778 (92%)	72 (8%)	10	36

All (72) 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	155	SER
1	A	198	PHE
1	A	204	GLU
1	A	219	LEU
1	A	257	MET
1	A	270	PHE

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Mol	Chain	Res	Type
1	A	274	ASP
1	A	283	LEU
1	A	290	LEU
1	A	334	GLU
1	A	347	LEU
1	A	353	ILE
1	A	355	LYS
1	A	357	ILE
1	A	361	PRO
1	A	376	ARG
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	573	ARG
1	A	574	THR
1	A	600	LEU
1	A	605	GLN
1	B	263	ILE
1	B	268	LEU
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
1	B	353	ILE

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Mol	Chain	Res	Type
1	B	361	PRO
1	B	396	ASN
1	B	418	LYS
1	B	422	LYS
1	B	424	LYS
1	B	439	CYS
1	B	440	LEU
1	B	446	LYS
1	B	453	LEU
1	B	478	LYS
1	B	490	LEU
1	B	495	GLU
1	B	501	ILE
1	B	514	LEU
1	B	515	LEU
1	B	546	ILE
1	B	550	GLN
1	B	553	LEU
1	B	555	GLN
1	B	558	ILE
1	B	566	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) 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	377	ASN
1	A	384	ASN
1	A	395	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

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Mol	Chain	Res	Type
1	A	554	GLN
1	A	580	GLN
1	A	605	GLN
1	B	108	GLN
1	B	123	ASN
1	B	137	ASN
1	B	195	ASN
1	B	212	ASN
1	B	214	GLN
1	B	277	ASN
1	B	315	GLN
1	B	377	ASN
1	B	384	ASN
1	B	396	ASN
1	B	402	HIS
1	B	405	GLN
1	B	407	ASN
1	B	415	GLN
1	B	430	ASN
1	B	436	GLN
1	B	479	ASN
1	B	496	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 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 [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	487/514 (94%)	-0.12	5 (1%)	79 59	40, 76, 125, 154	0
1	B	487/514 (94%)	-0.17	4 (0%)	82 64	36, 74, 123, 162	0
All	All	974/1028 (94%)	-0.14	9 (0%)	81 61	36, 75, 125, 162	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	438	ALA	4.7
1	B	438	ALA	4.7
1	B	439	CYS	3.5
1	A	439	CYS	3.2
1	A	490	LEU	2.6
1	B	200	ASP	2.5
1	A	489	ASP	2.3
1	B	437	LEU	2.2
1	A	198	PHE	2.2

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 oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers ⓘ

There are no such residues in this entry.