



Full wwPDB X-ray Structure Validation Report ⓘ

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PDB ID : 2OVP / pdb_00002ovp
Title : Structure of the Skp1-Fbw7 complex
Authors : Hao, B.; Oehlmann, S.; Sowa, M.E.; Harper, J.W.; Pavletich, N.P.
Deposited on : 2007-02-14
Resolution : 2.90 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

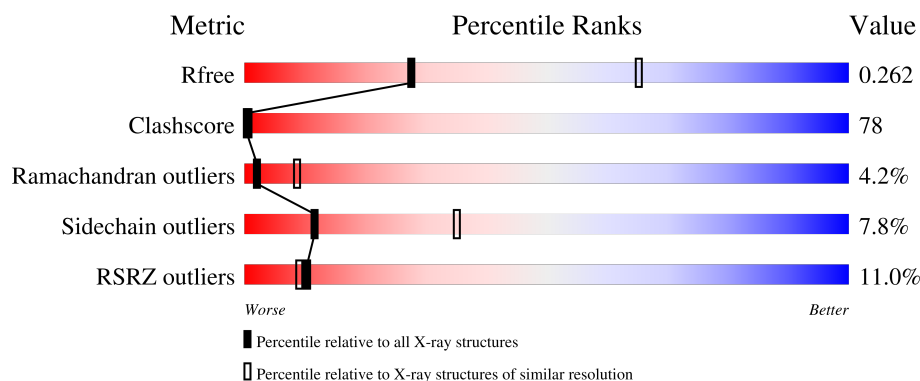
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.90 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	2481 (2.90-2.90)
Clashscore	190562	2690 (2.90-2.90)
Ramachandran outliers	187476	2623 (2.90-2.90)
Sidechain outliers	187428	2625 (2.90-2.90)
RSRZ outliers	180081	2481 (2.90-2.90)

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	149	15% 14% 69% 6% 10%
2	B	445	9% 18% 70% 10% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4676 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 S-phase kinase-associated protein 1A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	134	Total	C	N	O	S	0	0	0
			1073	686	174	208	5			

There are 18 discrepancies between the modelled and reference sequences:

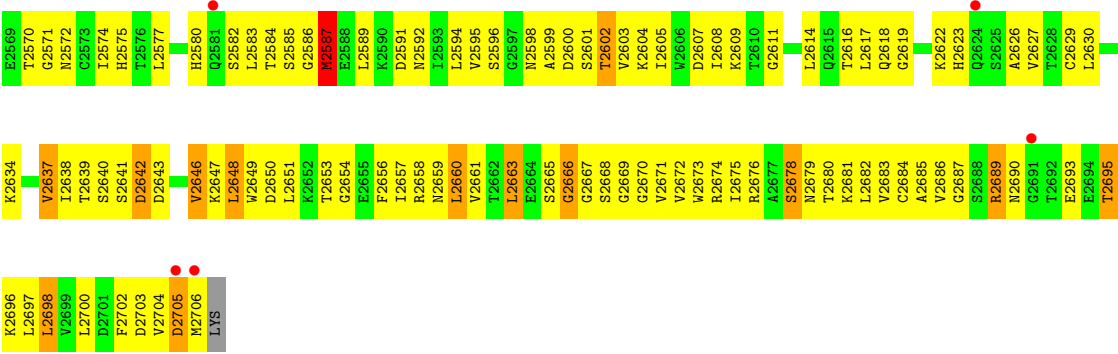
Chain	Residue	Modelled	Actual	Comment	Reference
A	?	-	ASP	deletion	UNP P63208
A	?	-	ASP	deletion	UNP P63208
A	?	-	GLU	deletion	UNP P63208
A	?	-	GLY	deletion	UNP P63208
A	?	-	ASP	deletion	UNP P63208
A	?	-	ASP	deletion	UNP P63208
A	?	-	PRO	deletion	UNP P63208
A	?	-	PRO	deletion	UNP P63208
A	?	-	PRO	deletion	UNP P63208
A	?	-	GLU	deletion	UNP P63208
A	?	-	ASP	deletion	UNP P63208
A	?	-	ASP	deletion	UNP P63208
A	?	-	GLU	deletion	UNP P63208
A	?	-	ASN	deletion	UNP P63208
A	1078	GLY	LYS	linker	UNP P63208
A	1079	GLY	GLU	linker	UNP P63208
A	1080	SER	LYS	linker	UNP P63208
A	1081	GLY	ARG	linker	UNP P63208

- Molecule 2 is a protein called F-box/WD repeat protein 7.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	441	Total	C	N	O	S	0	0	0
			3484	2187	627	648	22			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	10	Total 10	O 10	0	0
3	B	109	Total 109	O 109	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	I 41 2 2	Depositor
Cell constants a, b, c, α , β , γ	222.70Å 222.70Å 102.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.94 – 2.90 19.94 – 2.90	Depositor EDS
% Data completeness (in resolution range)	98.5 (19.94-2.90) 98.1 (19.94-2.90)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.10 (at 2.88Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.235 , 0.268 0.233 , 0.262	Depositor DCC
R_{free} test set	1959 reflections (6.72%)	wwPDB-VP
Wilson B-factor (Å ²)	37.8	Xtriage
Anisotropy	0.011	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	4676	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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	0.39	0/1091	0.94	3/1476 (0.2%)
2	B	0.62	0/3554	1.08	22/4815 (0.5%)
All	All	0.58	0/4645	1.05	25/6291 (0.4%)

There are no bond length outliers.

All (25) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2678	SER	N-CA-C	-8.62	97.01	110.36
2	B	2372	SER	CA-C-N	8.45	128.48	119.78
2	B	2372	SER	C-N-CA	8.45	128.48	119.78
2	B	2559	LEU	N-CA-C	-8.23	103.13	113.01
2	B	2371	LYS	N-CA-C	7.93	122.80	113.20
2	B	2554	VAL	N-CA-C	-6.74	98.72	108.36
2	B	2571	GLY	N-CA-C	-6.63	106.55	115.36
2	B	2637	VAL	N-CA-C	-6.54	98.10	107.77
2	B	2372	SER	N-CA-C	-6.47	95.52	109.81
2	B	2439	THR	N-CA-C	-6.37	104.77	112.54
1	A	1044	PRO	N-CA-C	-6.25	99.60	112.47
2	B	2400	ASP	N-CA-C	-6.16	105.61	112.57
2	B	2527	ASP	N-CA-C	-6.00	96.54	109.81
2	B	2326	LYS	N-CA-C	-5.95	106.11	113.19
2	B	2411	GLY	N-CA-C	-5.94	106.90	115.27
2	B	2289	ALA	N-CA-C	-5.77	104.99	111.28
1	A	1023	GLN	N-CA-C	-5.72	106.25	113.18
2	B	2443	LEU	N-CA-C	-5.68	102.88	110.55
2	B	2421	THR	N-CA-C	-5.68	106.52	113.50
2	B	2408	ALA	N-CA-C	-5.61	105.53	112.38
2	B	2646	VAL	N-CA-C	-5.52	99.20	107.37
2	B	2403	LEU	N-CA-C	-5.34	101.06	109.50
2	B	2265	VAL	N-CA-C	-5.24	105.29	111.00
2	B	2689	ARG	N-CA-C	-5.18	105.71	111.36
1	A	1026	THR	N-CA-C	-5.09	105.38	111.03

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	1073	0	1083	174	0
2	B	3484	0	3468	577	0
3	A	10	0	0	2	0
3	B	109	0	0	12	0
All	All	4676	0	4551	714	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 78.

All (714) 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)
2:B:2343:LYS:HB3	2:B:2344:PRO:HD2	1.16	1.13
2:B:2487:ASP:HB2	2:B:2494:LEU:HD11	1.29	1.12
1:A:1037:ASP:HB2	1:A:1044:PRO:HD3	1.27	1.09
2:B:2642:ASP:HA	2:B:2671:VAL:HG23	1.07	1.07
2:B:2554:VAL:HG13	2:B:2566:TRP:HB2	1.35	1.02
2:B:2642:ASP:HA	2:B:2671:VAL:CG2	1.88	1.01
2:B:2462:SER:OG	2:B:2479:ARG:HB2	1.61	1.01
2:B:2549:PHE:HE1	2:B:2568:VAL:HG21	1.23	0.99
1:A:1130:LYS:HG3	2:B:2303:GLN:HG3	1.46	0.98
1:A:1017:ASP:HB2	1:A:1020:ILE:HD12	1.47	0.97
2:B:2642:ASP:CA	2:B:2671:VAL:HG23	1.97	0.94
2:B:2468:HIS:HD2	2:B:2509:TYR:H	1.16	0.92
2:B:2468:HIS:CD2	2:B:2509:TYR:H	1.87	0.92
2:B:2334:LEU:H	2:B:2354:ALA:HB2	1.34	0.92
2:B:2390:CYS:HB2	2:B:2429:MET:HE3	1.51	0.92
2:B:2343:LYS:HB3	2:B:2344:PRO:CD	2.01	0.89
1:A:1020:ILE:HG21	1:A:1063:THR:HG22	1.56	0.88
2:B:2549:PHE:CE1	2:B:2568:VAL:HG21	2.09	0.87
2:B:2366:ARG:O	2:B:2658:ARG:HD2	1.73	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2513:ARG:HG2	2:B:2513:ARG:HH11	1.40	0.87
2:B:2382:HIS:H	2:B:2695:THR:HG21	1.38	0.86
2:B:2415:ARG:HD2	2:B:2451:GLY:HA3	1.57	0.86
1:A:1006:LEU:HD13	1:A:1055:LEU:HD11	1.57	0.86
2:B:2554:VAL:HG12	2:B:2568:VAL:HG22	1.58	0.86
2:B:2457:LEU:HB3	2:B:2486:TRP:CE3	2.13	0.83
2:B:2479:ARG:HA	2:B:2503:ALA:HB1	1.59	0.83
2:B:2648:LEU:HD13	2:B:2657:ILE:HD12	1.60	0.83
2:B:2352:LYS:HE2	2:B:2356:ILE:HD11	1.60	0.83
2:B:2334:LEU:HD23	2:B:2357:ARG:HD3	1.61	0.83
2:B:2325:CYS:HB3	2:B:2330:ILE:HB	1.61	0.82
2:B:2316:GLU:HG3	2:B:2346:PHE:CZ	2.15	0.81
2:B:2663:LEU:HD21	2:B:2686:VAL:HG13	1.61	0.81
2:B:2665:SER:OG	2:B:2693:GLU:HG2	1.79	0.81
1:A:1089:ASP:HB3	1:A:1118:VAL:HG11	1.63	0.81
2:B:2647:LYS:HG2	2:B:2659:ASN:ND2	1.95	0.80
2:B:2603:VAL:HG21	2:B:2639:THR:HG21	1.62	0.79
2:B:2272:ILE:HD12	2:B:2313:ILE:HD11	1.64	0.79
2:B:2672:VAL:HG22	2:B:2686:VAL:HG22	1.64	0.79
2:B:2404:LYS:HG2	2:B:2416:THR:HG23	1.65	0.79
2:B:2475:VAL:HG21	2:B:2514:VAL:HG22	1.64	0.79
1:A:1037:ASP:HB2	1:A:1044:PRO:CD	2.11	0.79
2:B:2486:TRP:CZ3	2:B:2493:CYS:HB2	2.18	0.78
2:B:2647:LYS:HG2	2:B:2659:ASN:HD22	1.47	0.78
2:B:2646:VAL:HG11	2:B:2682:LEU:HD21	1.64	0.78
2:B:2481:ALA:HB1	2:B:2500:HIS:O	1.84	0.77
2:B:2494:LEU:HD12	2:B:2494:LEU:H	1.49	0.77
2:B:2483:LEU:HD21	2:B:2516:SER:HB3	1.67	0.77
2:B:2521:PHE:HB3	2:B:2540:HIS:O	1.85	0.76
2:B:2388:GLN:HB3	2:B:2429:MET:HE2	1.67	0.76
1:A:1131:THR:HG21	1:A:1134:GLU:HG3	1.68	0.76
1:A:1130:LYS:HG3	2:B:2303:GLN:CG	2.15	0.75
2:B:2432:ASN:ND2	2:B:2449:GLU:H	1.84	0.75
2:B:2487:ASP:HB2	2:B:2494:LEU:CD1	2.14	0.75
2:B:2523:VAL:HB	2:B:2537:LEU:HB2	1.67	0.75
2:B:2318:ASN:ND2	2:B:2350:PRO:HD2	2.01	0.74
2:B:2443:LEU:HD21	2:B:2476:SER:HB3	1.69	0.74
2:B:2441:ARG:HG2	2:B:2461:THR:O	1.87	0.74
2:B:2580:HIS:HB3	2:B:2598:ASN:ND2	2.03	0.74
2:B:2686:VAL:HG21	2:B:2698:LEU:HD22	1.69	0.74
2:B:2567:ASP:HB2	2:B:2574:ILE:HD11	1.70	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2414:LEU:O	2:B:2415:ARG:HG2	1.88	0.73
2:B:2513:ARG:HG2	2:B:2513:ARG:NH1	2.03	0.72
2:B:2682:LEU:HD23	2:B:2700:LEU:HD12	1.72	0.72
2:B:2435:ILE:HG12	2:B:2488:ILE:CD1	2.20	0.72
2:B:2647:LYS:NZ	2:B:2659:ASN:HD21	1.88	0.72
2:B:2426:SER:HA	3:B:114:HOH:O	1.89	0.72
2:B:2617:LEU:HD13	2:B:2649:TRP:CG	2.25	0.72
2:B:2513:ARG:HG3	3:B:8:HOH:O	1.89	0.72
1:A:1026:THR:HG22	1:A:1030:MET:HE2	1.72	0.71
2:B:2373:PRO:HB3	2:B:2700:LEU:HD23	1.72	0.71
2:B:2443:LEU:HB2	2:B:2457:LEU:HB2	1.73	0.71
1:A:1131:THR:H	2:B:2303:GLN:HE21	1.36	0.71
2:B:2472:LYS:HD3	2:B:2472:LYS:H	1.56	0.70
1:A:1141:ILE:HD13	2:B:2307:THR:HG21	1.73	0.70
1:A:1009:SER:HB3	1:A:1048:PRO:O	1.92	0.69
2:B:2552:ILE:O	2:B:2568:VAL:HG23	1.92	0.69
1:A:1141:ILE:HG21	2:B:2307:THR:HG23	1.74	0.69
2:B:2523:VAL:HG21	2:B:2556:SER:HB3	1.75	0.69
2:B:2558:SER:HB3	2:B:2560:ASP:OD1	1.92	0.69
2:B:2634:LYS:HD3	3:B:94:HOH:O	1.91	0.69
2:B:2595:VAL:HG12	2:B:2630:LEU:HD22	1.74	0.69
2:B:2316:GLU:HG3	2:B:2346:PHE:HZ	1.58	0.68
2:B:2502:ALA:HB3	2:B:2520:ASP:N	2.07	0.68
1:A:1055:LEU:O	1:A:1055:LEU:HD23	1.93	0.68
1:A:1127:ILE:HB	2:B:2296:LEU:HD21	1.73	0.68
2:B:2324:LYS:O	2:B:2327:GLU:HB3	1.92	0.68
2:B:2426:SER:HB3	2:B:2465:ARG:O	1.92	0.68
2:B:2403:LEU:HD21	2:B:2436:SER:HB3	1.74	0.68
2:B:2559:LEU:HD23	2:B:2559:LEU:O	1.93	0.68
1:A:1141:ILE:HG21	2:B:2307:THR:CG2	2.24	0.68
2:B:2285:PRO:HD2	2:B:2288:LEU:HD12	1.74	0.68
2:B:2537:LEU:HD13	2:B:2566:TRP:CG	2.27	0.68
1:A:1133:GLU:CD	1:A:1133:GLU:H	2.02	0.68
2:B:2530:THR:OG1	2:B:2532:THR:HG22	1.93	0.68
1:A:1017:ASP:HB2	1:A:1020:ILE:CD1	2.22	0.68
2:B:2484:ARG:HG2	2:B:2496:VAL:HG22	1.76	0.68
2:B:2342:ILE:HG13	2:B:2343:LYS:H	1.58	0.67
2:B:2333:PRO:HB3	2:B:2351:TRP:CD2	2.29	0.67
2:B:2426:SER:HB2	2:B:2467:MET:HG2	1.74	0.67
1:A:1003:SER:HA	1:A:1018:VAL:H	1.59	0.67
2:B:2282:SER:HA	2:B:2310:TYR:CE2	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2398:SER:HB3	2:B:2400:ASP:OD1	1.94	0.67
2:B:2432:ASN:HA	2:B:2448:ALA:HB3	1.77	0.67
2:B:2502:ALA:H	2:B:2520:ASP:HB3	1.60	0.67
2:B:2540:HIS:ND1	2:B:2558:SER:HB2	2.09	0.67
1:A:1037:ASP:CB	1:A:1044:PRO:HD3	2.10	0.66
2:B:2268:MET:HE1	2:B:2346:PHE:CD1	2.30	0.66
2:B:2357:ARG:NH2	3:B:4:HOH:O	2.29	0.66
2:B:2546:SER:OG	2:B:2587:MET:HE2	1.96	0.66
2:B:2472:LYS:HE3	2:B:2473:ARG:HG3	1.76	0.66
1:A:1055:LEU:O	1:A:1059:ILE:HG12	1.96	0.66
1:A:1141:ILE:HD13	2:B:2307:THR:CG2	2.26	0.66
2:B:2415:ARG:HE	2:B:2450:THR:C	2.04	0.66
2:B:2473:ARG:HB2	2:B:2509:TYR:HE2	1.60	0.66
1:A:1062:CYS:C	1:A:1064:HIS:H	2.01	0.66
2:B:2342:ILE:HG13	2:B:2343:LYS:N	2.10	0.66
2:B:2433:ILE:HG21	2:B:2488:ILE:HG21	1.78	0.66
2:B:2363:THR:HG23	2:B:2367:ARG:CZ	2.25	0.65
1:A:1122:THR:O	1:A:1126:MET:HG3	1.97	0.65
2:B:2522:MET:SD	2:B:2538:GLN:HG2	2.37	0.65
1:A:1006:LEU:HD12	1:A:1006:LEU:O	1.97	0.65
2:B:2280:PHE:HE2	2:B:2284:LEU:HD11	1.62	0.65
2:B:2430:ARG:HB2	2:B:2469:LEU:HD21	1.79	0.65
1:A:1047:LEU:HD12	1:A:1055:LEU:HD11	1.79	0.64
1:A:1101:PHE:CE1	1:A:1105:LEU:HD11	2.32	0.64
2:B:2366:ARG:O	2:B:2658:ARG:CD	2.45	0.64
2:B:2479:ARG:HA	2:B:2503:ALA:CB	2.28	0.64
2:B:2524:LYS:HZ3	2:B:2536:THR:HG23	1.62	0.64
2:B:2523:VAL:CG1	2:B:2537:LEU:HD12	2.28	0.64
2:B:2647:LYS:HZ2	2:B:2659:ASN:HD21	1.46	0.64
2:B:2650:ASP:HB3	2:B:2653:THR:OG1	1.98	0.64
2:B:2379:HIS:HE1	2:B:2396:SER:OG	1.81	0.63
2:B:2445:VAL:HG12	2:B:2454:ILE:HD11	1.80	0.63
2:B:2483:LEU:HD21	2:B:2516:SER:CB	2.27	0.63
2:B:2494:LEU:HD12	2:B:2494:LEU:N	2.13	0.63
1:A:1130:LYS:HA	2:B:2303:GLN:HG3	1.80	0.63
2:B:2500:HIS:CE1	2:B:2524:LYS:HG3	2.34	0.63
2:B:2521:PHE:N	2:B:2521:PHE:HD2	1.96	0.63
2:B:2441:ARG:HA	2:B:2462:SER:O	1.98	0.63
2:B:2322:ARG:HA	2:B:2351:TRP:CD2	2.34	0.63
2:B:2604:LYS:HG2	2:B:2616:THR:HG23	1.81	0.62
2:B:2364:ASN:HA	2:B:2368:GLY:HA3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2455:HIS:ND1	2:B:2491:GLY:HA3	2.14	0.62
2:B:2333:PRO:HB3	2:B:2351:TRP:CE2	2.34	0.62
2:B:2481:ALA:O	2:B:2500:HIS:HB2	1.99	0.62
2:B:2524:LYS:NZ	2:B:2536:THR:OG1	2.32	0.62
2:B:2523:VAL:HG21	2:B:2556:SER:CB	2.30	0.62
2:B:2603:VAL:HG21	2:B:2639:THR:CG2	2.30	0.62
2:B:2684:CYS:HB2	2:B:2698:LEU:HB2	1.81	0.62
2:B:2382:HIS:CG	2:B:2400:ASP:HB3	2.34	0.62
2:B:2269:MET:HE3	2:B:2313:ILE:HD12	1.81	0.62
2:B:2417:LEU:HD13	2:B:2446:TRP:CG	2.35	0.62
2:B:2599:ALA:HA	2:B:2626:ALA:HB1	1.82	0.62
2:B:2605:ILE:HD13	2:B:2651:LEU:HD12	1.82	0.62
2:B:2281:ILE:HG12	2:B:2311:TRP:NE1	2.15	0.61
2:B:2273:GLU:N	2:B:2274:PRO:HD3	2.14	0.61
2:B:2522:MET:HE1	2:B:2538:GLN:HG2	1.80	0.61
2:B:2281:ILE:HG12	2:B:2311:TRP:CE2	2.35	0.61
2:B:2314:LEU:C	2:B:2316:GLU:H	2.05	0.61
2:B:2521:PHE:N	2:B:2521:PHE:CD2	2.67	0.61
1:A:1004:ILE:C	1:A:1004:ILE:HD12	2.26	0.61
2:B:2417:LEU:HB3	2:B:2446:TRP:CE3	2.35	0.61
2:B:2604:LYS:HE2	2:B:2616:THR:HG23	1.83	0.61
2:B:2422:GLY:N	2:B:2440:ASP:HB3	2.16	0.61
2:B:2343:LYS:O	2:B:2344:PRO:C	2.42	0.61
2:B:2364:ASN:O	2:B:2368:GLY:HA3	2.01	0.61
2:B:2469:LEU:HB2	2:B:2474:VAL:HG22	1.82	0.61
2:B:2374:LYS:HE2	2:B:2409:VAL:O	2.01	0.60
2:B:2392:ASN:N	2:B:2392:ASN:HD22	1.99	0.60
2:B:2439:THR:HA	2:B:2463:THR:OG1	2.02	0.60
1:A:1150:GLU:O	1:A:1154:ARG:HG3	2.01	0.60
2:B:2435:ILE:HG12	2:B:2488:ILE:HD12	1.82	0.60
2:B:2435:ILE:CD1	2:B:2469:LEU:HD22	2.32	0.60
2:B:2487:ASP:HB3	2:B:2490:THR:OG1	2.01	0.60
2:B:2646:VAL:HG23	2:B:2661:VAL:HB	1.83	0.60
2:B:2334:LEU:HD12	2:B:2334:LEU:O	2.02	0.60
2:B:2434:ILE:HB	2:B:2446:TRP:HB2	1.82	0.60
2:B:2334:LEU:HD12	2:B:2334:LEU:C	2.27	0.60
2:B:2483:LEU:HB2	2:B:2497:LEU:HD23	1.84	0.60
2:B:2469:LEU:HD12	2:B:2473:ARG:O	2.02	0.60
1:A:1139:PHE:HB3	2:B:2279:ASP:HB2	1.82	0.60
2:B:2370:LEU:HD22	2:B:2658:ARG:NH2	2.17	0.60
2:B:2457:LEU:HD13	2:B:2486:TRP:HB3	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2304:ALA:O	2:B:2307:THR:HB	2.02	0.59
2:B:2522:MET:CE	2:B:2538:GLN:HG2	2.32	0.59
1:A:1101:PHE:HE1	1:A:1105:LEU:HD11	1.67	0.59
1:A:1006:LEU:CD2	1:A:1027:ILE:HD13	2.31	0.59
2:B:2476:SER:O	2:B:2483:LEU:HA	2.01	0.59
1:A:1005:LYS:HB3	1:A:1015:GLU:OE1	2.01	0.59
2:B:2321:TRP:CE2	2:B:2352:LYS:HG3	2.37	0.59
1:A:1054:ILE:HG13	1:A:1102:GLU:HB3	1.83	0.59
2:B:2439:THR:HA	2:B:2463:THR:HG23	1.83	0.59
1:A:1057:LYS:NZ	1:A:1095:VAL:HG21	2.17	0.58
2:B:2334:LEU:N	2:B:2354:ALA:HB2	2.14	0.58
2:B:2360:ARG:NH1	2:B:2706:MET:HE3	2.19	0.58
2:B:2520:ASP:C	2:B:2522:MET:H	2.09	0.58
2:B:2357:ARG:CZ	2:B:2361:ILE:HD11	2.34	0.58
2:B:2515:VAL:HG12	2:B:2547:LEU:HD11	1.85	0.58
2:B:2334:LEU:HD23	2:B:2357:ARG:CD	2.31	0.58
2:B:2370:LEU:HD22	2:B:2658:ARG:HH21	1.69	0.58
2:B:2416:THR:O	2:B:2418:VAL:HG13	2.04	0.58
2:B:2518:ALA:C	2:B:2520:ASP:H	2.11	0.58
2:B:2595:VAL:HA	2:B:2604:LYS:O	2.02	0.58
2:B:2352:LYS:HE2	2:B:2356:ILE:CD1	2.31	0.58
2:B:2462:SER:HB3	2:B:2480:ASP:N	2.18	0.58
2:B:2495:HIS:HB3	2:B:2531:GLU:HG2	1.86	0.58
1:A:1055:LEU:HD23	1:A:1059:ILE:HG12	1.85	0.57
2:B:2309:ARG:O	2:B:2313:ILE:HG13	2.04	0.57
2:B:2457:LEU:HD13	2:B:2486:TRP:CB	2.34	0.57
2:B:2689:ARG:HD2	3:B:37:HOH:O	2.03	0.57
1:A:1057:LYS:HG3	1:A:1092:PHE:CZ	2.39	0.57
1:A:1095:VAL:HG12	1:A:1096:ASP:H	1.70	0.57
1:A:1136:ARG:O	1:A:1140:ASN:N	2.37	0.57
2:B:2650:ASP:O	2:B:2654:GLY:N	2.36	0.57
2:B:2454:ILE:HG13	2:B:2455:HIS:HD2	1.69	0.57
2:B:2386:CYS:SG	2:B:2427:SER:HB2	2.45	0.57
2:B:2525:VAL:HB	2:B:2535:HIS:HB2	1.86	0.57
2:B:2343:LYS:N	2:B:2343:LYS:HE3	2.20	0.57
2:B:2375:VAL:HG13	2:B:2696:LYS:CD	2.34	0.57
2:B:2394:ILE:HG21	2:B:2683:VAL:HG11	1.87	0.57
2:B:2483:LEU:CD2	2:B:2516:SER:HB3	2.34	0.57
2:B:2314:LEU:C	2:B:2316:GLU:N	2.62	0.57
2:B:2457:LEU:HB3	2:B:2486:TRP:CZ3	2.39	0.57
2:B:2684:CYS:O	2:B:2697:LEU:HA	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1024:SER:OG	1:A:1027:ILE:HG13	2.05	0.57
2:B:2417:LEU:N	2:B:2417:LEU:HD23	2.19	0.56
2:B:2554:VAL:CG1	2:B:2566:TRP:HB2	2.25	0.56
2:B:2561:THR:HG23	2:B:2580:HIS:O	2.05	0.56
2:B:2385:THR:OG1	2:B:2424:VAL:O	2.19	0.56
2:B:2509:TYR:CZ	2:B:2511:GLY:HA2	2.40	0.56
2:B:2560:ASP:O	2:B:2561:THR:HB	2.05	0.56
2:B:2475:VAL:HG21	2:B:2514:VAL:CG2	2.33	0.56
2:B:2641:SER:HB3	2:B:2643:ASP:OD2	2.06	0.56
2:B:2333:PRO:HD3	2:B:2351:TRP:CH2	2.40	0.56
2:B:2376:LEU:HB3	2:B:2406:TRP:CZ3	2.41	0.56
2:B:2400:ASP:O	2:B:2402:THR:HG23	2.06	0.56
2:B:2472:LYS:HD3	2:B:2472:LYS:N	2.21	0.56
1:A:1136:ARG:NH2	1:A:1143:ASN:HD22	2.03	0.56
2:B:2435:ILE:HG12	2:B:2488:ILE:HD11	1.88	0.56
2:B:2497:LEU:HB3	2:B:2526:TRP:CD2	2.41	0.56
2:B:2603:VAL:HB	2:B:2617:LEU:HB2	1.86	0.56
2:B:2522:MET:HE1	2:B:2538:GLN:CD	2.31	0.55
2:B:2640:SER:HB2	2:B:2672:VAL:CG1	2.36	0.55
2:B:2316:GLU:HG3	2:B:2346:PHE:CE2	2.41	0.55
2:B:2559:LEU:C	2:B:2561:THR:H	2.13	0.55
1:A:1058:VAL:HG23	1:A:1059:ILE:N	2.22	0.55
2:B:2272:ILE:HD12	2:B:2313:ILE:CD1	2.36	0.55
2:B:2280:PHE:CE2	2:B:2284:LEU:HD11	2.40	0.55
2:B:2318:ASN:HA	2:B:2349:SER:OG	2.07	0.55
2:B:2364:ASN:ND2	2:B:2702:PHE:HA	2.22	0.55
2:B:2549:PHE:CZ	2:B:2551:GLY:HA2	2.42	0.55
2:B:2554:VAL:HG22	2:B:2566:TRP:CD1	2.42	0.55
2:B:2269:MET:SD	2:B:2310:TYR:CE1	2.99	0.55
2:B:2439:THR:HG22	2:B:2463:THR:OG1	2.07	0.55
1:A:1006:LEU:HD12	1:A:1014:PHE:HB2	1.87	0.55
1:A:1153:VAL:HG11	2:B:2306:GLN:HA	1.88	0.55
2:B:2432:ASN:HD21	2:B:2449:GLU:H	1.56	0.54
2:B:2457:LEU:HD13	2:B:2486:TRP:CG	2.42	0.54
2:B:2630:LEU:HA	2:B:2638:ILE:O	2.07	0.54
1:A:1020:ILE:HG23	1:A:1063:THR:HA	1.89	0.54
1:A:1018:VAL:HG23	1:A:1022:LYS:HE3	1.90	0.54
1:A:1054:ILE:HG21	1:A:1106:ALA:HB2	1.89	0.54
2:B:2379:HIS:CD2	2:B:2398:SER:CB	2.91	0.54
2:B:2403:LEU:HD11	2:B:2436:SER:CB	2.38	0.54
2:B:2475:VAL:HG11	2:B:2514:VAL:CG1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2365:TRP:O	2:B:2658:ARG:NH1	2.40	0.54
1:A:1006:LEU:HA	1:A:1045:VAL:H	1.73	0.54
2:B:2603:VAL:HG22	2:B:2627:VAL:HG11	1.90	0.54
1:A:1018:VAL:O	1:A:1019:GLU:HB2	2.08	0.54
1:A:1144:ASP:OD1	2:B:2308:CYS:HB2	2.07	0.54
2:B:2325:CYS:C	2:B:2327:GLU:H	2.14	0.54
2:B:2475:VAL:HG11	2:B:2514:VAL:HG11	1.90	0.54
2:B:2500:HIS:CD2	2:B:2504:VAL:HG22	2.43	0.54
2:B:2472:LYS:H	2:B:2472:LYS:CD	2.21	0.53
2:B:2630:LEU:C	2:B:2630:LEU:HD12	2.32	0.53
2:B:2665:SER:O	2:B:2668:SER:N	2.41	0.53
2:B:2530:THR:OG1	2:B:2532:THR:CG2	2.56	0.53
1:A:1049:ASN:HB2	1:A:1109:TYR:CG	2.44	0.53
1:A:1062:CYS:C	1:A:1064:HIS:N	2.62	0.53
1:A:1131:THR:CG2	1:A:1134:GLU:HG3	2.39	0.53
2:B:2296:LEU:O	2:B:2301:LEU:HD21	2.08	0.53
2:B:2584:THR:HG23	2:B:2596:SER:HB2	1.89	0.53
2:B:2585:SER:OG	2:B:2586:GLY:N	2.40	0.53
2:B:2460:HIS:NE2	2:B:2476:SER:OG	2.35	0.53
2:B:2301:LEU:H	2:B:2301:LEU:HD22	1.73	0.53
2:B:2521:PHE:HA	2:B:2542:ASN:O	2.09	0.53
2:B:2623:HIS:ND1	2:B:2641:SER:HB3	2.24	0.53
1:A:1025:VAL:HA	1:A:1028:LYS:HB3	1.89	0.53
2:B:2470:HIS:CD2	2:B:2511:GLY:HA3	2.43	0.53
2:B:2365:TRP:CH2	2:B:2682:LEU:HB2	2.44	0.53
2:B:2398:SER:C	2:B:2400:ASP:H	2.17	0.53
2:B:2445:VAL:CG1	2:B:2454:ILE:HD11	2.39	0.53
2:B:2548:GLN:HB2	2:B:2555:VAL:HB	1.91	0.53
1:A:1030:MET:HA	1:A:1034:LEU:HD23	1.91	0.52
2:B:2330:ILE:C	2:B:2332:GLU:H	2.16	0.52
2:B:2444:LYS:O	2:B:2446:TRP:CD1	2.62	0.52
2:B:2663:LEU:HD21	2:B:2686:VAL:CG1	2.35	0.52
2:B:2474:VAL:HG23	2:B:2488:ILE:HG12	1.91	0.52
1:A:1136:ARG:NH1	1:A:1143:ASN:HB2	2.24	0.52
2:B:2375:VAL:HG13	2:B:2696:LYS:HD2	1.91	0.52
2:B:2532:THR:O	2:B:2532:THR:HG23	2.09	0.52
1:A:1136:ARG:NH2	1:A:1143:ASN:ND2	2.58	0.52
2:B:2312:ARG:HG2	2:B:2346:PHE:CZ	2.44	0.52
2:B:2580:HIS:CE1	2:B:2602:THR:HG22	2.45	0.52
2:B:2357:ARG:NH1	2:B:2703:ASP:OD1	2.43	0.52
2:B:2434:ILE:O	2:B:2446:TRP:N	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2467:MET:HA	2:B:2476:SER:HA	1.91	0.52
2:B:2540:HIS:C	2:B:2542:ASN:H	2.17	0.52
2:B:2417:LEU:HB3	2:B:2446:TRP:CD2	2.44	0.52
2:B:2600:ASP:CG	2:B:2602:THR:HB	2.35	0.52
2:B:2648:LEU:HD13	2:B:2657:ILE:CD1	2.37	0.52
1:A:1029:THR:O	1:A:1033:ASP:HB2	2.10	0.52
1:A:1130:LYS:HD3	2:B:2299:LYS:HE2	1.91	0.52
2:B:2629:CYS:HB2	2:B:2674:ARG:HA	1.91	0.52
1:A:1006:LEU:HD11	1:A:1055:LEU:HD21	1.92	0.52
1:A:1047:LEU:HD12	1:A:1055:LEU:CD1	2.40	0.52
2:B:2293:LEU:O	2:B:2301:LEU:HD11	2.10	0.52
2:B:2325:CYS:C	2:B:2327:GLU:N	2.68	0.52
2:B:2465:ARG:NH2	3:B:1:HOH:O	2.30	0.52
2:B:2468:HIS:HD2	2:B:2509:TYR:N	1.98	0.52
1:A:1136:ARG:NH1	1:A:1143:ASN:HD22	2.07	0.51
1:A:1157:ASN:HB3	2:B:2302:LEU:HB3	1.93	0.51
1:A:1136:ARG:HH22	1:A:1143:ASN:ND2	2.08	0.51
2:B:2512:ARG:NH1	2:B:2513:ARG:NE	2.58	0.51
2:B:2600:ASP:OD1	2:B:2602:THR:HB	2.11	0.51
1:A:1024:SER:HB2	1:A:1112:ILE:HD11	1.93	0.51
2:B:2518:ALA:C	2:B:2520:ASP:N	2.67	0.51
2:B:2565:VAL:HB	2:B:2575:HIS:HB2	1.92	0.51
1:A:1021:ALA:C	1:A:1023:GLN:H	2.19	0.51
1:A:1131:THR:HG22	1:A:1134:GLU:H	1.76	0.51
2:B:2285:PRO:O	2:B:2286:LYS:C	2.54	0.51
2:B:2403:LEU:CD2	2:B:2436:SER:HB3	2.41	0.51
2:B:2598:ASN:HB3	2:B:2600:ASP:OD1	2.09	0.51
2:B:2360:ARG:HB3	2:B:2704:VAL:HG21	1.91	0.51
2:B:2430:ARG:HD3	3:B:79:HOH:O	2.10	0.51
2:B:2269:MET:HE3	2:B:2313:ILE:CD1	2.40	0.51
2:B:2334:LEU:HD13	2:B:2336:ILE:HG23	1.91	0.51
2:B:2416:THR:O	2:B:2418:VAL:N	2.44	0.51
2:B:2545:TYR:HB2	2:B:2583:LEU:HD21	1.92	0.51
2:B:2554:VAL:HG22	2:B:2566:TRP:HD1	1.75	0.51
2:B:2577:LEU:HD21	2:B:2611:GLY:HA2	1.93	0.51
1:A:1036:MET:O	1:A:1037:ASP:C	2.54	0.51
1:A:1044:PRO:O	1:A:1046:PRO:HD3	2.10	0.51
2:B:2307:THR:HG22	2:B:2308:CYS:N	2.25	0.51
2:B:2365:TRP:HA	2:B:2702:PHE:CD1	2.45	0.51
2:B:2445:VAL:HB	2:B:2455:HIS:HB2	1.93	0.51
2:B:2673:TRP:CH2	2:B:2687:GLY:HA3	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1006:LEU:CD1	1:A:1055:LEU:HD11	2.36	0.51
1:A:1156:GLU:O	2:B:2356:ILE:HD13	2.11	0.51
2:B:2288:LEU:O	2:B:2292:VAL:HG23	2.11	0.51
2:B:2334:LEU:CD1	2:B:2336:ILE:HG23	2.40	0.51
2:B:2544:VAL:HA	2:B:2558:SER:HA	1.92	0.51
1:A:1006:LEU:HD22	1:A:1027:ILE:HD13	1.93	0.50
2:B:2376:LEU:HB3	2:B:2406:TRP:CE3	2.46	0.50
2:B:2474:VAL:HG23	2:B:2488:ILE:CG1	2.41	0.50
2:B:2522:MET:HE1	2:B:2538:GLN:CG	2.41	0.50
2:B:2318:ASN:HD21	2:B:2350:PRO:HD2	1.75	0.50
1:A:1020:ILE:CG2	1:A:1063:THR:HG22	2.36	0.50
2:B:2303:GLN:OE1	2:B:2303:GLN:HA	2.09	0.50
2:B:2415:ARG:HD2	2:B:2451:GLY:CA	2.35	0.50
2:B:2268:MET:HG2	2:B:2347:ILE:HD12	1.93	0.50
1:A:1006:LEU:CD1	1:A:1014:PHE:HB2	2.41	0.50
1:A:1130:LYS:CG	2:B:2303:GLN:HE21	2.25	0.50
2:B:2384:ILE:HB	2:B:2685:ALA:HB1	1.93	0.50
1:A:1102:GLU:HA	1:A:1102:GLU:OE1	2.10	0.50
2:B:2386:CYS:SG	2:B:2397:GLY:HA3	2.51	0.50
1:A:1055:LEU:O	1:A:1058:VAL:HG22	2.12	0.50
1:A:1057:LYS:HZ3	1:A:1095:VAL:HG21	1.75	0.50
1:A:1061:TRP:O	1:A:1064:HIS:HB3	2.11	0.50
1:A:1114:GLY:O	1:A:1118:VAL:HG23	2.12	0.50
1:A:1153:VAL:HG12	2:B:2306:GLN:HG2	1.94	0.50
2:B:2648:LEU:O	2:B:2657:ILE:HB	2.12	0.50
2:B:2321:TRP:C	2:B:2323:GLU:N	2.67	0.50
2:B:2618:GLN:C	2:B:2622:LYS:HB3	2.37	0.50
2:B:2333:PRO:HD3	2:B:2351:TRP:CZ2	2.47	0.49
1:A:1049:ASN:HB2	1:A:1109:TYR:CD2	2.46	0.49
1:A:1136:ARG:CZ	1:A:1143:ASN:HD22	2.25	0.49
2:B:2365:TRP:HH2	2:B:2682:LEU:HB2	1.76	0.49
2:B:2418:VAL:HG23	2:B:2418:VAL:O	2.11	0.49
1:A:1085:ILE:HD11	1:A:1125:ASN:ND2	2.26	0.49
2:B:2296:LEU:HB3	2:B:2300:ASP:HB2	1.94	0.49
2:B:2430:ARG:O	2:B:2431:ASP:O	2.29	0.49
2:B:2269:MET:HG3	2:B:2286:LYS:HE2	1.95	0.49
2:B:2407:SER:C	2:B:2409:VAL:N	2.67	0.49
2:B:2435:ILE:HD13	2:B:2474:VAL:HG21	1.94	0.49
2:B:2519:TYR:CD1	2:B:2543:ARG:HD3	2.47	0.49
2:B:2523:VAL:HG11	2:B:2537:LEU:HD12	1.94	0.49
2:B:2599:ALA:HA	2:B:2626:ALA:CB	2.43	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2514:VAL:HB	2:B:2526:TRP:HB2	1.93	0.49
2:B:2540:HIS:HD1	2:B:2558:SER:HB2	1.76	0.49
2:B:2494:LEU:HD21	3:B:113:HOH:O	2.12	0.49
2:B:2669:GLY:HA3	2:B:2690:ASN:HD21	1.77	0.49
2:B:2405:VAL:HG22	2:B:2434:ILE:CD1	2.42	0.49
2:B:2473:ARG:NH1	2:B:2529:GLU:OE2	2.45	0.49
2:B:2584:THR:CG2	2:B:2596:SER:HB2	2.42	0.49
2:B:2665:SER:OG	2:B:2670:GLY:HA3	2.12	0.49
1:A:1095:VAL:HG12	1:A:1096:ASP:N	2.28	0.49
1:A:1107:ALA:O	1:A:1111:ASP:N	2.46	0.49
2:B:2629:CYS:HB3	2:B:2675:ILE:HG12	1.93	0.49
1:A:1061:TRP:HB2	1:A:1092:PHE:CZ	2.48	0.48
1:A:1085:ILE:HG22	1:A:1090:GLN:HB2	1.95	0.48
2:B:2382:HIS:N	2:B:2695:THR:HG21	2.17	0.48
1:A:1142:LYS:NZ	3:A:56:HOH:O	2.45	0.48
2:B:2364:ASN:HD22	2:B:2702:PHE:C	2.20	0.48
2:B:2368:GLY:O	2:B:2658:ARG:NH2	2.44	0.48
2:B:2376:LEU:HD13	2:B:2406:TRP:CE3	2.48	0.48
2:B:2379:HIS:CD2	2:B:2398:SER:HB2	2.48	0.48
2:B:2515:VAL:HG12	2:B:2547:LEU:CD1	2.43	0.48
2:B:2520:ASP:O	2:B:2522:MET:HG2	2.13	0.48
2:B:2300:ASP:O	2:B:2301:LEU:C	2.56	0.48
2:B:2439:THR:HA	2:B:2463:THR:CG2	2.44	0.48
1:A:1132:PRO:O	1:A:1136:ARG:HG3	2.13	0.48
2:B:2264:GLN:HG2	2:B:2347:ILE:HG21	1.96	0.48
2:B:2375:VAL:HG13	2:B:2696:LYS:HD3	1.94	0.48
1:A:1010:ASP:OD2	1:A:1051:ASN:HB2	2.14	0.48
1:A:1030:MET:O	1:A:1035:GLY:N	2.47	0.48
1:A:1106:ALA:O	1:A:1110:LEU:HG	2.14	0.48
2:B:2274:PRO:HG2	2:B:2313:ILE:HD12	1.95	0.48
2:B:2474:VAL:HG21	2:B:2488:ILE:HD11	1.96	0.48
2:B:2520:ASP:C	2:B:2522:MET:N	2.72	0.48
2:B:2343:LYS:CB	2:B:2344:PRO:HD2	2.09	0.48
2:B:2379:HIS:O	2:B:2380:ASP:C	2.56	0.48
2:B:2430:ARG:HB2	2:B:2469:LEU:CD2	2.42	0.48
2:B:2450:THR:OG1	2:B:2452:GLU:HG2	2.13	0.48
2:B:2465:ARG:HG3	2:B:2465:ARG:HH11	1.79	0.48
2:B:2607:ASP:OD1	2:B:2609:LYS:HB2	2.14	0.48
2:B:2589:LEU:HD11	2:B:2608:ILE:HD13	1.95	0.48
2:B:2604:LYS:HE2	2:B:2616:THR:CG2	2.43	0.48
1:A:1057:LYS:HD2	1:A:1060:GLN:NE2	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2480:ASP:O	2:B:2481:ALA:HB3	2.13	0.48
2:B:2494:LEU:H	2:B:2494:LEU:CD1	2.21	0.48
2:B:2321:TRP:CZ2	2:B:2352:LYS:HG3	2.49	0.47
2:B:2408:ALA:HB1	2:B:2681:LYS:HD2	1.96	0.47
2:B:2665:SER:O	2:B:2666:GLY:C	2.56	0.47
2:B:2473:ARG:HD2	2:B:2509:TYR:OH	2.13	0.47
2:B:2619:GLY:O	2:B:2622:LYS:HD2	2.14	0.47
2:B:2321:TRP:O	2:B:2322:ARG:C	2.57	0.47
2:B:2505:ARG:HG2	2:B:2545:TYR:CD1	2.50	0.47
2:B:2314:LEU:O	2:B:2316:GLU:N	2.47	0.47
2:B:2435:ILE:HD13	2:B:2474:VAL:CG2	2.45	0.47
1:A:1051:ASN:OD1	1:A:1053:ALA:HB3	2.13	0.47
1:A:1136:ARG:HH22	1:A:1143:ASN:HD22	1.60	0.47
2:B:2420:HIS:NE2	2:B:2444:LYS:HB2	2.29	0.47
2:B:2567:ASP:CB	2:B:2574:ILE:HD11	2.41	0.47
2:B:2646:VAL:HG21	2:B:2684:CYS:SG	2.54	0.47
2:B:2290:LEU:C	2:B:2292:VAL:N	2.72	0.47
2:B:2432:ASN:O	2:B:2447:ASN:HA	2.14	0.47
2:B:2439:THR:HA	2:B:2463:THR:CB	2.45	0.47
2:B:2646:VAL:HG22	2:B:2672:VAL:HG11	1.96	0.47
2:B:2268:MET:HE1	2:B:2346:PHE:CG	2.50	0.47
2:B:2390:CYS:CB	2:B:2429:MET:HE3	2.34	0.47
2:B:2408:ALA:HB1	2:B:2681:LYS:CD	2.44	0.47
1:A:1018:VAL:O	1:A:1019:GLU:CB	2.63	0.46
2:B:2469:LEU:HD13	2:B:2474:VAL:CG2	2.45	0.46
2:B:2497:LEU:HB3	2:B:2526:TRP:CE2	2.50	0.46
1:A:1034:LEU:HD22	1:A:1034:LEU:H	1.80	0.46
1:A:1131:THR:O	1:A:1135:ILE:HG13	2.15	0.46
2:B:2296:LEU:O	2:B:2324:LYS:NZ	2.41	0.46
2:B:2469:LEU:HD13	2:B:2474:VAL:HG23	1.98	0.46
2:B:2523:VAL:HG12	2:B:2537:LEU:HD12	1.95	0.46
1:A:1093:LEU:HD13	1:A:1119:THR:HA	1.97	0.46
2:B:2447:ASN:O	2:B:2451:GLY:N	2.48	0.46
2:B:2520:ASP:OD1	2:B:2522:MET:HB2	2.15	0.46
2:B:2605:ILE:HD13	2:B:2651:LEU:CD1	2.44	0.46
2:B:2648:LEU:HB2	2:B:2660:LEU:CD2	2.46	0.46
2:B:2308:CYS:SG	2:B:2311:TRP:CD1	3.09	0.46
2:B:2352:LYS:O	2:B:2356:ILE:HG13	2.16	0.46
2:B:2373:PRO:HB3	2:B:2700:LEU:CD2	2.44	0.46
1:A:1142:LYS:HE3	2:B:2278:ARG:HH11	1.81	0.46
2:B:2376:LEU:HD22	2:B:2411:GLY:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2394:ILE:CG2	2:B:2683:VAL:HG11	2.45	0.46
2:B:2439:THR:C	2:B:2441:ARG:H	2.24	0.46
2:B:2470:HIS:O	2:B:2471:GLU:HB2	2.14	0.46
2:B:2495:HIS:NE2	2:B:2529:GLU:HA	2.30	0.46
2:B:2496:VAL:HG12	2:B:2498:MET:HG3	1.97	0.46
2:B:2592:ASN:O	2:B:2608:ILE:HG12	2.16	0.46
1:A:1141:ILE:HG12	2:B:2279:ASP:HB3	1.97	0.46
1:A:1143:ASN:HD21	1:A:1150:GLU:CD	2.23	0.46
2:B:2317:ASP:O	2:B:2320:LEU:HB3	2.16	0.46
2:B:2383:VAL:HG13	2:B:2673:TRP:CE2	2.50	0.46
2:B:2506:CYS:HB2	3:B:102:HOH:O	2.14	0.46
2:B:2512:ARG:HG2	2:B:2513:ARG:HG3	1.97	0.46
1:A:1099:THR:O	1:A:1102:GLU:HB2	2.15	0.46
2:B:2269:MET:CE	2:B:2313:ILE:HD12	2.45	0.46
2:B:2546:SER:HB3	2:B:2585:SER:O	2.16	0.46
2:B:2574:ILE:HG22	2:B:2575:HIS:CD2	2.51	0.46
1:A:1024:SER:OG	1:A:1110:LEU:HB3	2.16	0.46
2:B:2355:TYR:C	2:B:2355:TYR:CD2	2.93	0.46
2:B:2392:ASN:N	2:B:2392:ASN:ND2	2.62	0.46
2:B:2552:ILE:C	2:B:2568:VAL:HG23	2.40	0.46
2:B:2640:SER:HB2	2:B:2672:VAL:HG12	1.97	0.46
1:A:1034:LEU:HD22	1:A:1034:LEU:N	2.31	0.45
1:A:1149:GLU:O	1:A:1150:GLU:C	2.57	0.45
2:B:2330:ILE:O	2:B:2332:GLU:N	2.49	0.45
2:B:2425:TRP:CD1	2:B:2439:THR:HG23	2.51	0.45
2:B:2440:ASP:OD1	2:B:2440:ASP:C	2.59	0.45
1:A:1024:SER:HB3	1:A:1027:ILE:HD12	1.99	0.45
1:A:1137:LYS:NZ	1:A:1137:LYS:HB3	2.31	0.45
2:B:2311:TRP:O	2:B:2312:ARG:C	2.59	0.45
2:B:2647:LYS:NZ	2:B:2659:ASN:ND2	2.61	0.45
1:A:1055:LEU:HD23	1:A:1055:LEU:C	2.40	0.45
1:A:1135:ILE:O	1:A:1139:PHE:HD2	2.00	0.45
2:B:2316:GLU:OE2	2:B:2352:LYS:HD3	2.16	0.45
1:A:1085:ILE:HG13	1:A:1121:LYS:HD2	1.97	0.45
1:A:1018:VAL:HG22	1:A:1019:GLU:N	2.32	0.45
2:B:2273:GLU:C	2:B:2275:GLN:H	2.24	0.45
2:B:2390:CYS:O	2:B:2391:GLY:O	2.35	0.45
2:B:2440:ASP:O	2:B:2441:ARG:HB2	2.17	0.45
2:B:2475:VAL:CG1	2:B:2507:VAL:HG21	2.47	0.45
2:B:2623:HIS:ND1	2:B:2641:SER:CB	2.80	0.45
2:B:2665:SER:OG	2:B:2693:GLU:CG	2.58	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2685:ALA:HA	2:B:2697:LEU:HD13	1.99	0.45
1:A:1004:ILE:HD12	1:A:1004:ILE:O	2.17	0.45
1:A:1025:VAL:HG13	1:A:1111:ASP:HB3	1.98	0.45
2:B:2526:TRP:CZ3	2:B:2533:CYS:HB2	2.52	0.45
2:B:2638:ILE:HG22	2:B:2675:ILE:HD12	1.98	0.45
2:B:2663:LEU:CD2	2:B:2686:VAL:HG13	2.39	0.45
2:B:2318:ASN:CG	2:B:2350:PRO:HD2	2.41	0.45
2:B:2422:GLY:H	2:B:2440:ASP:HB3	1.81	0.45
2:B:2475:VAL:HG23	2:B:2509:TYR:CG	2.51	0.45
2:B:2360:ARG:CB	2:B:2704:VAL:HG21	2.47	0.45
2:B:2540:HIS:NE2	2:B:2564:ARG:HB2	2.31	0.45
1:A:1156:GLU:OE1	2:B:2348:HIS:CE1	2.69	0.45
1:A:1159:TRP:HA	2:B:2359:HIS:NE2	2.32	0.45
2:B:2407:SER:O	2:B:2411:GLY:N	2.48	0.45
2:B:2436:SER:O	2:B:2443:LEU:HA	2.16	0.45
2:B:2580:HIS:CE1	2:B:2604:LYS:HG3	2.52	0.45
1:A:1064:HIS:HD2	1:A:1065:HIS:CE1	2.35	0.45
1:A:1136:ARG:C	1:A:1138:THR:N	2.72	0.45
2:B:2490:THR:O	2:B:2492:GLN:NE2	2.50	0.45
2:B:2460:HIS:HE1	2:B:2482:THR:O	1.99	0.44
1:A:1101:PHE:HB2	2:B:2280:PHE:CE1	2.51	0.44
2:B:2356:ILE:O	2:B:2357:ARG:C	2.60	0.44
2:B:2364:ASN:CA	2:B:2368:GLY:HA3	2.46	0.44
2:B:2483:LEU:HD12	2:B:2483:LEU:N	2.32	0.44
2:B:2487:ASP:CG	2:B:2490:THR:HG23	2.43	0.44
2:B:2617:LEU:HB3	2:B:2649:TRP:CD2	2.52	0.44
2:B:2618:GLN:HB3	2:B:2622:LYS:HE2	2.00	0.44
2:B:2660:LEU:HB3	2:B:2700:LEU:CD1	2.47	0.44
2:B:2665:SER:O	2:B:2667:GLY:N	2.50	0.44
1:A:1115:LEU:HD23	1:A:1119:THR:HG23	1.99	0.44
1:A:1136:ARG:HH12	1:A:1143:ASN:HD22	1.65	0.44
2:B:2392:ASN:O	2:B:2407:SER:HA	2.17	0.44
2:B:2396:SER:O	2:B:2403:LEU:HA	2.18	0.44
1:A:1130:LYS:CG	1:A:1131:THR:H	2.30	0.44
1:A:1136:ARG:C	1:A:1138:THR:H	2.26	0.44
2:B:2294:SER:HA	2:B:2320:LEU:HD11	1.98	0.44
2:B:2547:LEU:HD23	2:B:2555:VAL:O	2.17	0.44
1:A:1130:LYS:HG2	2:B:2303:GLN:HE21	1.82	0.44
2:B:2269:MET:CE	2:B:2269:MET:HA	2.48	0.44
2:B:2342:ILE:CG1	2:B:2343:LYS:N	2.80	0.44
2:B:2379:HIS:CD2	2:B:2398:SER:HB3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2473:ARG:HA	2:B:2486:TRP:O	2.17	0.44
2:B:2479:ARG:NH2	3:B:9:HOH:O	2.50	0.44
2:B:2504:VAL:HA	2:B:2518:ALA:HA	2.00	0.44
2:B:2545:TYR:HE2	2:B:2559:LEU:HD12	1.82	0.44
2:B:2607:ASP:O	2:B:2611:GLY:N	2.44	0.44
1:A:1132:PRO:HD3	2:B:2303:GLN:NE2	2.33	0.44
2:B:2279:ASP:OD2	2:B:2282:SER:N	2.42	0.44
2:B:2443:LEU:HD11	2:B:2476:SER:CB	2.47	0.44
2:B:2512:ARG:HG2	2:B:2513:ARG:CG	2.47	0.44
2:B:2561:THR:HA	2:B:2582:SER:O	2.18	0.44
2:B:2486:TRP:CE3	2:B:2493:CYS:HB2	2.53	0.44
2:B:2649:TRP:CZ3	2:B:2656:PHE:HB2	2.52	0.44
2:B:2401:ASN:O	2:B:2420:HIS:HB2	2.18	0.44
2:B:2443:LEU:HD22	2:B:2457:LEU:HD12	1.99	0.44
2:B:2388:GLN:HE22	2:B:2676:ARG:NH2	2.16	0.43
2:B:2527:ASP:HB2	2:B:2534:LEU:HD11	2.00	0.43
2:B:2647:LYS:HZ3	2:B:2659:ASN:HD21	1.63	0.43
1:A:1064:HIS:C	1:A:1065:HIS:ND1	2.76	0.43
2:B:2396:SER:HB3	2:B:2697:LEU:HD21	2.01	0.43
2:B:2426:SER:HB3	2:B:2466:CYS:HA	2.00	0.43
2:B:2475:VAL:HG22	2:B:2485:VAL:HG22	1.99	0.43
2:B:2599:ALA:C	2:B:2601:SER:H	2.26	0.43
1:A:1130:LYS:CG	2:B:2303:GLN:HG3	2.33	0.43
1:A:1131:THR:HG23	1:A:1133:GLU:OE1	2.18	0.43
2:B:2277:GLN:HB3	2:B:2279:ASP:OD1	2.19	0.43
2:B:2364:ASN:O	2:B:2368:GLY:CA	2.66	0.43
2:B:2383:VAL:O	2:B:2398:SER:HA	2.19	0.43
2:B:2467:MET:O	2:B:2467:MET:HG3	2.17	0.43
2:B:2647:LYS:HZ3	2:B:2659:ASN:ND2	2.15	0.43
1:A:1018:VAL:HG13	1:A:1019:GLU:HG2	2.01	0.43
1:A:1153:VAL:CG1	2:B:2306:GLN:HA	2.49	0.43
2:B:2320:LEU:O	2:B:2324:LYS:HG2	2.19	0.43
2:B:2483:LEU:HD11	2:B:2500:HIS:HD2	1.82	0.43
2:B:2617:LEU:HB3	2:B:2649:TRP:CE3	2.53	0.43
1:A:1146:THR:OG1	1:A:1149:GLU:HG3	2.19	0.43
2:B:2401:ASN:HA	2:B:2422:GLY:O	2.18	0.43
2:B:2540:HIS:CE1	2:B:2556:SER:OG	2.72	0.43
2:B:2550:ASP:C	2:B:2552:ILE:H	2.26	0.43
2:B:2605:ILE:HG22	2:B:2614:LEU:HD12	2.01	0.43
1:A:1084:ASP:O	1:A:1086:PRO:HD3	2.19	0.43
1:A:1101:PHE:HA	2:B:2280:PHE:CZ	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1132:PRO:CG	2:B:2306:GLN:HB2	2.49	0.43
2:B:2530:THR:O	2:B:2531:GLU:C	2.61	0.43
2:B:2556:SER:O	2:B:2563:ILE:HA	2.19	0.43
1:A:1084:ASP:N	1:A:1121:LYS:NZ	2.66	0.43
2:B:2401:ASN:H	2:B:2423:GLY:HA2	1.83	0.43
2:B:2440:ASP:O	2:B:2441:ARG:CB	2.67	0.43
2:B:2605:ILE:HD11	2:B:2637:VAL:HG21	2.01	0.43
2:B:2663:LEU:C	2:B:2665:SER:N	2.75	0.43
2:B:2395:VAL:CG2	2:B:2429:MET:SD	3.07	0.43
2:B:2475:VAL:HG12	2:B:2507:VAL:HG21	2.00	0.43
2:B:2555:VAL:HG11	2:B:2594:LEU:HD22	2.00	0.43
2:B:2583:LEU:HD13	2:B:2583:LEU:O	2.19	0.43
2:B:2308:CYS:O	2:B:2309:ARG:C	2.61	0.42
2:B:2503:ALA:O	2:B:2519:TYR:N	2.44	0.42
2:B:2515:VAL:HG21	2:B:2549:PHE:CG	2.55	0.42
2:B:2527:ASP:O	2:B:2528:PRO:C	2.62	0.42
2:B:2559:LEU:C	2:B:2561:THR:N	2.77	0.42
1:A:1006:LEU:HD12	1:A:1006:LEU:C	2.45	0.42
1:A:1093:LEU:C	1:A:1095:VAL:H	2.28	0.42
1:A:1093:LEU:CD1	1:A:1118:VAL:HG12	2.49	0.42
1:A:1100:LEU:O	1:A:1104:ILE:HG12	2.19	0.42
1:A:1125:ASN:HA	1:A:1128:LYS:HD2	2.00	0.42
1:A:1025:VAL:CG1	1:A:1111:ASP:CG	2.92	0.42
1:A:1139:PHE:HB2	1:A:1141:ILE:CD1	2.49	0.42
2:B:2298:PRO:HA	2:B:2301:LEU:HD23	2.00	0.42
2:B:2420:HIS:HE1	2:B:2442:THR:O	2.02	0.42
1:A:1142:LYS:HE3	2:B:2278:ARG:CD	2.50	0.42
1:A:1158:GLN:HG3	1:A:1159:TRP:N	2.34	0.42
2:B:2389:PHE:CZ	2:B:2681:LYS:HG3	2.55	0.42
2:B:2443:LEU:HD13	2:B:2486:TRP:CE2	2.55	0.42
2:B:2454:ILE:HG13	2:B:2455:HIS:CD2	2.50	0.42
2:B:2506:CYS:SG	2:B:2547:LEU:HB2	2.59	0.42
2:B:2520:ASP:O	2:B:2522:MET:N	2.51	0.42
2:B:2575:HIS:CD2	2:B:2608:ILE:O	2.72	0.42
2:B:2582:SER:OG	2:B:2583:LEU:N	2.51	0.42
2:B:2280:PHE:CD2	2:B:2280:PHE:C	2.98	0.42
2:B:2441:ARG:CG	2:B:2461:THR:O	2.65	0.42
2:B:2505:ARG:HG3	2:B:2505:ARG:HH11	1.84	0.42
2:B:2514:VAL:O	2:B:2526:TRP:HD1	2.02	0.42
2:B:2567:ASP:HB2	2:B:2574:ILE:CD1	2.46	0.42
2:B:2594:LEU:O	2:B:2605:ILE:HA	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1019:GLU:HA	1:A:1022:LYS:HB2	2.01	0.42
1:A:1130:LYS:HG3	2:B:2303:GLN:NE2	2.34	0.42
2:B:2321:TRP:HB2	2:B:2351:TRP:HB2	2.01	0.42
2:B:2398:SER:C	2:B:2400:ASP:N	2.78	0.42
2:B:2403:LEU:HB2	2:B:2417:LEU:HB2	2.00	0.42
2:B:2503:ALA:O	2:B:2518:ALA:HA	2.19	0.42
1:A:1139:PHE:CD1	2:B:2280:PHE:HB3	2.55	0.42
2:B:2298:PRO:O	2:B:2302:LEU:HG	2.20	0.42
2:B:2386:CYS:SG	2:B:2427:SER:CB	3.08	0.42
2:B:2503:ALA:O	2:B:2518:ALA:HB1	2.20	0.42
2:B:2516:SER:O	2:B:2523:VAL:HA	2.20	0.42
1:A:1093:LEU:C	1:A:1095:VAL:N	2.76	0.42
2:B:2417:LEU:HB3	2:B:2446:TRP:CZ3	2.54	0.42
1:A:1028:LYS:HG2	1:A:1032:GLU:OE1	2.20	0.42
1:A:1108:ASN:ND2	2:B:2288:LEU:HD11	2.34	0.42
1:A:1139:PHE:HD1	2:B:2280:PHE:HB3	1.85	0.42
1:A:1142:LYS:HE3	2:B:2278:ARG:HD3	2.02	0.42
2:B:2389:PHE:CE2	2:B:2678:SER:HB3	2.55	0.42
1:A:1021:ALA:C	1:A:1023:GLN:N	2.77	0.41
1:A:1104:ILE:HD13	1:A:1119:THR:OG1	2.20	0.41
2:B:2269:MET:SD	2:B:2286:LYS:HE3	2.59	0.41
2:B:2342:ILE:CG1	2:B:2343:LYS:H	2.28	0.41
2:B:2515:VAL:HG11	2:B:2554:VAL:CG2	2.50	0.41
2:B:2522:MET:HE1	2:B:2538:GLN:OE1	2.20	0.41
2:B:2553:HIS:HD2	2:B:2574:ILE:HD12	1.85	0.41
1:A:1058:VAL:CG2	1:A:1059:ILE:N	2.83	0.41
1:A:1116:LEU:HD12	1:A:1120:CYS:SG	2.59	0.41
2:B:2307:THR:HG22	2:B:2308:CYS:SG	2.59	0.41
2:B:2508:GLN:HB3	2:B:2549:PHE:HB3	2.02	0.41
2:B:2395:VAL:HG21	2:B:2429:MET:SD	2.61	0.41
2:B:2469:LEU:HD11	2:B:2471:GLU:O	2.20	0.41
1:A:1085:ILE:CG2	1:A:1090:GLN:HB2	2.50	0.41
1:A:1097:GLN:O	1:A:1098:GLY:C	2.63	0.41
1:A:1158:GLN:HB3	3:A:35:HOH:O	2.19	0.41
2:B:2580:HIS:CB	2:B:2598:ASN:ND2	2.79	0.41
1:A:1117:ASP:OD2	2:B:2291:TYR:CE2	2.73	0.41
2:B:2297:GLU:O	2:B:2298:PRO:C	2.61	0.41
2:B:2540:HIS:C	2:B:2542:ASN:N	2.78	0.41
2:B:2704:VAL:HG12	2:B:2705:ASP:N	2.36	0.41
1:A:1020:ILE:CG2	1:A:1063:THR:HA	2.51	0.41
1:A:1055:LEU:HA	1:A:1058:VAL:HG22	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1006:LEU:CB	1:A:1045:VAL:HB	2.50	0.41
2:B:2265:VAL:O	2:B:2269:MET:HG2	2.21	0.41
2:B:2432:ASN:ND2	2:B:2449:GLU:N	2.63	0.41
2:B:2441:ARG:HB3	2:B:2460:HIS:O	2.21	0.41
2:B:2467:MET:HA	2:B:2475:VAL:O	2.21	0.41
2:B:2547:LEU:HD23	2:B:2556:SER:HA	2.03	0.41
2:B:2649:TRP:CE3	2:B:2656:PHE:HA	2.55	0.41
2:B:2476:SER:O	2:B:2483:LEU:CA	2.69	0.41
2:B:2524:LYS:HZ3	2:B:2524:LYS:HG2	1.80	0.41
2:B:2570:THR:OG1	2:B:2572:ASN:HB2	2.21	0.41
1:A:1062:CYS:O	1:A:1064:HIS:N	2.54	0.41
2:B:2334:LEU:C	2:B:2334:LEU:CD1	2.94	0.41
2:B:2379:HIS:O	2:B:2695:THR:HG21	2.21	0.41
2:B:2391:GLY:C	2:B:2393:ARG:H	2.29	0.41
2:B:2394:ILE:HB	2:B:2406:TRP:HB2	2.03	0.41
2:B:2497:LEU:HD22	2:B:2497:LEU:H	1.86	0.41
2:B:2583:LEU:HD13	2:B:2583:LEU:C	2.46	0.41
2:B:2704:VAL:HA	3:B:60:HOH:O	2.20	0.41
1:A:1054:ILE:CD1	1:A:1102:GLU:HB3	2.51	0.41
1:A:1141:ILE:CG1	2:B:2279:ASP:HB3	2.51	0.41
1:A:1085:ILE:CD1	1:A:1125:ASN:ND2	2.84	0.40
1:A:1097:GLN:HB3	2:B:2280:PHE:HD1	1.87	0.40
2:B:2443:LEU:HG	2:B:2464:VAL:HG11	2.04	0.40
2:B:2453:CYS:SG	2:B:2455:HIS:O	2.78	0.40
2:B:2482:THR:CG2	2:B:2498:MET:HG2	2.51	0.40
2:B:2368:GLY:O	2:B:2658:ARG:NH1	2.52	0.40
2:B:2279:ASP:OD1	2:B:2282:SER:OG	2.35	0.40
2:B:2497:LEU:HD22	2:B:2497:LEU:N	2.36	0.40
2:B:2537:LEU:HB3	2:B:2566:TRP:CE3	2.57	0.40
1:A:1018:VAL:CG2	1:A:1022:LYS:HE3	2.52	0.40
1:A:1130:LYS:HG2	1:A:1131:THR:H	1.85	0.40
2:B:2341:VAL:HA	3:B:72:HOH:O	2.22	0.40
2:B:2357:ARG:NH1	2:B:2361:ILE:HD11	2.36	0.40
2:B:2428:GLN:HG2	2:B:2467:MET:HG3	2.03	0.40
2:B:2530:THR:C	2:B:2532:THR:N	2.78	0.40
1:A:1104:ILE:HD13	1:A:1119:THR:CB	2.51	0.40
2:B:2488:ILE:HD13	2:B:2488:ILE:HA	1.73	0.40
2:B:2509:TYR:CE1	2:B:2511:GLY:HA2	2.57	0.40
2:B:2563:ILE:HD11	2:B:2584:THR:HG21	2.03	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	130/149 (87%)	102 (78%)	19 (15%)	9 (7%)	1	2
2	B	437/445 (98%)	360 (82%)	62 (14%)	15 (3%)	3	12
All	All	567/594 (96%)	462 (82%)	81 (14%)	24 (4%)	2	9

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	2275	GLN
2	B	2344	PRO
2	B	2366	ARG
2	B	2391	GLY
2	B	2431	ASP
1	A	1088	TRP
1	A	1128	LYS
1	A	1141	ILE
2	B	2276	PHE
2	B	2343	LYS
2	B	2417	LEU
1	A	1044	PRO
1	A	1129	GLY
1	A	1131	THR
1	A	1140	ASN
2	B	2372	SER
2	B	2666	GLY
2	B	2315	ALA
2	B	2499	GLY
1	A	1147	GLU
2	B	2531	GLU
2	B	2587	MET
1	A	1087	VAL
2	B	2539	GLY

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	122/134 (91%)	118 (97%)	4 (3%)	33	67
2	B	391/395 (99%)	355 (91%)	36 (9%)	8	27
All	All	513/529 (97%)	473 (92%)	40 (8%)	11	35

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1013	ILE
1	A	1095	VAL
1	A	1099	THR
1	A	1137	LYS
2	B	2264	GLN
2	B	2269	MET
2	B	2281	ILE
2	B	2298	PRO
2	B	2307	THR
2	B	2334	LEU
2	B	2343	LYS
2	B	2344	PRO
2	B	2352	LYS
2	B	2370	LEU
2	B	2388	GLN
2	B	2430	ARG
2	B	2431	ASP
2	B	2439	THR
2	B	2461	THR
2	B	2472	LYS
2	B	2513	ARG
2	B	2521	PHE
2	B	2541	THR
2	B	2544	VAL
2	B	2554	VAL
2	B	2560	ASP
2	B	2561	THR

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Mol	Chain	Res	Type
2	B	2568	VAL
2	B	2587	MET
2	B	2591	ASP
2	B	2602	THR
2	B	2642	ASP
2	B	2648	LEU
2	B	2660	LEU
2	B	2663	LEU
2	B	2679	ASN
2	B	2680	THR
2	B	2695	THR
2	B	2698	LEU
2	B	2705	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	1060	GLN
1	A	1064	HIS
1	A	1108	ASN
1	A	1140	ASN
1	A	1143	ASN
2	B	2264	GLN
2	B	2270	GLN
2	B	2275	GLN
2	B	2303	GLN
2	B	2306	GLN
2	B	2318	ASN
2	B	2348	HIS
2	B	2379	HIS
2	B	2382	HIS
2	B	2388	GLN
2	B	2392	ASN
2	B	2432	ASN
2	B	2468	HIS
2	B	2470	HIS
2	B	2538	GLN
2	B	2553	HIS
2	B	2572	ASN
2	B	2581	GLN
2	B	2615	GLN
2	B	2659	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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	134/149 (89%)	0.97	23 (17%) 4 3	34, 58, 83, 91	0
2	B	441/445 (99%)	0.50	40 (9%) 15 12	9, 36, 73, 89	0
All	All	575/594 (96%)	0.61	63 (10%) 10 9	9, 41, 77, 91	0

All (63) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1087	VAL	9.2
2	B	2341	VAL	5.7
2	B	2342	ILE	4.4
2	B	2343	LYS	4.1
2	B	2691	GLY	4.1
1	A	1130	LYS	3.9
1	A	1037	ASP	3.9
1	A	1002	PRO	3.8
2	B	2267	HIS	3.8
1	A	1142	LYS	3.8
2	B	2277	GLN	3.5
2	B	2271	VAL	3.4
1	A	1133	GLU	3.3
2	B	2278	ARG	3.2
2	B	2371	LYS	3.1
2	B	2274	PRO	3.1
2	B	2441	ARG	3.1
2	B	2336	ILE	3.1
2	B	2624	GLN	3.0
2	B	2705	ASP	3.0
2	B	2264	GLN	3.0
2	B	2367	ARG	3.0
2	B	2268	MET	3.0
2	B	2326	LYS	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	1020	ILE	2.9
2	B	2337	LYS	2.9
2	B	2331	ASP	2.9
2	B	2322	ARG	2.9
2	B	2319	LEU	2.8
1	A	1137	LYS	2.7
2	B	2432	ASN	2.7
1	A	1159	TRP	2.7
2	B	2706	MET	2.6
2	B	2465	ARG	2.6
2	B	2492	GLN	2.6
2	B	2330	ILE	2.5
1	A	1085	ILE	2.4
2	B	2344	PRO	2.4
2	B	2368	GLY	2.4
2	B	2462	SER	2.4
1	A	1158	GLN	2.4
1	A	1089	ASP	2.4
1	A	1086	PRO	2.4
2	B	2581	GLN	2.3
2	B	2479	ARG	2.3
1	A	1063	THR	2.3
1	A	1129	GLY	2.3
1	A	1005	LYS	2.3
1	A	1015	GLU	2.2
1	A	1095	VAL	2.2
1	A	1143	ASN	2.2
2	B	2461	THR	2.2
2	B	2539	GLY	2.1
2	B	2276	PHE	2.1
1	A	1131	THR	2.1
1	A	1019	GLU	2.1
2	B	2481	ALA	2.1
2	B	2315	ALA	2.1
2	B	2350	PRO	2.0
1	A	1140	ASN	2.0
2	B	2283	LEU	2.0
2	B	2345	GLY	2.0
1	A	1148	GLU	2.0

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 [i](#)

There are no such residues in this entry.