



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 13, 2017 – 04:52 pm GMT

PDB ID : 2OVP
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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity	:	4.02b-467
Xtriage (Phenix)	:	1.9-1692
EDS	:	trunk28620
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	recalc28949

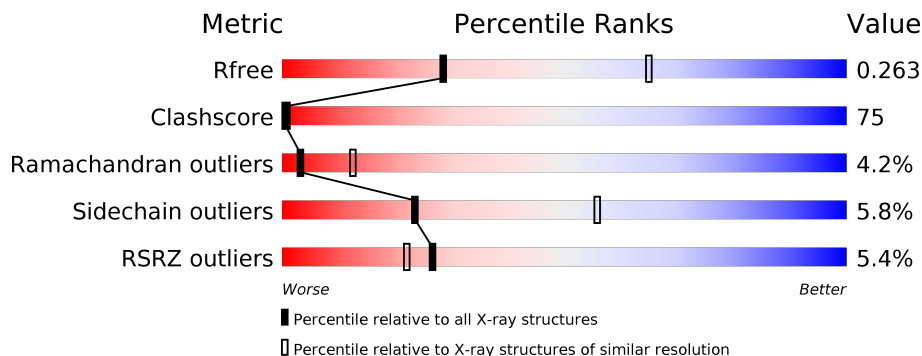
1 Overall quality at a glance

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}	100719	1586 (2.90-2.90)
Clashscore	112137	1807 (2.90-2.90)
Ramachandran outliers	110173	1768 (2.90-2.90)
Sidechain outliers	110143	1770 (2.90-2.90)
RSRZ outliers	101464	1596 (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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	149	<div> <div>11%</div> <div> <div>16%</div> <div>69%</div> <div>5%</div> <div>10%</div> </div> </div>
2	B	445	<div> <div>3%</div> <div> <div>20%</div> <div>71%</div> <div>7%</div> <div>••</div> </div> </div>

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			

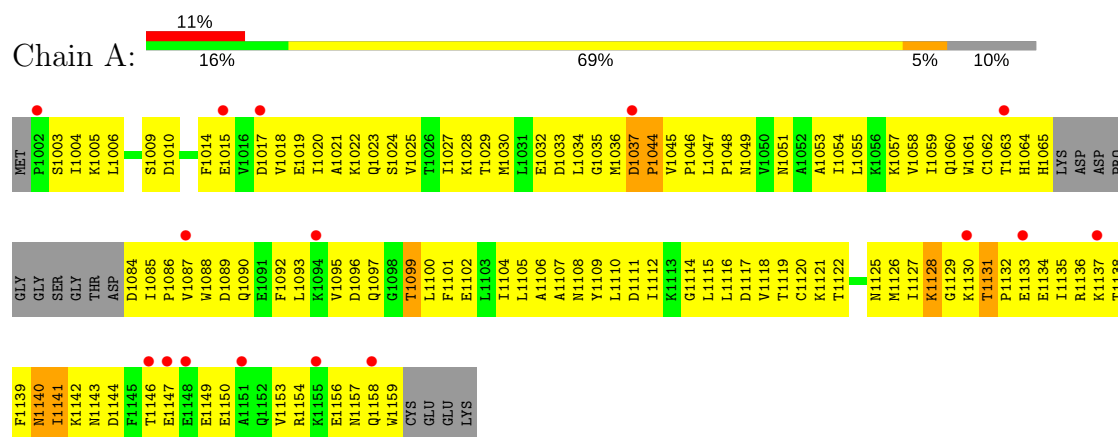
- Molecule 3 is water.

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

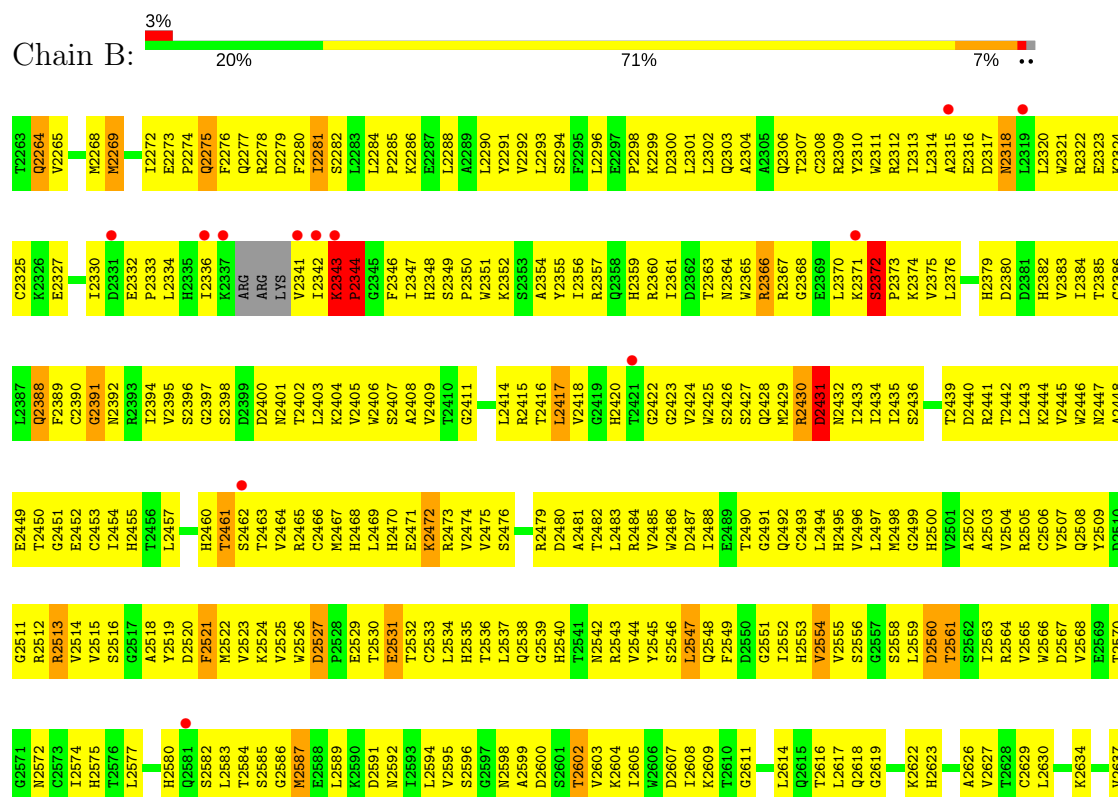
3 Residue-property plots

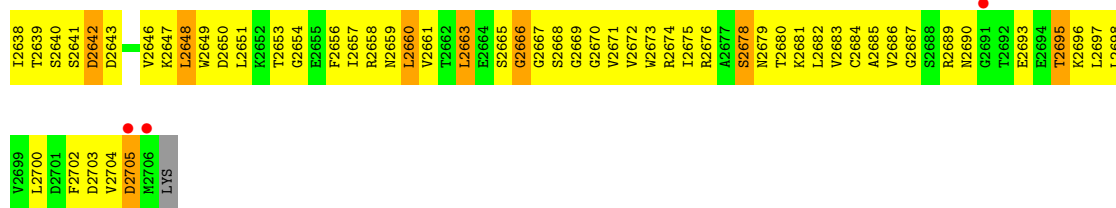
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: S-phase kinase-associated protein 1A



• Molecule 2: F-box/WD repeat protein 7





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 – 2.88	Depositor EDS
% Data completeness (in resolution range)	98.5 (19.94-2.90) 97.9 (19.94-2.88)	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 0.234 , 0.263	Depositor DCC
R_{free} test set	1959 reflections (6.91%)	DCC
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 , 42.6	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 [i](#)

5.1 Standard geometry [i](#)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.34	0/1091	0.61	0/1476
2	B	0.48	0/3554	0.76	3/4815 (0.1%)
All	All	0.45	0/4645	0.73	3/6291 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2372	SER	N-CA-C	-5.73	95.52	111.00
2	B	2527	ASP	N-CA-C	-5.36	96.54	111.00
2	B	2678	SER	N-CA-C	-5.18	97.01	111.00

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1073	0	1083	168	0
2	B	3484	0	3468	557	0
3	A	10	0	0	2	0
3	B	109	0	0	12	0
All	All	4676	0	4551	687	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 75.

All (687) 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: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
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:2388:GLN:HB3	2:B:2429:MET:HE1	1.60	0.83
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1055:LEU:HD23	1:A:1055:LEU:O	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
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
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:2357:ARG:NH2	3:B:4:HOH:O	2.29	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:2473:ARG:HB2	2:B:2509:TYR:HE2	1.60	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:O	1:A:1006:LEU:HD12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2494:LEU:N	2:B:2494:LEU:HD12	2.13	0.63
2:B:2483:LEU:HD21	2:B:2516:SER:CB	2.27	0.63
1:A:1133:GLU:CD	1:A:1133:GLU:H	2.02	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
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: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
1:A:1062:CYS:C	1:A:1064:HIS:H	2.01	0.61
2:B:2273:GLU:N	2:B:2274:PRO:HD3	2.14	0.61
2:B:2415:ARG:HE	2:B:2450:THR:C	2.04	0.61
2:B:2281:ILE:HG12	2:B:2311:TRP:CE2	2.35	0.61
2:B:2521:PHE:N	2:B:2521:PHE:CD2	2.67	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: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:2392:ASN:HD22	2:B:2392:ASN:N	1.99	0.60
2:B:2374:LYS:HE2	2:B:2409:VAL:O	2.01	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:CD1	2:B:2469:LEU:HD22	2.32	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2487:ASP:HB3	2:B:2490:THR:OG1	2.01	0.60
2:B:2435:ILE:HG12	2:B:2488:ILE:HD12	1.82	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: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
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:2357:ARG:CZ	2:B:2361:ILE:HD11	2.34	0.58
2:B:2314:LEU:C	2:B:2316:GLU:H	2.05	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:2416:THR:O	2:B:2418:VAL:HG13	2.04	0.58
2:B:2595:VAL:HA	2:B:2604:LYS:O	2.02	0.58
2:B:2370:LEU:HD22	2:B:2658:ARG:HH21	1.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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
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:2561:THR:HG23	2:B:2580:HIS:O	2.05	0.56
2:B:2554:VAL:CG1	2:B:2566:TRP:HB2	2.25	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
1:A:1004:ILE:C	1:A:1004:ILE:HD12	2.26	0.56
2:B:2641:SER:HB3	2:B:2643:ASP:OD2	2.06	0.56
2:B:2475:VAL:HG21	2:B:2514:VAL:CG2	2.33	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
2:B:2343:LYS:O	2:B:2344:PRO:C	2.42	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:2334:LEU:HD12	2:B:2334:LEU:C	2.27	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:2520:ASP:C	2:B:2522:MET:H	2.09	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:2500:HIS:CD2	2:B:2504:VAL:HG22	2.43	0.54
2:B:2475:VAL:HG11	2:B:2514:VAL:HG11	1.90	0.54
2:B:2472:LYS:CD	2:B:2472:LYS:H	2.21	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: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:2314:LEU:C	2:B:2316:GLU:N	2.62	0.53
2:B:2585:SER:OG	2:B:2586:GLY:N	2.40	0.53
2:B:2584:THR:HG23	2:B:2596:SER:HB2	1.89	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:2518:ALA:C	2:B:2520:ASP:H	2.11	0.53
2:B:2470:HIS:CD2	2:B:2511:GLY:HA3	2.43	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
2:B:2365:TRP:CH2	2:B:2682:LEU:HB2	2.44	0.53
1:A:1030:MET:HA	1:A:1034:LEU:HD23	1.91	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:1062:CYS:C	1:A:1064:HIS:N	2.62	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
2:B:2467:MET:HA	2:B:2476:SER:HA	1.91	0.52
2:B:2417:LEU:HB3	2:B:2446:TRP:CD2	2.44	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: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:2565:VAL:HB	2:B:2575:HIS:HB2	1.92	0.51
1:A:1131:THR:HG22	1:A:1134:GLU:H	1.76	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:2430:ARG:HD3	3:B:79:HOH:O	2.10	0.51
2:B:2360:ARG:HB3	2:B:2704:VAL:HG21	1.91	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: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: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
2:B:2365:TRP:HA	2:B:2702:PHE:CD1	2.45	0.51
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:2559:LEU:C	2:B:2561:THR:H	2.13	0.51
1:A:1006:LEU:HD22	1:A:1027:ILE:HD13	1.93	0.50
2:B:2269:MET:HE3	2:B:2269:MET:HA	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: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:2390:CYS:HB2	2:B:2429:MET:CE	2.41	0.50
2:B:2386:CYS:SG	2:B:2397:GLY:HA3	2.51	0.50
2:B:2630:LEU:C	2:B:2630:LEU:HD12	2.32	0.50
1:A:1057:LYS:HZ3	1:A:1095:VAL:HG21	1.75	0.50
1:A:1055:LEU:O	1:A:1058:VAL:HG22	2.12	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: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:2325:CYS:C	2:B:2327:GLU:H	2.14	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:1085:ILE:HG22	1:A:1090:GLN:HB2	1.95	0.48
1:A:1061:TRP:HB2	1:A:1092:PHE:CZ	2.48	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:2368:GLY:O	2:B:2658:ARG:NH2	2.44	0.48
2:B:2379:HIS:CD2	2:B:2398:SER:HB2	2.48	0.48
2:B:2376:LEU:HD13	2:B:2406:TRP:CE3	2.48	0.48
2:B:2520:ASP:O	2:B:2522:MET:HG2	2.13	0.48
2:B:2515:VAL:HG12	2:B:2547:LEU:CD1	2.43	0.48
2:B:2439:THR:HA	2:B:2463:THR:CG2	2.44	0.48
2:B:2480:ASP:O	2:B:2481:ALA:HB3	2.13	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
2:B:2398:SER:C	2:B:2400:ASP:H	2.17	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:2343:LYS:CB	2:B:2344:PRO:HD2	2.09	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:2430:ARG:HB2	2:B:2469:LEU:CD2	2.42	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
2:B:2330:ILE:C	2:B:2332:GLU:H	2.16	0.48
2:B:2494:LEU:CD1	2:B:2494:LEU:H	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2540:HIS:C	2:B:2542:ASN:H	2.17	0.47
1:A:1061:TRP:HE3	1:A:1062:CYS:HG	1.60	0.47
2:B:2505:ARG:HG2	2:B:2545:TYR:CD1	2.50	0.47
2:B:2600:ASP:CG	2:B:2602:THR:HB	2.35	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:1136:ARG:HH22	1:A:1143:ASN:HD22	1.60	0.47
2:B:2325:CYS:C	2:B:2327:GLU:N	2.68	0.47
1:A:1051:ASN:OD1	1:A:1053:ALA:HB3	2.13	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: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:2518:ALA:C	2:B:2520:ASP:N	2.67	0.47
2:B:2646:VAL:HG22	2:B:2672:VAL:HG11	1.96	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:1021:ALA:C	1:A:1023:GLN:H	2.19	0.46
1:A:1034:LEU:H	1:A:1034:LEU:HD22	1.80	0.46
1:A:1131:THR:O	1:A:1135:ILE:HG13	2.15	0.46
2:B:2269:MET:CE	2:B:2313:ILE:HD12	2.45	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:2285:PRO:O	2:B:2286:LYS:C	2.54	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:1036:MET:O	1:A:1037:ASP:C	2.54	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
2:B:2394:ILE:CG2	2:B:2683:VAL:HG11	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:2574:ILE:HG22	2:B:2575:HIS:CD2	2.51	0.46
2:B:2546:SER:HB3	2:B:2585:SER:O	2.16	0.46
1:A:1024:SER:OG	1:A:1110:LEU:HB3	2.16	0.46
2:B:2392:ASN:ND2	2:B:2392:ASN:N	2.62	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
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
1:A:1024:SER:HB3	1:A:1027:ILE:HD12	1.99	0.45
1:A:1137:LYS:HB3	1:A:1137:LYS:NZ	2.31	0.45
2:B:2647:LYS:NZ	2:B:2659:ASN:ND2	2.61	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: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
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:2321:TRP:C	2:B:2323:GLU:N	2.67	0.45
2:B:2460:HIS:CD2	2:B:2476:SER:HG	2.31	0.45
2:B:2526:TRP:CZ3	2:B:2533:CYS:HB2	2.52	0.45
2:B:2618:GLN:C	2:B:2622:LYS:HB3	2.37	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C	2:B:2409:VAL:N	2.67	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
2:B:2385:THR:OG1	2:B:2424:VAL:O	2.19	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: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:2618:GLN:HB3	2:B:2622:LYS:HE2	2.00	0.44
2:B:2617:LEU:HB3	2:B:2649:TRP:CD2	2.52	0.44
2:B:2665:SER:O	2:B:2667:GLY:N	2.50	0.44
2:B:2660:LEU:HB3	2:B:2700:LEU:CD1	2.47	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
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
2:B:2479:ARG:NH2	3:B:9:HOH:O	2.50	0.44
2:B:2473:ARG:HA	2:B:2486:TRP:O	2.17	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:1117:ASP:OD2	2:B:2291:TYR:OH	2.33	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:2269:MET:HE3	2:B:2313:ILE:HD12	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2269:MET:HE2	2:B:2274:PRO:HD2	1.99	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:2300:ASP:O	2:B:2301:LEU:C	2.56	0.43
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
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:2396:SER:HB3	2:B:2697:LEU:HD21	2.01	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
1:A:1130:LYS:CG	2:B:2303:GLN:HG3	2.33	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:HG3	2:B:2467:MET:O	2.17	0.43
2:B:2520:ASP:C	2:B:2522:MET:N	2.72	0.43
2:B:2379:HIS:O	2:B:2380:ASP:C	2.56	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:1136:ARG:C	1:A:1138:THR:N	2.72	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
2:B:2364:ASN:HD22	2:B:2702:PHE:C	2.20	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: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
1:A:1132:PRO:CG	2:B:2306:GLN:HB2	2.49	0.43
2:B:2556:SER:O	2:B:2563:ILE:HA	2.19	0.43
2:B:2665:SER:O	2:B:2666:GLY:C	2.56	0.43
1:A:1084:ASP:N	1:A:1121:LYS:NZ	2.66	0.43
1:A:1149:GLU:O	1:A:1150:GLU:C	2.57	0.43
2:B:2401:ASN:H	2:B:2423:GLY:HA2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2395:VAL:CG2	2:B:2429:MET:SD	3.07	0.43
2:B:2460:HIS:NE2	2:B:2476:SER:OG	2.35	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: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
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
2:B:2321:TRP:O	2:B:2322:ARG:C	2.57	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:1158:GLN:HG3	1:A:1159:TRP:N	2.34	0.42
1:A:1142:LYS:HE3	2:B:2278:ARG:CD	2.50	0.42
2:B:2389:PHE:CZ	2:B:2681:LYS:HG3	2.55	0.42
2:B:2443:LEU:CD2	2:B:2467:MET:HE2	2.50	0.42
2:B:2454:ILE:HG13	2:B:2455:HIS:CD2	2.50	0.42
2:B:2443:LEU:HD13	2:B:2486:TRP:CE2	2.55	0.42
2:B:2520:ASP:O	2:B:2522:MET:N	2.51	0.42
2:B:2506:CYS:SG	2:B:2547:LEU:HB2	2.59	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:2290:LEU:C	2:B:2292:VAL:N	2.72	0.42
2:B:2441:ARG:CG	2:B:2461:THR:O	2.65	0.42
2:B:2505:ARG:HH11	2:B:2505:ARG:HG3	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
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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2516:SER:O	2:B:2523:VAL:HA	2.20	0.42
2:B:2390:CYS:HB2	2:B:2429:MET:HE2	2.01	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
2:B:2268:MET:HE3	2:B:2346:PHE:CD1	2.55	0.42
1:A:1142:LYS:HE3	2:B:2278:ARG:HD3	2.02	0.42
1:A:1139:PHE:HD1	2:B:2280:PHE:HB3	1.85	0.42
1:A:1108:ASN:ND2	2:B:2288:LEU:HD11	2.34	0.42
2:B:2389:PHE:CE2	2:B:2678:SER:HB3	2.55	0.42
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:2371:LYS:O	2:B:2372:SER:OG	2.29	0.41
2:B:2553:HIS:HD2	2:B:2574:ILE:HD12	1.85	0.41
2:B:2515:VAL:HG11	2:B:2554:VAL:CG2	2.50	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:1084:ASP:N	1:A:1121:LYS:HZ2	2.17	0.41
1:A:1085:ILE:CG2	1:A:1090:GLN:HB2	2.50	0.41
1:A:1158:GLN:HB3	3:A:35:HOH:O	2.19	0.41
2:B:2439:THR:C	2:B:2441:ARG:H	2.24	0.41
2:B:2580:HIS:CB	2:B:2598:ASN:ND2	2.79	0.41
1:A:1143:ASN:HD21	1:A:1150:GLU:CD	2.23	0.41
1:A:1117:ASP:OD2	2:B:2291:TYR:CE2	2.73	0.41
2:B:2704:VAL:HG12	2:B:2705:ASP:N	2.36	0.41
1:A:1055:LEU:HA	1:A:1058:VAL:HG22	2.01	0.41
1:A:1020:ILE:CG2	1:A:1063:THR:HA	2.51	0.41
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:2552:ILE:C	2:B:2568:VAL:HG23	2.40	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2355:TYR:CD2	2:B:2355:TYR:C	2.93	0.41
2:B:2440:ASP:OD1	2:B:2440:ASP:C	2.59	0.41
2:B:2379:HIS:O	2:B:2695:THR:HG21	2.21	0.41
2:B:2394:ILE:HB	2:B:2406:TRP:HB2	2.03	0.41
2:B:2497:LEU:H	2:B:2497:LEU:HD22	1.86	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:1055:LEU:HD23	1:A:1055:LEU:C	2.40	0.41
1:A:1141:ILE:CG1	2:B:2279:ASP:HB3	2.51	0.41
2:B:2296:LEU:O	2:B:2324:LYS:NZ	2.41	0.41
2:B:2311:TRP:O	2:B:2312:ARG:C	2.59	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:2273:GLU:C	2:B:2275:GLN:H	2.24	0.40
2:B:2368:GLY:O	2:B:2658:ARG:NH1	2.52	0.40
2:B:2497:LEU:N	2:B:2497:LEU:HD22	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:2318:ASN:CG	2:B:2350:PRO:HD2	2.41	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
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	3
2	B	437/445 (98%)	360 (82%)	62 (14%)	15 (3%)	4	18
All	All	567/594 (96%)	462 (82%)	81 (14%)	24 (4%)	3	12

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%)	120 (98%)	2 (2%)	68	90
2	B	391/395 (99%)	363 (93%)	28 (7%)	17	43
All	All	513/529 (97%)	483 (94%)	30 (6%)	23	56

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1037	ASP
1	A	1099	THR
2	B	2264	GLN
2	B	2269	MET
2	B	2281	ILE
2	B	2318	ASN
2	B	2343	LYS
2	B	2344	PRO
2	B	2388	GLN
2	B	2430	ARG
2	B	2431	ASP
2	B	2461	THR
2	B	2472	LYS
2	B	2513	ARG
2	B	2521	PHE
2	B	2547	LEU
2	B	2554	VAL
2	B	2560	ASP
2	B	2561	THR
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	2705	ASP

Some 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	1143	ASN
2	B	2275	GLN
2	B	2303	GLN
2	B	2306	GLN
2	B	2318	ASN
2	B	2348	HIS
2	B	2364	ASN
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	2540	HIS
2	B	2553	HIS
2	B	2572	ASN
2	B	2581	GLN
2	B	2612	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

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%)	0.40	16 (11%) 5 3	34, 58, 83, 91	0
2	B	441/445 (99%)	0.09	15 (3%) 46 39	9, 36, 73, 89	0
All	All	575/594 (96%)	0.16	31 (5%) 26 22	9, 41, 77, 91	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1087	VAL	5.1
2	B	2341	VAL	4.9
1	A	1002	PRO	4.2
2	B	2343	LYS	4.0
2	B	2705	ASP	3.3
2	B	2421	THR	3.2
1	A	1130	LYS	3.2
1	A	1148	GLU	3.0
1	A	1137	LYS	2.9
2	B	2342	ILE	2.9
2	B	2331	ASP	2.8
1	A	1133	GLU	2.7
1	A	1146	THR	2.7
2	B	2706	MET	2.6
1	A	1151	ALA	2.6
2	B	2319	LEU	2.5
2	B	2371	LYS	2.5
2	B	2315	ALA	2.4
2	B	2336	ILE	2.4
2	B	2691	GLY	2.3
1	A	1037	ASP	2.3
1	A	1094	LYS	2.3
2	B	2337	LYS	2.2
1	A	1158	GLN	2.2

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Mol	Chain	Res	Type	RSRZ
2	B	2581	GLN	2.2
1	A	1147	GLU	2.1
1	A	1017	ASP	2.1
1	A	1155	LYS	2.1
1	A	1015	GLU	2.1
1	A	1063	THR	2.0
2	B	2462	SER	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 carbohydrates in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.