



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 12:06 am BST

PDB ID : 1MJE
Title : STRUCTURE OF A BRCA2-DSS1-SSDNA COMPLEX
Authors : Yang, H.; Jeffrey, P.D.; Miller, J.; Kinnucan, E.; Sun, Y.; Thoma, N.H.; Zheng, N.; Chen, P.L.; Lee, W.H.; Pavletich, N.P.
Deposited on : 2002-08-27
Resolution : 3.50 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

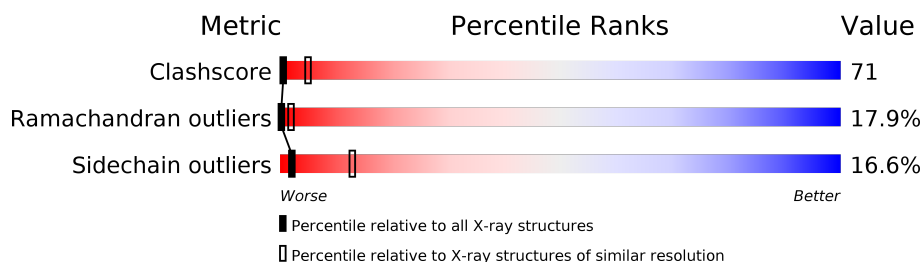
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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))
Clashscore	141614	1036 (3.58-3.42)
Ramachandran outliers	138981	1005 (3.58-3.42)
Sidechain outliers	138945	1006 (3.58-3.42)

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 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 $\leq 5\%$.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	6	
2	B	70	
3	A	649	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5198 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 DNA chain called 5'-D(P*TP*TP*TP*TP*TP*T)-3'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	6	Total	C	N	O	P	16	0	0
			121	60	12	43	6			

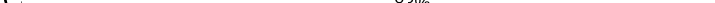
- Molecule 2 is a protein called Deleted in split hand/split foot protein 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	B	42	Total	C	N	O	0	0	0
			335	209	50	76			

- Molecule 3 is a protein called breast cancer 2.

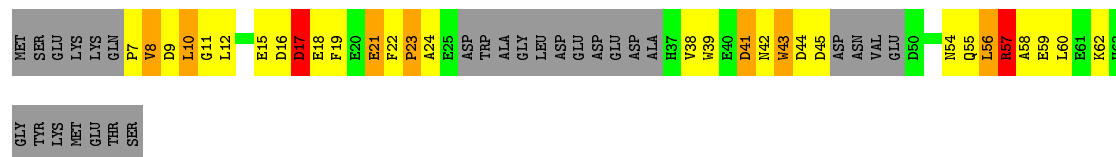
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	600	Total	C	N	O	S	0	0	0
			4742	3025	824	877	16			

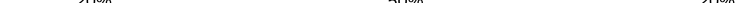
Note EDS was not executed.

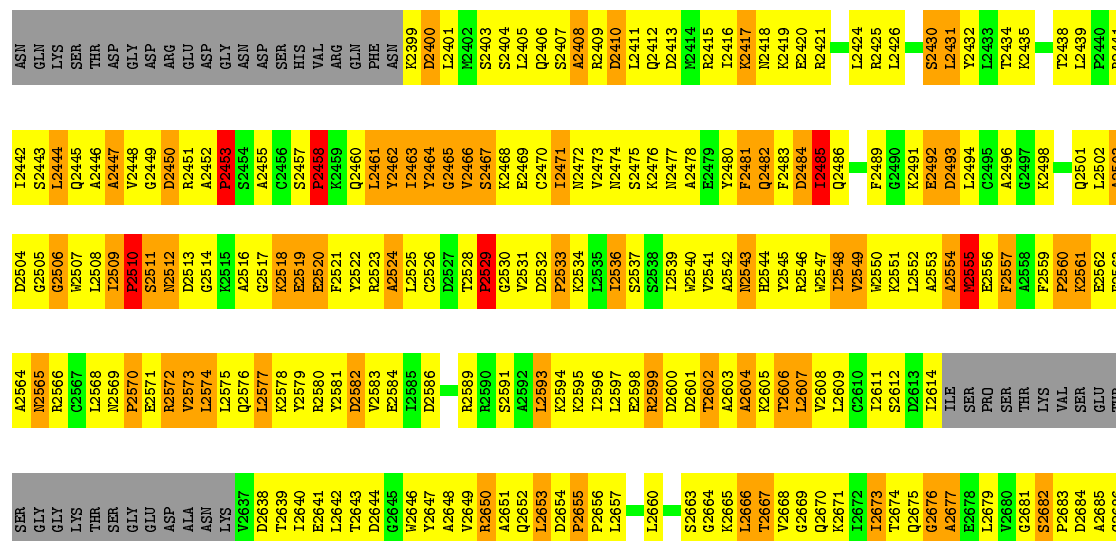
- Chain C:  83% 17%



- Chain B:  17% 30% 10% 5% 40%



- Chain A: 



WORLDWIDE
PDB
PROTEIN DATA BANK

4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	I 4 2 2	Depositor
Cell constants a, b, c, α , β , γ	198.87Å 198.87Å 200.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	15.00 – 3.50	Depositor
% Data completeness (in resolution range)	(Not available) (15.00-3.50)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.245 , 0.278	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5198	wwPDB-VP
Average B, all atoms (Å ²)	105.0	wwPDB-VP

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	C	0.96	1/132 (0.8%)	0.85	0/200
2	B	0.66	0/340	0.88	1/460 (0.2%)
3	A	0.66	2/4843 (0.0%)	0.92	10/6557 (0.2%)
All	All	0.67	3/5315 (0.1%)	0.92	11/7217 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
3	A	0	1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	2790	VAL	CA-CB	7.32	1.70	1.54
1	C	501	DT	OP3-P	-6.11	1.53	1.61
3	A	2789	LYS	CG-CD	5.09	1.69	1.52

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	A	3005	GLY	N-CA-C	-8.10	92.84	113.10
3	A	2889	VAL	CB-CA-C	-6.88	98.32	111.40
3	A	2458	PRO	N-CA-CB	5.79	110.25	103.30
3	A	2741	ILE	CB-CA-C	-5.75	100.10	111.60
3	A	2905	LEU	CA-CB-CG	-5.63	102.34	115.30
2	B	7	PRO	N-CA-CB	5.51	109.92	103.30
3	A	2769	GLU	N-CA-C	-5.33	96.61	111.00
3	A	2791	HIS	N-CA-C	5.26	125.22	111.00
3	A	2957	LEU	CA-CB-CG	-5.26	103.21	115.30
3	A	2926	ARG	N-CA-C	-5.10	97.23	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2790	VAL	CG1-CB-CG2	-5.04	102.83	110.90

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	3072	TYR	Sidechain

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	C	121	0	73	10	0
2	B	335	0	262	46	0
3	A	4742	0	4783	706	0
All	All	5198	0	5118	730	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 71.

All (730) 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:56:LEU:HD23	2:B:57:ARG:H	1.02	1.17
3:A:2604:ALA:HB1	3:A:2677:ALA:HB3	1.27	1.17
3:A:3040:ALA:HB1	3:A:3043:LEU:HD11	1.27	1.12
3:A:2691:ALA:HB1	3:A:2692:PRO:HD2	1.25	1.11
2:B:10:LEU:HD11	3:A:2566:ARG:HH21	1.12	1.10
3:A:2749:LEU:CD2	3:A:2750:GLN:H	1.66	1.09
3:A:2974:LEU:CD2	3:A:2976:PHE:H	1.68	1.06
3:A:2747:TYR:HB3	3:A:2748:PRO:HD2	1.35	1.05
3:A:2482:GLN:HG2	3:A:2517:GLY:HA3	1.38	1.04
3:A:2485:ILE:HD13	3:A:2510:PRO:HB3	1.38	1.01
3:A:2412:GLN:HA	3:A:2415:ARG:HH21	1.28	0.99
3:A:2974:LEU:HD23	3:A:2975:HIS:N	1.78	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:3028:LEU:O	3:A:3030:GLU:N	1.97	0.98
3:A:2681:GLY:HA3	3:A:2695:LEU:HA	1.45	0.98
3:A:2451:ARG:HE	3:A:2452:ALA:H	1.05	0.97
3:A:2749:LEU:HD23	3:A:2750:GLN:H	1.29	0.96
2:B:56:LEU:CD2	2:B:57:ARG:H	1.78	0.96
3:A:2548:ILE:HG22	3:A:2552:LEU:HD11	1.47	0.96
2:B:10:LEU:HD11	3:A:2566:ARG:NH2	1.80	0.94
3:A:2674:THR:HB	3:A:2704:THR:HG22	1.47	0.93
3:A:2768:GLU:O	3:A:2768:GLU:HG3	1.66	0.93
3:A:2974:LEU:HD23	3:A:2976:PHE:H	1.34	0.92
3:A:2691:ALA:HB1	3:A:2692:PRO:CD	2.00	0.92
3:A:2723:PRO:C	3:A:2724:LEU:HD12	1.90	0.91
3:A:2611:ILE:HD11	3:A:2667:THR:O	1.69	0.91
3:A:2927:ILE:HG22	3:A:2930:LEU:HD21	1.52	0.90
3:A:2549:VAL:HA	3:A:2552:LEU:HD12	1.54	0.90
3:A:2572:ARG:O	3:A:2575:LEU:HB2	1.71	0.89
3:A:2729:LEU:HD21	3:A:2736:VAL:HG22	1.52	0.89
3:A:2604:ALA:CB	3:A:2677:ALA:HB3	2.03	0.88
3:A:2596:ILE:HD11	3:A:2603:ALA:HA	1.54	0.88
3:A:2691:ALA:CB	3:A:2692:PRO:HD2	2.04	0.87
3:A:2675:GLN:NE2	3:A:2721:PRO:HA	1.89	0.87
3:A:2763:ARG:HG3	3:A:2763:ARG:HH11	1.40	0.87
3:A:2740:ASP:OD2	3:A:2897:TYR:HB2	1.75	0.87
2:B:56:LEU:HD23	2:B:57:ARG:N	1.87	0.86
3:A:2453:PRO:HD3	3:A:2559:PHE:CZ	2.10	0.86
3:A:2526:CYS:HB3	3:A:2533:PRO:HG3	1.56	0.86
3:A:2679:LEU:HD11	3:A:2695:LEU:HD21	1.57	0.85
3:A:2653:LEU:HD13	3:A:2657:LEU:HB3	1.58	0.85
3:A:2442:ILE:HD12	3:A:2442:ILE:N	1.92	0.85
2:B:55:GLN:HG3	3:A:2670:GLN:HA	1.59	0.85
2:B:43:TRP:CZ3	3:A:2704:THR:O	2.30	0.85
3:A:2747:TYR:HB3	3:A:2748:PRO:CD	2.05	0.84
3:A:2444:LEU:H	3:A:2444:LEU:HD12	1.41	0.84
3:A:3019:LEU:HD22	3:A:3019:LEU:N	1.93	0.84
3:A:2473:VAL:HA	3:A:2477:ASN:HD21	1.40	0.84
3:A:2961:SER:O	3:A:2965:LEU:HD13	1.77	0.84
3:A:2674:THR:CB	3:A:2704:THR:HG22	2.08	0.84
3:A:2939:PHE:O	3:A:2940:GLU:HG3	1.77	0.83
3:A:3040:ALA:CB	3:A:3043:LEU:HD11	2.07	0.83
3:A:2573:VAL:HG12	3:A:2577:LEU:CD1	2.07	0.83
3:A:2695:LEU:HD23	3:A:2696:ARG:N	1.94	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:3001:VAL:HG12	3:A:3003:PRO:HD3	1.61	0.82
3:A:2412:GLN:HA	3:A:2415:ARG:NH2	1.95	0.82
3:A:2975:HIS:O	3:A:2976:PHE:HB2	1.78	0.82
2:B:43:TRP:HZ3	3:A:2704:THR:O	1.62	0.82
3:A:3081:LYS:O	3:A:3085:GLU:HG2	1.78	0.82
3:A:2565:ASN:HA	3:A:2568:LEU:HD13	1.61	0.82
3:A:2729:LEU:CD2	3:A:2736:VAL:HG22	2.09	0.81
3:A:3030:GLU:C	3:A:3032:ILE:H	1.81	0.81
3:A:2742:ILE:HD13	3:A:2923:LYS:O	1.80	0.81
3:A:2573:VAL:HG12	3:A:2577:LEU:HD11	1.61	0.80
3:A:2509:ILE:O	3:A:2511:SER:N	2.15	0.79
3:A:2749:LEU:HD22	3:A:2750:GLN:H	1.47	0.79
3:A:2526:CYS:SG	3:A:2533:PRO:HB3	2.23	0.79
3:A:2773:LEU:HD23	3:A:2774:ARG:N	1.97	0.79
3:A:2560:PRO:C	3:A:2562:GLU:H	1.86	0.79
3:A:2608:VAL:O	3:A:2609:LEU:HD23	1.82	0.79
3:A:2470:CYS:SG	3:A:2471:ILE:N	2.55	0.79
3:A:2726:LEU:HA	3:A:2729:LEU:HD12	1.65	0.78
3:A:2986:PRO:HB2	3:A:2987:PRO:HD2	1.63	0.78
3:A:2650:ARG:HH22	3:A:2695:LEU:HB3	1.49	0.78
3:A:2753:GLU:HG3	3:A:2886:VAL:HG23	1.66	0.78
3:A:2768:GLU:CG	3:A:2768:GLU:O	2.31	0.78
3:A:3037:LEU:CD1	3:A:3080:LEU:HD23	2.14	0.77
3:A:2675:GLN:HE22	3:A:2721:PRO:HA	1.47	0.77
3:A:2892:LEU:HD12	3:A:2906:LEU:O	1.83	0.77
3:A:2749:LEU:HD23	3:A:2750:GLN:N	1.98	0.77
3:A:2654:ASP:OD1	3:A:2656:PRO:HD2	1.85	0.77
3:A:3028:LEU:C	3:A:3030:GLU:H	1.88	0.77
3:A:2773:LEU:HD23	3:A:2773:LEU:C	2.06	0.76
3:A:3081:LYS:HA	3:A:3084:ILE:HD12	1.68	0.76
3:A:3020:LEU:O	3:A:3020:LEU:HD23	1.84	0.76
3:A:2451:ARG:HE	3:A:2452:ALA:N	1.83	0.76
3:A:2502:LEU:HD13	3:A:2570:PRO:HB2	1.68	0.76
3:A:2611:ILE:HD13	3:A:2666:LEU:HD23	1.68	0.75
3:A:3050:THR:HB	3:A:3053:VAL:HG13	1.67	0.75
3:A:2485:ILE:HD13	3:A:2510:PRO:CB	2.17	0.75
3:A:2571:GLU:HG3	3:A:2572:ARG:H	1.52	0.75
3:A:2448:VAL:HG11	3:A:2559:PHE:CE1	2.21	0.75
3:A:2521:PHE:HA	3:A:2524:ALA:HB3	1.69	0.74
3:A:2451:ARG:NE	3:A:2452:ALA:H	1.84	0.74
3:A:2406:GLN:HA	3:A:2409:ARG:HB3	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2408:ALA:HA	3:A:2411:LEU:HB3	1.69	0.74
3:A:2554:ALA:O	3:A:2557:PHE:N	2.21	0.74
3:A:2769:GLU:O	3:A:2772:ALA:HB3	1.88	0.73
3:A:2596:ILE:HD11	3:A:2603:ALA:CA	2.18	0.73
3:A:2650:ARG:HE	3:A:2650:ARG:H	1.36	0.73
3:A:2710:HIS:O	3:A:2711:SER:HB2	1.89	0.73
3:A:3050:THR:HB	3:A:3053:VAL:CG1	2.19	0.72
3:A:2605:LYS:HG3	3:A:2606:THR:H	1.53	0.72
3:A:2895:THR:HG22	3:A:2901:GLU:OE1	1.88	0.72
3:A:2747:TYR:CB	3:A:2748:PRO:HD2	2.18	0.71
3:A:2485:ILE:CD1	3:A:2510:PRO:HB3	2.18	0.71
3:A:2549:VAL:CA	3:A:2552:LEU:HD12	2.20	0.71
3:A:2607:LEU:HD23	3:A:2609:LEU:HD21	1.73	0.71
3:A:2596:ILE:HD11	3:A:2604:ALA:N	2.05	0.71
3:A:2788:THR:HG22	3:A:2788:THR:O	1.89	0.71
3:A:2653:LEU:HD13	3:A:2657:LEU:CB	2.21	0.71
3:A:2611:ILE:HG13	3:A:2668:VAL:HA	1.73	0.71
3:A:2408:ALA:O	3:A:2412:GLN:HB2	1.90	0.70
3:A:2462:TYR:HB3	3:A:2466:VAL:HG22	1.71	0.70
3:A:2462:TYR:CD1	3:A:2462:TYR:N	2.60	0.70
3:A:3089:ASP:C	3:A:3091:PHE:H	1.93	0.70
3:A:2473:VAL:HA	3:A:2477:ASN:ND2	2.06	0.70
3:A:2573:VAL:C	3:A:2577:LEU:HD12	2.12	0.70
3:A:2548:ILE:O	3:A:2552:LEU:HG	1.92	0.70
3:A:2596:ILE:CD1	3:A:2603:ALA:HA	2.22	0.70
3:A:3078:ASN:HA	3:A:3081:LYS:HB2	1.72	0.70
3:A:2749:LEU:HD23	3:A:2889:VAL:O	1.90	0.70
3:A:2560:PRO:O	3:A:2562:GLU:N	2.25	0.69
3:A:2671:LYS:HE3	3:A:2709:TRP:O	1.91	0.69
2:B:57:ARG:HG2	3:A:2550:TRP:CZ2	2.27	0.69
3:A:2654:ASP:HB2	3:A:2655:PRO:HD2	1.74	0.69
3:A:2892:LEU:HD12	3:A:2892:LEU:H	1.57	0.69
3:A:2910:ARG:O	3:A:2911:PRO:O	2.09	0.69
3:A:2763:ARG:NH1	3:A:2763:ARG:HG3	2.08	0.69
3:A:2417:LYS:HA	3:A:2420:GLU:HG2	1.74	0.69
3:A:2689:LEU:HD13	3:A:2690:GLU:N	2.08	0.69
3:A:2929:HIS:O	3:A:2930:LEU:HD23	1.93	0.69
3:A:2967:VAL:HG23	3:A:2968:TYR:H	1.58	0.69
2:B:12:LEU:C	3:A:2441:ARG:HH21	1.97	0.68
3:A:2641:GLU:HG2	3:A:2648:ALA:HB1	1.76	0.68
3:A:2462:TYR:H	3:A:2462:TYR:HD1	1.41	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2695:LEU:HD23	3:A:2696:ARG:H	1.59	0.68
3:A:3055:THR:HG22	3:A:3056:LEU:H	1.59	0.68
3:A:2424:LEU:HD12	3:A:2532:ASP:HB2	1.75	0.68
3:A:2927:ILE:CG2	3:A:2930:LEU:HD21	2.24	0.67
3:A:2749:LEU:CD2	3:A:2750:GLN:N	2.48	0.66
3:A:2976:PHE:HE2	3:A:3020:LEU:HD22	1.59	0.66
3:A:2608:VAL:C	3:A:2609:LEU:HD23	2.16	0.66
3:A:2675:GLN:HE22	3:A:2721:PRO:CA	2.09	0.65
3:A:2682:SER:OG	3:A:2695:LEU:HD12	1.96	0.65
3:A:2702:ASN:ND2	3:A:2733:GLY:O	2.29	0.65
3:A:3030:GLU:C	3:A:3032:ILE:N	2.50	0.65
3:A:3096:GLU:O	3:A:3100:ILE:HG13	1.97	0.65
3:A:2406:GLN:HG2	3:A:2410:ASP:HB2	1.79	0.65
3:A:2532:ASP:OD1	3:A:2534:LYS:HB3	1.97	0.64
3:A:2787:PHE:C	3:A:2789:LYS:H	1.99	0.64
3:A:2919:LEU:N	3:A:2919:LEU:HD23	2.13	0.64
3:A:2582:ASP:O	3:A:2586:ASP:HB2	1.97	0.64
3:A:2915:LEU:O	3:A:2915:LEU:HD23	1.97	0.64
3:A:2987:PRO:O	3:A:2989:SER:N	2.30	0.64
3:A:3017:LEU:O	3:A:3098:LYS:HE3	1.97	0.64
3:A:2478:ALA:HB3	3:A:2546:ARG:HG3	1.80	0.64
3:A:3012:LEU:CD1	3:A:3020:LEU:HD21	2.27	0.64
3:A:3078:ASN:HD22	3:A:3079:ASN:N	1.95	0.64
3:A:2441:ARG:C	3:A:2442:ILE:HD12	2.19	0.63
3:A:3037:LEU:HD11	3:A:3080:LEU:HD23	1.80	0.63
3:A:2614:ILE:HA	3:A:2640:ILE:HG22	1.78	0.63
3:A:3045:CYS:O	3:A:3046:GLN:HG2	1.98	0.63
3:A:2528:THR:HB	3:A:2531:VAL:HG21	1.80	0.63
3:A:2723:PRO:HG3	3:A:2926:ARG:NH2	2.14	0.62
3:A:2532:ASP:O	3:A:2534:LYS:N	2.31	0.62
3:A:2568:LEU:HD12	3:A:2568:LEU:N	2.14	0.62
3:A:2611:ILE:HG22	3:A:2642:LEU:CD2	2.29	0.62
3:A:2503:ALA:C	3:A:2505:GLY:H	2.03	0.62
3:A:2667:THR:O	3:A:2670:GLN:HG3	1.99	0.62
3:A:3077:VAL:HG12	3:A:3078:ASN:N	2.14	0.62
3:A:2543:ASN:OD1	3:A:2544:HIS:N	2.32	0.62
3:A:2922:GLY:O	3:A:2923:LYS:HD3	2.00	0.62
3:A:2987:PRO:C	3:A:2989:SER:H	2.03	0.62
3:A:2764:SER:HB3	3:A:2767:GLU:HB3	1.82	0.62
3:A:2413:ASP:HA	3:A:2416:ILE:HD12	1.81	0.62
3:A:3057:PHE:C	3:A:3057:PHE:CD1	2.73	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2539:ILE:O	3:A:2542:ALA:N	2.26	0.61
3:A:2906:LEU:HA	3:A:2946:LEU:O	1.99	0.61
3:A:2532:ASP:C	3:A:2534:LYS:H	2.03	0.61
3:A:2790:VAL:HG12	3:A:2791:HIS:CE1	2.35	0.61
3:A:2790:VAL:HG12	3:A:2791:HIS:ND1	2.15	0.61
3:A:2892:LEU:O	3:A:2905:LEU:HD12	2.01	0.61
3:A:2756:VAL:HG23	3:A:2757:SER:N	2.14	0.61
3:A:2551:LYS:O	3:A:2554:ALA:HB3	2.01	0.60
3:A:2723:PRO:O	3:A:2724:LEU:HD12	2.00	0.60
3:A:2906:LEU:HD12	3:A:2946:LEU:O	2.00	0.60
3:A:3055:THR:HG22	3:A:3056:LEU:N	2.16	0.60
1:C:503:DT:O4	3:A:2891:LYS:HE3	2.01	0.60
3:A:2444:LEU:CD1	3:A:2444:LEU:H	2.10	0.60
3:A:2503:ALA:O	3:A:2505:GLY:N	2.35	0.60
3:A:2724:LEU:N	3:A:2724:LEU:HD12	2.14	0.60
3:A:2974:LEU:CD2	3:A:2976:PHE:N	2.53	0.60
3:A:2974:LEU:HD23	3:A:2976:PHE:N	2.10	0.60
3:A:3074:GLN:HA	3:A:3077:VAL:HB	1.82	0.60
3:A:2976:PHE:CE2	3:A:3020:LEU:HD13	2.37	0.60
3:A:2412:GLN:OE1	3:A:2509:ILE:HD11	2.01	0.60
3:A:2892:LEU:N	3:A:2892:LEU:HD12	2.14	0.60
3:A:2415:ARG:O	3:A:2419:LYS:HB2	2.02	0.60
3:A:2442:ILE:CG2	3:A:2447:ALA:HB2	2.32	0.60
3:A:2547:TRP:CE3	3:A:2547:TRP:HA	2.36	0.60
3:A:2730:PHE:HB3	3:A:2732:ASP:OD1	2.01	0.60
3:A:2738:CYS:HB2	3:A:2928:TYR:HD1	1.66	0.60
3:A:2895:THR:HG22	3:A:2903:SER:HA	1.84	0.60
3:A:3013:SER:HB2	3:A:3019:LEU:CD1	2.31	0.60
3:A:3048:GLU:N	3:A:3048:GLU:OE1	2.34	0.60
3:A:2560:PRO:C	3:A:2562:GLU:N	2.55	0.60
3:A:2599:ARG:NH2	3:A:2683:PRO:HA	2.17	0.60
3:A:2547:TRP:HA	3:A:2547:TRP:HE3	1.67	0.59
3:A:2922:GLY:HA2	3:A:2968:TYR:CE1	2.37	0.59
3:A:2695:LEU:O	3:A:2696:ARG:HD2	2.02	0.59
3:A:3050:THR:O	3:A:3051:SER:C	2.40	0.59
3:A:3057:PHE:HE1	3:A:3059:CYS:HA	1.67	0.59
2:B:42:ASN:O	2:B:43:TRP:O	2.21	0.59
3:A:3083:ALA:O	3:A:3086:ASN:HB3	2.02	0.59
3:A:2442:ILE:N	3:A:2442:ILE:CD1	2.62	0.59
3:A:2679:LEU:HD11	3:A:2695:LEU:CD2	2.31	0.59
3:A:2412:GLN:CD	3:A:2509:ILE:HD11	2.23	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2987:PRO:C	3:A:2988:CYS:SG	2.81	0.59
2:B:16:ASP:OD1	2:B:16:ASP:O	2.20	0.59
3:A:2890:TRP:HZ3	3:A:2915:LEU:HD23	1.68	0.59
3:A:2897:TYR:CE1	3:A:2924:ARG:CZ	2.85	0.59
3:A:2502:LEU:O	3:A:2503:ALA:O	2.21	0.59
3:A:2723:PRO:HG3	3:A:2926:ARG:HH21	1.68	0.59
3:A:2523:ARG:C	3:A:2525:LEU:H	2.06	0.58
3:A:2733:GLY:O	3:A:2734:GLY:O	2.21	0.58
3:A:2898:LYS:O	3:A:2899:LYS:HB3	2.03	0.58
3:A:3012:LEU:HD12	3:A:3020:LEU:HD21	1.82	0.58
3:A:3041:SER:O	3:A:3042:ASN:HB2	2.02	0.58
3:A:2430:SER:HB3	3:A:2575:LEU:CD2	2.33	0.58
3:A:2650:ARG:NH1	3:A:2695:LEU:O	2.35	0.58
3:A:2968:TYR:CG	3:A:2969:GLN:N	2.70	0.58
3:A:2569:ASN:HB3	3:A:2571:GLU:HG2	1.85	0.58
3:A:2745:ARG:NH2	3:A:2971:ARG:HA	2.19	0.58
3:A:2576:GLN:O	3:A:2579:TYR:HB3	2.04	0.58
3:A:2573:VAL:O	3:A:2577:LEU:HD12	2.03	0.58
3:A:2611:ILE:CD1	3:A:2667:THR:O	2.48	0.58
3:A:2405:LEU:C	3:A:2407:SER:H	2.05	0.58
3:A:3091:PHE:C	3:A:3093:LYS:H	2.07	0.58
2:B:22:PHE:O	2:B:24:ALA:N	2.37	0.58
3:A:2552:LEU:HA	3:A:2555:MET:HG3	1.86	0.58
3:A:2442:ILE:HG22	3:A:2447:ALA:HB2	1.85	0.58
3:A:2478:ALA:HB3	3:A:2546:ARG:CG	2.34	0.58
3:A:2607:LEU:O	3:A:2673:ILE:HA	2.04	0.58
3:A:2742:ILE:HG22	3:A:2895:THR:OG1	2.04	0.58
3:A:3059:CYS:O	3:A:3062:SER:HB2	2.03	0.58
3:A:2526:CYS:HB3	3:A:2533:PRO:CG	2.31	0.58
3:A:2690:GLU:HA	3:A:2690:GLU:OE2	2.03	0.57
3:A:2779:GLN:HA	3:A:2779:GLN:NE2	2.18	0.57
2:B:21:GLU:CD	3:A:2589:ARG:HG2	2.24	0.57
3:A:2745:ARG:HH11	3:A:2745:ARG:HG2	1.69	0.57
3:A:2502:LEU:CD1	3:A:2570:PRO:HB2	2.34	0.57
3:A:2409:ARG:HH11	3:A:2409:ARG:HB2	1.70	0.57
3:A:2492:GLU:HG3	3:A:2493:ASP:H	1.69	0.57
3:A:2717:ARG:HH11	3:A:2717:ARG:HG2	1.69	0.57
3:A:2508:LEU:HA	3:A:2524:ALA:HB2	1.86	0.57
3:A:2889:VAL:HG13	3:A:2909:TRP:CD2	2.40	0.57
3:A:3008:PRO:C	3:A:3009:LEU:HD12	2.24	0.57
3:A:2539:ILE:C	3:A:2542:ALA:H	2.08	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2417:LYS:O	3:A:2420:GLU:HG2	2.05	0.57
3:A:2551:LYS:HG2	3:A:2552:LEU:N	2.20	0.57
3:A:2935:SER:HB3	3:A:2941:ARG:O	2.04	0.57
3:A:2412:GLN:CA	3:A:2415:ARG:HH21	2.10	0.57
3:A:2552:LEU:O	3:A:2555:MET:HB2	2.04	0.57
3:A:2761:ILE:HG21	3:A:2763:ARG:NH2	2.19	0.57
3:A:2960:SER:OG	3:A:2963:THR:OG1	2.23	0.57
3:A:2978:ARG:HD3	3:A:2984:PHE:CE1	2.40	0.57
3:A:2417:LYS:O	3:A:2420:GLU:N	2.34	0.57
3:A:2516:ALA:HA	3:A:2520:GLU:OE2	2.04	0.57
3:A:2611:ILE:O	3:A:2668:VAL:HG13	2.05	0.57
3:A:2508:LEU:O	3:A:2510:PRO:HD3	2.05	0.56
3:A:2560:PRO:HA	3:A:2563:PHE:O	2.05	0.56
3:A:2596:ILE:C	3:A:2598:GLU:H	2.08	0.56
3:A:2741:ILE:HD13	3:A:2927:ILE:HG12	1.87	0.56
3:A:3091:PHE:C	3:A:3093:LYS:N	2.58	0.56
3:A:2574:LEU:HA	3:A:2577:LEU:HD13	1.85	0.56
3:A:2607:LEU:HD23	3:A:2609:LEU:HD11	1.87	0.56
3:A:2925:TYR:HA	3:A:2955:GLN:O	2.06	0.56
3:A:2485:ILE:HG21	3:A:2510:PRO:HB3	1.87	0.56
3:A:2744:GLN:C	3:A:2745:ARG:HD2	2.26	0.56
3:A:2988:CYS:O	3:A:2989:SER:HB2	2.05	0.56
3:A:2693:ASP:O	3:A:2696:ARG:NH1	2.38	0.56
3:A:2749:LEU:O	3:A:2750:GLN:HG2	2.05	0.56
3:A:2963:THR:O	3:A:2967:VAL:HG22	2.05	0.56
3:A:2994:VAL:HG21	3:A:3077:VAL:HG23	1.88	0.56
3:A:3055:THR:O	3:A:3056:LEU:HD23	2.05	0.56
2:B:10:LEU:HD12	2:B:10:LEU:N	2.20	0.56
3:A:2597:LEU:O	3:A:2686:CYS:HB3	2.06	0.56
3:A:2702:ASN:HD21	3:A:2730:PHE:H	1.52	0.56
3:A:2754:LYS:HG2	3:A:2760:TYR:CE2	2.41	0.56
3:A:3020:LEU:HD23	3:A:3020:LEU:N	2.20	0.56
3:A:2568:LEU:HD12	3:A:2568:LEU:H	1.69	0.56
1:C:505:DT:C6	3:A:3057:PHE:CE2	2.94	0.56
3:A:3102:VAL:HG12	3:A:3103:LEU:N	2.20	0.55
3:A:2409:ARG:HB2	3:A:2409:ARG:NH1	2.21	0.55
3:A:2764:SER:HB3	3:A:2767:GLU:OE1	2.05	0.55
3:A:2909:TRP:C	3:A:2911:PRO:HD3	2.25	0.55
3:A:2729:LEU:CD2	3:A:2736:VAL:CG2	2.84	0.55
3:A:2593:LEU:HG	3:A:2644:ASP:HB3	1.87	0.55
3:A:2924:ARG:HD3	3:A:2957:LEU:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:16:ASP:CG	2:B:16:ASP:O	2.44	0.55
3:A:2607:LEU:CD2	3:A:2609:LEU:HD21	2.35	0.55
3:A:2898:LYS:O	3:A:2899:LYS:CB	2.55	0.55
3:A:2417:LYS:CA	3:A:2420:GLU:HG2	2.37	0.55
2:B:55:GLN:NE2	3:A:2671:LYS:HD2	2.21	0.55
3:A:2883:SER:OG	3:A:2884:ARG:N	2.40	0.55
3:A:2574:LEU:HA	3:A:2577:LEU:CD1	2.37	0.54
3:A:2890:TRP:HZ3	3:A:2915:LEU:CD2	2.20	0.54
3:A:2501:GLN:HB2	3:A:2507:TRP:CH2	2.42	0.54
3:A:2750:GLN:OE1	3:A:2762:PHE:HD1	1.90	0.54
3:A:3019:LEU:CD2	3:A:3019:LEU:N	2.68	0.54
3:A:3020:LEU:HD23	3:A:3020:LEU:H	1.72	0.54
3:A:3057:PHE:CD1	3:A:3058:ALA:N	2.76	0.54
3:A:2688:PRO:O	3:A:2689:LEU:C	2.46	0.54
2:B:16:ASP:O	2:B:17:ASP:HB3	2.06	0.54
3:A:2470:CYS:O	3:A:2473:VAL:N	2.40	0.54
3:A:2964:LEU:O	3:A:2966:GLN:N	2.40	0.54
3:A:3036:VAL:HG12	3:A:3038:ILE:HG12	1.90	0.54
3:A:2474:ASN:O	3:A:2476:LYS:N	2.40	0.54
3:A:2753:GLU:HA	3:A:2885:ASP:O	2.08	0.54
3:A:2652:GLN:HB3	3:A:2698:LYS:HA	1.89	0.53
3:A:3108:PRO:O	3:A:3110:TRP:N	2.41	0.53
3:A:2430:SER:HB3	3:A:2575:LEU:HD22	1.89	0.53
3:A:2463:ILE:O	3:A:2465:GLY:N	2.41	0.53
3:A:2937:SER:O	3:A:2939:PHE:N	2.41	0.53
3:A:3089:ASP:C	3:A:3091:PHE:N	2.60	0.53
3:A:2432:TYR:C	3:A:2432:TYR:CD2	2.82	0.53
3:A:2605:LYS:HG3	3:A:2606:THR:N	2.21	0.53
3:A:2902:LYS:O	3:A:2903:SER:O	2.27	0.53
2:B:56:LEU:CG	2:B:57:ARG:N	2.71	0.53
3:A:2765:GLU:C	3:A:2767:GLU:H	2.11	0.53
3:A:2896:SER:O	3:A:2897:TYR:O	2.26	0.53
2:B:56:LEU:CG	2:B:57:ARG:H	2.22	0.53
3:A:2444:LEU:N	3:A:2444:LEU:HD12	2.16	0.53
3:A:2677:ALA:HB1	3:A:2698:LYS:O	2.09	0.53
3:A:3011:TYR:CD2	3:A:3099:LEU:HD21	2.44	0.53
3:A:2448:VAL:HG12	3:A:2451:ARG:HB3	1.91	0.53
3:A:2570:PRO:HA	3:A:2573:VAL:HB	1.90	0.53
3:A:2922:GLY:CA	3:A:2968:TYR:CE1	2.92	0.53
3:A:3020:LEU:CD2	3:A:3020:LEU:N	2.71	0.53
3:A:2598:GLU:O	3:A:2600:ASP:N	2.42	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2751:TRP:CH2	3:A:2765:GLU:HG3	2.44	0.52
3:A:3019:LEU:HD22	3:A:3019:LEU:H	1.70	0.52
3:A:3049:SER:HB2	3:A:3055:THR:OG1	2.10	0.52
3:A:2736:VAL:HG11	3:A:2739:VAL:CG1	2.39	0.52
3:A:3093:LYS:HD3	3:A:3093:LYS:O	2.09	0.52
3:A:2578:LYS:O	3:A:2579:TYR:C	2.48	0.52
3:A:2578:LYS:O	3:A:2581:TYR:HB3	2.10	0.52
3:A:2596:ILE:HD11	3:A:2603:ALA:C	2.29	0.52
3:A:2710:HIS:N	3:A:2710:HIS:ND1	2.55	0.52
3:A:2986:PRO:HB2	3:A:2987:PRO:CD	2.39	0.52
3:A:2552:LEU:O	3:A:2553:ALA:C	2.47	0.52
3:A:2601:ASP:O	3:A:2602:THR:C	2.48	0.52
3:A:3086:ASN:OD1	3:A:3087:ILE:HD11	2.09	0.52
3:A:2405:LEU:C	3:A:2407:SER:N	2.63	0.52
3:A:2573:VAL:O	3:A:2575:LEU:N	2.43	0.52
3:A:2961:SER:HB2	3:A:2962:GLU:OE2	2.09	0.52
3:A:2689:LEU:HD13	3:A:2690:GLU:H	1.75	0.52
2:B:55:GLN:HE22	3:A:2671:LYS:HD2	1.74	0.52
3:A:2743:VAL:HG12	3:A:2743:VAL:O	2.09	0.52
3:A:2928:TYR:O	3:A:2952:THR:HA	2.09	0.52
3:A:3089:ASP:O	3:A:3091:PHE:N	2.43	0.52
1:C:505:DT:H72	3:A:2939:PHE:HZ	1.75	0.52
3:A:2519:GLU:O	3:A:2522:TYR:HB3	2.10	0.52
3:A:2569:ASN:HB3	3:A:2571:GLU:CG	2.39	0.52
3:A:3075:GLU:O	3:A:3079:ASN:HB2	2.09	0.52
3:A:3099:LEU:O	3:A:3100:ILE:C	2.47	0.52
1:C:501:DT:C6	1:C:501:DT:H5'	2.45	0.52
3:A:2654:ASP:OD2	3:A:2700:SER:HA	2.09	0.51
3:A:2967:VAL:HG23	3:A:2968:TYR:N	2.24	0.51
3:A:2523:ARG:C	3:A:2525:LEU:N	2.63	0.51
3:A:2544:HIS:O	3:A:2548:ILE:HG13	2.10	0.51
3:A:2598:GLU:O	3:A:2599:ARG:C	2.48	0.51
3:A:3008:PRO:HG2	3:A:3024:PHE:HB2	1.91	0.51
2:B:60:LEU:HD21	3:A:2473:VAL:O	2.10	0.51
3:A:2674:THR:HB	3:A:2704:THR:CG2	2.31	0.51
3:A:2968:TYR:O	3:A:2969:GLN:HB2	2.11	0.51
3:A:2988:CYS:O	3:A:2989:SER:CB	2.58	0.51
3:A:2556:GLU:HG3	3:A:2564:ALA:HA	1.93	0.51
3:A:3077:VAL:O	3:A:3080:LEU:HB3	2.10	0.51
3:A:2728:SER:O	3:A:2729:LEU:HB2	2.11	0.51
3:A:3089:ASP:HA	3:A:3092:TYR:CD1	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2517:GLY:H	3:A:2520:GLU:CD	2.14	0.51
3:A:2749:LEU:C	3:A:2750:GLN:HG2	2.31	0.51
3:A:2992:ASP:O	3:A:2993:VAL:HG13	2.10	0.51
3:A:2745:ARG:HD2	3:A:2745:ARG:N	2.25	0.51
3:A:2559:PHE:O	3:A:2563:PHE:HB2	2.11	0.51
3:A:2446:ALA:C	3:A:2448:VAL:H	2.14	0.51
3:A:3074:GLN:O	3:A:3078:ASN:ND2	2.44	0.51
3:A:2992:ASP:OD1	3:A:3041:SER:HA	2.10	0.50
3:A:2997:VAL:CG1	3:A:3034:PRO:HA	2.41	0.50
2:B:10:LEU:HD21	3:A:2566:ARG:NE	2.26	0.50
3:A:2501:GLN:HB2	3:A:2507:TRP:CZ2	2.46	0.50
3:A:2910:ARG:N	3:A:2911:PRO:HD3	2.26	0.50
3:A:2735:ASN:N	3:A:2735:ASN:OD1	2.44	0.50
3:A:3017:LEU:CD1	3:A:3091:PHE:HE1	2.23	0.50
2:B:54:ASN:HB3	3:A:2453:PRO:HB2	1.93	0.50
3:A:2537:SER:O	3:A:2541:VAL:HG23	2.11	0.50
3:A:2729:LEU:HD22	3:A:2736:VAL:HG22	1.93	0.50
3:A:2561:LYS:O	3:A:2561:LYS:HG2	2.12	0.50
3:A:2936:LYS:O	3:A:2936:LYS:HG3	2.11	0.50
3:A:2467:SER:C	3:A:2469:GLU:H	2.14	0.50
3:A:2408:ALA:CA	3:A:2411:LEU:HB3	2.37	0.50
3:A:2893:ARG:NH1	3:A:2905:LEU:HD13	2.26	0.50
2:B:43:TRP:CH2	3:A:2705:ARG:HA	2.46	0.50
3:A:2551:LYS:CG	3:A:2552:LEU:N	2.72	0.50
3:A:2449:GLY:O	3:A:2450:ASP:C	2.50	0.50
3:A:2724:LEU:CD1	3:A:2724:LEU:N	2.74	0.50
3:A:2738:CYS:SG	3:A:2739:VAL:N	2.83	0.50
3:A:2521:PHE:CE2	3:A:2570:PRO:HB3	2.47	0.49
3:A:2571:GLU:HG3	3:A:2572:ARG:N	2.25	0.49
3:A:2974:LEU:HD23	3:A:2975:HIS:H	1.70	0.49
3:A:2578:LYS:HZ3	3:A:2581:TYR:HD2	1.58	0.49
3:A:2484:ASP:O	3:A:2486:GLN:N	2.45	0.49
3:A:2736:VAL:HG12	3:A:2738:CYS:H	1.77	0.49
1:C:502:DT:O4	3:A:2947:THR:HG23	2.12	0.49
3:A:2952:THR:HG22	3:A:2953:GLN:N	2.26	0.49
3:A:2424:LEU:HD12	3:A:2532:ASP:CB	2.43	0.49
3:A:2890:TRP:CZ3	3:A:2915:LEU:CD2	2.96	0.49
3:A:2927:ILE:HD12	3:A:2954:TYR:HD1	1.78	0.49
3:A:2960:SER:O	3:A:2963:THR:N	2.46	0.49
3:A:3006:LEU:O	3:A:3007:ALA:HB3	2.13	0.49
3:A:3019:LEU:HD21	3:A:3098:LYS:HG2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2674:THR:HG22	3:A:2704:THR:CG2	2.42	0.49
3:A:2751:TRP:CG	3:A:2768:GLU:HG2	2.47	0.49
3:A:2906:LEU:HD13	3:A:2946:LEU:HB3	1.94	0.49
3:A:2987:PRO:O	3:A:2988:CYS:SG	2.71	0.49
3:A:2924:ARG:HB3	3:A:2957:LEU:O	2.13	0.49
3:A:2591:SER:O	3:A:2595:LYS:HB2	2.11	0.49
3:A:2596:ILE:HD11	3:A:2604:ALA:H	1.76	0.49
3:A:2964:LEU:C	3:A:2966:GLN:H	2.15	0.49
3:A:2453:PRO:HD3	3:A:2559:PHE:HZ	1.68	0.49
3:A:2532:ASP:OD1	3:A:2534:LYS:CB	2.61	0.49
3:A:2603:ALA:O	3:A:2605:LYS:N	2.45	0.49
3:A:2763:ARG:NH1	3:A:2763:ARG:CG	2.73	0.49
3:A:2576:GLN:HA	3:A:2579:TYR:HB2	1.95	0.49
3:A:2596:ILE:C	3:A:2598:GLU:N	2.64	0.49
3:A:2764:SER:OG	3:A:2765:GLU:N	2.45	0.49
3:A:2439:LEU:N	3:A:2439:LEU:HD23	2.27	0.48
3:A:2910:ARG:NH1	3:A:2910:ARG:HG3	2.28	0.48
3:A:2593:LEU:HD12	3:A:2647:TYR:O	2.13	0.48
3:A:2650:ARG:HE	3:A:2650:ARG:N	2.08	0.48
3:A:2787:PHE:C	3:A:2789:LYS:N	2.67	0.48
3:A:2955:GLN:CG	3:A:2957:LEU:HD21	2.42	0.48
3:A:3057:PHE:CE1	3:A:3058:ALA:C	2.87	0.48
3:A:2452:ALA:HB1	3:A:2453:PRO:HD2	1.94	0.48
3:A:2560:PRO:HG2	3:A:2561:LYS:H	1.78	0.48
3:A:2569:ASN:O	3:A:2571:GLU:N	2.47	0.48
3:A:2909:TRP:O	3:A:2910:ARG:C	2.52	0.48
3:A:3020:LEU:C	3:A:3020:LEU:HD23	2.32	0.48
3:A:2638:ASP:O	3:A:2639:THR:HG23	2.13	0.48
3:A:2790:VAL:O	3:A:2790:VAL:CG1	2.62	0.48
3:A:2974:LEU:C	3:A:2974:LEU:HD23	2.32	0.48
3:A:3009:LEU:N	3:A:3009:LEU:HD12	2.29	0.48
3:A:2483:PHE:CD2	3:A:2570:PRO:HG3	2.48	0.48
3:A:2481:PHE:HD2	3:A:2545:TYR:OH	1.97	0.48
3:A:2571:GLU:O	3:A:2572:ARG:C	2.52	0.48
3:A:2682:SER:C	3:A:2684:ASP:H	2.17	0.48
2:B:56:LEU:CD2	2:B:57:ARG:N	2.60	0.48
3:A:2399:LYS:N	3:A:2494:LEU:HD21	2.28	0.48
3:A:2431:LEU:O	3:A:2432:TYR:C	2.51	0.48
3:A:2582:ASP:HA	3:A:2586:ASP:HB2	1.95	0.48
3:A:2611:ILE:HG22	3:A:2642:LEU:HD21	1.94	0.48
3:A:2675:GLN:O	3:A:2677:ALA:N	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2649:VAL:HG23	3:A:2650:ARG:N	2.29	0.47
3:A:2788:THR:O	3:A:2788:THR:CG2	2.58	0.47
3:A:2897:TYR:CD2	3:A:2898:LYS:N	2.82	0.47
3:A:3070:GLU:HB3	3:A:3072:TYR:CE2	2.49	0.47
3:A:2689:LEU:O	3:A:2690:GLU:HG2	2.14	0.47
1:C:503:DT:H2"	1:C:504:DT:H5"	1.96	0.47
2:B:10:LEU:CD1	3:A:2566:ARG:NH2	2.67	0.47
2:B:41:ASP:O	3:A:2705:ARG:NE	2.47	0.47
3:A:2681:GLY:HA3	3:A:2695:LEU:CA	2.31	0.47
1:C:505:DT:H72	3:A:2939:PHE:CZ	2.49	0.47
3:A:3099:LEU:O	3:A:3103:LEU:HB2	2.15	0.47
2:B:60:LEU:CD2	3:A:2473:VAL:O	2.62	0.47
2:B:8:VAL:HG12	2:B:9:ASP:O	2.13	0.47
3:A:2485:ILE:HA	3:A:2489:PHE:CE1	2.49	0.47
3:A:2717:ARG:NH1	3:A:2717:ARG:HG2	2.28	0.47
3:A:2751:TRP:CZ3	3:A:2765:GLU:HA	2.49	0.47
3:A:2426:LEU:HD23	3:A:2586:ASP:OD2	2.14	0.47
3:A:2897:TYR:HE1	3:A:2924:ARG:CZ	2.26	0.47
3:A:2974:LEU:HD13	3:A:2979:LEU:HD11	1.97	0.47
3:A:2455:ALA:HB1	3:A:2557:PHE:HE2	1.80	0.47
3:A:2783:LEU:O	3:A:2784:GLU:C	2.53	0.47
3:A:3034:PRO:C	3:A:3035:ARG:HG3	2.35	0.47
3:A:3053:VAL:HG23	3:A:3054:PRO:HD2	1.97	0.47
3:A:2522:TYR:O	3:A:2525:LEU:HB3	2.15	0.47
3:A:2736:VAL:HG11	3:A:2739:VAL:HG12	1.97	0.47
3:A:3013:SER:HB2	3:A:3019:LEU:HD13	1.97	0.47
2:B:15:GLU:HB2	2:B:18:GLU:HG2	1.96	0.47
3:A:2528:THR:O	3:A:2531:VAL:HB	2.15	0.47
3:A:2674:THR:CA	3:A:2704:THR:HG22	2.45	0.47
3:A:2704:THR:O	3:A:2705:ARG:HG3	2.15	0.47
3:A:2927:ILE:CG2	3:A:2930:LEU:HD11	2.45	0.47
3:A:3009:LEU:CD1	3:A:3009:LEU:N	2.78	0.47
3:A:2460:GLN:HA	3:A:2462:TYR:CE1	2.50	0.46
3:A:2507:TRP:O	3:A:2524:ALA:HA	2.15	0.46
3:A:2675:GLN:O	3:A:2676:GLY:C	2.54	0.46
3:A:2557:PHE:C	3:A:2559:PHE:H	2.19	0.46
3:A:2569:ASN:O	3:A:2572:ARG:N	2.48	0.46
3:A:2674:THR:HA	3:A:2704:THR:HA	1.97	0.46
3:A:2531:VAL:HG12	3:A:2533:PRO:HD3	1.96	0.46
3:A:2457:SER:O	3:A:2458:PRO:CB	2.64	0.46
3:A:2755:THR:O	3:A:2756:VAL:C	2.54	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2756:VAL:CG2	3:A:2757:SER:N	2.77	0.46
3:A:2766:ARG:HG3	3:A:2766:ARG:O	2.15	0.46
3:A:2470:CYS:O	3:A:2471:ILE:C	2.54	0.46
3:A:2541:VAL:O	3:A:2541:VAL:HG12	2.15	0.46
3:A:2889:VAL:HG13	3:A:2909:TRP:CE3	2.51	0.46
3:A:2449:GLY:O	3:A:2451:ARG:N	2.49	0.46
3:A:2529:PRO:O	3:A:2531:VAL:HG23	2.15	0.46
3:A:2573:VAL:C	3:A:2575:LEU:N	2.67	0.46
3:A:2607:LEU:HD23	3:A:2609:LEU:CD2	2.44	0.46
3:A:2689:LEU:O	3:A:2690:GLU:CB	2.63	0.46
3:A:2750:GLN:OE1	3:A:2762:PHE:CD1	2.68	0.46
3:A:3085:GLU:O	3:A:3086:ASN:C	2.54	0.46
3:A:2460:GLN:HA	3:A:2462:TYR:HE1	1.81	0.46
3:A:3040:ALA:HA	3:A:3063:ILE:O	2.16	0.46
3:A:2526:CYS:CB	3:A:2533:PRO:HB3	2.46	0.46
3:A:2555:MET:CE	3:A:2555:MET:HA	2.46	0.46
3:A:2594:LYS:HD2	3:A:2647:TYR:CE1	2.51	0.46
3:A:2764:SER:HB3	3:A:2767:GLU:CB	2.46	0.46
3:A:2593:LEU:O	3:A:2596:ILE:HG22	2.15	0.46
3:A:2554:ALA:O	3:A:2555:MET:C	2.54	0.45
3:A:2573:VAL:HG12	3:A:2577:LEU:HD12	1.95	0.45
3:A:2604:ALA:HB1	3:A:2677:ALA:CB	2.19	0.45
3:A:2650:ARG:CZ	3:A:2695:LEU:O	2.64	0.45
3:A:2651:ALA:HA	3:A:2697:LEU:O	2.16	0.45
3:A:2421:ARG:HB3	3:A:2421:ARG:NH1	2.31	0.45
3:A:2512:ASN:O	3:A:2514:GLY:N	2.50	0.45
3:A:2612:SER:O	3:A:2668:VAL:HG11	2.16	0.45
3:A:2647:TYR:HB3	3:A:2689:LEU:HG	1.97	0.45
3:A:2786:LEU:HD23	3:A:2786:LEU:HA	1.63	0.45
3:A:2927:ILE:HG21	3:A:2930:LEU:HD11	1.98	0.45
3:A:2976:PHE:O	3:A:2977:SER:C	2.55	0.45
3:A:3080:LEU:O	3:A:3084:ILE:HG13	2.16	0.45
2:B:17:ASP:C	2:B:17:ASP:OD1	2.54	0.45
3:A:2498:LYS:HD3	3:A:2498:LYS:HA	1.79	0.45
3:A:2529:PRO:O	3:A:2531:VAL:N	2.50	0.45
3:A:2576:GLN:O	3:A:2579:TYR:N	2.49	0.45
3:A:2668:VAL:HG12	3:A:2669:GLY:N	2.30	0.45
3:A:2769:GLU:C	3:A:2772:ALA:HB3	2.36	0.45
3:A:3014:ASP:CG	3:A:3018:ASN:HD22	2.18	0.45
3:A:2446:ALA:O	3:A:2448:VAL:N	2.50	0.45
3:A:2465:GLY:O	3:A:2466:VAL:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2732:ASP:OD1	3:A:2732:ASP:N	2.47	0.45
3:A:2906:LEU:HD12	3:A:2946:LEU:C	2.36	0.45
3:A:2539:ILE:HA	3:A:2542:ALA:HB2	1.98	0.45
3:A:2611:ILE:CD1	3:A:2666:LEU:HD23	2.43	0.45
3:A:2673:ILE:HG23	3:A:2673:ILE:O	2.17	0.45
3:A:2997:VAL:HB	3:A:3034:PRO:HA	1.97	0.45
3:A:3030:GLU:O	3:A:3031:ASP:HB2	2.17	0.45
3:A:2430:SER:HB3	3:A:2575:LEU:HD21	1.98	0.45
3:A:3017:LEU:HD11	3:A:3091:PHE:CE1	2.52	0.45
3:A:3096:GLU:O	3:A:3097:LYS:C	2.54	0.45
3:A:2539:ILE:C	3:A:2541:VAL:N	2.68	0.45
3:A:2702:ASN:CG	3:A:2729:LEU:HD23	2.37	0.45
3:A:2485:ILE:HD11	3:A:2514:GLY:HA2	1.99	0.45
3:A:2761:ILE:HG21	3:A:2763:ARG:CZ	2.46	0.45
3:A:2937:SER:O	3:A:2938:LYS:C	2.55	0.45
3:A:2443:SER:O	3:A:2444:LEU:C	2.54	0.45
3:A:2400:ASP:CG	3:A:2401:LEU:H	2.19	0.45
3:A:2684:ASP:O	3:A:2686:CYS:N	2.50	0.45
3:A:2448:VAL:HG12	3:A:2448:VAL:O	2.17	0.44
3:A:2470:CYS:O	3:A:2472:ASN:N	2.49	0.44
3:A:2660:LEU:O	3:A:2664:GLY:N	2.49	0.44
3:A:2939:PHE:C	3:A:2940:GLU:HG3	2.38	0.44
3:A:3030:GLU:O	3:A:3032:ILE:HG13	2.17	0.44
3:A:3099:LEU:HD12	3:A:3103:LEU:HD12	1.99	0.44
3:A:2539:ILE:HA	3:A:2542:ALA:CB	2.47	0.44
3:A:2776:ALA:O	3:A:2780:GLN:HB2	2.18	0.44
3:A:2746:VAL:CG2	3:A:2892:LEU:HD23	2.48	0.44
3:A:2946:LEU:HD12	3:A:2946:LEU:HA	1.70	0.44
3:A:2987:PRO:C	3:A:2989:SER:N	2.68	0.44
3:A:3024:PHE:HA	3:A:3058:ALA:HB3	1.98	0.44
3:A:2426:LEU:H	3:A:2426:LEU:HD12	1.83	0.44
2:B:59:GLU:HG3	3:A:2453:PRO:HB3	1.99	0.44
3:A:2697:LEU:HA	3:A:2697:LEU:HD12	1.61	0.44
3:A:3038:ILE:HD13	3:A:3038:ILE:HA	1.81	0.44
3:A:2568:LEU:H	3:A:2568:LEU:CD1	2.31	0.44
3:A:2575:LEU:HD23	3:A:2575:LEU:HA	1.77	0.44
3:A:2968:TYR:CE2	3:A:2970:PRO:HB3	2.52	0.44
3:A:2466:VAL:O	3:A:2467:SER:CB	2.65	0.44
3:A:2789:LYS:C	3:A:2791:HIS:H	2.21	0.44
3:A:2910:ARG:HG3	3:A:2910:ARG:HH11	1.82	0.44
3:A:2691:ALA:CB	3:A:2692:PRO:CD	2.72	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2955:GLN:HG2	3:A:2957:LEU:HD21	1.98	0.44
3:A:3012:LEU:HD13	3:A:3020:LEU:HD21	1.97	0.44
3:A:3030:GLU:HA	3:A:3030:GLU:OE1	2.16	0.44
3:A:2470:CYS:O	3:A:2473:VAL:HG12	2.17	0.44
3:A:2519:GLU:O	3:A:2520:GLU:C	2.56	0.44
3:A:2560:PRO:O	3:A:2563:PHE:N	2.51	0.44
3:A:2789:LYS:O	3:A:2791:HIS:N	2.51	0.44
3:A:2994:VAL:HG11	3:A:3077:VAL:HG22	1.99	0.44
3:A:2409:ARG:CB	3:A:2409:ARG:HH11	2.30	0.44
3:A:2471:ILE:C	3:A:2473:VAL:H	2.21	0.43
3:A:2484:ASP:C	3:A:2486:GLN:H	2.21	0.43
3:A:2593:LEU:O	3:A:2596:ILE:N	2.43	0.43
3:A:3078:ASN:C	3:A:3078:ASN:HD22	2.20	0.43
3:A:3078:ASN:HA	3:A:3081:LYS:CB	2.46	0.43
2:B:57:ARG:CG	3:A:2550:TRP:CE2	3.01	0.43
3:A:2483:PHE:CE1	3:A:2521:PHE:CZ	3.06	0.43
3:A:2521:PHE:H	3:A:2521:PHE:HD1	1.66	0.43
3:A:2710:HIS:O	3:A:2711:SER:CB	2.59	0.43
3:A:2582:ASP:C	3:A:2586:ASP:HB2	2.39	0.43
3:A:2689:LEU:O	3:A:2690:GLU:HB2	2.18	0.43
3:A:2924:ARG:O	3:A:2956:GLN:HA	2.18	0.43
3:A:2529:PRO:C	3:A:2531:VAL:H	2.22	0.43
3:A:2483:PHE:CE2	3:A:2570:PRO:HG3	2.53	0.43
3:A:2614:ILE:HD13	3:A:2640:ILE:HG21	2.00	0.43
3:A:2675:GLN:HE22	3:A:2721:PRO:CB	2.31	0.43
3:A:2518:LYS:HE3	3:A:2542:ALA:HB2	2.00	0.43
3:A:2594:LYS:HB2	3:A:2647:TYR:CD1	2.53	0.43
3:A:2593:LEU:HD13	3:A:2649:VAL:HG13	2.00	0.43
3:A:2981:ASP:OD1	3:A:2982:PRO:HD2	2.18	0.43
3:A:2525:LEU:O	3:A:2531:VAL:HG11	2.19	0.43
3:A:3028:LEU:C	3:A:3030:GLU:N	2.52	0.43
3:A:3038:ILE:CG2	3:A:3039:ALA:N	2.82	0.43
3:A:3020:LEU:HA	3:A:3053:VAL:CG2	2.48	0.43
2:B:19:PHE:HE2	3:A:2646:TRP:CE2	2.37	0.43
3:A:2523:ARG:O	3:A:2525:LEU:N	2.51	0.43
3:A:2540:TRP:O	3:A:2544:HIS:HD2	2.01	0.43
3:A:2641:GLU:O	3:A:2642:LEU:HD23	2.18	0.43
3:A:2522:TYR:CE1	3:A:2536:ILE:HD11	2.53	0.43
3:A:2580:ARG:HD3	3:A:2646:TRP:CZ3	2.54	0.43
3:A:2941:ARG:HB2	3:A:2942:PRO:HD3	2.01	0.43
2:B:42:ASN:C	2:B:43:TRP:O	2.55	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2438:THR:O	3:A:2438:THR:HG22	2.18	0.43
3:A:2441:ARG:HA	3:A:2442:ILE:HD12	2.01	0.43
3:A:2503:ALA:C	3:A:2505:GLY:N	2.70	0.43
3:A:2997:VAL:HG12	3:A:3034:PRO:HA	1.99	0.43
3:A:3013:SER:HA	3:A:3018:ASN:O	2.17	0.43
3:A:2446:ALA:C	3:A:2448:VAL:N	2.72	0.43
3:A:2473:VAL:HG11	3:A:2553:ALA:CB	2.49	0.42
3:A:2536:ILE:HG13	3:A:2537:SER:N	2.33	0.42
3:A:3020:LEU:HA	3:A:3053:VAL:HG23	2.00	0.42
3:A:3046:GLN:NE2	3:A:3057:PHE:HB2	2.33	0.42
1:C:506:DT:O5'	3:A:3007:ALA:HB3	2.19	0.42
3:A:2539:ILE:HG13	3:A:2540:TRP:H	1.83	0.42
3:A:2540:TRP:O	3:A:2544:HIS:CD2	2.72	0.42
3:A:2729:LEU:HD21	3:A:2736:VAL:CG2	2.34	0.42
3:A:2789:LYS:C	3:A:2791:HIS:N	2.73	0.42
3:A:2941:ARG:NH1	3:A:2941:ARG:HG2	2.34	0.42
3:A:3103:LEU:HD23	3:A:3103:LEU:HA	1.81	0.42
2:B:43:TRP:O	2:B:44:ASP:C	2.58	0.42
1:C:505:DT:C6	3:A:3057:PHE:HE2	2.34	0.42
3:A:2554:ALA:O	3:A:2556:GLU:N	2.52	0.42
3:A:2650:ARG:NH2	3:A:2695:LEU:HD22	2.33	0.42
3:A:2768:GLU:O	3:A:2772:ALA:HB2	2.19	0.42
3:A:2461:LEU:CB	3:A:2464:TYR:HE2	2.32	0.42
3:A:2539:ILE:HG13	3:A:2540:TRP:N	2.34	0.42
3:A:2968:TYR:HE2	3:A:2970:PRO:HB3	1.83	0.42
3:A:3000:VAL:O	3:A:3000:VAL:HG12	2.19	0.42
2:B:44:ASP:O	2:B:45:ASP:HB3	2.20	0.42
3:A:2442:ILE:HG21	3:A:2447:ALA:HB2	2.01	0.42
2:B:62:LYS:O	3:A:2457:SER:HA	2.20	0.42
3:A:2522:TYR:HE1	3:A:2536:ILE:CG1	2.33	0.42
3:A:2736:VAL:HG23	3:A:2932:VAL:HG21	2.02	0.42
2:B:9:ASP:OD2	2:B:12:LEU:N	2.47	0.42
3:A:2400:ASP:OD2	3:A:2401:LEU:N	2.51	0.42
3:A:2572:ARG:O	3:A:2575:LEU:CB	2.56	0.42
3:A:2593:LEU:O	3:A:2594:LYS:C	2.57	0.42
2:B:55:GLN:NE2	3:A:2671:LYS:H	2.18	0.42
3:A:2771:GLU:O	3:A:2772:ALA:C	2.56	0.42
3:A:2906:LEU:CD1	3:A:2946:LEU:HB3	2.50	0.42
3:A:3057:PHE:CE1	3:A:3058:ALA:O	2.73	0.42
3:A:2462:TYR:CB	3:A:2466:VAL:HG22	2.45	0.42
3:A:2519:GLU:O	3:A:2522:TYR:N	2.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2571:GLU:CG	3:A:2572:ARG:H	2.28	0.42
3:A:2897:TYR:CE1	3:A:2924:ARG:NE	2.88	0.42
3:A:2443:SER:O	3:A:2446:ALA:N	2.53	0.42
3:A:2605:LYS:O	3:A:2675:GLN:HA	2.19	0.42
3:A:3017:LEU:N	3:A:3017:LEU:HD12	2.35	0.41
3:A:2473:VAL:HG11	3:A:2553:ALA:HB1	2.02	0.41
3:A:2579:TYR:O	3:A:2580:ARG:C	2.59	0.41
3:A:2584:GLU:OE2	3:A:2647:TYR:OH	2.36	0.41
2:B:11:GLY:O	3:A:2435:LYS:HE2	2.20	0.41
3:A:2991:VAL:HG23	3:A:2992:ASP:N	2.34	0.41
3:A:3091:PHE:O	3:A:3093:LYS:N	2.53	0.41
3:A:2745:ARG:NH1	3:A:2745:ARG:HG2	2.35	0.41
3:A:2611:ILE:HD13	3:A:2666:LEU:CD2	2.46	0.41
3:A:2736:VAL:O	3:A:2737:GLY:C	2.58	0.41
3:A:2783:LEU:O	3:A:2786:LEU:N	2.53	0.41
3:A:2642:LEU:O	3:A:2648:ALA:HA	2.20	0.41
3:A:2941:ARG:HB2	3:A:2942:PRO:CD	2.50	0.41
2:B:43:TRP:CZ2	3:A:2706:PRO:HD3	2.55	0.41
3:A:2509:ILE:O	3:A:2509:ILE:HG22	2.19	0.41
3:A:2548:ILE:O	3:A:2549:VAL:C	2.58	0.41
1:C:506:DT:O5'	3:A:3007:ALA:CB	2.69	0.41
3:A:2505:GLY:O	3:A:2506:GLY:O	2.38	0.41
3:A:2532:ASP:C	3:A:2534:LYS:N	2.72	0.41
3:A:2573:VAL:O	3:A:2574:LEU:C	2.59	0.41
3:A:2736:VAL:O	3:A:2738:CYS:N	2.53	0.41
3:A:2779:GLN:O	3:A:2782:LYS:HB3	2.21	0.41
3:A:3017:LEU:CD1	3:A:3091:PHE:CE1	3.03	0.41
3:A:2466:VAL:HG12	3:A:2467:SER:N	2.34	0.41
3:A:2485:ILE:O	3:A:2489:PHE:CD1	2.73	0.41
3:A:2657:LEU:O	3:A:2660:LEU:HB2	2.21	0.41
3:A:2552:LEU:H	3:A:2552:LEU:HG	1.35	0.41
3:A:2597:LEU:HA	3:A:2597:LEU:HD23	1.82	0.41
3:A:2663:SER:OG	3:A:2665:LYS:HG2	2.20	0.41
3:A:3011:TYR:CD2	3:A:3021:VAL:HG13	2.56	0.41
3:A:2443:SER:C	3:A:2445:GLN:N	2.71	0.41
3:A:2688:PRO:O	3:A:2689:LEU:O	2.39	0.41
3:A:2724:LEU:HB3	3:A:2725:PRO:HD2	2.03	0.41
3:A:2773:LEU:HD23	3:A:2774:ARG:CA	2.50	0.41
3:A:2905:LEU:HD12	3:A:2905:LEU:HA	1.28	0.41
3:A:2926:ARG:HD2	3:A:2957:LEU:HD11	2.02	0.41
3:A:2926:ARG:HD3	3:A:2928:TYR:OH	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2960:SER:O	3:A:2962:GLU:N	2.54	0.41
3:A:3048:GLU:N	3:A:3048:GLU:CD	2.75	0.41
2:B:57:ARG:HB2	2:B:57:ARG:HE	1.40	0.41
3:A:2569:ASN:C	3:A:2571:GLU:N	2.74	0.40
3:A:2576:GLN:O	3:A:2577:LEU:C	2.59	0.40
3:A:2768:GLU:CD	3:A:2884:ARG:HH22	2.24	0.40
3:A:3086:ASN:OD1	3:A:3087:ILE:CD1	2.69	0.40
3:A:3089:ASP:OD1	3:A:3089:ASP:C	2.59	0.40
3:A:2924:ARG:HD2	3:A:2959:VAL:HG22	2.02	0.40
2:B:56:LEU:O	2:B:58:ALA:N	2.54	0.40
2:B:56:LEU:HD23	2:B:57:ARG:HB2	2.03	0.40
3:A:2434:THR:HG22	3:A:2435:LYS:N	2.36	0.40
3:A:2674:THR:CG2	3:A:2704:THR:CG2	2.99	0.40
3:A:2531:VAL:O	3:A:2533:PRO:HD2	2.21	0.40
3:A:2722:PHE:CD2	3:A:2724:LEU:HD11	2.57	0.40
3:A:2747:TYR:CB	3:A:2748:PRO:CD	2.79	0.40
3:A:2783:LEU:HA	3:A:2786:LEU:HB2	2.03	0.40
3:A:2964:LEU:HB3	3:A:2965:LEU:H	1.77	0.40
3:A:3074:GLN:O	3:A:3075:GLU:C	2.60	0.40
3:A:2540:TRP:CE3	3:A:2541:VAL:HG22	2.57	0.40
3:A:2670:GLN:HE21	3:A:2670:GLN:HB3	1.57	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	
2	B	36/70 (51%)	23 (64%)	5 (14%)	8 (22%)	0	1
3	A	594/649 (92%)	372 (63%)	117 (20%)	105 (18%)	0	2
All	All	630/719 (88%)	395 (63%)	122 (19%)	113 (18%)	0	2

All (113) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	17	ASP
2	B	23	PRO
2	B	38	VAL
2	B	41	ASP
2	B	43	TRP
3	A	2400	ASP
3	A	2408	ALA
3	A	2453	PRO
3	A	2458	PRO
3	A	2461	LEU
3	A	2463	ILE
3	A	2464	TYR
3	A	2466	VAL
3	A	2467	SER
3	A	2475	SER
3	A	2492	GLU
3	A	2503	ALA
3	A	2510	PRO
3	A	2512	ASN
3	A	2555	MET
3	A	2561	LYS
3	A	2599	ARG
3	A	2604	ALA
3	A	2690	GLU
3	A	2692	PRO
3	A	2734	GLY
3	A	2759	LEU
3	A	2897	TYR
3	A	2899	LYS
3	A	2903	SER
3	A	2911	PRO
3	A	2913	SER
3	A	2941	ARG
3	A	2965	LEU
3	A	2968	TYR
3	A	2969	GLN
3	A	2988	CYS
3	A	3006	LEU
3	A	3029	ASN
3	A	3050	THR
3	A	3090	THR
3	A	2417	LYS

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Mol	Chain	Res	Type
3	A	2418	ASN
3	A	2447	ALA
3	A	2471	ILE
3	A	2485	ILE
3	A	2491	LYS
3	A	2504	ASP
3	A	2506	GLY
3	A	2513	ASP
3	A	2518	LYS
3	A	2530	GLY
3	A	2533	PRO
3	A	2549	VAL
3	A	2573	VAL
3	A	2676	GLY
3	A	2685	ALA
3	A	2715	PHE
3	A	2721	PRO
3	A	2744	GLN
3	A	2749	LEU
3	A	2936	LYS
3	A	2938	LYS
3	A	2952	THR
3	A	2976	PHE
3	A	3028	LEU
3	A	3049	SER
3	A	3051	SER
3	A	3109	LYS
2	B	21	GLU
2	B	57	ARG
3	A	2450	ASP
3	A	2465	GLY
3	A	2480	TYR
3	A	2482	GLN
3	A	2496	ALA
3	A	2511	SER
3	A	2519	GLU
3	A	2520	GLU
3	A	2560	PRO
3	A	2655	PRO
3	A	2677	ALA
3	A	2702	ASN
3	A	2712	ARG

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Mol	Chain	Res	Type
3	A	2756	VAL
3	A	2961	SER
3	A	2974	LEU
3	A	2989	SER
3	A	3047	PRO
3	A	2403	SER
3	A	2431	LEU
3	A	2468	LYS
3	A	2481	PHE
3	A	2554	ALA
3	A	2574	LEU
3	A	2689	LEU
3	A	2691	ALA
3	A	2710	HIS
3	A	2729	LEU
3	A	2524	ALA
3	A	2529	PRO
3	A	2602	THR
3	A	2713	LEU
3	A	2430	SER
3	A	2548	ILE
3	A	2593	LEU
3	A	2682	SER
3	A	3087	ILE
3	A	3084	ILE
2	B	8	VAL
3	A	2509	ILE
3	A	2790	VAL
3	A	2570	PRO

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	
2	B	33/63 (52%)	27 (82%)	6 (18%)	1	9
3	A	521/572 (91%)	435 (84%)	86 (16%)	2	13

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	554/635 (87%)	462 (83%)	92 (17%)	2 13

All (92) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	10	LEU
2	B	17	ASP
2	B	23	PRO
2	B	39	TRP
2	B	56	LEU
2	B	57	ARG
3	A	2404	SER
3	A	2410	ASP
3	A	2425	ARG
3	A	2444	LEU
3	A	2453	PRO
3	A	2462	TYR
3	A	2484	ASP
3	A	2485	ILE
3	A	2493	ASP
3	A	2510	PRO
3	A	2529	PRO
3	A	2536	ILE
3	A	2543	ASN
3	A	2555	MET
3	A	2557	PHE
3	A	2565	ASN
3	A	2572	ARG
3	A	2577	LEU
3	A	2582	ASP
3	A	2583	VAL
3	A	2606	THR
3	A	2607	LEU
3	A	2643	THR
3	A	2650	ARG
3	A	2653	LEU
3	A	2666	LEU
3	A	2667	THR
3	A	2673	ILE
3	A	2689	LEU
3	A	2696	ARG
3	A	2706	PRO

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Mol	Chain	Res	Type
3	A	2708	ARG
3	A	2710	HIS
3	A	2721	PRO
3	A	2725	PRO
3	A	2731	SER
3	A	2732	ASP
3	A	2735	ASN
3	A	2738	CYS
3	A	2740	ASP
3	A	2741	ILE
3	A	2742	ILE
3	A	2744	GLN
3	A	2745	ARG
3	A	2746	VAL
3	A	2749	LEU
3	A	2773	LEU
3	A	2780	GLN
3	A	2786	LEU
3	A	2787	PHE
3	A	2789	LYS
3	A	2792	THR
3	A	2886	VAL
3	A	2887	THR
3	A	2889	VAL
3	A	2892	LEU
3	A	2897	TYR
3	A	2901	GLU
3	A	2903	SER
3	A	2907	SER
3	A	2933	SER
3	A	2946	LEU
3	A	2947	THR
3	A	2951	ARG
3	A	2954	TYR
3	A	2969	GLN
3	A	2998	VAL
3	A	3012	LEU
3	A	3013	SER
3	A	3019	LEU
3	A	3020	LEU
3	A	3021	VAL
3	A	3028	LEU

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Mol	Chain	Res	Type
3	A	3031	ASP
3	A	3041	SER
3	A	3045	CYS
3	A	3048	GLU
3	A	3055	THR
3	A	3074	GLN
3	A	3078	ASN
3	A	3079	ASN
3	A	3087	ILE
3	A	3089	ASP
3	A	3097	LYS
3	A	3099	LEU
3	A	3103	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	55	GLN
3	A	2486	GLN
3	A	2652	GLN
3	A	2675	GLN
3	A	2779	GLN
3	A	2945	GLN
3	A	2956	GLN
3	A	3018	ASN
3	A	3042	ASN
3	A	3060	HIS
3	A	3078	ASN
3	A	3079	ASN

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 [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 ⓘ

EDS was not executed - this section is therefore empty.

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

EDS was not executed - this section is therefore empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.