Full wwPDB X-ray Structure Validation Report ⓘ

May 28, 2020 – 07:58 pm BST

PDB ID	:	1MIU
Title	:	Structure of a BRCA2-DSS1 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	:	2002-08-23
Resolution	:	3.10 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:

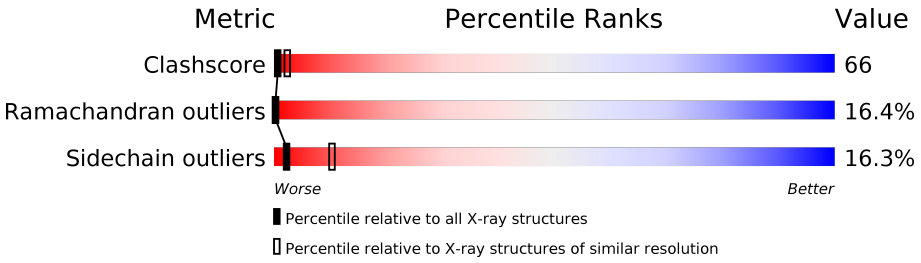
MolProbity	:	4.02b-467
Xtriage (Phenix)	:	NOT EXECUTED
EDS	:	NOT EXECUTED
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)

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 <=5%

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	B	70	23% 29% 6% • 40%
2	A	738	23% 47% 19% • 9%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 5647 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 Deleted in split hand/split foot protein 1.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
1	B	42	348	217	53	78	0	0	0

- Molecule 2 is a protein called Breast Cancer type 2 susceptibility protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
2	A	671	5294	3361	925	991	17	0	0	0

- Molecule 3 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Hg		
3	A	5	5	5	0	0

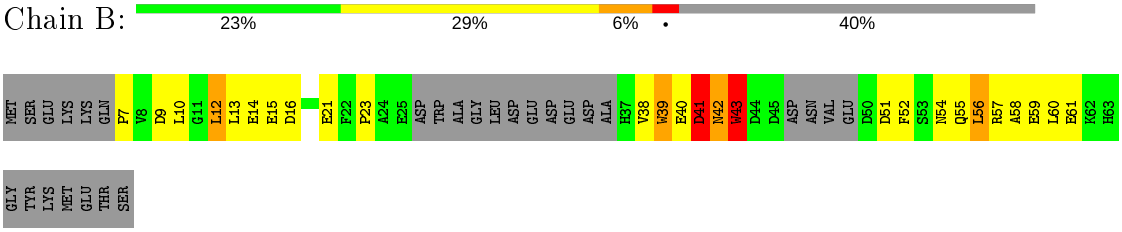
3 Residue-property plots (i)

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. 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. 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.

Note EDS was not executed.

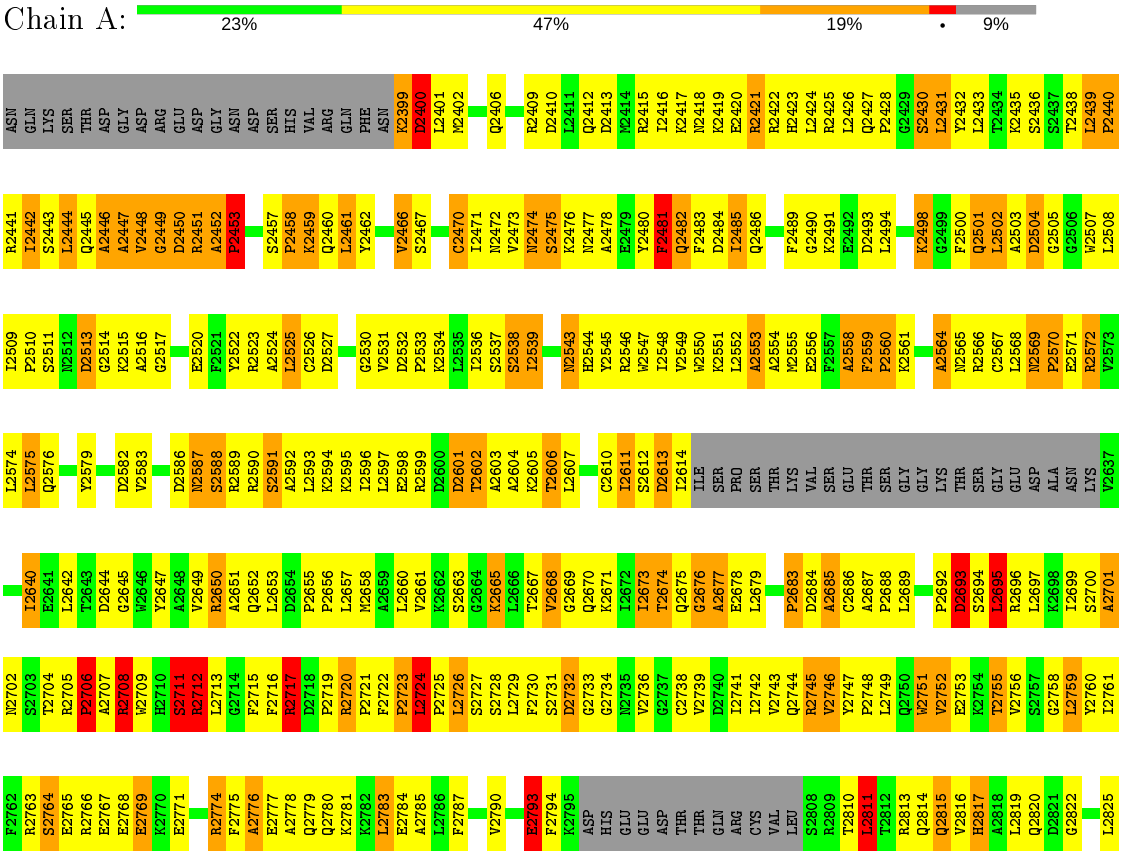
- Molecule 1: Deleted in split hand/split foot protein 1

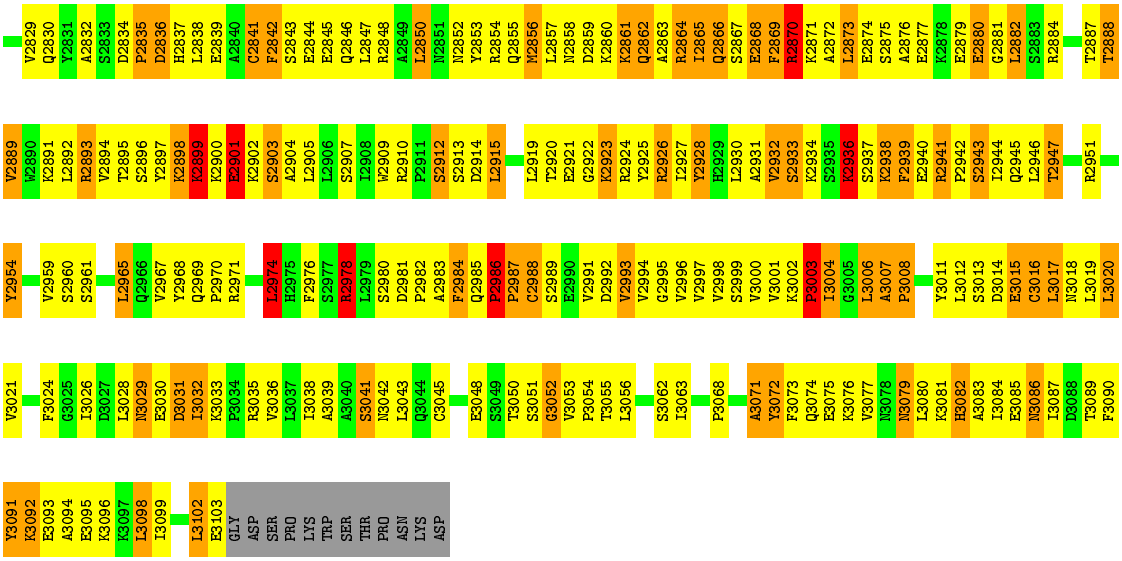
Chain B:



- Molecule 2: Breast Cancer type 2 susceptibility protein

Chain A:




V2829 Q2830 Y2831 A2832 S2833 D2834 P2835 D2836 H2837 L2838 E2839 A2840 C2841 F2842 S2843 E2844 E2845 Q2846 L2847 R2848 A2849 L2850 N2851 N2852 Y2853 R2854 Q2855 M2856 L2857 N2858 D2859 K2860 K2861 Q2862 A2863 R2864 I2865 Q2866 S2867 E2868 F2869 R2870 K2871 A2872 L2873 E2874 S2875 A2876 E2877 K2878 E2879 E2880 G2881 L2882 S2883 R2884 T2887 T2888
V2889 W2890 K2891 L2892 R2893 V2894 T2895 S2896 Y2897 K2898 K2899 K2900 E2901 K2902 S2903 A2904 L2905 L2906 S2907 I2908 W2909 R2910 P2911 S2912 S2913 D2914 L2915 L2919 T2920 E2921 G2922 K2923 R2924 Y2925 R2926 I2927 Y2928 H2929 L2930 A2931 V2932 S2933 K2934 S2935 K2936 S2937 K2938 F2939 E2940 R2941 P2942 S2943 I2944 Q2945 L2946 T2947 R2951
Y2954 V2959 S2960 S2961 L2965 Q2966 V2967 Y2968 Q2969 P2970 R2971 L2974 H2975 F2976 S2977 R2978 L2979 S2980 D2981 P2982 A2983 F2984 Q2985 P2986 P2987 C2988 S2989 E2990 V2991 D2992 V2993 V2994 G2995 V2996 V2997 V2998 S2999 V3000 V3001 K3002 P3003 I3004 G3005 L3006 A3007 P3008 Y3011 L3012 S3013 D3014 E3015 C3016 L3017 N3018 L3019 L3020
V3021 F3024 G3025 I3026 D3027 L3028 N3029 E3030 D3031 I3032 K3033 P3034 R3035 V3036 L3037 I3038 A3039 A3040 S3041 N3042 L3043 Q3044 C3045 E3048 S3049 T3050 S3051 G3052 V3053 P3054 T3055 L3056 S3062 I3063 P3068 A3071 Y3072 F3073 Q3074 E3075 K3076 V3077 N3078 N3079 L3080 K3081 H3082 A3083 I3084 E3085 N3086 I3087 D3088 T3089 F3090
Y3091 K3092 E3093 A3094 E3095 K3096 R3097 L3098 I3099 L3102 E3103 GLY ASP SER PRO LYS TRP SER THR PRO ASN LYS ASP

4 Data and refinement statistics (i)

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

Property	Value	Source
Space group	C 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	160.51Å 228.27Å 81.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 3.10	Depositor
% Data completeness (in resolution range)	(Not available) (20.00-3.10)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
Refinement program	CNS	Depositor
R, R_{free}	0.256 , 0.310	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	5647	wwPDB-VP
Average B, all atoms (Å^2)	107.0	wwPDB-VP

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HG

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	B	0.57	0/354	0.85	2/478 (0.4%)
2	A	0.59	6/5399 (0.1%)	0.86	9/7303 (0.1%)
All	All	0.59	6/5753 (0.1%)	0.85	11/7781 (0.1%)

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
2	A	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2712	ARG	CZ-NH1	6.55	1.41	1.33
2	A	2712	ARG	CZ-NH2	6.13	1.41	1.33
2	A	2978	ARG	CZ-NH1	5.45	1.40	1.33
2	A	2978	ARG	CZ-NH2	5.41	1.40	1.33
2	A	3045	CYS	CB-SG	5.15	1.91	1.82
2	A	2472	ASN	CG-OD1	5.13	1.35	1.24

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2978	ARG	NE-CZ-NH1	11.80	126.20	120.30
2	A	2458	PRO	N-CA-CB	5.95	110.44	103.30
2	A	2811	LEU	CA-CB-CG	5.82	128.69	115.30
2	A	2724	LEU	CA-CB-CG	5.76	128.54	115.30
1	B	7	PRO	N-CA-CB	5.45	109.83	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	12	LEU	CA-CB-CG	-5.36	102.96	115.30
2	A	2505	GLY	N-CA-C	-5.35	99.73	113.10
2	A	2926	ARG	N-CA-C	-5.34	96.57	111.00
2	A	2978	ARG	NE-CZ-NH2	-5.09	117.75	120.30
2	A	2986	PRO	N-CA-CB	5.04	109.34	103.30
2	A	2695	LEU	CA-CB-CG	5.04	126.88	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	A	2853	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	B	348	0	281	59	0
2	A	5294	0	5280	722	0
3	A	5	0	0	0	0
All	All	5647	0	5561	744	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 66.

All (744) 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:A:2936:LYS:HD3	2:A:2936:LYS:H	1.02	1.15
2:A:3001:VAL:HG12	2:A:3003:PRO:HD3	1.34	1.05
2:A:2426:LEU:H	2:A:2426:LEU:HD12	1.20	1.01
1:B:9:ASP:HB3	1:B:12:LEU:HD12	1.42	0.99
2:A:3020:LEU:HA	2:A:3054:PRO:HD2	1.47	0.97
2:A:2502:LEU:HD23	2:A:2503:ALA:H	1.28	0.97
2:A:2430:SER:HB3	2:A:2575:LEU:HD21	1.48	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2611:ILE:HD11	2:A:2670:GLN:HB3	1.50	0.93
2:A:2548:ILE:HG23	2:A:2576:GLN:HE21	1.32	0.92
1:B:21:GLU:O	1:B:23:PRO:HD3	1.69	0.92
2:A:2650:ARG:HH11	2:A:2650:ARG:HB2	1.34	0.90
2:A:2502:LEU:HD23	2:A:2503:ALA:N	1.87	0.90
2:A:2420:GLU:HB3	2:A:2533:PRO:HG2	1.55	0.89
2:A:2936:LYS:HD3	2:A:2936:LYS:N	1.87	0.89
2:A:2548:ILE:HG23	2:A:2576:GLN:NE2	1.88	0.88
2:A:2862:GLN:HE21	2:A:2866:GLN:HE21	1.19	0.88
2:A:2502:LEU:HD21	2:A:2571:GLU:HG2	1.54	0.88
2:A:2612:SER:O	2:A:2668:VAL:HG22	1.74	0.88
2:A:2656:PRO:HD3	2:A:2732:ASP:HB2	1.56	0.87
2:A:2448:VAL:HG21	2:A:2559:PHE:CE1	2.08	0.87
2:A:2811:LEU:HA	2:A:2814:GLN:NE2	1.90	0.87
2:A:2558:ALA:C	2:A:2559:PHE:HD2	1.78	0.87
2:A:2678:GLU:HG2	2:A:2679:LEU:N	1.90	0.87
2:A:2452:ALA:HB1	2:A:2453:PRO:HD2	1.58	0.85
2:A:2485:ILE:HG21	2:A:2510:PRO:HB3	1.58	0.85
2:A:3092:LYS:O	2:A:3096:LYS:HG3	1.76	0.85
2:A:2843:SER:HA	2:A:2847:LEU:HD22	1.56	0.85
2:A:2862:GLN:NE2	2:A:2866:GLN:HE21	1.75	0.84
2:A:2995:GLY:HA2	2:A:3080:LEU:HD23	1.58	0.84
2:A:2462:TYR:HB3	2:A:2466:VAL:HG22	1.59	0.84
2:A:2811:LEU:HA	2:A:2814:GLN:HE21	1.41	0.84
2:A:2503:ALA:O	2:A:2504:ASP:HB2	1.79	0.82
2:A:2572:ARG:O	2:A:2576:GLN:HG3	1.78	0.82
2:A:2861:LYS:O	2:A:2863:ALA:N	2.13	0.82
2:A:3002:LYS:HE2	2:A:3028:LEU:HD12	1.58	0.82
1:B:41:ASP:O	2:A:2705:ARG:HD2	1.80	0.81
2:A:2723:PRO:HG3	2:A:2926:ARG:HH21	1.45	0.81
2:A:2931:ALA:O	2:A:2933:SER:N	2.13	0.81
2:A:2428:PRO:HB2	2:A:2433:LEU:HG	1.63	0.80
2:A:2441:ARG:O	2:A:2442:ILE:HG13	1.82	0.80
2:A:2485:ILE:HD12	2:A:2486:GLN:N	1.97	0.80
2:A:2614:ILE:HD11	2:A:2668:VAL:HG23	1.64	0.80
2:A:2746:VAL:HG22	2:A:2892:LEU:HD22	1.63	0.80
2:A:2415:ARG:NH1	2:A:2527:ASP:OD1	2.15	0.80
2:A:2845:GLU:HG3	2:A:2846:GLN:HG3	1.61	0.80
2:A:2650:ARG:HH11	2:A:2650:ARG:CB	1.94	0.79
2:A:2483:PHE:HB2	2:A:2516:ALA:HB3	1.63	0.79
2:A:2543:ASN:HD21	2:A:2547:TRP:HE1	1.30	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2678:GLU:O	2:A:2697:LEU:HD12	1.82	0.79
2:A:2651:ALA:HB1	2:A:2699:ILE:HD13	1.65	0.79
2:A:2675:GLN:NE2	2:A:2722:PHE:H	1.79	0.79
2:A:2421:ARG:CZ	2:A:2422:ARG:HG3	2.12	0.79
2:A:2543:ASN:ND2	2:A:2547:TRP:HE1	1.81	0.79
2:A:2553:ALA:O	2:A:2556:GLU:HB2	1.84	0.78
2:A:2544:HIS:O	2:A:2548:ILE:HG13	1.84	0.78
2:A:2448:VAL:HG21	2:A:2559:PHE:HE1	1.47	0.77
2:A:2869:PHE:O	2:A:2870:ARG:C	2.22	0.77
2:A:2476:LYS:HD2	2:A:2613:ASP:OD2	1.84	0.77
2:A:2724:LEU:HB2	2:A:2725:PRO:HD2	1.64	0.77
2:A:2892:LEU:O	2:A:2905:LEU:HD12	1.83	0.77
2:A:2868:GLU:HA	2:A:2868:GLU:OE2	1.84	0.76
2:A:3095:GLU:O	2:A:3099:ILE:HG22	1.85	0.76
2:A:2650:ARG:HB2	2:A:2650:ARG:NH1	1.97	0.76
1:B:56:LEU:O	1:B:56:LEU:HG	1.85	0.76
2:A:2675:GLN:HG3	2:A:2722:PHE:CE1	2.19	0.76
2:A:2565:ASN:C	2:A:2567:CYS:H	1.86	0.76
2:A:2601:ASP:O	2:A:2603:ALA:N	2.19	0.76
2:A:2673:ILE:CG1	2:A:2707:ALA:HB2	2.16	0.76
2:A:2674:THR:CG2	2:A:2699:ILE:HG23	2.14	0.76
2:A:2587:ASN:H	2:A:2587:ASN:HD22	1.35	0.75
2:A:2532:ASP:OD2	2:A:2534:LYS:HE3	1.86	0.75
2:A:2748:PRO:HG3	2:A:3063:ILE:HD11	1.69	0.75
2:A:2480:TYR:O	2:A:2482:GLN:HG2	1.85	0.75
2:A:2834:ASP:OD1	2:A:2837:HIS:HB2	1.86	0.75
2:A:2869:PHE:O	2:A:2871:LYS:N	2.20	0.75
2:A:2687:ALA:O	2:A:2689:LEU:N	2.20	0.75
2:A:2726:LEU:HA	2:A:2729:LEU:HG	1.68	0.75
2:A:2768:GLU:O	2:A:2768:GLU:HG3	1.87	0.75
2:A:3008:PRO:HG2	2:A:3024:PHE:HB2	1.68	0.75
2:A:2995:GLY:HA2	2:A:3080:LEU:CD2	2.16	0.74
2:A:2516:ALA:HA	2:A:2520:GLU:HG2	1.68	0.74
2:A:2399:LYS:O	2:A:2400:ASP:HB2	1.84	0.74
2:A:2915:LEU:HD11	2:A:2954:TYR:CE1	2.23	0.74
2:A:2409:ARG:NH2	2:A:2511:SER:HA	2.02	0.74
1:B:9:ASP:CB	1:B:12:LEU:HD12	2.16	0.74
2:A:3081:LYS:O	2:A:3085:GLU:HG2	1.88	0.74
2:A:2564:ALA:HB3	2:A:2566:ARG:HG2	1.69	0.73
2:A:2751:TRP:HB3	2:A:2768:GLU:HG2	1.69	0.73
2:A:3012:LEU:HB2	2:A:3020:LEU:HD21	1.71	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2415:ARG:HD2	2:A:2527:ASP:OD2	1.87	0.73
2:A:2745:ARG:HH21	2:A:2971:ARG:HA	1.52	0.73
2:A:2898:LYS:O	2:A:2899:LYS:O	2.07	0.72
1:B:58:ALA:O	1:B:61:GLU:HB2	1.89	0.72
2:A:2419:LYS:HE3	2:A:2526:CYS:O	1.90	0.72
2:A:2936:LYS:CD	2:A:2936:LYS:H	1.90	0.72
2:A:3035:ARG:NE	2:A:3092:LYS:HD3	2.04	0.72
2:A:3015:GLU:OE1	2:A:3079:ASN:HB3	1.89	0.72
2:A:2452:ALA:HB1	2:A:2453:PRO:CD	2.20	0.71
2:A:2502:LEU:HD21	2:A:2571:GLU:CG	2.19	0.71
2:A:2614:ILE:HG23	2:A:2640:ILE:HG22	1.72	0.71
2:A:2656:PRO:CD	2:A:2732:ASP:HB2	2.21	0.71
2:A:3052:GLY:O	2:A:3054:PRO:HD3	1.91	0.70
2:A:2711:SER:O	2:A:2712:ARG:HB2	1.89	0.70
2:A:2602:THR:O	2:A:2603:ALA:C	2.30	0.70
2:A:2400:ASP:C	2:A:2402:MET:H	1.93	0.70
2:A:2653:LEU:HD22	2:A:2657:LEU:HD13	1.73	0.70
2:A:2723:PRO:HG3	2:A:2926:ARG:NH2	2.06	0.70
2:A:2819:LEU:HD13	2:A:2842:PHE:CD2	2.26	0.70
2:A:3032:ILE:O	2:A:3032:ILE:HG22	1.92	0.69
2:A:2745:ARG:HE	2:A:2971:ARG:CG	2.04	0.69
2:A:2976:PHE:CE2	2:A:3020:LEU:HD22	2.27	0.69
2:A:2475:SER:HB2	2:A:2550:TRP:NE1	2.06	0.69
2:A:2902:LYS:HE2	2:A:2943:SER:HA	1.74	0.69
1:B:12:LEU:CD2	2:A:2439:LEU:HD22	2.23	0.68
2:A:2475:SER:HB2	2:A:2550:TRP:CE2	2.28	0.68
2:A:2484:ASP:O	2:A:2486:GLN:N	2.27	0.68
2:A:2954:TYR:N	2:A:2954:TYR:HD2	1.90	0.68
2:A:2571:GLU:O	2:A:2575:LEU:HB2	1.93	0.68
2:A:2418:ASN:O	2:A:2421:ARG:HB3	1.94	0.68
2:A:2895:THR:CG2	2:A:2903:SER:HB3	2.24	0.67
2:A:2485:ILE:HG21	2:A:2510:PRO:CB	2.24	0.67
2:A:2702:ASN:ND2	2:A:2733:GLY:O	2.27	0.67
2:A:2745:ARG:HD3	2:A:2921:GLU:OE2	1.93	0.67
2:A:2845:GLU:HG3	2:A:2846:GLN:N	2.09	0.67
2:A:2723:PRO:CG	2:A:2926:ARG:HH21	2.06	0.67
2:A:2984:PHE:O	2:A:2986:PRO:N	2.28	0.67
2:A:2676:GLY:O	2:A:2677:ALA:O	2.13	0.67
2:A:2653:LEU:CD2	2:A:2657:LEU:HD13	2.25	0.67
2:A:3014:ASP:HA	2:A:3080:LEU:HD22	1.76	0.67
2:A:2431:LEU:HD21	2:A:2575:LEU:HD13	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2915:LEU:HD21	2:A:2954:TYR:CZ	2.30	0.66
2:A:2450:ASP:O	2:A:2451:ARG:HB2	1.93	0.66
2:A:2900:LYS:O	2:A:2901:GLU:HB3	1.96	0.66
1:B:39:TRP:CZ2	2:A:2722:PHE:HB2	2.31	0.66
2:A:2678:GLU:HG2	2:A:2679:LEU:H	1.58	0.66
2:A:2587:ASN:H	2:A:2587:ASN:ND2	1.92	0.66
2:A:2938:LYS:O	2:A:2939:PHE:HB2	1.95	0.66
2:A:2954:TYR:N	2:A:2954:TYR:CD2	2.62	0.66
2:A:2822:GLY:HA2	2:A:2825:LEU:HB2	1.78	0.66
1:B:54:ASN:HB3	2:A:2453:PRO:HD2	1.78	0.66
2:A:2766:ARG:NE	2:A:2766:ARG:HA	2.10	0.65
1:B:57:ARG:HB3	2:A:2550:TRP:CH2	2.32	0.65
2:A:2675:GLN:NE2	2:A:2722:PHE:N	2.44	0.65
2:A:2745:ARG:NE	2:A:2971:ARG:HG3	2.11	0.65
2:A:3012:LEU:HB2	2:A:3020:LEU:CD2	2.26	0.65
2:A:2421:ARG:O	2:A:2421:ARG:NE	2.30	0.65
2:A:2684:ASP:O	2:A:2685:ALA:O	2.15	0.65
2:A:2775:PHE:O	2:A:2777:GLU:N	2.30	0.65
2:A:2858:ASN:O	2:A:2860:LYS:N	2.30	0.65
1:B:40:GLU:HB2	1:B:52:PHE:CZ	2.32	0.65
2:A:3002:LYS:HE2	2:A:3028:LEU:CD1	2.27	0.64
2:A:2445:GLN:HE21	2:A:2450:ASP:HA	1.62	0.64
2:A:2864:ARG:HH11	2:A:2864:ARG:HG3	1.60	0.64
2:A:2611:ILE:HG13	2:A:2669:GLY:H	1.60	0.64
2:A:2845:GLU:HA	2:A:2848:ARG:HE	1.62	0.64
2:A:2474:ASN:H	2:A:2477:ASN:HD21	1.43	0.64
2:A:2768:GLU:CG	2:A:2768:GLU:O	2.46	0.64
1:B:52:PHE:CE1	2:A:2708:ARG:NH1	2.65	0.64
1:B:12:LEU:HD22	2:A:2439:LEU:HD22	1.80	0.64
2:A:2936:LYS:HE3	2:A:2942:PRO:O	1.98	0.64
2:A:2675:GLN:HG3	2:A:2722:PHE:HE1	1.62	0.63
2:A:2996:VAL:HG21	2:A:3084:ILE:HD11	1.79	0.63
2:A:2872:ALA:O	2:A:2875:SER:N	2.24	0.63
2:A:2459:LYS:C	2:A:2461:LEU:N	2.48	0.63
2:A:2667:THR:O	2:A:2668:VAL:C	2.36	0.63
2:A:2844:GLU:HG2	2:A:2846:GLN:H	1.64	0.63
2:A:2919:LEU:HD21	2:A:2954:TYR:HD1	1.64	0.63
2:A:2865:ILE:O	2:A:2866:GLN:C	2.37	0.63
2:A:2742:ILE:HD12	2:A:2923:LYS:O	1.99	0.63
2:A:3081:LYS:NZ	2:A:3085:GLU:HB3	2.14	0.63
1:B:16:ASP:OD1	1:B:57:ARG:NH2	2.32	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2640:ILE:HD13	2:A:2640:ILE:H	1.63	0.63
2:A:2675:GLN:O	2:A:2677:ALA:N	2.32	0.62
2:A:3031:ASP:O	2:A:3033:LYS:N	2.31	0.62
2:A:3099:ILE:HD11	2:A:3103:GLU:OE1	1.99	0.62
2:A:2891:LYS:O	2:A:2892:LEU:HD23	1.98	0.62
2:A:2425:ARG:HE	2:A:2426:LEU:CD1	2.12	0.62
2:A:2830:GLN:C	2:A:2832:ALA:H	2.03	0.62
2:A:2969:GLN:HE22	2:A:2987:PRO:CB	2.11	0.62
2:A:3020:LEU:HB2	2:A:3054:PRO:HB2	1.82	0.62
2:A:2606:THR:HG22	2:A:2716:PHE:HB3	1.80	0.62
2:A:2653:LEU:HB3	2:A:2657:LEU:CB	2.30	0.62
2:A:2783:LEU:HD12	2:A:2879:GLU:CG	2.30	0.62
2:A:2591:SER:OG	2:A:2592:ALA:N	2.30	0.61
2:A:2745:ARG:HA	2:A:2921:GLU:OE2	2.00	0.61
2:A:2604:ALA:HB1	2:A:2677:ALA:HB3	1.80	0.61
2:A:2994:VAL:HG22	2:A:3073:PHE:HD2	1.65	0.61
2:A:3087:ILE:C	2:A:3089:THR:H	2.04	0.61
2:A:2611:ILE:HG13	2:A:2670:GLN:H	1.65	0.61
2:A:2474:ASN:H	2:A:2477:ASN:ND2	1.98	0.61
2:A:2674:THR:HG21	2:A:2699:ILE:HG23	1.83	0.61
2:A:2432:TYR:O	2:A:2436:SER:HB2	2.00	0.61
2:A:2751:TRP:CB	2:A:2768:GLU:HG2	2.31	0.61
2:A:2522:TYR:HE2	2:A:2523:ARG:HH21	1.49	0.60
2:A:2745:ARG:NH2	2:A:2971:ARG:HA	2.16	0.60
2:A:2891:LYS:C	2:A:2892:LEU:HD23	2.21	0.60
2:A:3001:VAL:HG12	2:A:3003:PRO:CD	2.22	0.60
2:A:3032:ILE:H	2:A:3032:ILE:HD12	1.67	0.60
2:A:2932:VAL:O	2:A:2933:SER:C	2.39	0.60
2:A:2976:PHE:CD1	2:A:3014:ASP:HB3	2.37	0.60
2:A:2974:LEU:HD11	2:A:2993:VAL:HG12	1.84	0.60
2:A:2543:ASN:O	2:A:2546:ARG:HB3	2.01	0.60
1:B:55:GLN:CD	2:A:2670:GLN:HG3	2.22	0.60
2:A:3002:LYS:CE	2:A:3028:LEU:HD12	2.31	0.60
2:A:2825:LEU:O	2:A:2829:VAL:HG23	2.02	0.60
2:A:2900:LYS:O	2:A:2901:GLU:CB	2.50	0.60
2:A:2552:LEU:O	2:A:2553:ALA:C	2.41	0.59
2:A:2441:ARG:C	2:A:2442:ILE:HG13	2.22	0.59
2:A:2904:ALA:HB1	2:A:2944:ILE:O	2.01	0.59
2:A:2565:ASN:C	2:A:2567:CYS:N	2.56	0.59
2:A:2653:LEU:HB3	2:A:2657:LEU:HB2	1.84	0.59
2:A:2775:PHE:C	2:A:2777:GLU:H	2.05	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2850:LEU:HD21	2:A:2854:ARG:NH2	2.18	0.59
2:A:2656:PRO:CG	2:A:2732:ASP:HB2	2.33	0.58
2:A:2416:ILE:HG22	2:A:2533:PRO:HG3	1.85	0.58
2:A:2559:PHE:CD2	2:A:2559:PHE:N	2.69	0.58
2:A:2856:MET:SD	2:A:2856:MET:O	2.61	0.58
2:A:2897:TYR:OH	2:A:2959:VAL:HG13	2.03	0.58
2:A:2491:LYS:HA	2:A:2494:LEU:HB2	1.84	0.58
2:A:2838:LEU:HD23	2:A:2838:LEU:O	2.03	0.58
2:A:2657:LEU:O	2:A:2661:VAL:HG23	2.03	0.58
2:A:2421:ARG:CZ	2:A:2422:ARG:CG	2.82	0.58
2:A:2587:ASN:ND2	2:A:2587:ASN:N	2.51	0.58
2:A:2431:LEU:HD23	2:A:2431:LEU:N	2.18	0.58
2:A:2611:ILE:HA	2:A:2642:LEU:HD23	1.85	0.58
2:A:2934:LYS:O	2:A:2945:GLN:HB3	2.03	0.58
2:A:2819:LEU:HD11	2:A:2844:GLU:OE2	2.04	0.58
2:A:3019:LEU:CD2	2:A:3099:ILE:HB	2.34	0.58
2:A:2783:LEU:HD12	2:A:2879:GLU:HG2	1.86	0.58
2:A:2861:LYS:O	2:A:2864:ARG:N	2.37	0.58
2:A:3062:SER:C	2:A:3063:ILE:HD13	2.24	0.58
2:A:2766:ARG:HH22	2:A:2769:GLU:HG3	1.69	0.57
2:A:3071:ALA:O	2:A:3073:PHE:N	2.37	0.57
2:A:2559:PHE:HD2	2:A:2559:PHE:N	2.02	0.57
2:A:2596:ILE:HD11	2:A:2715:PHE:HZ	1.69	0.57
2:A:2895:THR:HG22	2:A:2903:SER:HB3	1.87	0.57
2:A:2984:PHE:C	2:A:2986:PRO:N	2.56	0.57
2:A:2675:GLN:HE22	2:A:2722:PHE:N	2.00	0.57
2:A:2884:ARG:HH11	2:A:2884:ARG:HG2	1.69	0.57
2:A:2678:GLU:CG	2:A:2679:LEU:N	2.67	0.57
2:A:2858:ASN:C	2:A:2860:LYS:H	2.08	0.57
2:A:3051:SER:C	2:A:3053:VAL:H	2.07	0.57
2:A:2508:LEU:HD23	2:A:2508:LEU:O	2.04	0.57
2:A:2889:VAL:HG13	2:A:2909:TRP:CD2	2.40	0.57
2:A:2969:GLN:NE2	2:A:2987:PRO:CB	2.68	0.57
1:B:55:GLN:CG	2:A:2670:GLN:HG3	2.35	0.57
2:A:2553:ALA:O	2:A:2556:GLU:N	2.30	0.57
2:A:2559:PHE:N	2:A:2560:PRO:HD3	2.19	0.57
2:A:2699:ILE:HD12	2:A:2699:ILE:N	2.20	0.57
2:A:2819:LEU:HG	2:A:2846:GLN:CB	2.35	0.57
2:A:2459:LYS:C	2:A:2461:LEU:H	2.08	0.56
2:A:2976:PHE:HE2	2:A:3020:LEU:HD22	1.70	0.56
1:B:41:ASP:O	2:A:2705:ARG:CD	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:51:ASP:HB3	2:A:2708:ARG:HG3	1.88	0.56
2:A:2931:ALA:N	2:A:2947:THR:O	2.35	0.56
1:B:55:GLN:HG3	2:A:2670:GLN:HG3	1.86	0.56
2:A:2758:GLY:O	2:A:2759:LEU:O	2.23	0.56
2:A:2998:VAL:CG2	2:A:2999:SER:N	2.69	0.56
2:A:2406:GLN:HG2	2:A:2410:ASP:OD2	2.06	0.56
2:A:3032:ILE:N	2:A:3032:ILE:HD12	2.19	0.56
2:A:3075:GLU:O	2:A:3077:VAL:N	2.39	0.56
2:A:2416:ILE:HG23	2:A:2526:CYS:HB3	1.88	0.56
2:A:2723:PRO:O	2:A:2724:LEU:CB	2.53	0.56
2:A:3093:GLU:O	2:A:3096:LYS:HB2	2.06	0.56
2:A:2427:GLN:HB2	2:A:2530:GLY:HA3	1.87	0.56
2:A:2556:GLU:O	2:A:2558:ALA:N	2.37	0.56
2:A:2586:ASP:C	2:A:2588:SER:H	2.08	0.56
2:A:2755:THR:OG1	2:A:2758:GLY:O	2.23	0.56
2:A:2784:GLU:HG3	2:A:2785:ALA:N	2.20	0.56
1:B:10:LEU:HD12	2:A:2572:ARG:HD3	1.87	0.56
2:A:2442:ILE:O	2:A:2442:ILE:HG22	2.05	0.55
2:A:2462:TYR:HB3	2:A:2466:VAL:CG2	2.35	0.55
2:A:2864:ARG:O	2:A:2868:GLU:N	2.24	0.55
2:A:2976:PHE:CZ	2:A:3020:LEU:HD22	2.40	0.55
2:A:2612:SER:O	2:A:2668:VAL:CG2	2.51	0.55
2:A:2739:VAL:HG23	2:A:2739:VAL:O	2.05	0.55
2:A:2776:ALA:O	2:A:2780:GLN:HG3	2.05	0.55
2:A:2745:ARG:HE	2:A:2971:ARG:HG3	1.72	0.55
2:A:2415:ARG:HH11	2:A:2527:ASP:CG	2.09	0.55
2:A:2647:TYR:CE2	2:A:2689:LEU:HD21	2.42	0.55
2:A:2845:GLU:CG	2:A:2846:GLN:HG3	2.34	0.55
2:A:2994:VAL:HG22	2:A:3073:PHE:CD2	2.41	0.55
2:A:2466:VAL:HG23	2:A:2467:SER:N	2.22	0.55
2:A:2723:PRO:O	2:A:2724:LEU:HG	2.06	0.55
2:A:2476:LYS:O	2:A:2476:LYS:HG2	2.05	0.55
2:A:2548:ILE:CG2	2:A:2576:GLN:HE21	2.13	0.55
2:A:2406:GLN:HA	2:A:2409:ARG:HB2	1.88	0.55
2:A:2895:THR:HG22	2:A:2903:SER:CA	2.36	0.55
2:A:2817:HIS:C	2:A:2819:LEU:H	2.10	0.55
2:A:2747:TYR:HD2	2:A:3042:ASN:ND2	2.05	0.55
2:A:2501:GLN:HG2	2:A:2507:TRP:CE2	2.42	0.54
2:A:2550:TRP:HH2	2:A:2669:GLY:HA2	1.72	0.54
2:A:2673:ILE:HG13	2:A:2707:ALA:HB2	1.87	0.54
2:A:2842:PHE:HB2	2:A:2844:GLU:OE2	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3079:ASN:O	2:A:3082:HIS:HB2	2.07	0.54
2:A:2474:ASN:HB2	2:A:2477:ASN:OD1	2.08	0.54
2:A:2889:VAL:HG13	2:A:2909:TRP:CE3	2.43	0.54
2:A:2655:PRO:O	2:A:2658:MET:HB2	2.07	0.54
2:A:2889:VAL:HG22	2:A:2909:TRP:CZ3	2.43	0.54
2:A:2994:VAL:HG12	2:A:2995:GLY:N	2.22	0.54
2:A:3052:GLY:C	2:A:3054:PRO:HD3	2.27	0.54
2:A:3102:LEU:N	2:A:3102:LEU:HD23	2.22	0.54
2:A:2775:PHE:HD2	2:A:2776:ALA:N	2.06	0.54
2:A:2749:LEU:HD22	2:A:2888:THR:OG1	2.06	0.54
2:A:3051:SER:O	2:A:3053:VAL:HG12	2.08	0.54
2:A:2443:SER:C	2:A:2445:GLN:N	2.59	0.54
2:A:2485:ILE:HG13	2:A:2514:GLY:O	2.08	0.54
2:A:2655:PRO:HB2	2:A:2656:PRO:HD3	1.90	0.54
2:A:2743:VAL:HA	2:A:2894:VAL:HG12	1.90	0.54
2:A:2579:TYR:O	2:A:2583:VAL:HG23	2.08	0.53
2:A:2592:ALA:O	2:A:2596:ILE:HG12	2.08	0.53
2:A:2430:SER:HB3	2:A:2575:LEU:CD2	2.30	0.53
2:A:2551:LYS:O	2:A:2555:MET:HG3	2.08	0.53
2:A:2872:ALA:O	2:A:2874:GLU:N	2.42	0.53
2:A:2988:CYS:O	2:A:2989:SER:HB3	2.09	0.53
2:A:2552:LEU:O	2:A:2555:MET:N	2.41	0.53
2:A:3019:LEU:HD21	2:A:3099:ILE:HB	1.91	0.53
2:A:2994:VAL:CG2	2:A:3073:PHE:HD2	2.22	0.53
2:A:2867:SER:O	2:A:2871:LYS:HB2	2.09	0.53
1:B:21:GLU:CG	2:A:2595:LYS:HE3	2.38	0.53
1:B:52:PHE:HE1	2:A:2708:ARG:NH1	2.05	0.53
2:A:2745:ARG:HE	2:A:2971:ARG:HG2	1.72	0.53
2:A:3006:LEU:O	2:A:3007:ALA:CB	2.55	0.53
1:B:55:GLN:C	1:B:57:ARG:H	2.12	0.53
2:A:2927:ILE:CG2	2:A:2930:LEU:HD11	2.39	0.53
2:A:2915:LEU:HD11	2:A:2954:TYR:CD1	2.44	0.52
2:A:2819:LEU:HA	2:A:2825:LEU:HD21	1.91	0.52
2:A:2687:ALA:C	2:A:2689:LEU:H	2.13	0.52
2:A:2539:ILE:H	2:A:2539:ILE:HD13	1.74	0.52
2:A:2558:ALA:O	2:A:2559:PHE:HD2	1.92	0.52
2:A:2974:LEU:HD11	2:A:2993:VAL:CB	2.40	0.52
1:B:10:LEU:C	1:B:12:LEU:H	2.13	0.52
2:A:2443:SER:O	2:A:2445:GLN:N	2.43	0.52
2:A:2660:LEU:HD22	2:A:2665:LYS:CB	2.40	0.52
2:A:2509:ILE:HG22	2:A:2510:PRO:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2998:VAL:HG23	2:A:2999:SER:N	2.24	0.52
2:A:2844:GLU:N	2:A:2844:GLU:OE1	2.41	0.52
2:A:3015:GLU:CA	2:A:3080:LEU:HD13	2.40	0.52
2:A:3035:ARG:HD2	2:A:3092:LYS:HB3	1.92	0.52
2:A:2836:ASP:HA	2:A:2839:GLU:HG2	1.92	0.52
2:A:2482:GLN:OE1	2:A:2515:LYS:HD3	2.10	0.52
2:A:2793:GLU:O	2:A:2794:PHE:HD1	1.93	0.52
2:A:2892:LEU:HD11	2:A:2919:LEU:HD13	1.91	0.52
2:A:2774:ARG:NH1	2:A:2775:PHE:HA	2.25	0.51
2:A:2872:ALA:O	2:A:2873:LEU:C	2.48	0.51
2:A:2931:ALA:CB	2:A:2947:THR:O	2.58	0.51
2:A:3039:ALA:HB2	2:A:3068:PRO:HG3	1.92	0.51
2:A:3098:LEU:HD13	2:A:3102:LEU:HD21	1.91	0.51
2:A:2862:GLN:O	2:A:2862:GLN:HG3	2.09	0.51
2:A:2431:LEU:HD23	2:A:2431:LEU:H	1.74	0.51
2:A:2744:GLN:HA	2:A:2744:GLN:OE1	2.10	0.51
2:A:2968:TYR:CE2	2:A:2970:PRO:HG3	2.46	0.51
2:A:2467:SER:O	2:A:2471:ILE:HD13	2.11	0.51
2:A:2502:LEU:HD21	2:A:2571:GLU:CB	2.41	0.51
2:A:2532:ASP:OD2	2:A:2534:LYS:CE	2.57	0.51
2:A:2882:LEU:O	2:A:2882:LEU:HD23	2.11	0.51
2:A:2747:TYR:HB3	2:A:2748:PRO:HD2	1.92	0.51
2:A:2895:THR:HG22	2:A:2903:SER:HA	1.93	0.51
2:A:2400:ASP:C	2:A:2402:MET:N	2.63	0.51
2:A:2651:ALA:HB1	2:A:2699:ILE:CD1	2.38	0.51
2:A:2747:TYR:HD2	2:A:3042:ASN:HD21	1.56	0.51
2:A:2513:ASP:CB	2:A:2515:LYS:HE3	2.41	0.51
2:A:2502:LEU:CD2	2:A:2571:GLU:HG2	2.33	0.51
2:A:2793:GLU:O	2:A:2794:PHE:CD1	2.64	0.51
2:A:2835:PRO:C	2:A:2837:HIS:H	2.13	0.51
1:B:39:TRP:HB3	2:A:2673:ILE:HD12	1.93	0.51
2:A:2532:ASP:CG	2:A:2534:LYS:HE3	2.31	0.51
2:A:2775:PHE:C	2:A:2777:GLU:N	2.64	0.51
2:A:2919:LEU:HA	2:A:2925:TYR:OH	2.10	0.50
2:A:3000:VAL:HG12	2:A:3001:VAL:N	2.26	0.50
2:A:2448:VAL:C	2:A:2450:ASP:H	2.14	0.50
2:A:2725:PRO:HG2	2:A:2728:SER:OG	2.11	0.50
2:A:3015:GLU:HA	2:A:3080:LEU:HD13	1.94	0.50
2:A:2604:ALA:HB3	2:A:2677:ALA:O	2.12	0.50
2:A:2847:LEU:HG	2:A:2847:LEU:O	2.12	0.50
2:A:2583:VAL:O	2:A:2589:ARG:HB2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2675:GLN:CG	2:A:2722:PHE:CE1	2.94	0.50
2:A:2656:PRO:HG3	2:A:2732:ASP:OD1	2.11	0.50
2:A:2974:LEU:HD11	2:A:2993:VAL:CG1	2.41	0.50
1:B:39:TRP:CE2	2:A:2722:PHE:HB2	2.46	0.50
2:A:2652:GLN:N	2:A:2697:LEU:O	2.45	0.50
2:A:2965:LEU:HD12	2:A:2965:LEU:H	1.75	0.50
2:A:2425:ARG:HE	2:A:2426:LEU:HD13	1.75	0.50
1:B:60:LEU:HD11	2:A:2554:ALA:N	2.27	0.49
2:A:2790:VAL:O	2:A:2790:VAL:HG12	2.12	0.49
2:A:2593:LEU:O	2:A:2597:LEU:HD23	2.11	0.49
2:A:2909:TRP:O	2:A:2910:ARG:C	2.50	0.49
2:A:3099:ILE:CD1	2:A:3103:GLU:OE1	2.60	0.49
2:A:2419:LYS:HD3	2:A:2531:VAL:O	2.12	0.49
2:A:2543:ASN:ND2	2:A:2547:TRP:NE1	2.57	0.49
2:A:2559:PHE:N	2:A:2560:PRO:CD	2.76	0.49
2:A:3031:ASP:OD1	2:A:3031:ASP:N	2.45	0.49
1:B:59:GLU:C	1:B:61:GLU:H	2.16	0.49
2:A:2478:ALA:C	2:A:2480:TYR:H	2.16	0.49
2:A:2912:SER:OG	2:A:2914:ASP:HB2	2.12	0.49
2:A:2978:ARG:C	2:A:2980:SER:H	2.14	0.49
2:A:2423:HIS:C	2:A:2424:LEU:HG	2.33	0.49
2:A:2760:TYR:C	2:A:2761:ILE:HD12	2.33	0.49
2:A:2763:ARG:O	2:A:2764:SER:O	2.30	0.49
1:B:42:ASN:HA	2:A:2728:SER:HB2	1.93	0.49
2:A:2675:GLN:NE2	2:A:2722:PHE:CD1	2.81	0.49
2:A:3020:LEU:HD12	2:A:3056:LEU:HG	1.94	0.49
1:B:52:PHE:CD1	1:B:52:PHE:N	2.80	0.49
2:A:2443:SER:C	2:A:2445:GLN:H	2.15	0.49
2:A:2829:VAL:O	2:A:2832:ALA:HB3	2.11	0.49
2:A:2865:ILE:HG22	2:A:2866:GLN:N	2.26	0.49
2:A:2446:ALA:C	2:A:2448:VAL:H	2.16	0.49
1:B:55:GLN:HG3	2:A:2670:GLN:CB	2.43	0.49
2:A:3018:ASN:C	2:A:3019:LEU:HD12	2.32	0.49
2:A:2660:LEU:HD22	2:A:2665:LYS:HB2	1.95	0.49
2:A:2671:LYS:HD3	2:A:2711:SER:HB2	1.95	0.49
2:A:2474:ASN:C	2:A:2476:LYS:H	2.16	0.49
1:B:55:GLN:HG3	2:A:2670:GLN:CG	2.42	0.49
2:A:2997:VAL:O	2:A:3035:ARG:N	2.44	0.49
2:A:2500:PHE:CE2	2:A:2510:PRO:HG3	2.47	0.48
2:A:2550:TRP:CH2	2:A:2669:GLY:HA2	2.48	0.48
2:A:2723:PRO:O	2:A:2724:LEU:CG	2.61	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3014:ASP:HA	2:A:3080:LEU:CD2	2.43	0.48
2:A:2483:PHE:O	2:A:2485:ILE:N	2.46	0.48
2:A:2523:ARG:HA	2:A:2523:ARG:NE	2.28	0.48
2:A:2981:ASP:O	2:A:2983:ALA:N	2.42	0.48
2:A:2981:ASP:C	2:A:2983:ALA:H	2.15	0.48
1:B:14:GLU:HG2	2:A:2441:ARG:HB3	1.95	0.48
2:A:2412:GLN:O	2:A:2416:ILE:HG13	2.13	0.48
2:A:2426:LEU:HD12	2:A:2426:LEU:N	2.06	0.48
2:A:2683:PRO:HG2	2:A:2684:ASP:H	1.77	0.48
2:A:2413:ASP:OD1	2:A:2523:ARG:NH1	2.45	0.48
2:A:2574:LEU:HG	2:A:2574:LEU:O	2.13	0.48
2:A:2590:ARG:HG2	2:A:2594:LYS:HD3	1.94	0.48
1:B:43:TRP:CH2	2:A:2657:LEU:HD21	2.48	0.48
2:A:2869:PHE:O	2:A:2872:ALA:N	2.41	0.48
2:A:2611:ILE:CG1	2:A:2670:GLN:H	2.26	0.48
2:A:2673:ILE:HD11	2:A:2707:ALA:HB2	1.96	0.48
1:B:51:ASP:HB2	2:A:2708:ARG:HH11	1.77	0.48
2:A:2856:MET:SD	2:A:2856:MET:C	2.91	0.48
2:A:3019:LEU:O	2:A:3054:PRO:CD	2.61	0.48
2:A:2868:GLU:O	2:A:2869:PHE:O	2.31	0.48
2:A:2423:HIS:O	2:A:2424:LEU:HG	2.13	0.48
2:A:2459:LYS:O	2:A:2461:LEU:N	2.47	0.48
2:A:2708:ARG:HD3	2:A:2708:ARG:H	1.79	0.48
2:A:3011:TYR:CD2	2:A:3099:ILE:HD13	2.49	0.48
1:B:10:LEU:C	1:B:12:LEU:N	2.67	0.48
2:A:2742:ILE:CG2	2:A:2895:THR:OG1	2.62	0.48
2:A:2787:PHE:CD1	2:A:2787:PHE:N	2.82	0.48
1:B:59:GLU:OE2	2:A:2453:PRO:HG2	2.14	0.48
2:A:2524:ALA:O	2:A:2526:CYS:N	2.47	0.48
2:A:2696:ARG:HH11	2:A:2696:ARG:HG3	1.79	0.48
2:A:2835:PRO:O	2:A:2837:HIS:N	2.46	0.48
2:A:2915:LEU:HD21	2:A:2954:TYR:OH	2.14	0.48
2:A:3091:TYR:O	2:A:3093:GLU:N	2.47	0.48
2:A:2549:VAL:HG12	2:A:2550:TRP:N	2.29	0.48
2:A:2974:LEU:HD11	2:A:2993:VAL:HB	1.96	0.48
2:A:2861:LYS:HE2	2:A:2861:LYS:HB3	1.71	0.47
2:A:2924:ARG:HB2	2:A:2959:VAL:CG2	2.43	0.47
2:A:3004:ILE:H	2:A:3004:ILE:HG13	1.47	0.47
1:B:59:GLU:C	1:B:61:GLU:N	2.65	0.47
2:A:2474:ASN:N	2:A:2477:ASN:HD21	2.12	0.47
2:A:2489:PHE:HB3	2:A:2493:ASP:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2524:ALA:C	2:A:2526:CYS:H	2.17	0.47
2:A:2545:TYR:O	2:A:2549:VAL:HG23	2.14	0.47
2:A:2861:LYS:C	2:A:2863:ALA:N	2.65	0.47
2:A:2775:PHE:CD2	2:A:2776:ALA:N	2.81	0.47
2:A:2855:GLN:HG3	2:A:2855:GLN:O	2.14	0.47
2:A:2876:ALA:O	2:A:2880:GLU:HG2	2.14	0.47
2:A:3001:VAL:C	2:A:3003:PRO:HD3	2.34	0.47
2:A:2467:SER:OG	2:A:2470:CYS:HB3	2.14	0.47
2:A:2752:VAL:HG12	2:A:2887:THR:HG22	1.96	0.47
2:A:2996:VAL:CG2	2:A:3084:ILE:HD11	2.44	0.47
2:A:3033:LYS:O	2:A:3036:VAL:HG22	2.14	0.47
2:A:2445:GLN:O	2:A:2447:ALA:N	2.48	0.47
2:A:2597:LEU:C	2:A:2599:ARG:H	2.17	0.47
2:A:2745:ARG:NE	2:A:2971:ARG:CG	2.70	0.47
2:A:2936:LYS:HD2	2:A:2944:ILE:HA	1.96	0.47
1:B:55:GLN:O	1:B:57:ARG:N	2.45	0.47
2:A:2399:LYS:HE3	2:A:2399:LYS:HA	1.97	0.47
2:A:3016:CYS:C	2:A:3017:LEU:HD12	2.35	0.47
2:A:2842:PHE:O	2:A:2842:PHE:HD1	1.98	0.47
2:A:2960:SER:O	2:A:2961:SER:C	2.52	0.47
2:A:2462:TYR:CG	2:A:2466:VAL:HG21	2.49	0.47
2:A:2576:GLN:O	2:A:2579:TYR:N	2.48	0.47
2:A:2764:SER:OG	2:A:2767:GLU:HG3	2.14	0.47
2:A:2815:GLN:NE2	2:A:2841:CYS:O	2.46	0.47
2:A:2879:GLU:O	2:A:2881:GLY:N	2.48	0.47
2:A:2902:LYS:O	2:A:2903:SER:C	2.53	0.47
2:A:2905:LEU:HD12	2:A:2905:LEU:HA	1.71	0.47
2:A:3091:TYR:O	2:A:3094:ALA:N	2.47	0.47
2:A:2815:GLN:O	2:A:2819:LEU:HB2	2.14	0.47
2:A:2976:PHE:HE1	2:A:2994:VAL:O	1.98	0.47
1:B:12:LEU:HD21	2:A:2439:LEU:HD22	1.96	0.47
2:A:2445:GLN:HG3	2:A:2450:ASP:OD1	2.14	0.47
2:A:2548:ILE:O	2:A:2552:LEU:HG	2.15	0.47
2:A:2559:PHE:O	2:A:2561:LYS:N	2.48	0.47
2:A:2774:ARG:HD2	2:A:2774:ARG:O	2.14	0.47
2:A:2416:ILE:CG2	2:A:2526:CYS:HB3	2.45	0.46
2:A:2525:LEU:O	2:A:2531:VAL:HG11	2.15	0.46
2:A:2558:ALA:C	2:A:2559:PHE:CD2	2.69	0.46
2:A:2753:GLU:OE1	2:A:2884:ARG:NH2	2.48	0.46
2:A:2861:LYS:O	2:A:2862:GLN:C	2.54	0.46
2:A:2931:ALA:CB	2:A:2947:THR:HB	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:3089:THR:C	2:A:3091:TYR:H	2.19	0.46
2:A:2601:ASP:O	2:A:2602:THR:C	2.53	0.46
2:A:2742:ILE:HG22	2:A:2895:THR:O	2.14	0.46
2:A:3051:SER:O	2:A:3053:VAL:N	2.47	0.46
2:A:2736:VAL:HG11	2:A:2739:VAL:CG1	2.46	0.46
2:A:2936:LYS:NZ	2:A:2944:ILE:HD12	2.30	0.46
2:A:2420:GLU:C	2:A:2422:ARG:H	2.18	0.46
2:A:2838:LEU:HD23	2:A:2838:LEU:C	2.36	0.46
2:A:2944:ILE:HG13	2:A:2945:GLN:H	1.81	0.46
2:A:2569:ASN:C	2:A:2571:GLU:H	2.19	0.46
2:A:2644:ASP:C	2:A:2713:LEU:HD13	2.35	0.46
2:A:2673:ILE:CD1	2:A:2707:ALA:HB2	2.45	0.46
2:A:2526:CYS:SG	2:A:2536:ILE:HD11	2.56	0.46
2:A:2607:LEU:O	2:A:2673:ILE:HA	2.14	0.46
2:A:2597:LEU:HD21	2:A:2649:VAL:HG11	1.97	0.46
2:A:2656:PRO:HG3	2:A:2732:ASP:HB2	1.96	0.46
2:A:2844:GLU:H	2:A:2844:GLU:CD	2.19	0.46
2:A:2901:GLU:OE1	2:A:2901:GLU:C	2.54	0.46
2:A:2931:ALA:HB3	2:A:2947:THR:HB	1.98	0.46
2:A:2520:GLU:O	2:A:2523:ARG:HB2	2.16	0.46
2:A:3039:ALA:CB	2:A:3068:PRO:HG3	2.45	0.46
2:A:2431:LEU:O	2:A:2435:LYS:HG3	2.16	0.46
2:A:2544:HIS:O	2:A:2548:ILE:CG1	2.60	0.46
2:A:2558:ALA:H	2:A:2560:PRO:HD3	1.80	0.46
2:A:2467:SER:HB3	2:A:2470:CYS:SG	2.55	0.45
2:A:2554:ALA:C	2:A:2556:GLU:H	2.19	0.45
2:A:2988:CYS:O	2:A:2989:SER:CB	2.64	0.45
2:A:2480:TYR:O	2:A:2481:PHE:C	2.54	0.45
2:A:2484:ASP:O	2:A:2485:ILE:C	2.54	0.45
2:A:2409:ARG:HH22	2:A:2511:SER:HA	1.78	0.45
2:A:2586:ASP:C	2:A:2586:ASP:OD2	2.53	0.45
2:A:2611:ILE:HG12	2:A:2611:ILE:H	1.36	0.45
2:A:2678:GLU:CG	2:A:2679:LEU:H	2.26	0.45
2:A:2705:ARG:O	2:A:2706:PRO:O	2.33	0.45
2:A:2746:VAL:HG12	2:A:2746:VAL:O	2.16	0.45
2:A:2751:TRP:CG	2:A:2768:GLU:HG2	2.52	0.45
2:A:2993:VAL:HG11	2:A:3056:LEU:HD11	1.98	0.45
2:A:2451:ARG:O	2:A:2451:ARG:HG2	2.16	0.45
2:A:2779:GLN:OE1	2:A:2882:LEU:HD21	2.16	0.45
2:A:3099:ILE:O	2:A:3103:GLU:HG2	2.16	0.45
1:B:42:ASN:O	1:B:43:TRP:C	2.55	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2420:GLU:HB3	2:A:2533:PRO:CG	2.35	0.45
2:A:2576:GLN:O	2:A:2579:TYR:HB3	2.16	0.45
2:A:2892:LEU:HD11	2:A:2919:LEU:CD1	2.47	0.45
2:A:2406:GLN:O	2:A:2410:ASP:N	2.36	0.45
2:A:2420:GLU:CB	2:A:2533:PRO:HG2	2.36	0.45
2:A:2720:ARG:HD3	2:A:2720:ARG:HA	1.84	0.45
2:A:2751:TRP:CZ3	2:A:2765:GLU:HB2	2.52	0.45
2:A:2992:ASP:OD1	2:A:3042:ASN:N	2.43	0.45
2:A:3011:TYR:CE2	2:A:3021:VAL:CG2	3.00	0.45
2:A:2483:PHE:CB	2:A:2516:ALA:HB3	2.42	0.45
2:A:2470:CYS:SG	2:A:2556:GLU:OE2	2.75	0.45
2:A:3020:LEU:HA	2:A:3054:PRO:CD	2.33	0.45
2:A:2731:SER:HB2	2:A:2944:ILE:HD11	1.97	0.45
2:A:2922:GLY:HA3	2:A:2968:TYR:CZ	2.51	0.45
2:A:2998:VAL:HG22	2:A:3011:TYR:CB	2.47	0.45
2:A:3082:HIS:C	2:A:3084:ILE:H	2.20	0.45
2:A:3091:TYR:O	2:A:3092:LYS:C	2.54	0.45
2:A:2558:ALA:C	2:A:2560:PRO:HD3	2.38	0.45
2:A:2699:ILE:HG22	2:A:2700:SER:N	2.32	0.45
2:A:2931:ALA:HB3	2:A:2947:THR:O	2.15	0.45
2:A:2605:LYS:HE3	2:A:2715:PHE:CE1	2.52	0.45
2:A:2726:LEU:CA	2:A:2729:LEU:HG	2.43	0.45
2:A:2409:ARG:HH21	2:A:2511:SER:HA	1.75	0.45
2:A:2692:PRO:C	2:A:2694:SER:H	2.20	0.45
2:A:2701:ALA:O	2:A:2705:ARG:NH1	2.47	0.45
2:A:2738:CYS:SG	2:A:2926:ARG:HG2	2.57	0.45
2:A:2490:GLY:O	2:A:2494:LEU:HD12	2.18	0.44
2:A:2524:ALA:C	2:A:2526:CYS:N	2.71	0.44
2:A:2830:GLN:C	2:A:2832:ALA:N	2.69	0.44
2:A:2783:LEU:HD11	2:A:2880:GLU:N	2.32	0.44
2:A:2951:ARG:HH11	2:A:2951:ARG:HG2	1.82	0.44
2:A:2442:ILE:O	2:A:2443:SER:C	2.56	0.44
2:A:2572:ARG:HA	2:A:2575:LEU:HB2	1.98	0.44
2:A:2967:VAL:HG23	2:A:2968:TYR:H	1.81	0.44
2:A:2687:ALA:C	2:A:2689:LEU:N	2.69	0.44
1:B:52:PHE:CE2	2:A:2706:PRO:O	2.70	0.44
2:A:2644:ASP:O	2:A:2713:LEU:CB	2.65	0.44
2:A:2978:ARG:C	2:A:2980:SER:N	2.71	0.44
2:A:2451:ARG:O	2:A:2451:ARG:CG	2.65	0.44
2:A:2498:LYS:HE3	2:A:2498:LYS:O	2.17	0.44
2:A:2694:SER:OG	2:A:2695:LEU:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2723:PRO:O	2:A:2724:LEU:HB3	2.16	0.44
2:A:2937:SER:O	2:A:2938:LYS:HB2	2.18	0.44
1:B:12:LEU:HD22	2:A:2439:LEU:O	2.17	0.44
2:A:2426:LEU:H	2:A:2426:LEU:CD1	1.97	0.44
2:A:2448:VAL:O	2:A:2450:ASP:N	2.50	0.44
2:A:2524:ALA:O	2:A:2527:ASP:N	2.46	0.44
2:A:2676:GLY:O	2:A:2677:ALA:C	2.55	0.44
2:A:3011:TYR:CE2	2:A:3021:VAL:HG21	2.53	0.44
1:B:56:LEU:C	1:B:57:ARG:HG3	2.37	0.44
2:A:2522:TYR:HE1	2:A:2537:SER:CA	2.31	0.44
2:A:2815:GLN:OE1	2:A:2842:PHE:HD2	2.00	0.44
2:A:2895:THR:HG22	2:A:2903:SER:CB	2.47	0.44
2:A:2898:LYS:NZ	2:A:2898:LYS:HB3	2.31	0.44
2:A:2483:PHE:CD2	2:A:2570:PRO:HB3	2.53	0.44
2:A:2748:PRO:HG3	2:A:3063:ILE:CD1	2.45	0.44
2:A:2766:ARG:NH2	2:A:2769:GLU:HG3	2.33	0.44
2:A:2899:LYS:O	2:A:2900:LYS:C	2.55	0.44
2:A:2967:VAL:HG23	2:A:2968:TYR:N	2.32	0.44
2:A:2742:ILE:HA	2:A:2923:LYS:O	2.17	0.44
2:A:2870:ARG:O	2:A:2871:LYS:C	2.56	0.44
2:A:2783:LEU:HD21	2:A:2880:GLU:HB3	2.00	0.44
2:A:2412:GLN:NE2	2:A:2507:TRP:O	2.51	0.43
2:A:2640:ILE:HD11	2:A:2651:ALA:HB3	1.99	0.43
2:A:2653:LEU:HB3	2:A:2657:LEU:HB3	1.99	0.43
1:B:52:PHE:HE2	2:A:2706:PRO:O	2.01	0.43
2:A:2726:LEU:HD22	2:A:2904:ALA:HB3	2.00	0.43
2:A:2817:HIS:C	2:A:2819:LEU:N	2.72	0.43
2:A:2674:THR:HG21	2:A:2699:ILE:HG13	2.00	0.43
2:A:3077:VAL:O	2:A:3081:LYS:N	2.48	0.43
2:A:2445:GLN:O	2:A:2448:VAL:N	2.51	0.43
2:A:2459:LYS:O	2:A:2460:GLN:C	2.56	0.43
2:A:2474:ASN:CB	2:A:2477:ASN:OD1	2.66	0.43
1:B:52:PHE:O	2:A:2670:GLN:NE2	2.52	0.43
2:A:2816:VAL:O	2:A:2819:LEU:HB3	2.19	0.43
2:A:3041:SER:HB2	2:A:3042:ASN:OD1	2.17	0.43
1:B:43:TRP:CH2	2:A:2704:THR:HB	2.52	0.43
2:A:2884:ARG:HH11	2:A:2884:ARG:CG	2.31	0.43
1:B:54:ASN:CB	2:A:2452:ALA:HB1	2.48	0.43
2:A:2611:ILE:HG13	2:A:2669:GLY:N	2.31	0.43
2:A:2940:GLU:HB2	2:A:2942:PRO:HD2	2.00	0.43
2:A:3028:LEU:HD23	2:A:3028:LEU:HA	1.75	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:ASP:OD1	1:B:57:ARG:NE	2.51	0.43
2:A:2484:ASP:C	2:A:2486:GLN:N	2.71	0.43
2:A:2485:ILE:CG2	2:A:2516:ALA:HB2	2.48	0.43
2:A:2604:ALA:O	2:A:2675:GLN:O	2.37	0.43
2:A:2445:GLN:HE22	2:A:2709:TRP:HE1	1.65	0.43
1:B:56:LEU:O	1:B:56:LEU:CG	2.60	0.43
2:A:2549:VAL:O	2:A:2550:TRP:C	2.55	0.43
2:A:2700:SER:HB3	2:A:2734:GLY:CA	2.49	0.43
2:A:2766:ARG:CZ	2:A:2766:ARG:HA	2.47	0.43
2:A:3020:LEU:O	2:A:3020:LEU:HD23	2.18	0.43
2:A:2448:VAL:HG21	2:A:2559:PHE:CD1	2.52	0.43
2:A:2857:LEU:HD23	2:A:2857:LEU:HA	1.67	0.43
2:A:2858:ASN:C	2:A:2860:LYS:N	2.70	0.43
1:B:13:LEU:HD11	2:A:2444:LEU:CD1	2.48	0.43
2:A:2432:TYR:OH	2:A:2589:ARG:NH2	2.31	0.43
2:A:2448:VAL:HG11	2:A:2559:PHE:CD1	2.53	0.43
2:A:2449:GLY:O	2:A:2450:ASP:CB	2.66	0.43
2:A:2462:TYR:CD1	2:A:2466:VAL:HG11	2.54	0.43
2:A:2517:GLY:N	2:A:2520:GLU:OE1	2.51	0.43
2:A:2708:ARG:H	2:A:2708:ARG:CD	2.32	0.43
2:A:2645:GLY:N	2:A:2713:LEU:HD13	2.34	0.43
2:A:2655:PRO:HB2	2:A:2732:ASP:CB	2.49	0.43
2:A:2727:SER:HA	2:A:2902:LYS:CD	2.49	0.43
2:A:2760:TYR:O	2:A:2761:ILE:HD12	2.19	0.43
2:A:2987:PRO:O	2:A:2989:SER:N	2.52	0.43
2:A:3029:ASN:O	2:A:3030:GLU:HB2	2.19	0.43
2:A:3053:VAL:HG13	2:A:3053:VAL:O	2.19	0.43
2:A:2647:TYR:CD2	2:A:2689:LEU:HD21	2.54	0.42
2:A:3016:CYS:HB3	2:A:3018:ASN:ND2	2.34	0.42
2:A:2860:LYS:HA	2:A:2860:LYS:HD2	1.88	0.42
2:A:2452:ALA:CB	2:A:2453:PRO:CD	2.90	0.42
2:A:2596:ILE:HD11	2:A:2715:PHE:CZ	2.50	0.42
2:A:2596:ILE:HD12	2:A:2602:THR:O	2.19	0.42
2:A:2705:ARG:O	2:A:2706:PRO:C	2.58	0.42
2:A:2717:ARG:O	2:A:2719:PRO:HD3	2.19	0.42
2:A:2892:LEU:CD1	2:A:2919:LEU:HD13	2.49	0.42
1:B:13:LEU:HG	1:B:15:GLU:HG3	2.01	0.42
2:A:2522:TYR:HE1	2:A:2537:SER:HA	1.84	0.42
1:B:51:ASP:CB	2:A:2708:ARG:HG3	2.50	0.42
2:A:3086:ASN:CG	2:A:3087:ILE:N	2.72	0.42
2:A:2745:ARG:HA	2:A:2745:ARG:HD3	1.51	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2864:ARG:HA	2:A:2864:ARG:HD2	1.62	0.42
2:A:2892:LEU:O	2:A:2905:LEU:CD1	2.61	0.42
2:A:2675:GLN:HE21	2:A:2721:PRO:HA	1.85	0.42
2:A:2861:LYS:C	2:A:2863:ALA:H	2.21	0.42
2:A:3000:VAL:CG1	2:A:3001:VAL:N	2.82	0.42
2:A:2742:ILE:HD12	2:A:2923:LYS:C	2.40	0.42
2:A:2893:ARG:HA	2:A:2905:LEU:HD12	2.01	0.42
2:A:2640:ILE:CD1	2:A:2640:ILE:H	2.29	0.42
2:A:2650:ARG:NH1	2:A:2650:ARG:CB	2.69	0.42
2:A:2729:LEU:C	2:A:2730:PHE:HD1	2.23	0.42
2:A:2845:GLU:HA	2:A:2848:ARG:HH21	1.83	0.42
2:A:2865:ILE:O	2:A:2868:GLU:N	2.53	0.42
2:A:2941:ARG:N	2:A:2942:PRO:HD2	2.34	0.42
2:A:2763:ARG:CZ	2:A:2771:GLU:HG2	2.50	0.42
1:B:43:TRP:HZ3	2:A:2701:ALA:HA	1.84	0.42
2:A:2466:VAL:O	2:A:2467:SER:HB2	2.19	0.42
2:A:2873:LEU:HD23	2:A:2873:LEU:C	2.40	0.42
1:B:16:ASP:CG	1:B:57:ARG:HH21	2.20	0.42
2:A:2676:GLY:C	2:A:2677:ALA:O	2.58	0.41
2:A:2420:GLU:C	2:A:2422:ARG:N	2.73	0.41
2:A:2726:LEU:HD12	2:A:2896:SER:OG	2.19	0.41
2:A:2926:ARG:HB3	2:A:2928:TYR:CE2	2.56	0.41
2:A:2587:ASN:O	2:A:2588:SER:C	2.57	0.41
2:A:2941:ARG:N	2:A:2942:PRO:CD	2.83	0.41
2:A:3013:SER:HA	2:A:3018:ASN:O	2.19	0.41
1:B:59:GLU:OE2	2:A:2453:PRO:CG	2.69	0.41
2:A:2674:THR:HG23	2:A:2699:ILE:HG23	2.01	0.41
2:A:2819:LEU:HD21	2:A:2844:GLU:OE2	2.20	0.41
2:A:2864:ARG:O	2:A:2868:GLU:HB2	2.20	0.41
2:A:2976:PHE:HB2	2:A:3014:ASP:OD2	2.19	0.41
2:A:2747:TYR:CD2	2:A:3042:ASN:ND2	2.87	0.41
2:A:2513:ASP:HB3	2:A:2515:LYS:HE3	2.01	0.41
2:A:2679:LEU:CD2	2:A:2697:LEU:HD13	2.50	0.41
2:A:2965:LEU:CD1	2:A:2965:LEU:H	2.33	0.41
2:A:3050:THR:O	2:A:3050:THR:HG22	2.20	0.41
2:A:3051:SER:C	2:A:3053:VAL:N	2.74	0.41
2:A:3015:GLU:N	2:A:3080:LEU:HD13	2.35	0.41
2:A:2605:LYS:HE3	2:A:2715:PHE:CD1	2.56	0.41
2:A:2783:LEU:HD11	2:A:2880:GLU:H	1.84	0.41
1:B:13:LEU:HD11	2:A:2444:LEU:HD12	2.02	0.41
2:A:2481:PHE:O	2:A:2482:GLN:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2647:TYR:HE2	2:A:2689:LEU:HD21	1.84	0.41
2:A:2902:LYS:HE2	2:A:2943:SER:CA	2.46	0.41
2:A:2694:SER:O	2:A:2695:LEU:C	2.59	0.41
2:A:2673:ILE:HG12	2:A:2707:ALA:HB2	2.00	0.41
2:A:2951:ARG:HG2	2:A:2951:ARG:NH1	2.35	0.41
2:A:2534:LYS:HE3	2:A:2534:LYS:HB2	1.91	0.41
2:A:2684:ASP:HB3	2:A:2685:ALA:H	1.58	0.41
2:A:2700:SER:HB3	2:A:2734:GLY:HA3	2.03	0.41
2:A:3011:TYR:CZ	2:A:3021:VAL:HG21	2.55	0.41
1:B:10:LEU:O	1:B:12:LEU:N	2.54	0.41
2:A:2864:ARG:O	2:A:2865:ILE:O	2.38	0.41
2:A:3062:SER:O	2:A:3063:ILE:HD13	2.21	0.41
2:A:2445:GLN:HB3	2:A:2446:ALA:H	1.77	0.41
2:A:2458:PRO:O	2:A:2459:LYS:O	2.38	0.41
2:A:2819:LEU:HG	2:A:2846:GLN:CD	2.40	0.41
2:A:2965:LEU:HD12	2:A:2965:LEU:N	2.36	0.41
2:A:2415:ARG:HH11	2:A:2415:ARG:HD2	1.74	0.40
2:A:2582:ASP:O	2:A:2587:ASN:ND2	2.48	0.40
2:A:2660:LEU:HD22	2:A:2665:LYS:HG2	2.02	0.40
2:A:2927:ILE:HB	2:A:2930:LEU:HD11	2.03	0.40
2:A:3054:PRO:O	2:A:3055:THR:OG1	2.35	0.40
2:A:2445:GLN:O	2:A:2446:ALA:C	2.59	0.40
2:A:2610:CYS:O	2:A:2642:LEU:HA	2.21	0.40
2:A:2751:TRP:HZ3	2:A:2765:GLU:HB2	1.86	0.40
2:A:3042:ASN:O	2:A:3043:LEU:HD23	2.21	0.40
2:A:3091:TYR:CD1	2:A:3092:LYS:N	2.89	0.40
2:A:2522:TYR:CE1	2:A:2538:SER:N	2.89	0.40
2:A:2864:ARG:CG	2:A:2864:ARG:HH11	2.32	0.40
2:A:2912:SER:O	2:A:2914:ASP:N	2.54	0.40
2:A:3014:ASP:C	2:A:3014:ASP:OD1	2.59	0.40
2:A:2993:VAL:O	2:A:3073:PHE:HE2	2.04	0.40
2:A:3087:ILE:C	2:A:3089:THR:N	2.73	0.40
2:A:2778:ALA:O	2:A:2781:LYS:HB2	2.21	0.40
2:A:2423:HIS:CD2	2:A:2423:HIS:O	2.75	0.40
2:A:2471:ILE:C	2:A:2473:VAL:H	2.25	0.40
2:A:2481:PHE:O	2:A:2482:GLN:HB2	2.21	0.40
2:A:2693:ASP:OD1	2:A:2693:ASP:N	2.52	0.40
2:A:2644:ASP:O	2:A:2713:LEU:HB3	2.21	0.40
2:A:2993:VAL:HG23	2:A:2994:VAL:N	2.37	0.40
1:B:9:ASP:CG	1:B:12:LEU:HD12	2.40	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	36/70 (51%)	25 (69%)	7 (19%)	4 (11%)	0 2
2	A	665/738 (90%)	427 (64%)	127 (19%)	111 (17%)	0 0
All	All	701/808 (87%)	452 (64%)	134 (19%)	115 (16%)	0 0

All (115) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	41	ASP
1	B	56	LEU
2	A	2440	PRO
2	A	2451	ARG
2	A	2453	PRO
2	A	2457	SER
2	A	2481	PHE
2	A	2485	ILE
2	A	2564	ALA
2	A	2602	THR
2	A	2677	ALA
2	A	2683	PRO
2	A	2685	ALA
2	A	2688	PRO
2	A	2706	PRO
2	A	2708	ARG
2	A	2711	SER
2	A	2712	ARG
2	A	2724	LEU
2	A	2759	LEU
2	A	2764	SER
2	A	2810	THR
2	A	2835	PRO
2	A	2862	GLN
2	A	2865	ILE

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Mol	Chain	Res	Type
2	A	2869	PHE
2	A	2870	ARG
2	A	2899	LYS
2	A	2901	GLU
2	A	2932	VAL
2	A	2974	LEU
2	A	2984	PHE
2	A	2986	PRO
2	A	2987	PRO
2	A	3007	ALA
2	A	3072	TYR
2	A	3074	GLN
2	A	3076	LYS
1	B	43	TRP
2	A	2446	ALA
2	A	2449	GLY
2	A	2461	LEU
2	A	2588	SER
2	A	2601	ASP
2	A	2668	VAL
2	A	2676	GLY
2	A	2695	LEU
2	A	2701	ALA
2	A	2723	PRO
2	A	2776	ALA
2	A	2836	ASP
2	A	2873	LEU
2	A	2880	GLU
2	A	2933	SER
2	A	2939	PHE
2	A	2965	LEU
2	A	2985	GLN
2	A	2988	CYS
2	A	3006	LEU
2	A	3032	ILE
2	A	3092	LYS
2	A	2400	ASP
2	A	2430	SER
2	A	2444	LEU
2	A	2447	ALA
2	A	2450	ASP
2	A	2452	ALA

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Mol	Chain	Res	Type
2	A	2459	LYS
2	A	2504	ASP
2	A	2513	ASP
2	A	2525	LEU
2	A	2558	ALA
2	A	2591	SER
2	A	2606	THR
2	A	2686	CYS
2	A	2717	ARG
2	A	2793	GLU
2	A	2861	LYS
2	A	2903	SER
2	A	2936	LYS
2	A	2943	SER
2	A	2978	ARG
2	A	3003	PRO
2	A	3071	ALA
2	A	2482	GLN
2	A	2553	ALA
2	A	2693	ASP
2	A	2820	GLN
2	A	2859	ASP
2	A	2982	PRO
2	A	3091	TYR
2	A	2401	LEU
2	A	2439	LEU
2	A	2475	SER
2	A	2598	GLU
2	A	2673	ILE
2	A	2811	LEU
2	A	2866	GLN
2	A	2913	SER
2	A	3029	ASN
2	A	3090	PHE
2	A	2466	VAL
2	A	2560	PRO
2	A	2938	LYS
2	A	3083	ALA
2	A	2570	PRO
2	A	2756	VAL
2	A	2442	ILE
2	A	2448	VAL

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Mol	Chain	Res	Type
2	A	2941	ARG
2	A	3008	PRO
2	A	3052	GLY
1	B	38	VAL
2	A	3026	ILE
2	A	3004	ILE

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	B	36/63 (57%)	32 (89%)	4 (11%)	6 24
2	A	571/649 (88%)	476 (83%)	95 (17%)	2 9
All	All	607/712 (85%)	508 (84%)	99 (16%)	2 10

All (99) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	39	TRP
1	B	41	ASP
1	B	42	ASN
1	B	43	TRP
2	A	2399	LYS
2	A	2400	ASP
2	A	2417	LYS
2	A	2421	ARG
2	A	2431	LEU
2	A	2438	THR
2	A	2440	PRO
2	A	2453	PRO
2	A	2470	CYS
2	A	2474	ASN
2	A	2481	PHE
2	A	2498	LYS
2	A	2501	GLN

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Mol	Chain	Res	Type
2	A	2502	LEU
2	A	2538	SER
2	A	2539	ILE
2	A	2543	ASN
2	A	2559	PHE
2	A	2568	LEU
2	A	2569	ASN
2	A	2572	ARG
2	A	2575	LEU
2	A	2587	ASN
2	A	2611	ILE
2	A	2613	ASP
2	A	2640	ILE
2	A	2650	ARG
2	A	2663	SER
2	A	2665	LYS
2	A	2674	THR
2	A	2693	ASP
2	A	2706	PRO
2	A	2708	ARG
2	A	2711	SER
2	A	2717	ARG
2	A	2720	ARG
2	A	2726	LEU
2	A	2732	ASP
2	A	2741	ILE
2	A	2745	ARG
2	A	2746	VAL
2	A	2751	TRP
2	A	2752	VAL
2	A	2755	THR
2	A	2769	GLU
2	A	2774	ARG
2	A	2783	LEU
2	A	2793	GLU
2	A	2813	ARG
2	A	2815	GLN
2	A	2817	HIS
2	A	2841	CYS
2	A	2842	PHE
2	A	2850	LEU
2	A	2852	ASN

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Mol	Chain	Res	Type
2	A	2856	MET
2	A	2864	ARG
2	A	2868	GLU
2	A	2870	ARG
2	A	2877	GLU
2	A	2882	LEU
2	A	2888	THR
2	A	2889	VAL
2	A	2893	ARG
2	A	2898	LYS
2	A	2899	LYS
2	A	2901	GLU
2	A	2907	SER
2	A	2912	SER
2	A	2915	LEU
2	A	2920	THR
2	A	2923	LYS
2	A	2928	TYR
2	A	2936	LYS
2	A	2946	LEU
2	A	2947	THR
2	A	2954	TYR
2	A	2974	LEU
2	A	2991	VAL
2	A	2993	VAL
2	A	3003	PRO
2	A	3015	GLU
2	A	3016	CYS
2	A	3017	LEU
2	A	3020	LEU
2	A	3031	ASP
2	A	3038	ILE
2	A	3041	SER
2	A	3048	GLU
2	A	3072	TYR
2	A	3079	ASN
2	A	3082	HIS
2	A	3086	ASN
2	A	3098	LEU
2	A	3102	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	2423	HIS
2	A	2486	GLN
2	A	2543	ASN
2	A	2565	ASN
2	A	2569	ASN
2	A	2576	GLN
2	A	2587	ASN
2	A	2670	GLN
2	A	2675	GLN
2	A	2814	GLN
2	A	2855	GLN
2	A	2862	GLN
2	A	2929	HIS
2	A	2956	GLN
2	A	2969	GLN
2	A	3018	ASN
2	A	3044	GLN
2	A	3078	ASN
2	A	3079	ASN
2	A	3086	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

There are no carbohydrates in this entry.

5.6 Ligand geometry

Of 5 ligands modelled in this entry, 5 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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.