



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:23 PM UTC

PDB ID : 1MJE / pdb_00001mje
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

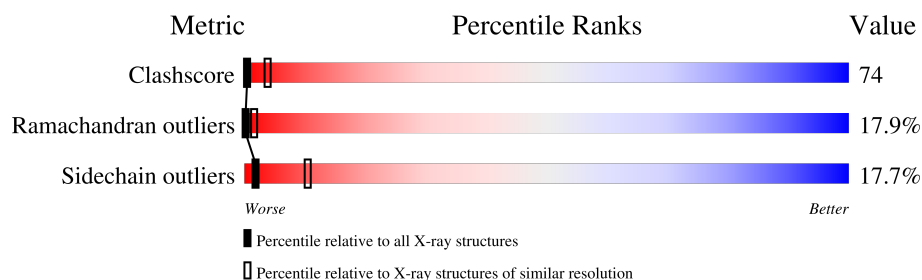
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 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	190562	1140 (3.54-3.46)
Ramachandran outliers	187476	1113 (3.54-3.46)
Sidechain outliers	187428	1114 (3.54-3.46)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	C	6	100%
2	B	70	14% 26% 17% . 40%
3	A	649	17% 45% 25% 5% 8%

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.

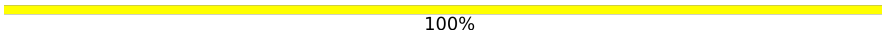
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	A	600	Total	C	N	O	S	0	0	0
			4742	3025	824	877	16			

3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. 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.

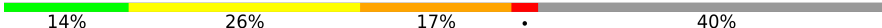
Note EDS was not executed.

- Molecule 1: 5'-D(P*TP*TP*TP*TP*TP*T)-3'

Chain C: 

T501
T502
T503
T504
T505
T506

- Molecule 2: Deleted in split hand/split foot protein 1

Chain B: 

MET SER GLY TYR MET THR SER
P7 V8 D9 L10 G11 G12
E15 D16 D17 E18 F19 E20 E21 E22 P23 A24 E25
ASP TRP ALA GLY LEU ASP ASP ASP ASP ASP
H37 Y38 Y39 F40 D41 N42 W43 D44 D45
ASP ASN VAL GLU D50
S53 N54 Q55 L56 R57 A58 E59 L60 E61 K62

- Molecule 3: breast cancer 2

Chain A: 

ASN GLN LYS THR ASP GLY ARG GLU ASP GLY ASN
K2399 D2400 L2401 K2402 S2403 S2404 L2405 Q2406 S2407 A2408 R2409 D2410 L2411 Q2412 D2413 K2414 R2415 I2416 N2417 N2418 K2419 E2420 R2421
L2424 R2425 L2426 S2430 L2431 Y2432 L2433 T2434 K2435 T2438 L2439 L2502 F2503
D2504 G2505 G2506 W2507 Q2508 L2509 N2510 S2511 N2512 D2513 L2514 A2515 R2516 S2517 R2518 E2519 R2520 F2521 Y2522 Q2523 L2524 A2525 C2526 G2527 V2528 P2529 G2530 V2531 D2532 D2533 K2534 L2535 L2536 S2537 R2538 N2539 V2540 A2541 A2542 N2543 H2544 T2545 R2546 L2547 Q2548 F2549 W2550 K2551 L2552 A2553 R2554 R2555 C2556 F2557 A2558 K2559 P2560 R2561 E2562 F2563
A2564 N2565 R2566 C2567 L2568 N2569 P2570 E2571 R2572 L2573 L2574 L2575 Q2576 L2577 R2578 Y2579 R2580 Y2581 D2582 D2583 E2584 I2585 L2586 R2587 L2588 R2589 R2590 D2600 D2601 T2602 A2603 A2604 T2605 T2606 L2607 V2608 L2609 C2610 I2611 S2612 Q2613 I2614 ILE SER PRO SER THR LYS VAL SER GLU THR
SER GLY GLY LYS THR SER GLY ASP ALA ASN LYS D2637 D2638 T2639 I2640 E2641 L2642 T2643 D2644 D2645 G2646 Y2647 Y2648 A2649 V2649 R2650 A2651 Q2652 L2653 D2654 D2655 P2656 L2657 L2660 S2663 G2664 L2665 T2666 T2667 T2668 G2669 Q2670 K2671 L2672 T2673 T2674 Q2675 G2676 A2677 E2678 L2679 V2680 G2681 S2682 P2683 D2684 A2685 C2686

Y3092	K3093	E3094	A3095	E3096	K3097	K3098	L3099	L3100	H3101	V3102	L3103		D3106	S3107	P3108	K3109	W3110	SER	THR	PRO	ASN																																							
L3028	N3029	E3030	D3031	I3032	K3033	P3034	R3035	V3036	L3037	L3038	A3039	A3040	S3041	N3042	L3043	Q3044	G3045	Q3046	P3047	E3048	S3049	T3050	S3051	G3052	V3053	P3054	L3055	F3056	F3057	A3058	C3059	H3060	S3061	I3062	I3063		S3067		E3070	A3071	V3072	F3073	Q3074	E3075	K3076	V3077	N3078	N3079	L3080	K3081	H3082	A3083	I3084	E3085	N3086	I3087	D3089	T3090	F3091	
E2962	T2963	L2964	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		V2997	V2998	S2999	V3000	V3001	A3002	P3003	I3004	G3005	L3006	A3007	P3008	L3009	V3010	Y3011	L3012	S3013	D3014		L3017	N3018	L3019	L3020	V3021		F3024		
S2896	Y2897	K2898	K2899	K2900	E2901	K2902	A2903	L2904	L2905	L2906	S2907	T2908	W2909	R2910	P2911	S2912	S2913	D2914	L2915		L2919		G2922	K2923	R2924	Y2925	R2926	L2927	Y2928	H2929	L2930	A2931	V2932	S2933	K2934	S2935	K2936	S2937	K2938	F2939	E2940	R2941	P2942		Q2945	L2946	T2947		R2951	T2952	Q2953	Y2954	Q2955	Q2956	L2957	P2958	V2959	S2960	S2961	
P2748	L2749	Q2750	W2751	V2752	E2753	K2754	T2755	V2756	S2757	G2758	L2759	Y2760	I2761	F2762	K2763	S2764	E2765	R2766	E2767	E2768	E2769	K2770	E2771	A2772	L2773	R2774	F2775	A2776		Q2779	Q2780	K2781	K2782	L2783	E2784	A2785	L2786	F2787	T2788	K2789	V2790	L2791	T2792	GLU	GLY	L2882	S2883	R2884	D2885	V2886	T2887	V2888	V2889	W2890	L2742	K2891	L2892	R2893	V2894	T2895
A2687	P2688	L2689	E2690	A2691	P2692	D2693	S2694	L2695	R2696	L2697	K2698	S2700	A2701	N2702	S2703	T2704	R2705	P2706	A2707	R2708	W2709	S2710	S2711	R2712	L2713	G2714	F2715	E2716	R2717		R2720	P2721	F2722	P2723	L2724	P2725	L2726	S2727	S2728	L2729	F2730	S2731	D2732	G2733	N2735	V2736	G2737	C2738	V2739	D2740	L2741	L2742	V2743	Q2744	R2745	V2746	Y2747			

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	0.52	0/132	0.97	0/200
2	B	0.74	0/340	1.24	7/460 (1.5%)
3	A	0.81	3/4843 (0.1%)	1.39	81/6557 (1.2%)
All	All	0.80	3/5315 (0.1%)	1.37	88/7217 (1.2%)

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	11.52	1.70	1.54
3	A	2789	LYS	CG-CD	5.76	1.69	1.52
3	A	3055	THR	CA-CB	-5.17	1.45	1.53

All (88) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2769	GLU	N-CA-C	-12.46	96.61	113.18
3	A	2452	ALA	CA-C-N	11.50	134.21	119.84
3	A	2452	ALA	C-N-CA	11.50	134.21	119.84
3	A	3089	ASP	N-CA-C	-11.48	101.54	114.62
3	A	2768	GLU	N-CA-C	-10.40	97.57	110.88
3	A	3079	ASN	N-CA-C	-9.79	100.69	111.36
3	A	3053	VAL	CA-C-N	9.28	129.22	120.03
3	A	3053	VAL	C-N-CA	9.28	129.22	120.03
3	A	3060	HIS	N-CA-C	-9.13	101.23	111.82
3	A	3005	GLY	N-CA-C	-8.58	92.84	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	2717	ARG	N-CA-C	8.37	121.15	111.11
3	A	2791	HIS	N-CA-C	8.31	125.22	114.75
3	A	2655	PRO	N-CA-C	8.24	120.76	110.70
3	A	2442	ILE	N-CA-C	7.78	119.69	108.48
3	A	2571	GLU	N-CA-C	-7.42	102.80	111.03
3	A	2896	SER	N-CA-C	-7.33	99.91	110.24
3	A	2657	LEU	N-CA-C	-7.25	103.31	111.14
3	A	2741	ILE	CB-CA-C	-7.25	100.10	110.82
3	A	2406	GLN	N-CA-C	-7.16	104.67	113.19
3	A	2993	VAL	N-CA-C	7.08	117.80	107.75
3	A	2779	GLN	N-CA-C	-7.05	103.59	111.28
3	A	2963	THR	N-CA-C	-7.04	103.96	112.54
3	A	2889	VAL	CB-CA-C	-7.02	98.32	111.30
3	A	3053	VAL	N-CA-C	7.01	115.54	109.02
3	A	2439	LEU	N-CA-C	6.97	119.52	109.48
3	A	2926	ARG	N-CA-C	-6.92	97.23	108.52
3	A	2741	ILE	N-CA-C	6.89	118.86	108.80
3	A	2613	ASP	N-CA-C	6.81	119.11	108.96
3	A	2654	ASP	CA-C-N	6.77	127.36	120.38
3	A	2654	ASP	C-N-CA	6.77	127.36	120.38
3	A	3094	GLU	N-CA-C	-6.70	104.05	111.82
3	A	2458	PRO	N-CA-CB	6.66	110.25	103.25
3	A	2411	LEU	N-CA-C	-6.56	105.40	113.41
3	A	2545	TYR	N-CA-C	-6.56	103.82	110.97
3	A	2720	ARG	CA-C-N	6.55	128.02	119.84
3	A	2720	ARG	C-N-CA	6.55	128.02	119.84
3	A	3067	SER	CA-C-N	6.52	127.03	119.99
3	A	3067	SER	C-N-CA	6.52	127.03	119.99
3	A	2908	ILE	CB-CA-C	-6.50	102.20	111.31
2	B	22	PHE	CA-C-N	6.44	127.89	119.84
2	B	22	PHE	C-N-CA	6.44	127.89	119.84
3	A	2478	ALA	N-CA-C	-6.42	106.02	114.31
3	A	3033	LYS	N-CA-C	-6.39	100.32	110.10
3	A	2752	VAL	N-CA-C	6.31	116.94	108.11
2	B	7	PRO	N-CA-CB	6.29	109.92	103.00
3	A	2743	VAL	CB-CA-C	-6.12	105.70	112.68
2	B	12	LEU	N-CA-C	-6.04	105.95	113.38
3	A	2742	ILE	N-CA-C	-6.01	99.47	108.12
3	A	2945	GLN	N-CA-C	5.95	118.22	108.52
3	A	2912	SER	N-CA-C	5.91	117.68	107.93
3	A	2640	ILE	N-CA-C	5.90	117.42	108.80
3	A	3000	VAL	CB-CA-C	-5.88	104.77	111.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	3018	ASN	N-CA-C	-5.87	100.15	109.59
2	B	53	SER	N-CA-C	5.81	118.40	111.71
3	A	2540	TRP	N-CA-C	-5.81	104.78	112.34
3	A	3000	VAL	N-CA-C	5.79	114.69	106.53
2	B	38	VAL	N-CA-C	5.77	121.34	109.34
3	A	2939	PHE	N-CA-C	5.74	120.14	113.20
3	A	2705	ARG	N-CA-C	5.73	113.38	108.22
3	A	2883	SER	N-CA-C	5.71	115.83	108.34
3	A	2559	PHE	CA-C-N	5.68	126.94	119.84
3	A	2559	PHE	C-N-CA	5.68	126.94	119.84
3	A	2722	PHE	CA-C-N	5.47	125.23	119.76
3	A	2722	PHE	C-N-CA	5.47	125.23	119.76
3	A	2705	ARG	CA-C-N	5.46	125.38	119.76
3	A	2705	ARG	C-N-CA	5.46	125.38	119.76
3	A	2542	ALA	N-CA-C	-5.43	105.79	112.90
3	A	3007	ALA	CA-C-N	5.40	125.69	119.92
3	A	3007	ALA	C-N-CA	5.40	125.69	119.92
3	A	2952	THR	N-CA-C	5.33	122.16	110.80
3	A	2693	ASP	N-CA-C	-5.33	106.55	114.64
3	A	2935	SER	N-CA-C	5.32	117.89	111.40
3	A	3106	ASP	N-CA-C	5.26	120.05	111.37
3	A	2787	PHE	N-CA-C	5.25	119.40	112.89
3	A	3091	PHE	N-CA-C	-5.25	104.56	111.96
3	A	2572	ARG	N-CA-C	-5.24	102.77	111.37
3	A	2941	ARG	N-CA-C	5.23	121.36	109.81
3	A	2786	LEU	N-CA-C	-5.21	105.51	111.14
3	A	2979	LEU	N-CA-C	5.18	119.07	112.34
3	A	3038	ILE	N-CA-C	5.17	117.29	108.86
2	B	59	GLU	N-CA-C	-5.14	105.79	111.71
3	A	2410	ASP	N-CA-C	-5.09	106.84	113.16
3	A	2731	SER	N-CA-C	-5.09	105.62	111.07
3	A	3059	CYS	N-CA-C	5.09	117.10	110.53
3	A	3006	LEU	N-CA-C	5.08	121.63	110.80
3	A	2985	GLN	CA-C-N	5.08	125.62	120.38
3	A	2985	GLN	C-N-CA	5.08	125.62	120.38
3	A	2525	LEU	N-CA-C	-5.05	106.22	112.93

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 ⓘ

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	48	0
3	A	4742	0	4783	740	0
All	All	5198	0	5118	766	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 74.

All (766) 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
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:2723:PRO:C	3:A:2724:LEU:HD12	1.90	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:3030:GLU:C	3:A:3032:ILE:H	1.81	0.85
3:A:2653:LEU:HD13	3:A:2657:LEU:HB3	1.58	0.85
3:A:2442:ILE:N	3:A:2442:ILE:HD12	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:HD12	3:A:2444:LEU:H	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
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
3:A:2560:PRO:C	3:A:2562:GLU:H	1.86	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:3028:LEU:C	3:A:3030:GLU:H	1.88	0.81
3:A:2729:LEU:CD2	3:A:2736:VAL:HG22	2.09	0.81
3:A:2773:LEU:HD23	3:A:2773:LEU:C	2.06	0.81
3:A:2742:ILE:HD13	3:A:2923:LYS:O	1.80	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:O	3:A:2768:GLU:CG	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:3081:LYS:HA	3:A:3084:ILE:HD12	1.68	0.76
3:A:3020:LEU:HD23	3:A:3020:LEU:O	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:3089:ASP:C	3:A:3091:PHE:H	1.93	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:2573:VAL:C	3:A:2577:LEU:HD12	2.12	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
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
2:B:12:LEU:C	3:A:2441:ARG:HH21	1.97	0.73
3:A:2650:ARG:H	3:A:2650:ARG:HE	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2608:VAL:C	3:A:2609:LEU:HD23	2.16	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:N	3:A:2462:TYR:CD1	2.60	0.70
3:A:2473:VAL:HA	3:A:2477:ASN:ND2	2.06	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:HG3	3:A:2763:ARG:NH1	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
3:A:2441:ARG:C	3:A:2442:ILE:HD12	2.19	0.68
3:A:2641:GLU:HG2	3:A:2648:ALA:HB1	1.76	0.68
3:A:2787:PHE:C	3:A:2789:LYS:H	1.99	0.68
3:A:2462:TYR:HD1	3:A:2462:TYR:H	1.41	0.68
3:A:2695:LEU:HD23	3:A:2696:ARG:H	1.59	0.68
3:A:3030:GLU:C	3:A:3032:ILE:N	2.50	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:2503:ALA:C	3:A:2505:GLY:H	2.03	0.67
3:A:2987:PRO:C	3:A:2989:SER:H	2.03	0.67
3:A:3057:PHE:CD1	3:A:3057:PHE:C	2.73	0.66
3:A:2749:LEU:CD2	3:A:2750:GLN:N	2.48	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2532:ASP:C	3:A:2534:LYS:H	2.03	0.66
3:A:2976:PHE:HE2	3:A:3020:LEU:HD22	1.59	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: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:2560:PRO:C	3:A:2562:GLU:N	2.55	0.64
3:A:2710:HIS:HD1	3:A:2710:HIS:H	1.43	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:3050:THR:O	3:A:3051:SER:C	2.40	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:2412:GLN:CD	3:A:2509:ILE:HD11	2.23	0.64
3:A:2987:PRO:C	3:A:2988:CYS:SG	2.81	0.64
3:A:3037:LEU:HD11	3:A:3080:LEU:HD23	1.80	0.63
3:A:2523:ARG:C	3:A:2525:LEU:H	2.06	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:3091:PHE:C	3:A:3093:LYS:H	2.07	0.63
3:A:2723:PRO:HG3	3:A:2926:ARG:NH2	2.14	0.62
3:A:3008:PRO:C	3:A:3009:LEU:HD12	2.24	0.62
3:A:2532:ASP:O	3:A:2534:LYS:N	2.31	0.62
3:A:2568:LEU:N	3:A:2568:LEU:HD12	2.14	0.62
3:A:2405:LEU:C	3:A:2407:SER:H	2.05	0.62
3:A:2611:ILE:HG22	3:A:2642:LEU:CD2	2.29	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:2539:ILE:C	3:A:2542:ALA:H	2.08	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:2539:ILE:O	3:A:2542:ALA:N	2.26	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2906:LEU:HA	3:A:2946:LEU:O	1.99	0.61
3:A:2790:VAL:HG12	3:A:2791:HIS:CE1	2.35	0.61
2:B:21:GLU:CD	3:A:2589:ARG:HG2	2.24	0.61
3:A:2596:ILE:C	3:A:2598:GLU:H	2.08	0.61
3:A:2744:GLN:C	3:A:2745:ARG:HD2	2.26	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
1:C:503:DT:O4	3:A:2891:LYS:HE3	2.01	0.60
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
3:A:2444:LEU:H	3:A:2444:LEU:CD1	2.10	0.60
3:A:2503:ALA:O	3:A:2505:GLY:N	2.35	0.60
3:A:2724:LEU:HD12	3:A:2724:LEU:N	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:2756:VAL:HG23	3:A:2757:SER:N	2.14	0.60
3:A:2976:PHE:CE2	3:A:3020:LEU:HD13	2.37	0.60
3:A:2909:TRP:C	3:A:2911:PRO:HD3	2.25	0.60
3:A:2412:GLN:OE1	3:A:2509:ILE:HD11	2.01	0.60
3:A:2892:LEU:HD12	3:A:2892:LEU:N	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:HA	3:A:2547:TRP:CE3	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
2:B:16:ASP:O	2:B:16:ASP:CG	2.44	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
2:B:42:ASN:O	2:B:43:TRP:O	2.21	0.59
3:A:2695:LEU:O	3:A:2696:ARG:HD2	2.02	0.59
3:A:3057:PHE:HE1	3:A:3059:CYS:HA	1.67	0.59
3:A:3089:ASP:C	3:A:3091:PHE:N	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2679:LEU:HD11	3:A:2695:LEU:CD2	2.31	0.59
2:B:16:ASP:O	2:B:16:ASP:OD1	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:2688:PRO:O	3:A:2689:LEU:C	2.46	0.59
3:A:2723:PRO:HG3	3:A:2926:ARG:HH21	1.68	0.59
3:A:2733:GLY:O	3:A:2734:GLY:O	2.21	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: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:2573:VAL:O	3:A:2577:LEU:HD12	2.03	0.58
3:A:2576:GLN:O	3:A:2579:TYR:HB3	2.04	0.58
3:A:2611:ILE:CD1	3:A:2667:THR:O	2.48	0.58
2:B:22:PHE:O	2:B:24:ALA:N	2.37	0.58
3:A:2432:TYR:C	3:A:2432:TYR:CD2	2.82	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:OE2	3:A:2690:GLU:HA	2.03	0.57
3:A:2779:GLN:HA	3:A:2779:GLN:NE2	2.18	0.57
3:A:2745:ARG:HG2	3:A:2745:ARG:HH11	1.69	0.57
3:A:2765:GLU:C	3:A:2767:GLU:H	2.11	0.57
3:A:2898:LYS:O	3:A:2899:LYS:HB3	2.03	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:HG2	3:A:2717:ARG:HH11	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: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:2578:LYS:O	3:A:2579:TYR:C	2.48	0.57
3:A:2935:SER:HB3	3:A:2941:ARG:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2412:GLN:CA	3:A:2415:ARG:HH21	2.10	0.57
3:A:2596:ILE:HD11	3:A:2603:ALA:C	2.29	0.57
3:A:2552:LEU:O	3:A:2553:ALA:C	2.47	0.57
3:A:2552:LEU:O	3:A:2555:MET:HB2	2.04	0.57
3:A:2601:ASP:O	3:A:2602:THR:C	2.48	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:3028:LEU:C	3:A:3030:GLU:N	2.52	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: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:3099:LEU:O	3:A:3100:ILE:C	2.47	0.56
3:A:2485:ILE:HG21	3:A:2510:PRO:HB3	1.87	0.56
3:A:2988:CYS:O	3:A:2989:SER:HB2	2.05	0.56
3:A:2598:GLU:O	3:A:2599:ARG:C	2.48	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:2523:ARG:C	3:A:2525:LEU:N	2.63	0.56
3:A:2994:VAL:HG21	3:A:3077:VAL:HG23	1.88	0.56
2:B:10:LEU:N	2:B:10:LEU:HD12	2.20	0.56
3:A:2517:GLY:H	3:A:2520:GLU:CD	2.14	0.56
3:A:3055:THR:O	3:A:3056:LEU:HD23	2.05	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:2467:SER:C	3:A:2469:GLU:H	2.14	0.56
3:A:2749:LEU:C	3:A:2750:GLN:HG2	2.31	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2764:SER:HB3	3:A:2767:GLU:OE1	2.05	0.55
3:A:2446:ALA:C	3:A:2448:VAL:H	2.14	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
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
2:B:55:GLN:NE2	3:A:2671:LYS:HD2	2.21	0.55
3:A:2417:LYS:CA	3:A:2420:GLU:HG2	2.37	0.55
3:A:2405:LEU:C	3:A:2407:SER:N	2.63	0.54
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:2449:GLY:O	3:A:2450:ASP:C	2.50	0.54
3:A:2501:GLN:HB2	3:A:2507:TRP:CH2	2.42	0.54
3:A:2596:ILE:C	3:A:2598:GLU:N	2.64	0.54
3:A:2968:TYR:CG	3:A:2969:GLN:N	2.70	0.54
3:A:2750:GLN:OE1	3:A:2762:PHE:HD1	1.90	0.54
3:A:3019:LEU:N	3:A:3019:LEU:CD2	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
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:2964:LEU:C	3:A:2966:GLN:H	2.15	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: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
3:A:2787:PHE:C	3:A:2789:LYS:N	2.67	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
2:B:56:LEU:CG	2:B:57:ARG:N	2.71	0.53
3:A:2909:TRP:O	3:A:2910:ARG:C	2.52	0.53
3:A:3020:LEU:HD23	3:A:3020:LEU:C	2.32	0.53
3:A:2974:LEU:HD23	3:A:2974:LEU:C	2.32	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2444:LEU:HD12	3:A:2444:LEU:N	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:3057:PHE:CE1	3:A:3058:ALA:C	2.87	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:2571:GLU:O	3:A:2572:ARG:C	2.52	0.53
3:A:2682:SER:C	3:A:2684:ASP:H	2.17	0.53
3:A:2922:GLY:CA	3:A:2968:TYR:CE1	2.92	0.53
3:A:3020:LEU:N	3:A:3020:LEU:CD2	2.71	0.53
3:A:2598:GLU:O	3:A:2600:ASP:N	2.42	0.52
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:2431:LEU:O	3:A:2432:TYR:C	2.51	0.52
3:A:2736:VAL:HG11	3:A:2739:VAL:CG1	2.39	0.52
3:A:3093:LYS:O	3:A:3093:LYS:HD3	2.09	0.52
3:A:2578:LYS:O	3:A:2581:TYR:HB3	2.10	0.52
3:A:2710:HIS:ND1	3:A:2710:HIS:N	2.55	0.52
3:A:2986:PRO:HB2	3:A:2987:PRO:CD	2.39	0.52
3:A:3086:ASN:OD1	3:A:3087:ILE:HD11	2.09	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
1:C:501:DT:H5'	1:C:501:DT:C6	2.45	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:2783:LEU:O	3:A:2784:GLU:C	2.53	0.52
3:A:2883:SER:OG	3:A:2884:ARG:N	2.40	0.52
3:A:2987:PRO:C	3:A:2989:SER:N	2.68	0.52
3:A:3034:PRO:C	3:A:3035:ARG:HG3	2.35	0.52
3:A:3075:GLU:O	3:A:3079:ASN:HB2	2.09	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:2544:HIS:O	3:A:2548:ILE:HG13	2.10	0.51
3:A:3008:PRO:HG2	3:A:3024:PHE:HB2	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2557:PHE:C	3:A:2559:PHE:H	2.19	0.51
3:A:3077:VAL:O	3:A:3080:LEU:HB3	2.10	0.51
3:A:3089:ASP:HA	3:A:3092:TYR:CD1	2.45	0.51
3:A:2728:SER:O	3:A:2729:LEU:HB2	2.11	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:2470:CYS:O	3:A:2471:ILE:C	2.54	0.51
3:A:2559:PHE:O	3:A:2563:PHE:HB2	2.11	0.51
3:A:3074:GLN:O	3:A:3078:ASN:ND2	2.44	0.51
3:A:3085:GLU:O	3:A:3086:ASN:C	2.54	0.51
2:B:10:LEU:HD21	3:A:2566:ARG:NE	2.26	0.50
3:A:2573:VAL:C	3:A:2575:LEU:N	2.67	0.50
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
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:OD1	3:A:2735:ASN:N	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:2554:ALA:O	3:A:2555:MET:C	2.54	0.50
3:A:2675:GLN:O	3:A:2676:GLY:C	2.54	0.50
3:A:2729:LEU:HD22	3:A:2736:VAL:HG22	1.93	0.50
2:B:17:ASP:OD1	2:B:17:ASP:C	2.54	0.50
3:A:2503:ALA:C	3:A:2505:GLY:N	2.70	0.50
3:A:2561:LYS:O	3:A:2561:LYS:HG2	2.12	0.50
3:A:2936:LYS:HG3	3:A:2936:LYS:O	2.11	0.50
3:A:2976:PHE:O	3:A:2977:SER:C	2.55	0.50
3:A:2769:GLU:C	3:A:2772:ALA:HB3	2.36	0.50
3:A:3014:ASP:CG	3:A:3018:ASN:HD22	2.18	0.50
2:B:43:TRP:CH2	3:A:2705:ARG:HA	2.46	0.50
3:A:2408:ALA:CA	3:A:2411:LEU:HB3	2.37	0.50
3:A:2755:THR:O	3:A:2756:VAL:C	2.54	0.50
3:A:2893:ARG:NH1	3:A:2905:LEU:HD13	2.26	0.50
3:A:2906:LEU:HD12	3:A:2946:LEU:C	2.36	0.50
3:A:2551:LYS:CG	3:A:2552:LEU:N	2.72	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2465:GLY:O	3:A:2466:VAL:C	2.55	0.50
3:A:2702:ASN:CG	3:A:2729:LEU:HD23	2.37	0.50
3:A:2724:LEU:N	3:A:2724:LEU:CD1	2.74	0.50
3:A:2738:CYS:SG	3:A:2739:VAL:N	2.83	0.50
3:A:3096:GLU:O	3:A:3097:LYS:C	2.54	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:2937:SER:O	3:A:2938:LYS:C	2.55	0.49
1:C:502:DT:O4	3:A:2947:THR:HG23	2.12	0.49
3:A:2443:SER:O	3:A:2444:LEU:C	2.54	0.49
3:A:2484:ASP:O	3:A:2486:GLN:N	2.45	0.49
3:A:2539:ILE:C	3:A:2541:VAL:N	2.68	0.49
3:A:2736:VAL:HG12	3:A:2738:CYS:H	1.77	0.49
3:A:2952:THR:HG22	3:A:2953:GLN:N	2.26	0.49
3:A:2400:ASP:CG	3:A:2401:LEU:H	2.19	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:2939:PHE:C	3:A:2940:GLU:HG3	2.38	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
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: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: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:3078:ASN:HD22	3:A:3078:ASN:C	2.20	0.48
3:A:2519:GLU:O	3:A:2520:GLU:C	2.56	0.48
3:A:2773:LEU:C	3:A:2773:LEU:CD2	2.77	0.48
3:A:2582:ASP:C	3:A:2586:ASP:HB2	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2955:GLN:CG	3:A:2957:LEU:HD21	2.42	0.48
3:A:2452:ALA:HB1	3:A:2453:PRO:HD2	1.94	0.48
3:A:2484:ASP:C	3:A:2486:GLN:H	2.21	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:2638:ASP:O	3:A:2639:THR:HG23	2.13	0.48
3:A:2764:SER:OG	3:A:2765:GLU:N	2.45	0.48
3:A:2790:VAL:O	3:A:2790:VAL:CG1	2.62	0.48
3:A:3009:LEU:HD12	3:A:3009:LEU:N	2.29	0.48
3:A:2483:PHE:CD2	3:A:2570:PRO:HG3	2.48	0.48
3:A:2529:PRO:C	3:A:2531:VAL:H	2.22	0.48
3:A:2789:LYS:C	3:A:2791:HIS:H	2.21	0.48
2:B:56:LEU:CD2	2:B:57:ARG:N	2.60	0.48
3:A:2481:PHE:HD2	3:A:2545:TYR:OH	1.97	0.48
3:A:2399:LYS:N	3:A:2494:LEU:HD21	2.28	0.48
3:A:2471:ILE:C	3:A:2473:VAL:H	2.21	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
2:B:42:ASN:C	2:B:43:TRP:O	2.55	0.47
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
1:C:503:DT:H2"	1:C:504:DT:H5"	1.96	0.47
3:A:2689:LEU:O	3:A:2690:GLU:HG2	2.14	0.47
2:B:10:LEU:CD1	3:A:2566:ARG:NH2	2.67	0.47
3:A:2446:ALA:C	3:A:2448:VAL:N	2.72	0.47
2:B:41:ASP:O	3:A:2705:ARG:NE	2.47	0.47
1:C:505:DT:H72	3:A:2939:PHE:CZ	2.49	0.47
2:B:8:VAL:HG12	2:B:9:ASP:O	2.13	0.47
2:B:43:TRP:O	2:B:44:ASP:C	2.58	0.47
2:B:60:LEU:CD2	3:A:2473:VAL:O	2.62	0.47
3:A:2681:GLY:HA3	3:A:2695:LEU:CA	2.31	0.47
3:A:2789:LYS:C	3:A:2791:HIS:N	2.73	0.47
3:A:3099:LEU:O	3:A:3103:LEU:HB2	2.15	0.47
3:A:2485:ILE:HA	3:A:2489:PHE:CE1	2.49	0.47
3:A:2717:ARG:HG2	3:A:2717:ARG:NH1	2.28	0.47
3:A:2742:ILE:HG22	3:A:2895:THR:HG1	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2455:ALA:HB1	3:A:2557:PHE:HE2	1.80	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: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
2:B:15:GLU:HB2	2:B:18:GLU:HG2	1.96	0.47
3:A:2593:LEU:O	3:A:2594:LYS:C	2.57	0.47
3:A:3013:SER:HB2	3:A:3019:LEU:HD13	1.97	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:2771:GLU:O	3:A:2772:ALA:C	2.56	0.47
3:A:2927:ILE:CG2	3:A:2930:LEU:HD11	2.45	0.47
3:A:3009:LEU:N	3:A:3009:LEU:CD1	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: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:2579:TYR:O	3:A:2580:ARG:C	2.59	0.46
3:A:2457:SER:O	3:A:2458:PRO:CB	2.64	0.46
3:A:2756:VAL:CG2	3:A:2757:SER:N	2.77	0.46
3:A:2766:ARG:O	3:A:2766:ARG:HG3	2.15	0.46
3:A:2541:VAL:HG12	3:A:2541:VAL:O	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: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:2736:VAL:O	3:A:2737:GLY:C	2.58	0.46
3:A:2750:GLN:OE1	3:A:2762:PHE:CD1	2.68	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:2548:ILE:O	3:A:2549:VAL:C	2.58	0.46
3:A:2555:MET:HA	3:A:2555:MET:CE	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2573:VAL:O	3:A:2574:LEU:C	2.59	0.46
3:A:2593:LEU:O	3:A:2596:ILE:HG22	2.15	0.46
3:A:2573:VAL:HG12	3:A:2577:LEU:HD12	1.95	0.45
3:A:2578:LYS:NZ	3:A:2582:ASP:OD2	2.48	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:NH1	3:A:2421:ARG:HB3	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:3080:LEU:O	3:A:3084:ILE:HG13	2.16	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:3048:GLU:N	3:A:3048:GLU:CD	2.75	0.45
3:A:3089:ASP:C	3:A:3089:ASP:OD1	2.59	0.45
3:A:2446:ALA:O	3:A:2448:VAL:N	2.50	0.45
3:A:2576:GLN:O	3:A:2577:LEU:C	2.59	0.45
3:A:2668:VAL:HG12	3:A:2669:GLY:N	2.30	0.45
3:A:2732:ASP:OD1	3:A:2732:ASP:N	2.47	0.45
3:A:2768:GLU:CD	3:A:2884:ARG:HH22	2.24	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:2467:SER:C	3:A:2469:GLU:N	2.74	0.45
3:A:2569:ASN:C	3:A:2571:GLU:N	2.74	0.45
3:A:3017:LEU:HD11	3:A:3091:PHE:CE1	2.52	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:3074:GLN:O	3:A:3075:GLU:C	2.60	0.45
3:A:2929:HIS:C	3:A:2930:LEU:HD23	2.41	0.45
3:A:2684:ASP:O	3:A:2686:CYS:N	2.50	0.45
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:3030:GLU:O	3:A:3032:ILE:HG13	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2746:VAL:CG2	3:A:2892:LEU:HD23	2.48	0.44
3:A:2776:ALA:O	3:A:2780:GLN:HB2	2.18	0.44
3:A:2946:LEU:HD12	3:A:2946:LEU:HA	1.70	0.44
3:A:3024:PHE:HA	3:A:3058:ALA:HB3	1.98	0.44
2:B:59:GLU:HG3	3:A:2453:PRO:HB3	1.99	0.44
3:A:2426:LEU:HD12	3:A:2426:LEU:H	1.83	0.44
3:A:2613:ASP:CG	3:A:2614:ILE:H	2.25	0.44
3:A:2697:LEU:HD12	3:A:2697:LEU:HA	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:2736:VAL:C	3:A:2738:CYS:N	2.76	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: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
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:OE1	3:A:3030:GLU:HA	2.16	0.44
3:A:2470:CYS:O	3:A:2473:VAL:HG12	2.17	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:HH11	3:A:2409:ARG:CB	2.30	0.44
3:A:2448:VAL:HG12	3:A:2448:VAL:O	2.17	0.44
2:B:57:ARG:CG	3:A:2550:TRP:CE2	3.01	0.43
3:A:2593:LEU:O	3:A:2596:ILE:N	2.43	0.43
3:A:3078:ASN:HA	3:A:3081:LYS:CB	2.46	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:2611:ILE:HD11	3:A:2667:THR:C	2.38	0.43
3:A:2687:ALA:C	3:A:2688:PRO:O	2.60	0.43
3:A:2710:HIS:O	3:A:2711:SER:CB	2.59	0.43
3:A:2532:ASP:C	3:A:2532:ASP:OD1	2.59	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2964:LEU:C	3:A:2966:GLN:N	2.76	0.43
3:A:2518:LYS:HE3	3:A:2542:ALA:HB2	2.00	0.43
3:A:2593:LEU:HD13	3:A:2649:VAL:HG13	2.00	0.43
3:A:2594:LYS:HB2	3:A:2647:TYR:CD1	2.53	0.43
3:A:2981:ASP:OD1	3:A:2982:PRO:HD2	2.18	0.43
2:B:19:PHE:HE2	3:A:2646:TRP:CE2	2.37	0.43
3:A:2525:LEU:O	3:A:2531:VAL:HG11	2.19	0.43
3:A:2564:ALA:C	3:A:2566:ARG:H	2.27	0.43
3:A:3020:LEU:HA	3:A:3053:VAL:CG2	2.48	0.43
3:A:2443:SER:C	3:A:2445:GLN:N	2.71	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:2897:TYR:CD2	3:A:2897:TYR:C	2.97	0.43
3:A:2941:ARG:HB2	3:A:2942:PRO:HD3	2.01	0.43
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:2701:ALA:C	3:A:2703:SER:H	2.26	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
1:C:506:DT:O5'	3:A:3007:ALA:HB3	2.19	0.42
3:A:2473:VAL:HG11	3:A:2553:ALA:CB	2.49	0.42
3:A:2532:ASP:C	3:A:2534:LYS:N	2.72	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
3:A:2517:GLY:O	3:A:2518:LYS:C	2.62	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: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
1:C:505:DT:C6	3:A:3057:PHE:HE2	2.34	0.42
3:A:2773:LEU:O	3:A:2774:ARG:C	2.61	0.42
3:A:2509:ILE:O	3:A:2510:PRO:C	2.62	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:2449:GLY:C	3:A:2451:ARG:N	2.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2461:LEU:CB	3:A:2464:TYR:HE2	2.32	0.42
3:A:2508:LEU:C	3:A:2510:PRO:HD3	2.44	0.42
3:A:2539:ILE:HG13	3:A:2540:TRP:N	2.34	0.42
3:A:2555:MET:HA	3:A:2555:MET:HE2	2.00	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
2:B:9:ASP:OD2	2:B:12:LEU:N	2.47	0.42
2:B:62:LYS:O	3:A:2457:SER:HA	2.20	0.42
3:A:2442:ILE:HG21	3:A:2447:ALA:HB2	2.01	0.42
3:A:2522:TYR:HE1	3:A:2536:ILE:CG1	2.33	0.42
3:A:2582:ASP:HA	3:A:2586:ASP:CG	2.45	0.42
3:A:2736:VAL:HG23	3:A:2932:VAL:HG21	2.02	0.42
2:B:55:GLN:NE2	3:A:2671:LYS:H	2.18	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: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
3:A:2571:GLU:CG	3:A:2572:ARG:H	2.28	0.42
3:A:2765:GLU:C	3:A:2767:GLU:N	2.78	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:2611:ILE:CD1	3:A:2667:THR:C	2.92	0.42
3:A:2912:SER:O	3:A:2913:SER:C	2.62	0.42
2:B:58:ALA:C	2:B:60:LEU:N	2.76	0.41
3:A:3017:LEU:N	3:A:3017:LEU:HD12	2.35	0.41
2:B:11:GLY:O	3:A:2435:LYS:HE2	2.20	0.41
3:A:2473:VAL:HG11	3:A:2553:ALA:HB1	2.02	0.41
3:A:2584:GLU:OE2	3:A:2647:TYR:OH	2.36	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:HG2	3:A:2745:ARG:NH1	2.35	0.41
3:A:2433:LEU:O	3:A:2434:THR:C	2.63	0.41
3:A:2611:ILE:HD13	3:A:2666:LEU:CD2	2.46	0.41
3:A:2783:LEU:O	3:A:2786:LEU:N	2.53	0.41
2:B:20:GLU:O	2:B:21:GLU:C	2.63	0.41
2:B:43:TRP:CZ2	3:A:2706:PRO:HD3	2.55	0.41
3:A:2642:LEU:O	3:A:2648:ALA:HA	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2941:ARG:HB2	3:A:2942:PRO:CD	2.50	0.41
3:A:3045:CYS:C	3:A:3046:GLN:HG2	2.45	0.41
1:C:506:DT:O5'	3:A:3007:ALA:CB	2.69	0.41
3:A:2509:ILE:O	3:A:2509:ILE:HG22	2.19	0.41
3:A:3086:ASN:CG	3:A:3087:ILE:HG13	2.45	0.41
3:A:2505:GLY:O	3:A:2506:GLY:O	2.38	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:2915:LEU:HD23	3:A:2915:LEU:C	2.46	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:2552:LEU:HG	3:A:2552:LEU:H	1.35	0.41
3:A:2573:VAL:C	3:A:2575:LEU:H	2.29	0.41
3:A:2597:LEU:HD23	3:A:2597:LEU:HA	1.82	0.41
3:A:2657:LEU:O	3:A:2660:LEU:HB2	2.21	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
2:B:57:ARG:HE	2:B:57:ARG:HB2	1.40	0.41
3:A:2430:SER:O	3:A:2431:LEU:C	2.63	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
3:A:2960:SER:O	3:A:2962:GLU:N	2.54	0.41
3:A:2688:PRO:O	3:A:2689:LEU:O	2.39	0.40
3:A:3086:ASN:OD1	3:A:3087:ILE:CD1	2.69	0.40
2:B:56:LEU:HD23	2:B:57:ARG:HB2	2.03	0.40
2:B:56:LEU:O	2:B:58:ALA:N	2.54	0.40
3:A:2740:ASP:OD2	3:A:2740:ASP:C	2.64	0.40
3:A:2924:ARG:HD2	3:A:2959:VAL:HG22	2.02	0.40
3:A:2434:THR:HG22	3:A:2435:LYS:N	2.36	0.40
3:A:2474:ASN:O	3:A:2475:SER:C	2.64	0.40
3:A:2674:THR:CG2	3:A:2704:THR:CG2	2.99	0.40
3:A:2510:PRO:O	3:A:2511:SER:C	2.65	0.40
3:A:2531:VAL:O	3:A:2533:PRO:HD2	2.21	0.40
3:A:2650:ARG:NH2	3:A:2695:LEU:C	2.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:2964:LEU:HB3	3:A:2965:LEU:H	1.77	0.40
3:A:3098:LYS:O	3:A:3099:LEU:C	2.64	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 [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	
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	1
All	All	630/719 (88%)	395 (63%)	122 (19%)	113 (18%)	0	1

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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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%)	26 (79%)	7 (21%)	1	6
3	A	521/572 (91%)	430 (82%)	91 (18%)	2	11
All	All	554/635 (87%)	456 (82%)	98 (18%)	2	10

All (98) 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	53	SER
2	B	56	LEU
2	B	57	ARG
3	A	2404	SER

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Mol	Chain	Res	Type
3	A	2410	ASP
3	A	2434	THR
3	A	2439	LEU
3	A	2442	ILE
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	2540	TRP
3	A	2543	ASN
3	A	2555	MET
3	A	2565	ASN
3	A	2568	LEU
3	A	2572	ARG
3	A	2577	LEU
3	A	2583	VAL
3	A	2606	THR
3	A	2607	LEU
3	A	2643	THR
3	A	2649	VAL
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	2706	PRO
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	2738	CYS
3	A	2740	ASP
3	A	2741	ILE
3	A	2742	ILE

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Mol	Chain	Res	Type
3	A	2744	GLN
3	A	2746	VAL
3	A	2749	LEU
3	A	2773	LEU
3	A	2779	GLN
3	A	2780	GLN
3	A	2786	LEU
3	A	2789	LYS
3	A	2790	VAL
3	A	2792	THR
3	A	2886	VAL
3	A	2887	THR
3	A	2889	VAL
3	A	2892	LEU
3	A	2893	ARG
3	A	2901	GLU
3	A	2903	SER
3	A	2906	LEU
3	A	2907	SER
3	A	2919	LEU
3	A	2933	SER
3	A	2946	LEU
3	A	2947	THR
3	A	2951	ARG
3	A	2969	GLN
3	A	2991	VAL
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
3	A	3036	VAL
3	A	3041	SER
3	A	3045	CYS
3	A	3047	PRO
3	A	3048	GLU
3	A	3055	THR
3	A	3074	GLN
3	A	3077	VAL
3	A	3078	ASN

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Mol	Chain	Res	Type
3	A	3087	ILE
3	A	3089	ASP
3	A	3093	LYS
3	A	3097	LYS
3	A	3099	LEU
3	A	3103	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	55	GLN
3	A	2482	GLN
3	A	2486	GLN
3	A	2675	GLN
3	A	2779	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 [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers

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.