



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 04:43 AM UTC

PDB ID : 1MIU / pdb_00001miu
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 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

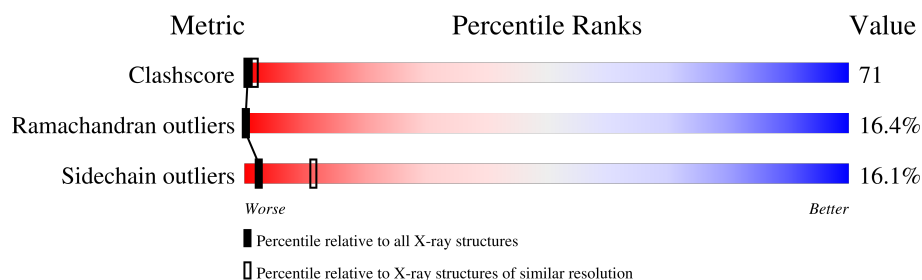
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 Å.

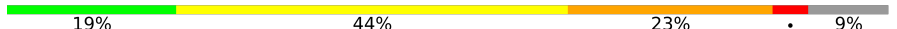
Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (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 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	B	70	
2	A	738	

2 Entry composition

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
1	B	42	Total	C	N	O	0	0	0
			348	217	53	78			

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

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

- Molecule 3 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

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

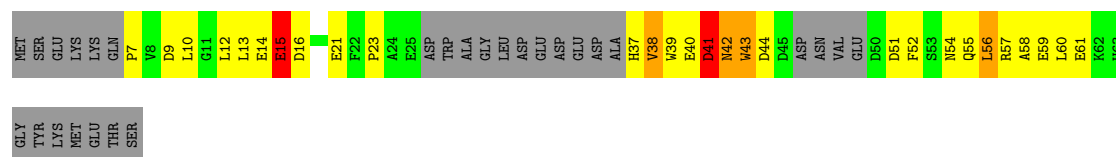
3 Residue-property plots

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.

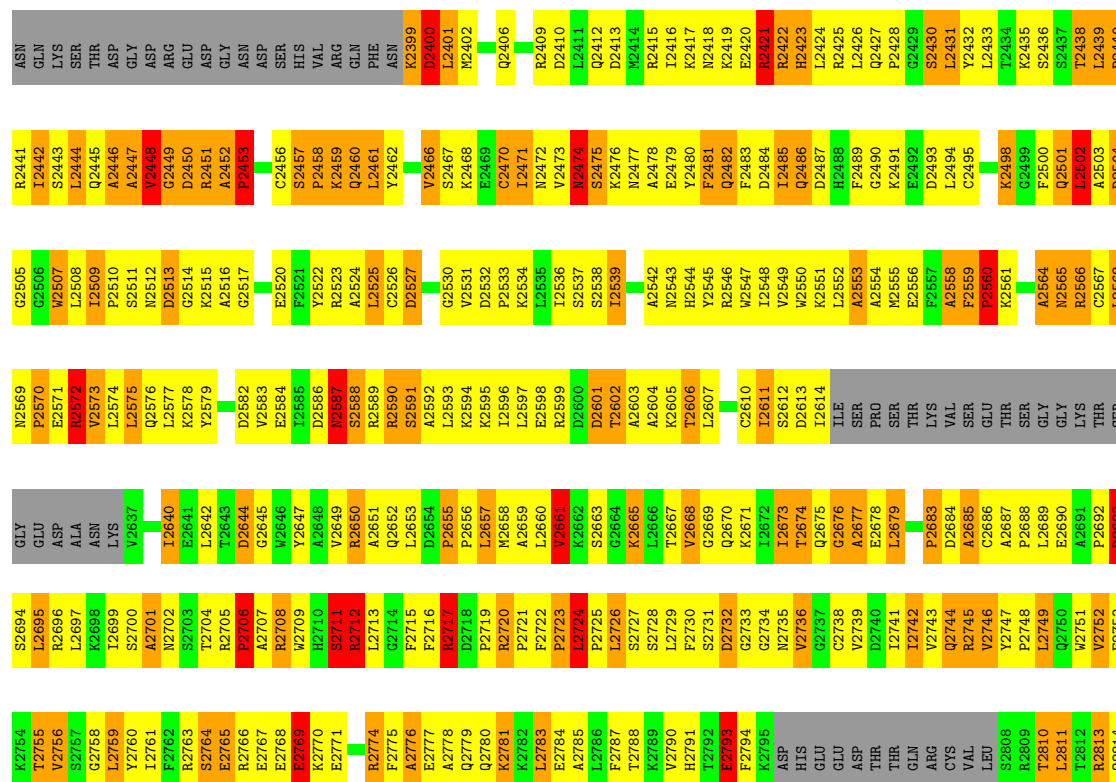
- Molecule 1: Deleted in split hand/split foot protein 1

Chain B: 



- Molecule 2: Breast Cancer type 2 susceptibility protein

Chain A: 



L3080	K3081	H3082	A3083	L3084	E3085	N3086	I3087	D3088	T3089	F3090	Y3091	K3092	E3093	A3094	E3095	K3096	K3097	L3098	I3099	L3102	E3103	GLY	ASP	SER	PRO	LYS	TRP	SER	THR	PRO	ASN	LYS	ASP																															
G3005	L3006	A3007	P3008	Y3011	L3012	S3013	D3014	E3015	L3016	T3017	K3018	L3019	L3020	V3021	F3024	G3025	I3026	D3027	L3028	N3029	E3030	D3031	I3032	K3033	P3034	R3035	V3036	L3037	I3038	A3039	S3041	N3042	L3043																															
S2937	K2938	F2939	E2940	R2941	P2942	S2943	I2944	Q2945	L2946	T2947	R2951	L2952	Q2953	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									
S2875	A2876	E2877	K2878	E2879	E2880	G2881	L2882	S2883	R2884	D2885	V2886	T2887	T2888	V2889	W2890	K2891	L2892	R2893	V2894	T2895	S2896	Y2897	K2898	K2899	K2900	E2901	K2902	F2842	S2843	A2904	L2905	L2906	S2907	L2847	R2848	A2849	R2910	L2850	P2851	S2852	Y2853	R2854	Q2855	K2856	L2857	W2858	D2859	E2921	D2859	K2860	K2861	Q2862	A2863	R2864	L2865	Q2866	S2867	E2868	F2869	R2870	K2871	A2872	L2873	E2874
Q2815	V2816	E2817	A2818	L2819	Q2820	D2821	G2822	A2823	E2824	L2825	Y2826	A2827	L2828	V2829	Q2830	Y2831	A2832	S2833	D2834	P2835	D2836	Y2837	L2838	E2839	A2840	G2841	F2842	S2843	A2844	E2845	Q2846	L2847	R2848	A2849	R2910	L2850	P2851	S2852	Y2853	R2854	Q2855	K2856	L2857	W2858	D2859	E2921	D2859	K2860	K2861	Q2862	A2863	R2864	L2865	Q2866	S2867	E2868	F2869	R2870	K2871	A2872	L2873	E2874		

4 Data and refinement statistics

Xtrriage (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.	Xtrriage
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	0.66	0/354	1.16	3/478 (0.6%)
2	A	0.74	6/5399 (0.1%)	1.29	78/7303 (1.1%)
All	All	0.74	6/5753 (0.1%)	1.28	81/7781 (1.0%)

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	6.30	1.41	1.32
2	A	2472	ASN	CG-OD1	6.15	1.35	1.23
2	A	2712	ARG	CZ-NH2	5.82	1.41	1.33
2	A	2978	ARG	NE-CZ	5.66	1.39	1.33
2	A	2978	ARG	CZ-NH1	5.27	1.40	1.32
2	A	2978	ARG	CZ-NH2	5.10	1.40	1.33

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2844	GLU	N-CA-C	11.50	118.21	108.78
2	A	2422	ARG	N-CA-C	10.70	122.83	108.07
2	A	2724	LEU	CA-C-N	8.88	129.58	119.99
2	A	2724	LEU	C-N-CA	8.88	129.58	119.99
2	A	2769	GLU	N-CA-C	-8.83	103.34	114.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2813	ARG	N-CA-C	-8.40	101.64	112.23
2	A	2849	ALA	N-CA-C	-8.30	103.67	113.88
2	A	2507	TRP	N-CA-C	8.29	121.94	109.25
2	A	2572	ARG	N-CA-C	-8.20	103.06	113.72
2	A	2565	ASN	N-CA-C	-8.20	101.31	113.61
2	A	2661	VAL	N-CA-C	-8.16	105.29	111.90
2	A	2573	VAL	N-CA-C	-8.15	103.32	110.74
2	A	2781	LYS	N-CA-C	-7.77	102.35	112.68
2	A	2495	CYS	N-CA-C	-7.70	103.77	113.01
1	B	15	GLU	N-CA-C	7.62	120.42	110.43
2	A	2726	LEU	N-CA-C	-7.56	103.04	111.28
2	A	2847	LEU	N-CA-C	-7.55	101.96	113.89
2	A	3035	ARG	N-CA-C	7.50	119.69	110.91
2	A	2502	LEU	N-CA-C	7.45	121.07	109.52
2	A	2886	VAL	N-CA-C	7.18	118.17	108.11
2	A	2527	ASP	N-CA-C	-6.98	104.24	112.89
2	A	2460	GLN	N-CA-C	-6.97	103.28	112.34
2	A	2644	ASP	N-CA-C	-6.94	104.42	113.17
2	A	2735	ASN	N-CA-C	-6.90	99.73	110.42
2	A	2770	LYS	N-CA-C	-6.85	102.40	111.24
2	A	2458	PRO	N-CA-CB	6.84	110.44	103.25
2	A	2788	THR	N-CA-C	-6.70	104.00	111.71
2	A	2968	TYR	N-CA-C	6.61	119.60	108.23
2	A	2848	ARG	N-CA-C	-6.55	103.70	112.94
2	A	3087	ILE	N-CA-C	-6.54	103.95	110.30
2	A	2986	PRO	N-CA-CB	6.46	109.34	103.08
2	A	2926	ARG	N-CA-C	-6.43	96.57	108.02
2	A	2998	VAL	N-CA-C	-6.37	104.65	110.82
2	A	2852	ASN	N-CA-C	-6.34	105.31	114.12
2	A	3081	LYS	N-CA-C	-6.33	105.53	113.18
2	A	2856	MET	N-CA-C	-6.33	105.39	113.23
2	A	2655	PRO	N-CA-C	6.27	118.35	110.70
1	B	44	ASP	N-CA-C	6.22	118.43	108.41
1	B	7	PRO	N-CA-CB	6.21	109.83	103.00
2	A	2765	GLU	N-CA-C	-6.16	103.18	112.04
2	A	2578	LYS	N-CA-C	-6.12	104.16	111.69
2	A	2566	ARG	N-CA-C	-6.09	104.97	113.37
2	A	2853	TYR	N-CA-C	-6.06	105.53	113.17
2	A	2423	HIS	N-CA-C	-6.00	98.86	109.06
2	A	2584	GLU	N-CA-C	6.00	120.61	113.12
2	A	2657	LEU	N-CA-C	-5.99	103.42	112.04
2	A	2509	ILE	N-CA-C	5.97	113.79	107.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	2590	ARG	N-CA-C	5.96	118.95	109.24
2	A	2679	LEU	N-CA-C	5.94	119.15	109.59
2	A	2992	ASP	N-CA-C	-5.86	99.46	109.24
2	A	2819	LEU	N-CA-C	-5.80	108.01	114.62
2	A	2421	ARG	N-CA-C	-5.76	106.34	113.19
2	A	3056	LEU	N-CA-C	-5.75	103.11	110.53
2	A	2844	GLU	CA-C-O	5.73	121.27	117.94
2	A	2505	GLY	N-CA-C	-5.67	99.73	113.18
2	A	2474	ASN	N-CA-C	5.67	118.31	109.52
2	A	2568	LEU	N-CA-C	5.65	119.70	113.21
2	A	2840	ALA	N-CA-C	-5.64	105.98	112.92
2	A	2791	HIS	N-CA-C	-5.56	104.85	111.69
2	A	3002	LYS	CA-C-N	5.53	126.76	119.84
2	A	3002	LYS	C-N-CA	5.53	126.76	119.84
2	A	2690	GLU	N-CA-C	-5.52	104.75	112.25
2	A	2993	VAL	N-CA-C	5.51	115.25	108.53
2	A	2486	GLN	N-CA-C	5.51	117.28	111.28
2	A	2810	THR	N-CA-C	5.50	122.51	110.80
2	A	2665	LYS	N-CA-C	-5.49	105.63	112.93
2	A	2577	LEU	N-CA-C	-5.45	105.44	111.71
2	A	2878	LYS	N-CA-C	-5.44	106.32	113.17
2	A	3078	ASN	N-CA-C	-5.43	105.46	111.71
2	A	2472	ASN	N-CA-C	-5.42	105.82	113.20
2	A	3095	GLU	N-CA-C	-5.41	104.62	111.11
2	A	2861	LYS	N-CA-C	-5.41	99.29	110.80
2	A	2987	PRO	N-CA-CB	5.37	108.89	103.25
2	A	2844	GLU	CB-CA-C	-5.33	109.40	117.07
2	A	2587	ASN	N-CA-C	-5.33	107.09	113.21
2	A	2834	ASP	CA-C-N	5.32	126.49	119.84
2	A	2834	ASP	C-N-CA	5.32	126.49	119.84
2	A	3024	PHE	N-CA-C	5.18	117.19	108.96
2	A	2479	GLU	N-CA-C	-5.13	107.08	113.19
2	A	2877	GLU	N-CA-C	-5.09	106.76	112.87
2	A	2487	ASP	N-CA-C	5.05	119.43	113.16

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 ⓘ

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	61	0
2	A	5294	0	5280	767	0
3	A	5	0	0	0	0
All	All	5647	0	5561	791	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 71.

All (791) 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:H	2:A:2936:LYS:HD3	1.02	1.15
2:A:3001:VAL:HG12	2:A:3003:PRO:HD3	1.34	1.05
2:A:2426:LEU:HD12	2:A:2426:LEU:H	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
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:2558:ALA:C	2:A:2559:PHE:HD2	1.78	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2869:PHE:O	2:A:2870:ARG:C	2.22	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:2565:ASN:C	2:A:2567:CYS:H	1.86	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
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: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:OE2	2:A:2868:GLU:HA	1.84	0.76
2:A:3095:GLU:O	2:A:3099:ILE:HG22	1.85	0.76
1:B:56:LEU:O	1:B:56:LEU:HG	1.85	0.76
2:A:2650:ARG:HB2	2:A:2650:ARG:NH1	1.97	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2675:GLN:HG3	2:A:2722:PHE:CE1	2.19	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:HD22	2:A:2587:ASN:H	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:2602:THR:O	2:A:2603:ALA:C	2.30	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:2400:ASP:C	2:A:2402:MET:H	1.93	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
1:B:9:ASP:CB	1:B:12:LEU:HD12	2.16	0.74
2:A:2409:ARG:NH2	2:A:2511:SER:HA	2.02	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
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:H	2:A:2936:LYS:CD	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:2653:LEU:HD22	2:A:2657:LEU:HD13	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HD2	2:A:2954:TYR:N	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:2667:THR:O	2:A:2668:VAL:C	2.36	0.68
2:A:2865:ILE:O	2:A:2866:GLN:C	2.37	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:2723:PRO:CG	2:A:2926:ARG:HH21	2.06	0.67
2:A:2845:GLU:HG3	2:A:2846:GLN:N	2.09	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:2459:LYS:C	2:A:2461:LEU:N	2.48	0.67
2:A:2653:LEU:CD2	2:A:2657:LEU:HD13	2.25	0.67
2:A:2830:GLN:C	2:A:2832:ALA:H	2.03	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
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:2558:ALA:C	2:A:2559:PHE:CD2	2.69	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:3087:ILE:C	2:A:3089:THR:H	2.04	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:HA	2:A:2766:ARG:NE	2.10	0.65
1:B:57:ARG:HB3	2:A:2550:TRP:CH2	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:2891:LYS:C	2:A:2892:LEU:HD23	2.21	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
2:A:2932:VAL:O	2:A:2933:SER:C	2.39	0.65
1:B:40:GLU:HB2	1:B:52:PHE:CZ	2.32	0.65
2:A:2900:LYS:O	2:A:2901:GLU:HB3	1.96	0.65
2:A:3002:LYS:HE2	2:A:3028:LEU:CD1	2.27	0.64
1:B:55:GLN:CD	2:A:2670:GLN:HG3	2.22	0.64
2:A:2445:GLN:HE21	2:A:2450:ASP:HA	1.62	0.64
2:A:2864:ARG:HG3	2:A:2864:ARG:HH11	1.60	0.64
2:A:2552:LEU:O	2:A:2553:ALA:C	2.41	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:2441:ARG:C	2:A:2442:ILE:HG13	2.22	0.64
2:A:2768:GLU:O	2:A:2768:GLU:CG	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:2565:ASN:C	2:A:2567:CYS:N	2.56	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:2775:PHE:C	2:A:2777:GLU:H	2.05	0.63
2:A:2872:ALA:O	2:A:2875:SER:N	2.24	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: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
2:A:2640:ILE:HD13	2:A:2640:ILE:H	1.63	0.63
2:A:3062:SER:C	2:A:3063:ILE:HD13	2.24	0.62
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2969:GLN:HE22	2:A:2987:PRO:CB	2.11	0.62
2:A:2984:PHE:C	2:A:2986:PRO:N	2.56	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:2858:ASN:C	2:A:2860:LYS:H	2.08	0.62
2:A:3051:SER:C	2:A:3053:VAL:H	2.07	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:2459:LYS:C	2:A:2461:LEU:H	2.08	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:3001:VAL:HG12	2:A:3003:PRO:CD	2.22	0.60
2:A:2415:ARG:HH11	2:A:2527:ASP:CG	2.09	0.60
2:A:3032:ILE:HD12	2:A:3032:ILE:H	1.67	0.60
2:A:2586:ASP:C	2:A:2588:SER:H	2.08	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
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:2817:HIS:C	2:A:2819:LEU:H	2.10	0.59
2:A:2904:ALA:HB1	2:A:2944:ILE:O	2.01	0.59
2:A:2653:LEU:HB3	2:A:2657:LEU:HB2	1.84	0.59
2:A:2850:LEU:HD21	2:A:2854:ARG:NH2	2.18	0.59
2:A:2443:SER:C	2:A:2445:GLN:N	2.59	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:O	2:A:2856:MET:SD	2.61	0.58
2:A:2897:TYR:OH	2:A:2959:VAL:HG13	2.03	0.58
2:A:3052:GLY:C	2:A:3054:PRO:HD3	2.27	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:N	2:A:2431:LEU:HD23	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: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
1:B:55:GLN:C	1:B:57:ARG:H	2.12	0.57
2:A:2895:THR:HG22	2:A:2903:SER:HB3	1.87	0.57
2:A:2675:GLN:HE22	2:A:2722:PHE:N	2.00	0.57
2:A:2884:ARG:HG2	2:A:2884:ARG:HH11	1.69	0.57
2:A:2678:GLU:CG	2:A:2679:LEU:N	2.67	0.57
2:A:2508:LEU:HD23	2:A:2508:LEU:O	2.04	0.57
2:A:2687:ALA:C	2:A:2689:LEU:H	2.13	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:10:LEU:C	1:B:12:LEU:H	2.13	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: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
1:B:51:ASP:HB3	2:A:2708:ARG:HG3	1.88	0.56
2:A:2872:ALA:O	2:A:2873:LEU:C	2.48	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:HD12	2:A:3032:ILE:N	2.19	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HG22	2:A:2442:ILE:O	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:2448:VAL:C	2:A:2450:ASP:H	2.14	0.55
2:A:2532:ASP:CG	2:A:2534:LYS:HE3	2.31	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:2835:PRO:C	2:A:2837:HIS:H	2.13	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:2747:TYR:HD2	2:A:3042:ASN:ND2	2.05	0.55
2:A:3018:ASN:C	2:A:3019:LEU:HD12	2.32	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
2:A:2909:TRP:O	2:A:2910:ARG:C	2.50	0.54
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
1:B:59:GLU:C	1:B:61:GLU:H	2.16	0.54
2:A:2760:TYR:C	2:A:2761:ILE:HD12	2.33	0.54
2:A:2889:VAL:HG13	2:A:2909:TRP:CE3	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2978:ARG:C	2:A:2980:SER:H	2.14	0.54
2:A:2423:HIS:C	2:A:2424:LEU:HG	2.33	0.54
2:A:2478:ALA:C	2:A:2480:TYR:H	2.16	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:3102:LEU:HD23	2:A:3102:LEU:N	2.22	0.54
2:A:2749:LEU:HD22	2:A:2888:THR:OG1	2.06	0.54
2:A:2775:PHE:HD2	2:A:2776:ALA:N	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:H	2.15	0.54
2:A:2446:ALA:C	2:A:2448:VAL:H	2.16	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:2861:LYS:C	2:A:2863:ALA:N	2.65	0.53
2:A:2430:SER:HB3	2:A:2575:LEU:CD2	2.30	0.53
2:A:2775:PHE:C	2:A:2777:GLU:N	2.64	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:2474:ASN:C	2:A:2476:LYS:H	2.16	0.53
2:A:2981:ASP:C	2:A:2983:ALA:H	2.15	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:2994:VAL:CG2	2:A:3073:PHE:HD2	2.22	0.53
2:A:3019:LEU:HD21	2:A:3099:ILE:HB	1.91	0.53
2:A:2856:MET:SD	2:A:2856:MET:C	2.91	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:10:LEU:C	1:B:12:LEU:N	2.67	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
1:B:59:GLU:C	1:B:61:GLU:N	2.65	0.52
2:A:2524:ALA:C	2:A:2526:CYS:H	2.17	0.52
2:A:2539:ILE:H	2:A:2539:ILE:HD13	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
2:A:2998:VAL:HG23	2:A:2999:SER:N	2.24	0.52
2:A:3001:VAL:C	2:A:3003:PRO:HD3	2.34	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:2400:ASP:C	2:A:2402:MET:N	2.63	0.52
2:A:2836:ASP:HA	2:A:2839:GLU:HG2	1.92	0.52
2:A:2597:LEU:C	2:A:2599:ARG:H	2.17	0.52
2:A:3016:CYS:C	2:A:3017:LEU:HD12	2.35	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:2902:LYS:O	2:A:2903:SER:C	2.53	0.52
2:A:2960:SER:O	2:A:2961:SER:C	2.52	0.52
2:A:2774:ARG:NH1	2:A:2775:PHE:HA	2.25	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:2861:LYS:O	2:A:2862:GLN:C	2.54	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:HD23	2:A:2882:LEU:O	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:3089:THR:C	2:A:3091:TYR:H	2.19	0.51
2:A:2601:ASP:O	2:A:2602:THR:C	2.53	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:2502:LEU:CD2	2:A:2571:GLU:HG2	2.33	0.51
2:A:2513:ASP:CB	2:A:2515:LYS:HE3	2.41	0.51
2:A:2793:GLU:O	2:A:2794:PHE:CD1	2.64	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:39:TRP:HB3	2:A:2673:ILE:HD12	1.93	0.51
2:A:2838:LEU:HD23	2:A:2838:LEU:C	2.36	0.51
2:A:2569:ASN:C	2:A:2571:GLU:H	2.19	0.51
2:A:2420:GLU:C	2:A:2422:ARG:H	2.18	0.50
2:A:2644:ASP:C	2:A:2713:LEU:HD13	2.35	0.50
2:A:2844:GLU:CD	2:A:2844:GLU:H	2.19	0.50
2:A:2901:GLU:C	2:A:2901:GLU:OE1	2.54	0.50
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: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:O	2:A:2847:LEU:HG	2.12	0.50
2:A:2480:TYR:O	2:A:2481:PHE:C	2.54	0.50
2:A:2484:ASP:O	2:A:2485:ILE:C	2.54	0.50
2:A:2554:ALA:C	2:A:2556:GLU:H	2.19	0.50
2:A:2583:VAL:O	2:A:2589:ARG:HB2	2.11	0.50
2:A:2586:ASP:C	2:A:2586:ASP:OD2	2.53	0.50
2:A:2656:PRO:HG3	2:A:2732:ASP:OD1	2.11	0.50
2:A:2675:GLN:CG	2:A:2722:PHE:CE1	2.94	0.50
1:B:39:TRP:CE2	2:A:2722:PHE:HB2	2.46	0.50
1:B:42:ASN:O	1:B:43:TRP:C	2.55	0.50
2:A:2974:LEU:HD11	2:A:2993:VAL:CG1	2.41	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:HG12	2:A:2790:VAL:O	2.12	0.49
2:A:3091:TYR:O	2:A:3092:LYS:C	2.54	0.49
2:A:2593:LEU:O	2:A:2597:LEU:HD23	2.11	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
2:A:2692:PRO:C	2:A:2694:SER:H	2.20	0.49
2:A:2912:SER:OG	2:A:2914:ASP:HB2	2.12	0.49
2:A:3082:HIS:C	2:A:3084:ILE:H	2.20	0.49
1:B:42:ASN:HA	2:A:2728:SER:HB2	1.93	0.49
2:A:2763:ARG:O	2:A:2764:SER:O	2.30	0.49
1:B:52:PHE:CD1	1:B:52:PHE:N	2.80	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2442:ILE:O	2:A:2443:SER:C	2.56	0.49
2:A:2675:GLN:NE2	2:A:2722:PHE:CD1	2.81	0.49
2:A:2687:ALA:C	2:A:2689:LEU:N	2.69	0.49
2:A:3020:LEU:HD12	2:A:3056:LEU:HG	1.94	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
1:B:55:GLN:HG3	2:A:2670:GLN:CB	2.43	0.49
2:A:2558:ALA:C	2:A:2560:PRO:HD3	2.38	0.49
2:A:2978:ARG:C	2:A:2980:SER:N	2.71	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:2861:LYS:C	2:A:2863:ALA:H	2.21	0.49
1:B:55:GLN:HG3	2:A:2670:GLN:CG	2.42	0.49
2:A:2676:GLY:O	2:A:2677:ALA:C	2.55	0.49
2:A:2997:VAL:O	2:A:3035:ARG:N	2.44	0.49
1:B:56:LEU:C	1:B:57:ARG:HG3	2.37	0.48
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
2:A:3014:ASP:HA	2:A:3080:LEU:CD2	2.43	0.48
1:B:14:GLU:HG2	2:A:2441:ARG:HB3	1.95	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:2899:LYS:O	2:A:2900:LYS:C	2.55	0.48
2:A:2981:ASP:O	2:A:2983:ALA:N	2.42	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
1:B:43:TRP:CH2	2:A:2657:LEU:HD21	2.48	0.48
2:A:2413:ASP:OD1	2:A:2523:ARG:NH1	2.45	0.48
2:A:2574:LEU:O	2:A:2574:LEU:HG	2.13	0.48
2:A:2590:ARG:HG2	2:A:2594:LYS:HD3	1.94	0.48
2:A:2869:PHE:O	2:A:2872:ALA:N	2.41	0.48
1:B:51:ASP:HB2	2:A:2708:ARG:HH11	1.77	0.48
2:A:2459:LYS:O	2:A:2460:GLN:C	2.56	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2708:ARG:H	2:A:2708:ARG:HD3	1.79	0.48
2:A:3011:TYR:CD2	2:A:3099:ILE:HD13	2.49	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
2:A:2817:HIS:C	2:A:2819:LEU:N	2.72	0.48
1:B:59:GLU:OE2	2:A:2453:PRO:HG2	2.14	0.48
2:A:2484:ASP:C	2:A:2486:GLN:N	2.71	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:2870:ARG:O	2:A:2871:LYS:C	2.56	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:2549:VAL:O	2:A:2550:TRP:C	2.55	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
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
2:A:2545:TYR:O	2:A:2549:VAL:HG23	2.14	0.47
2:A:2775:PHE:CD2	2:A:2776:ALA:N	2.81	0.47
2:A:2855:GLN:O	2:A:2855:GLN:HG3	2.14	0.47
2:A:2876:ALA:O	2:A:2880:GLU:HG2	2.14	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
1:B:55:GLN:O	1:B:57:ARG:N	2.45	0.47
2:A:2445:GLN:O	2:A:2447:ALA:N	2.48	0.47
2:A:2705:ARG:O	2:A:2706:PRO:C	2.58	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
2:A:2399:LYS:HE3	2:A:2399:LYS:HA	1.97	0.47
2:A:2842:PHE:HD1	2:A:2842:PHE:O	1.98	0.47
2:A:3086:ASN:CG	2:A:3087:ILE:N	2.72	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2879:GLU:O	2:A:2881:GLY:N	2.48	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:2742:ILE:HD12	2:A:2923:LYS:C	2.40	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:2729:LEU:C	2:A:2730:PHE:HD1	2.23	0.47
2:A:2774:ARG:HD2	2:A:2774:ARG:O	2.14	0.47
1:B:16:ASP:CG	1:B:57:ARG:HH21	2.20	0.46
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:2753:GLU:OE1	2:A:2884:ARG:NH2	2.48	0.46
2:A:2819:LEU:HG	2:A:2846:GLN:CD	2.40	0.46
2:A:2873:LEU:C	2:A:2873:LEU:HD23	2.40	0.46
2:A:2676:GLY:C	2:A:2677:ALA:O	2.58	0.46
2:A:2931:ALA:CB	2:A:2947:THR:HB	2.45	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:2587:ASN:O	2:A:2588:SER:C	2.57	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:2944:ILE:HG13	2:A:2945:GLN:H	1.81	0.46
2:A:2673:ILE:CD1	2:A:2707:ALA:HB2	2.45	0.46
2:A:3051:SER:C	2:A:3053:VAL:N	2.74	0.46
2:A:2526:CYS:SG	2:A:2536:ILE:HD11	2.56	0.46
2:A:2597:LEU:HD21	2:A:2649:VAL:HG11	1.97	0.46
2:A:2607:LEU:O	2:A:2673:ILE:HA	2.14	0.46
2:A:2656:PRO:HG3	2:A:2732:ASP:HB2	1.96	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:2694:SER:O	2:A:2695:LEU:C	2.59	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:2988:CYS:O	2:A:2989:SER:CB	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2409:ARG:HH22	2:A:2511:SER:HA	1.78	0.45
2:A:2611:ILE:H	2:A:2611:ILE:HG12	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:O	2:A:2746:VAL:HG12	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:2481:PHE:C	2:A:2481:PHE:CD1	2.95	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
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:2420:GLU:C	2:A:2422:ARG:N	2.73	0.45
2:A:2470:CYS:SG	2:A:2556:GLU:OE2	2.75	0.45
2:A:2483:PHE:CB	2:A:2516:ALA:HB3	2.42	0.45
2:A:3014:ASP:C	2:A:3014:ASP:OD1	2.59	0.45
2:A:3020:LEU:HA	2:A:3054:PRO:CD	2.33	0.45
2:A:3087:ILE:C	2:A:3089:THR:N	2.73	0.45
2:A:2731:SER:HB2	2:A:2944:ILE:HD11	1.97	0.45
2:A:2830:GLN:C	2:A:2832:ALA:N	2.69	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
1:B:9:ASP:CG	1:B:12:LEU:HD12	2.40	0.45
2:A:2471:ILE:C	2:A:2473:VAL:H	2.25	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:2445:GLN:O	2:A:2446:ALA:C	2.59	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:3000:VAL:C	2:A:3001:VAL:HG23	2.42	0.45
2:A:2409:ARG:HH21	2:A:2511:SER:HA	1.75	0.45
2:A:2427:GLN:O	2:A:2428:PRO:C	2.59	0.45
2:A:2701:ALA:O	2:A:2705:ARG:NH1	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2738:CYS:SG	2:A:2926:ARG:HG2	2.57	0.45
2:A:2438:THR:O	2:A:2439:LEU:C	2.60	0.44
2:A:2490:GLY:O	2:A:2494:LEU:HD12	2.18	0.44
2:A:2783:LEU:HD11	2:A:2880:GLU:N	2.32	0.44
2:A:2951:ARG:HG2	2:A:2951:ARG:HH11	1.82	0.44
2:A:2524:ALA:C	2:A:2526:CYS:N	2.71	0.44
2:A:2572:ARG:HA	2:A:2575:LEU:HB2	1.98	0.44
2:A:2775:PHE:C	2:A:2775:PHE:CD2	2.95	0.44
2:A:2967:VAL:HG23	2:A:2968:TYR:H	1.81	0.44
1:B:52:PHE:CE2	2:A:2706:PRO:O	2.70	0.44
2:A:2447:ALA:C	2:A:2448:VAL:CG2	2.90	0.44
2:A:2644:ASP:O	2:A:2713:LEU:CB	2.65	0.44
1:B:12:LEU:HD22	2:A:2439:LEU:O	2.17	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
2:A:2723:PRO:O	2:A:2724:LEU:HB3	2.16	0.44
2:A:2864:ARG:O	2:A:2865:ILE:C	2.60	0.44
2:A:2937:SER:O	2:A:2938:LYS:HB2	2.18	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:2478:ALA:C	2:A:2480:TYR:N	2.74	0.44
2:A:2468:LYS:C	2:A:2470:CYS:H	2.26	0.44
2:A:2524:ALA:O	2:A:2527:ASP:N	2.46	0.44
2:A:3011:TYR:CE2	2:A:3021:VAL:HG21	2.53	0.44
2:A:2522:TYR:HE1	2:A:2537:SER:CA	2.31	0.44
2:A:2675:GLN:C	2:A:2677:ALA:H	2.24	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
1:B:55:GLN:C	1:B:57:ARG:N	2.76	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:2835:PRO:C	2:A:2837:HIS:N	2.76	0.44
2:A:2967:VAL:HG23	2:A:2968:TYR:N	2.32	0.44
2:A:2656:PRO:HG3	2:A:2732:ASP:CG	2.43	0.44
2:A:2742:ILE:HA	2:A:2923:LYS:O	2.17	0.44
2:A:2783:LEU:HD21	2:A:2880:GLU:HB3	2.00	0.44
1:B:52:PHE:HE2	2:A:2706:PRO:O	2.01	0.43
2:A:2412:GLN:NE2	2:A:2507:TRP:O	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2554:ALA:C	2:A:2556:GLU:N	2.75	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
2:A:2726:LEU:HD22	2:A:2904:ALA:HB3	2.00	0.43
2:A:2559:PHE:O	2:A:2560:PRO:C	2.60	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
1:B:52:PHE:O	2:A:2670:GLN:NE2	2.52	0.43
2:A:2445:GLN:O	2:A:2448:VAL:N	2.51	0.43
2:A:2474:ASN:CB	2:A:2477:ASN:OD1	2.66	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
1:B:54:ASN:CB	2:A:2452:ALA:HB1	2.48	0.43
2:A:2884:ARG:HH11	2:A:2884:ARG:CG	2.31	0.43
1:B:16:ASP:OD1	1:B:57:ARG:NE	2.51	0.43
2:A:2611:ILE:HG13	2:A:2669:GLY:N	2.31	0.43
2:A:2834:ASP:CG	2:A:2837:HIS:HB2	2.41	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
1:B:56:LEU:O	1:B:56:LEU:CG	2.60	0.43
2:A:2445:GLN:HE22	2:A:2709:TRP:HE1	1.65	0.43
2:A:2485:ILE:CG2	2:A:2516:ALA:HB2	2.48	0.43
2:A:2597:LEU:C	2:A:2599:ARG:N	2.77	0.43
2:A:2604:ALA:O	2:A:2675:GLN:O	2.37	0.43
2:A:2542:ALA:O	2:A:2543:ASN:C	2.61	0.43
2:A:2700:SER:HB3	2:A:2734:GLY:CA	2.49	0.43
2:A:2766:ARG:HA	2:A:2766:ARG:CZ	2.47	0.43
2:A:3020:LEU:HD23	2:A:3020:LEU:O	2.18	0.43
1:B:13:LEU:HD11	2:A:2444:LEU:CD1	2.48	0.43
2:A:2448:VAL:HG21	2:A:2559:PHE:CD1	2.52	0.43
2:A:2838:LEU:C	2:A:2838:LEU:CD2	2.91	0.43
2:A:2857:LEU:HA	2:A:2857:LEU:HD23	1.67	0.43
2:A:3020:LEU:HD23	2:A:3020:LEU:C	2.44	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:2605:LYS:O	2:A:2606:THR:C	2.62	0.43
2:A:2645:GLY:N	2:A:2713:LEU:HD13	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2655:PRO:HB2	2:A:2732:ASP:CB	2.49	0.43
2:A:2708:ARG:H	2:A:2708:ARG:CD	2.32	0.43
2:A:2520:GLU:H	2:A:2520:GLU:CD	2.26	0.43
2:A:2586:ASP:C	2:A:2588:SER:N	2.76	0.43
2:A:2726:LEU:O	2:A:2727:SER:C	2.62	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:2821:ASP:HB3	2:A:2824:GLU:CD	2.43	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:HD2	2:A:2860:LYS:HA	1.88	0.42
2:A:3075:GLU:C	2:A:3077:VAL:N	2.76	0.42
1:B:13:LEU:HG	1:B:15:GLU:HG3	2.01	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: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:51:ASP:CB	2:A:2708:ARG:HG3	2.50	0.42
2:A:2522:TYR:HE1	2:A:2537:SER:HA	1.84	0.42
2:A:2511:SER:O	2:A:2512:ASN:C	2.60	0.42
2:A:2745:ARG:HD3	2:A:2745:ARG:HA	1.51	0.42
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:2953:GLN:C	2:A:2954:TYR:HD2	2.28	0.42
2:A:3071:ALA:O	2:A:3072:TYR:C	2.62	0.42
2:A:2675:GLN:HE21	2:A:2721:PRO:HA	1.85	0.42
2:A:3000:VAL:CG1	2:A:3001:VAL:N	2.82	0.42
2:A:2763:ARG:C	2:A:2764:SER:O	2.60	0.42
2:A:2893:ARG:HA	2:A:2905:LEU:HD12	2.01	0.42
1:B:37:HIS:C	1:B:38:VAL:HG23	2.44	0.42
2:A:2640:ILE:H	2:A:2640:ILE:CD1	2.29	0.42
2:A:2650:ARG:CB	2:A:2650:ARG:NH1	2.69	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
1:B:43:TRP:HZ3	2:A:2701:ALA:HA	1.84	0.42
2:A:2657:LEU:C	2:A:2659:ALA:N	2.76	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2763:ARG:CZ	2:A:2771:GLU:HG2	2.50	0.42
2:A:2466:VAL:O	2:A:2467:SER:HB2	2.19	0.42
2:A:2573:VAL:C	2:A:2575:LEU:H	2.26	0.42
2:A:3073:PHE:O	2:A:3074:GLN:C	2.63	0.41
2:A:3082:HIS:C	2:A:3084:ILE:N	2.78	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: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:2747:TYR:CD2	2:A:3042:ASN:ND2	2.87	0.41
2:A:2819:LEU:HD21	2:A:2844:GLU:OE2	2.20	0.41
2:A:2825:LEU:C	2:A:2850:LEU:HD12	2.46	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: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:H	2:A:2965:LEU:CD1	2.33	0.41
2:A:3015:GLU:N	2:A:3080:LEU:HD13	2.35	0.41
2:A:3050:THR:O	2:A:3050:THR:HG22	2.20	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
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:2673:ILE:HG12	2:A:2707:ALA:HB2	2.00	0.41
2:A:2712:ARG:O	2:A:2713:LEU:C	2.63	0.41
2:A:2850:LEU:C	2:A:2852:ASN:H	2.29	0.41
2:A:2951:ARG:HG2	2:A:2951:ARG:NH1	2.35	0.41
1:B:10:LEU:O	1:B:12:LEU:N	2.54	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:2864:ARG:O	2:A:2865:ILE:O	2.38	0.41
2:A:3011:TYR:CZ	2:A:3021:VAL:HG21	2.55	0.41
2:A:3062:SER:O	2:A:3063:ILE:HD13	2.21	0.41
2:A:3075:GLU:C	2:A:3077:VAL:H	2.28	0.41
2:A:3084:ILE:O	2:A:3088:ASP:CG	2.64	0.41
2:A:2445:GLN:HB3	2:A:2446:ALA:H	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:2458:PRO:O	2:A:2459:LYS:O	2.38	0.41
2:A:2755:THR:O	2:A:2756:VAL:C	2.64	0.41
2:A:2965:LEU:HD12	2:A:2965:LEU:N	2.36	0.41
2:A:2415:ARG:HD2	2:A:2415:ARG:HH11	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:2573:VAL:C	2:A:2575:LEU:N	2.78	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:2456:CYS:O	2:A:2457:SER:C	2.65	0.40
2:A:2522:TYR:CE1	2:A:2538:SER:N	2.89	0.40
2:A:2826:TYR:O	2:A:2827:ALA:C	2.64	0.40
2:A:2864:ARG:HH11	2:A:2864:ARG:CG	2.32	0.40
2:A:2912:SER:O	2:A:2914:ASP:N	2.54	0.40
2:A:2993:VAL:O	2:A:3073:PHE:HE2	2.04	0.40
2:A:2778:ALA:O	2:A:2781:LYS:HB2	2.21	0.40
2:A:2872:ALA:C	2:A:2874:GLU:N	2.78	0.40
2:A:2418:ASN:O	2:A:2419:LYS:C	2.65	0.40
2:A:2423:HIS:O	2:A:2423:HIS:CD2	2.75	0.40
2:A:2448:VAL:C	2:A:2450:ASP:N	2.78	0.40
2:A:2481:PHE:O	2:A:2482:GLN:HB2	2.21	0.40
2:A:2485:ILE:HD12	2:A:2485:ILE:C	2.45	0.40
2:A:2644:ASP:O	2:A:2713:LEU:HB3	2.21	0.40
2:A:2693:ASP:OD1	2:A:2693:ASP:N	2.52	0.40
2:A:3077:VAL:C	2:A:3079:ASN:N	2.79	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	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
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

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Mol	Chain	Res	Type
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
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

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Mol	Chain	Res	Type
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
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%)	33 (92%)	3 (8%)	10	35
2	A	571/649 (88%)	476 (83%)	95 (17%)	2	10
All	All	607/712 (85%)	509 (84%)	98 (16%)	2	11

All (98) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	15	GLU
1	B	41	ASP
1	B	42	ASN
2	A	2399	LYS
2	A	2400	ASP
2	A	2401	LEU
2	A	2417	LYS
2	A	2421	ARG
2	A	2431	LEU
2	A	2438	THR
2	A	2440	PRO
2	A	2448	VAL
2	A	2453	PRO
2	A	2470	CYS
2	A	2471	ILE
2	A	2474	ASN
2	A	2498	LYS
2	A	2501	GLN
2	A	2502	LEU
2	A	2539	ILE
2	A	2559	PHE
2	A	2560	PRO
2	A	2568	LEU
2	A	2572	ARG
2	A	2575	LEU
2	A	2587	ASN
2	A	2611	ILE

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Mol	Chain	Res	Type
2	A	2640	ILE
2	A	2650	ARG
2	A	2661	VAL
2	A	2663	SER
2	A	2674	THR
2	A	2693	ASP
2	A	2706	PRO
2	A	2711	SER
2	A	2717	ARG
2	A	2720	ARG
2	A	2732	ASP
2	A	2736	VAL
2	A	2741	ILE
2	A	2742	ILE
2	A	2744	GLN
2	A	2745	ARG
2	A	2746	VAL
2	A	2749	LEU
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	2838	LEU
2	A	2841	CYS
2	A	2852	ASN
2	A	2856	MET
2	A	2858	ASN
2	A	2864	ARG
2	A	2868	GLU
2	A	2877	GLU
2	A	2882	LEU
2	A	2888	THR
2	A	2889	VAL
2	A	2892	LEU
2	A	2898	LYS
2	A	2899	LYS
2	A	2901	GLU

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Mol	Chain	Res	Type
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	2969	GLN
2	A	2974	LEU
2	A	2991	VAL
2	A	2993	VAL
2	A	3003	PRO
2	A	3004	ILE
2	A	3015	GLU
2	A	3016	CYS
2	A	3017	LEU
2	A	3031	ASP
2	A	3038	ILE
2	A	3041	SER
2	A	3072	TYR
2	A	3079	ASN
2	A	3082	HIS
2	A	3097	LYS
2	A	3098	LEU
2	A	3099	ILE
2	A	3102	LEU

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

Mol	Chain	Res	Type
1	B	42	ASN
2	A	2423	HIS
2	A	2486	GLN
2	A	2543	ASN
2	A	2565	ASN
2	A	2576	GLN
2	A	2587	ASN
2	A	2670	GLN
2	A	2675	GLN

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Mol	Chain	Res	Type
2	A	2814	GLN
2	A	2846	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	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 oligosaccharides 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.