



Full wwPDB EM Validation Report ⓘ

Mar 5, 2026 – 09:32 PM UTC

PDB ID : 9OL5 / pdb_00009ol5
EMDB ID : EMD-70590
Title : Rabbit Ryanodine Receptor 1: Atorvastatin Bound Closed Conformation
Authors : Molinarolo, S.M.; Van Petegem, F.
Deposited on : 2025-05-12
Resolution : 3.56 Å(reported)
Based on initial model : 7TZC

This is a Full wwPDB EM 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/EMValidationReportHelp>
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:

EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMD archive up until May 2025)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

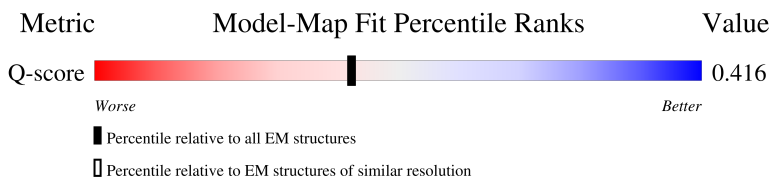
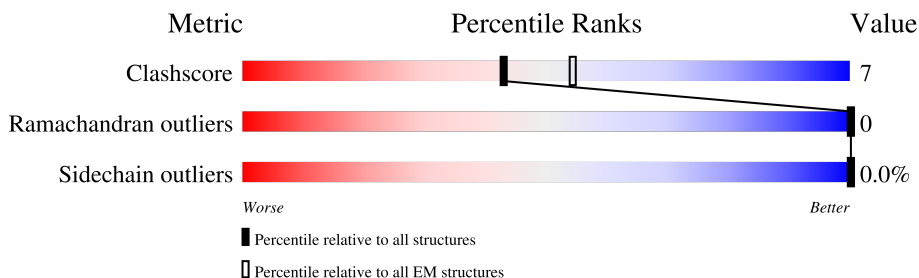
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 3.56 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)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	12750 (3.06 - 4.06)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	5037	11% 72% 11% 17%
1	G	5037	11% 72% 11% 17%
1	M	5037	10% 72% 11% 17%
1	S	5037	10% 72% 11% 17%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B	111	 77%20%•
2	H	111	 77%20%•
2	N	111	 77%19%•
2	T	111	 80%16%•

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 134812 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, 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 Ryanodine receptor 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4188	Total	C	N	O	S	0	0
			32850	20969	5669	5990	222		
1	G	4188	Total	C	N	O	S	0	0
			32850	20969	5669	5990	222		
1	M	4188	Total	C	N	O	S	0	0
			32850	20969	5669	5990	222		
1	S	4188	Total	C	N	O	S	0	0
			32850	20969	5669	5990	222		

- Molecule 2 is a protein called Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	107	Total	C	N	O	S	0	0
			810	512	143	151	4		
2	H	107	Total	C	N	O	S	0	0
			810	512	143	151	4		
2	N	107	Total	C	N	O	S	0	0
			810	512	143	151	4		
2	T	107	Total	C	N	O	S	0	0
			810	512	143	151	4		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	SER	-	expression tag	UNP P68106
B	-1	ASN	-	expression tag	UNP P68106
B	0	ALA	-	expression tag	UNP P68106
H	-2	SER	-	expression tag	UNP P68106
H	-1	ASN	-	expression tag	UNP P68106
H	0	ALA	-	expression tag	UNP P68106
N	-2	SER	-	expression tag	UNP P68106
N	-1	ASN	-	expression tag	UNP P68106
N	0	ALA	-	expression tag	UNP P68106

Continued on next page...

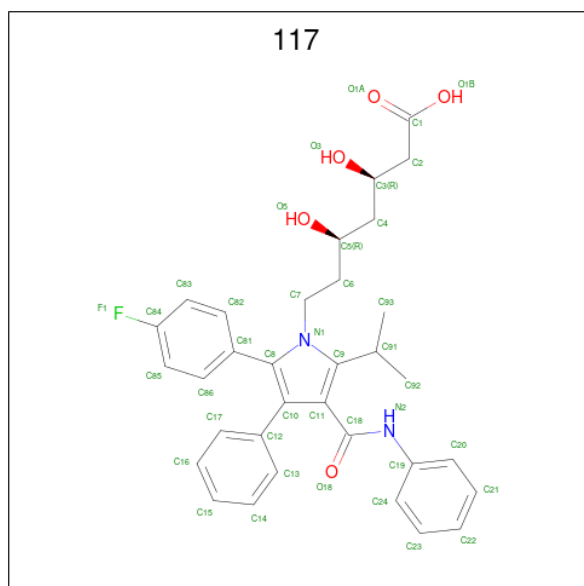
Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
T	-2	SER	-	expression tag	UNP P68106
T	-1	ASN	-	expression tag	UNP P68106
T	0	ALA	-	expression tag	UNP P68106

- Molecule 3 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	AltConf
3	A	1	Total Ca 1 1	0
3	G	1	Total Ca 1 1	0
3	M	1	Total Ca 1 1	0
3	S	1	Total Ca 1 1	0

- Molecule 4 is 7-[2-(4-FLUORO-PHENYL)-5-ISOPROPYL-3-PHENYL-4-PHENYLCARBA MOYL-PYRROL-1-YL]- 3,5-DIHYDROXY-HEPTANOIC ACID (CCD ID: 117) (formula: C₃₃H₃₅FN₂O₅) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	AltConf
4	A	1	Total C F N O 41 33 1 2 5	0
4	G	1	Total C F N O 41 33 1 2 5	0
4	M	1	Total C F N O 41 33 1 2 5	0

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					AltConf
4	S	1	Total	C	F	N	O	0
			41	33	1	2	5	

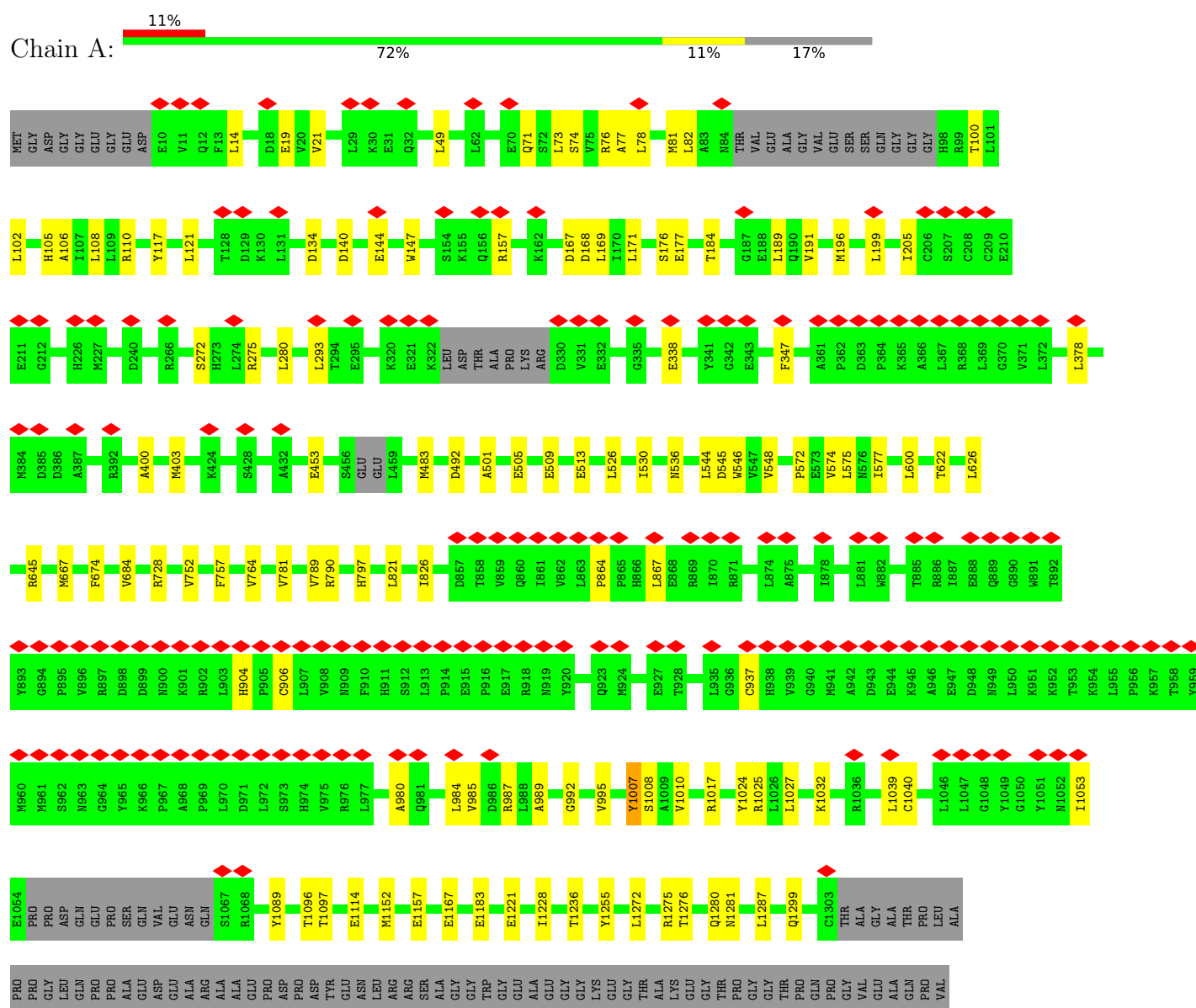
- Molecule 5 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		AltConf
5	A	1	Total	Zn	0
			1	1	
5	G	1	Total	Zn	0
			1	1	
5	M	1	Total	Zn	0
			1	1	
5	S	1	Total	Zn	0
			1	1	

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 and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

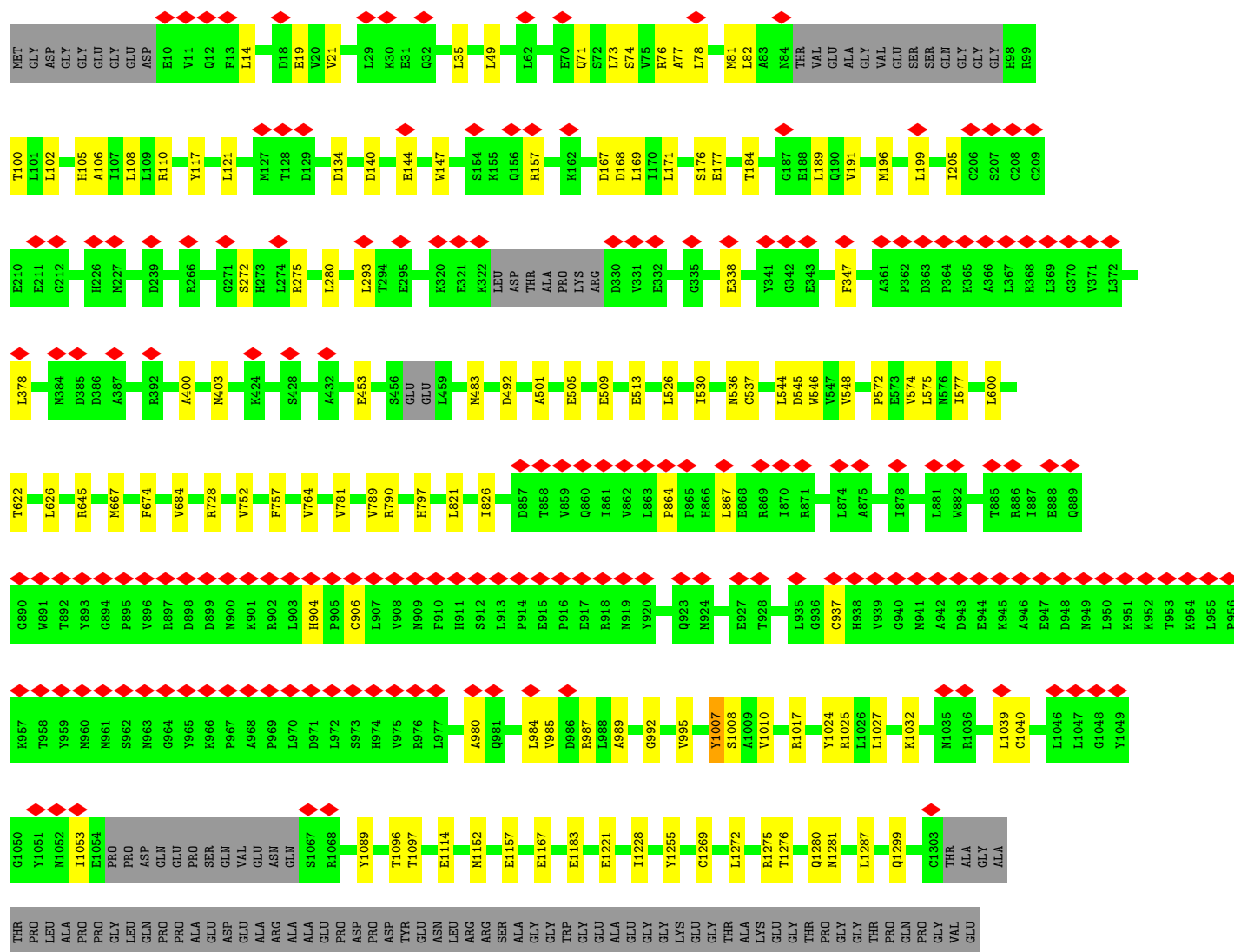
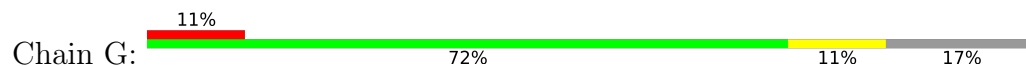
• Molecule 1: Ryanodine receptor 1



ARG	F1464	LYS	L2023	L2116	L3002	G2419	P2640	F2754	K2814	M2874	G2934
ALA	D1465	ALA	L2024	W2120	L3023	M2423	R2650	I2755	A2815	A2875	Y2935
GLU	V1474	VAL	E2025	L2123	L2313	C2651	C2651	M2756	M2816	E2876	A2936
ASP	D1478	GLU	R2028	L2124	Y2318	M2440	G2660	K2757	L2817	Q2877	V2937
LYS	G1481	LYS	L2031	W2125	N2324	D2465	V2666	F2758	A2818	L2878	T2938
ALA	C1489	GLU	Q2045	R2126	P2325	G2480	T2667	A2759	W2819	A2879	R2939
THR	L1815	GLU	L2046	Q2127	C2326	K2481	S2668	E2760	E2820	E2880	GLY
GLU	V1501	ALA	GLU	Y2128	G2327	E2484	E2670	Y2761	W2821	N2881	LEU
LYS	SER	PRO	GLU	E2150	G2328	A2484	E2671	E2762	T2822	Y2882	LYS
ASN	PRO	GLU	GLY	L2166	E2329	M2490	E2674	H2763	L2823	H2883	ASP
LYS	GLY	GLY	GLU	N2196	R2330	W2498	E2764	K2765	E2824	N2884	MET
ARG	GLN	GLU	GLU	L2197	V2339	H2498	K2766	A2767	K2825	T2885	GLU
GLY	GLY	GLU	GLU	L2198	E2347	K2499	W2768	W2766	A2826	W2886	LEU
PHE	ARG	ASP	PRO	R2199	E2348	M2502	D2769	A2766	R2827	Q2887	T2948
LEU	ILE	LEU	GLU	W2203	N2351	W2503	K2770	F2768	E2828	R2888	R2965
PHE	SER	LEU	GLU	T2206	V2354	Q2515	L2710	D2769	W2829	K2889	W2966
LYS	T1512	GLU	THR	V2210	R2355	L2519	P2711	K2771	E2830	K2890	T2969
ALA	D1513	GLU	LEU	W2211	C2363	D2523	A2717	Q2772	GLU	K2891	I2974
ALA	L1514	GLU	ARG	V2214	E2371	L2527	S2718	M2773	ARG	Q2892	T2977
ALA	E1535	SER	ARG	L2215	E2371	M2530	W2719	W2775	THR	E2893	GLU
MET	V1561	GLU	LEU	GLY	L2376	R2531	SER	W2776	ALA	L2894	GLY
THR	M1608	GLU	LEU	GLY	L2377	R2531	ALA	W2777	LYS	E2895	ALA
PRO	D1668	GLU	THR	THR	I2380	M2546	LYS	S2778	LYS	A2896	VAL
ALA	L1669	GLU	VAL	VAL	E2381	R2575	VAL	W2778	ALA	K2897	VAL
LEU	D1690	GLU	ARG	GLU	E2382	R2598	ASP	E2778	ASP	G2898	VAL
PRO	Q1693	GLU	VAL	P2226	R2392	A2598	ALA	E2779	GLY	E2899	SER
ARG	D1700	GLU	LYS	V2229	P2395	Q2599	GLY	E2780	ASN	G2900	GLY
ASP	R1727	GLU	GLU	T2230	VAL	R2601	GLY	E2781	PHE	T2901	THR
VAL	L1731	GLU	PRO	S2231	ARG	D2602	ASN	E2782	ASP	H2902	ALA
PRO	T1739	GLU	GLU	C2232	ASP	V2602	GLY	E2783	PRO	P2903	GLN
ALA	T1742	ASP	GLU	L2254	ARG	I2603	GLY	E2784	ARG	L2904	LYS
ASP	N1420	GLU	LEU	I2263	ARG	L2622	ASP	L2785	GLY	L2905	THR
R1421	R1422	GLU	GLU	G2264	ARG	L2623	P2737	L2786	R2738	D2906	SER
V1439	F1440	LYS	PRO	L2265	HIS	R2624	R2739	L2787	V2740	D2907	GLY
A1441	A1441	GLY	ALA	G2266	PHE	R2625	E2741	L2788	E2742	T2910	THR
T1454	N1756	ASP	LYS	W2267	GLY	L2626	L2742	H2788	L2743	T2911	ALA
P1455	A1757	GLU	GLU	Q2268	GLU	V2627	L2744	P2789	N2745	D2912	THR
D1456	P1787	GLU	GLU	Q2269	PRO	D2629	W2746	M2790	W2745	T2913	GLY
				S2270	PRO	L2632	I2747	L2791	I2746	A2914	GLY
				T2271	GLU	A2637	L2748	L2792	S2798	R2915	GLY
				D2274	ASN	K2638	E2749	L2793	E2799	D2916	GLY
				V2275	R2415	M2639	K2750	L2794	K2800	K2917	GLY
								L2795	D2801	A2918	GLY
								L2796	K2802	R2919	GLY
								L2797	L2803	L2920	GLY
								L2798	I2804	E2921	GLY
								L2799	Y2805	K2922	GLY
								L2800	E2806	A2923	GLY
								L2801	W2807	Q2924	GLY
								L2802	P2808	E2925	GLY
								L2803	I2809	L2926	GLY
								L2804	K2810	L2927	GLY
								L2805	E2811	K2928	GLY
								L2806	S2812	F2929	GLY
								L2807	S2813	L2930	GLY
								L2808		Q2931	GLY
								L2809		M2932	GLY
								L2810		N2933	GLY
								L2811			GLY
								L2812			GLY
								L2813			GLY
								L2814			GLY
								L2815			GLY
								L2816			GLY
								L2817			GLY
								L2818			GLY
								L2819			GLY
								L2820			GLY
								L2821			GLY
								L2822			GLY
								L2823			GLY
								L2824			GLY
								L2825			GLY
								L2826			GLY
								L2827			GLY
								L2828			GLY
								L2829			GLY
								L2830			GLY
								L2831			GLY
								L2832			GLY
								L2833			GLY
								L2834			GLY
								L2835			GLY
								L2836			GLY
								L2837			GLY
								L2838			GLY
								L2839			GLY
								L2840			GLY
								L2841			GLY
								L2842			GLY
								L2843			GLY
								L2844			GLY
								L2845			GLY
								L2846			GLY
								L2847			GLY
								L2848			GLY
								L2849			GLY
								L2850			GLY
								L2851			GLY
								L2852			GLY
								L2853			GLY
								L2854			GLY
								L2855			GLY
								L2856			GLY
								L2857			GLY
								L2858			GLY
								L2859			GLY
								L2860			GLY
								L2861			GLY
								L2862			GLY
								L2863			GLY
								L2864			GLY
								L2865			GLY
								L2866			GLY
								L2867			GLY
								L2868			GLY
								L2869			GLY
								L2870			GLY
								L2871			GLY
								L2872			GLY
								L2873			GLY
								L2874			GLY
								L2875			GLY
								L2876			GLY
								L2877			GLY
								L2878			GLY
								L2879			GLY
								L2880			GLY
								L2881			GLY
								L2882			GLY
								L2883			GLY
								L2884			GLY
								L2885			GLY
								L2886			GLY
								L2887			GLY
								L2888			GLY
								L2889			GLY
								L2890			GLY
								L2891			GLY
								L2892			GLY
								L2893			GLY
								L2894			GLY
								L2895			GLY
								L2896			GLY
								L2897			GLY
								L2898			GLY
								L2899			GLY
								L2900			GLY
								L2901			GLY
								L2902			GLY
								L2903			GLY
								L2904			GLY
								L2905			GLY
								L2906			GLY
								L2907			GLY
								L2908			GLY
								L2909			GLY
								L2910			GLY
								L2911			GLY
								L2912			GLY
								L2913			GLY
								L2914			GLY
								L2915			GLY
								L2916			GLY
								L2917			GLY
								L2918			GLY
								L2919			GLY
								L2920			GLY
								L2921			GLY
								L2922			GLY
								L2923	</		

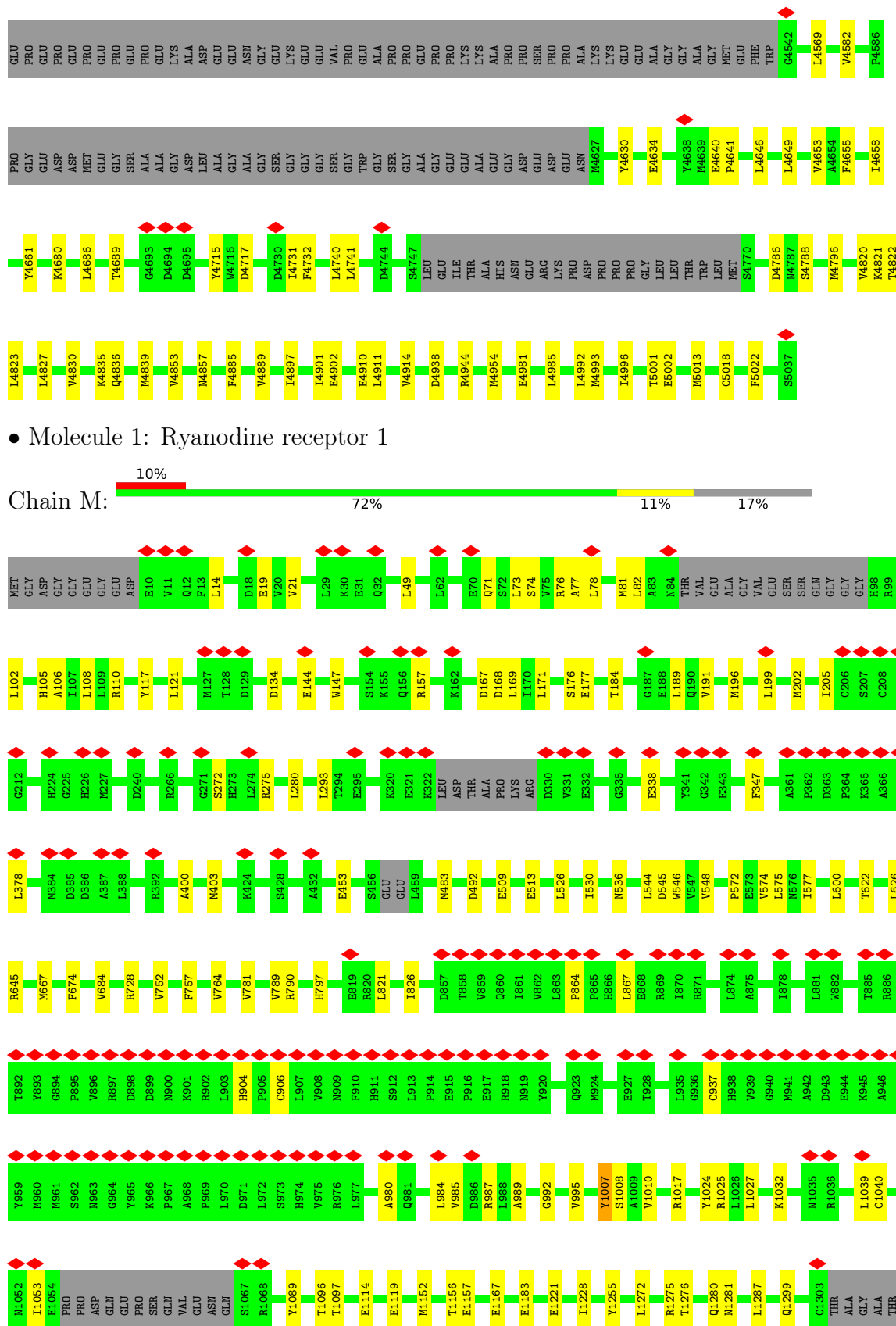


- Molecule 1: Ryanodine receptor 1



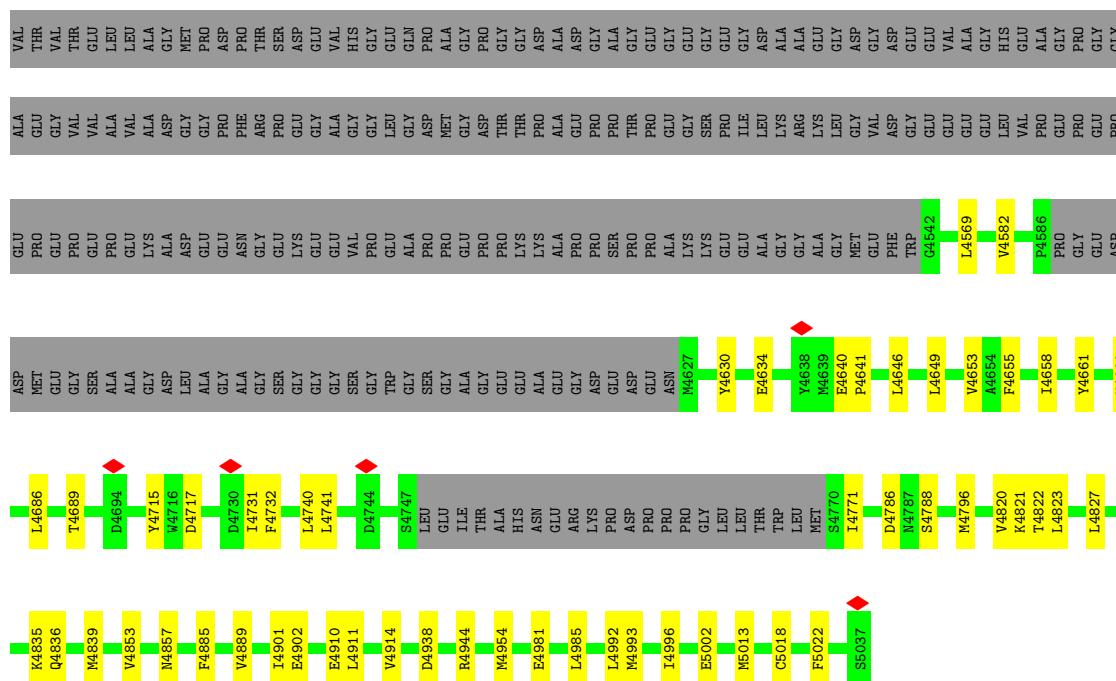




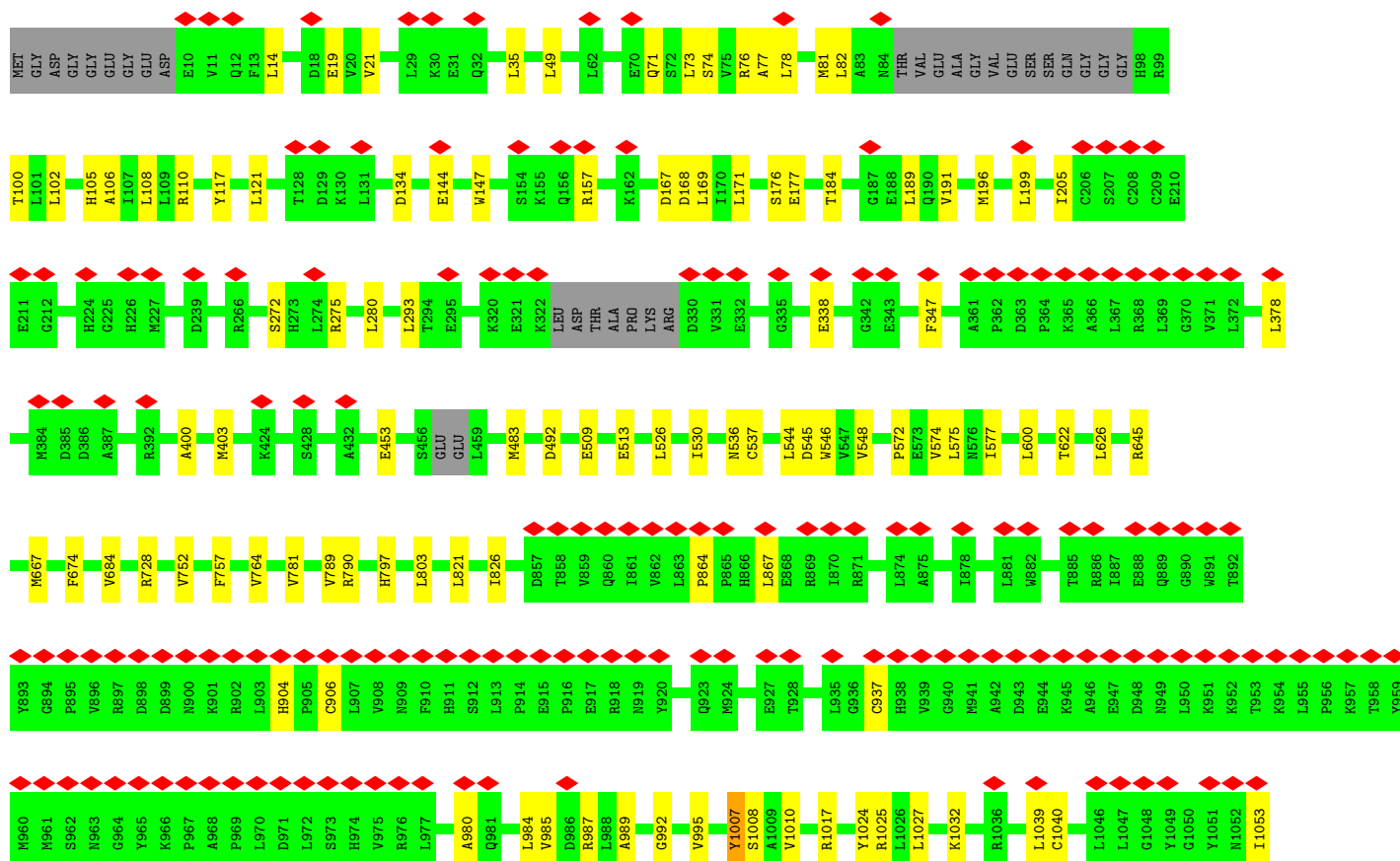






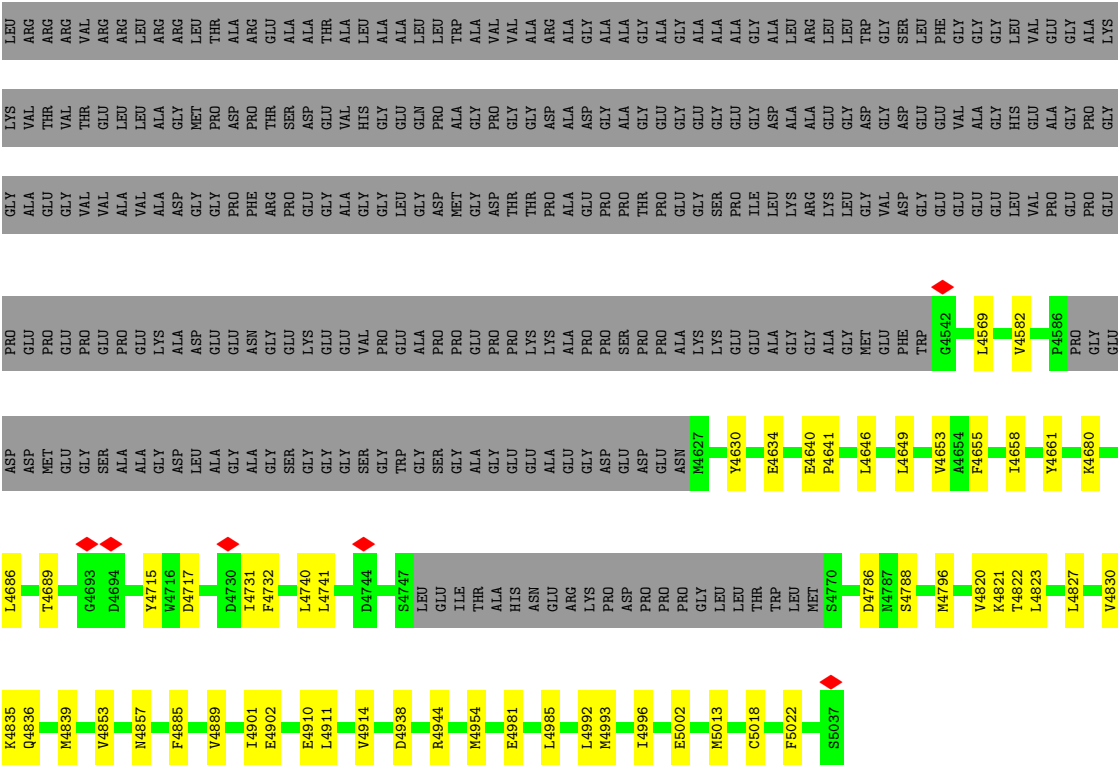


• Molecule 1: Ryanodine receptor 1

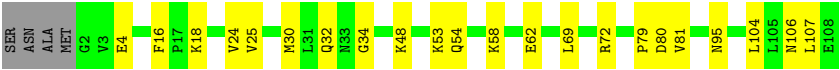








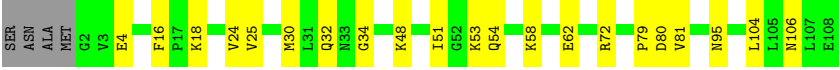
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



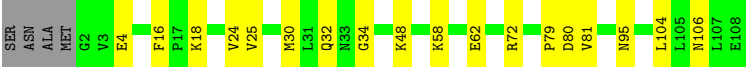
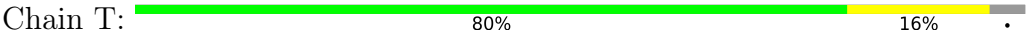
• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



• Molecule 2: Peptidyl-prolyl cis-trans isomerase FKBP1B



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C4	Depositor
Number of particles used	394024	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	500	Depositor
Maximum defocus (nm)	2500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON IV (4k x 4k)	Depositor
Maximum map value	0.773	Depositor
Minimum map value	0.000	Depositor
Average map value	0.003	Depositor
Map value standard deviation	0.021	Depositor
Recommended contour level	0.123	Depositor
Map size (Å)	491.52, 491.52, 491.52	wwPDB
Map dimensions	512, 512, 512	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.96, 0.96, 0.96	Depositor

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 117, CA, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.34	1/33591 (0.0%)	0.51	6/45545 (0.0%)
1	G	0.34	1/33591 (0.0%)	0.51	6/45545 (0.0%)
1	M	0.34	1/33591 (0.0%)	0.51	6/45545 (0.0%)
1	S	0.34	1/33591 (0.0%)	0.51	6/45545 (0.0%)
2	B	0.20	0/826	0.52	0/1112
2	H	0.20	0/826	0.52	0/1112
2	N	0.20	0/826	0.52	0/1112
2	T	0.20	0/826	0.52	0/1112
All	All	0.34	4/137668 (0.0%)	0.51	24/186628 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	3128	ASN	C-O	-6.11	1.17	1.24
1	G	3128	ASN	C-O	-6.11	1.17	1.24
1	A	3128	ASN	C-O	-6.10	1.17	1.24
1	S	3128	ASN	C-O	-6.06	1.17	1.24

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	4073	GLY	CA-C-O	-7.30	115.01	121.58
1	M	4073	GLY	CA-C-O	-7.28	115.02	121.58
1	S	4073	GLY	CA-C-O	-7.27	115.04	121.58
1	A	4073	GLY	CA-C-O	-7.24	115.06	121.58
1	A	1007	TYR	CA-C-O	-6.07	114.51	121.19
1	S	1007	TYR	CA-C-O	-6.07	114.51	121.19
1	M	1007	TYR	CA-C-O	-6.07	114.52	121.19
1	G	1007	TYR	CA-C-O	-6.05	114.53	121.19
1	M	76	ARG	N-CA-C	-5.92	104.74	111.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	76	ARG	N-CA-C	-5.92	104.75	111.14
1	A	76	ARG	N-CA-C	-5.89	104.78	111.14
1	G	76	ARG	N-CA-C	-5.88	104.78	111.14
1	A	3128	ASN	CA-C-O	-5.82	114.71	120.82
1	G	3128	ASN	CA-C-O	-5.76	114.77	120.82
1	M	3128	ASN	CA-C-O	-5.75	114.78	120.82
1	S	3128	ASN	CA-C-O	-5.75	114.78	120.82
1	S	4821	LYS	N-CA-C	5.21	116.81	111.03
1	G	4821	LYS	N-CA-C	5.20	116.80	111.03
1	A	4821	LYS	N-CA-C	5.18	116.78	111.03
1	M	4821	LYS	N-CA-C	5.18	116.78	111.03
1	A	3128	ASN	N-CA-C	-5.16	105.55	111.07
1	G	3128	ASN	N-CA-C	-5.14	105.57	111.07
1	M	3128	ASN	N-CA-C	-5.11	105.60	111.07
1	S	3128	ASN	N-CA-C	-5.11	105.60	111.07

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	32850	0	32148	435	0
1	G	32850	0	32148	432	0
1	M	32850	0	32148	425	0
1	S	32850	0	32148	431	0
2	B	810	0	812	27	0
2	H	810	0	812	27	0
2	N	810	0	812	26	0
2	T	810	0	812	24	0
3	A	1	0	0	0	0
3	G	1	0	0	0	0
3	M	1	0	0	0	0
3	S	1	0	0	0	0
4	A	41	0	34	3	0
4	G	41	0	34	3	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	M	41	0	34	3	0
4	S	41	0	34	3	0
5	A	1	0	0	0	0
5	G	1	0	0	0	0
5	M	1	0	0	0	0
5	S	1	0	0	0	0
All	All	134812	0	131976	1762	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 7.

All (1762) 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)
1:S:4820:VAL:HG21	4:S:5103:117:H85	1.43	1.00
1:A:4820:VAL:HG21	4:A:5103:117:H85	1.43	1.00
1:S:4242:ILE:HD13	1:S:4993:MET:HE3	1.45	0.99
1:M:4242:ILE:HD13	1:M:4993:MET:CE	1.94	0.98
1:M:4820:VAL:HG21	4:M:5103:117:H85	1.43	0.98
1:G:985:VAL:HG11	1:G:1040:CYS:SG	2.04	0.98
1:S:4242:ILE:HD13	1:S:4993:MET:CE	1.94	0.98
1:M:4242:ILE:HD13	1:M:4993:MET:HE3	1.45	0.98
1:S:985:VAL:HG11	1:S:1040:CYS:SG	2.04	0.97
1:A:4242:ILE:HD13	1:A:4993:MET:CE	1.94	0.97
1:A:985:VAL:HG11	1:A:1040:CYS:SG	2.04	0.97
1:G:4820:VAL:HG21	4:G:5103:117:H85	1.43	0.97
1:M:985:VAL:HG11	1:M:1040:CYS:SG	2.04	0.97
1:A:4242:ILE:HD13	1:A:4993:MET:HE3	1.45	0.96
1:G:4242:ILE:HD13	1:G:4993:MET:CE	1.94	0.96
1:G:4242:ILE:HD13	1:G:4993:MET:HE3	1.45	0.95
1:S:3443:ILE:O	1:S:3447:LYS:HG2	1.68	0.94
1:M:3443:ILE:O	1:M:3447:LYS:HG2	1.68	0.94
1:A:3443:ILE:O	1:A:3447:LYS:HG2	1.68	0.93
1:S:3563:VAL:O	1:S:3569:LEU:HD11	1.69	0.93
1:G:3443:ILE:O	1:G:3447:LYS:HG2	1.68	0.92
1:M:3563:VAL:O	1:M:3569:LEU:HD11	1.69	0.92
1:M:4839:MET:HE1	1:S:4822:THR:HG21	1.52	0.92
1:A:3563:VAL:O	1:A:3569:LEU:HD11	1.69	0.92
1:A:4822:THR:HG21	1:S:4839:MET:HE1	1.52	0.91
1:A:4839:MET:HE1	1:G:4822:THR:HG21	1.52	0.91
1:G:4839:MET:HE1	1:M:4822:THR:HG21	1.52	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3563:VAL:O	1:G:3569:LEU:HD11	1.69	0.91
1:M:1299:GLN:CG	2:N:32:GLN:HE22	1.85	0.90
1:G:1299:GLN:CG	2:H:32:GLN:HE22	1.84	0.90
1:S:1299:GLN:CG	2:T:32:GLN:HE22	1.85	0.90
1:S:73:LEU:HD12	1:S:74:SER:O	1.73	0.89
1:A:1299:GLN:CG	2:B:32:GLN:HE22	1.84	0.89
1:A:73:LEU:HD12	1:A:74:SER:O	1.73	0.88
1:G:73:LEU:HD12	1:G:74:SER:O	1.73	0.88
1:M:73:LEU:HD12	1:M:74:SER:O	1.73	0.88
1:G:3535:LEU:O	1:G:3538:THR:HG22	1.74	0.88
1:A:3535:LEU:O	1:A:3538:THR:HG22	1.74	0.88
1:M:1027:LEU:HD23	1:M:1032:LYS:CG	2.04	0.88
1:A:1027:LEU:HD23	1:A:1032:LYS:CG	2.04	0.88
1:G:1027:LEU:HD23	1:G:1032:LYS:CG	2.04	0.87
1:M:3533:ILE:HD13	1:M:3596:VAL:HG23	1.57	0.86
1:M:3535:LEU:O	1:M:3538:THR:HG22	1.74	0.86
1:S:1027:LEU:HD23	1:S:1032:LYS:CG	2.04	0.86
1:S:3535:LEU:O	1:S:3538:THR:HG22	1.74	0.86
1:A:3533:ILE:HD13	1:A:3596:VAL:HG23	1.57	0.85
1:A:1299:GLN:CG	2:B:32:GLN:NE2	2.40	0.85
1:M:1299:GLN:CG	2:N:32:GLN:NE2	2.40	0.84
1:S:1299:GLN:CG	2:T:32:GLN:NE2	2.40	0.84
1:G:1299:GLN:CG	2:H:32:GLN:NE2	2.40	0.84
1:G:3533:ILE:HD13	1:G:3596:VAL:HG23	1.57	0.83
1:A:1299:GLN:HG2	2:B:32:GLN:HE22	1.43	0.83
1:A:1027:LEU:HD23	1:A:1032:LYS:HG3	1.60	0.83
1:S:2324:ASN:OD1	1:S:2326:CYS:SG	2.37	0.83
1:M:1027:LEU:HD23	1:M:1032:LYS:HG3	1.60	0.83
1:G:1299:GLN:HG2	2:H:32:GLN:HE22	1.43	0.83
1:S:5002:GLU:OE1	1:S:5002:GLU:N	2.12	0.83
1:S:3533:ILE:HD13	1:S:3596:VAL:HG23	1.57	0.82
1:G:5002:GLU:N	1:G:5002:GLU:OE1	2.12	0.82
1:A:2324:ASN:OD1	1:A:2326:CYS:SG	2.37	0.82
1:A:5002:GLU:N	1:A:5002:GLU:OE1	2.12	0.82
2:B:24:VAL:HG12	2:B:48:LYS:HG2	1.61	0.82
1:G:1027:LEU:HD23	1:G:1032:LYS:HG3	1.59	0.82
1:G:2324:ASN:OD1	1:G:2326:CYS:SG	2.37	0.82
1:S:4954:MET:HE2	1:S:4954:MET:HA	1.62	0.82
2:T:24:VAL:HG12	2:T:48:LYS:HG2	1.61	0.82
1:S:1299:GLN:HG2	2:T:32:GLN:HE22	1.43	0.82
1:M:5002:GLU:OE1	1:M:5002:GLU:N	2.12	0.82

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:1027:LEU:HD23	1:S:1032:LYS:HG3	1.59	0.82
1:A:1280:GLN:O	1:A:1281:ASN:ND2	2.13	0.82
1:M:2324:ASN:OD1	1:M:2326:CYS:SG	2.37	0.82
1:G:1280:GLN:O	1:G:1281:ASN:ND2	2.13	0.81
1:A:4954:MET:HA	1:A:4954:MET:HE2	1.62	0.81
1:M:2624:ARG:O	1:M:2627:VAL:HG12	1.80	0.81
2:N:24:VAL:HG12	2:N:48:LYS:HG2	1.61	0.81
1:S:1280:GLN:O	1:S:1281:ASN:ND2	2.13	0.81
1:A:2624:ARG:O	1:A:2627:VAL:HG12	1.80	0.81
2:H:24:VAL:HG12	2:H:48:LYS:HG2	1.62	0.81
1:M:1299:GLN:HG2	2:N:32:GLN:HE22	1.43	0.81
1:G:4954:MET:HE2	1:G:4954:MET:HA	1.62	0.81
1:G:1299:GLN:HG2	2:H:32:GLN:NE2	1.96	0.80
1:M:1280:GLN:O	1:M:1281:ASN:ND2	2.13	0.80
1:M:1299:GLN:HG2	2:N:32:GLN:NE2	1.96	0.80
1:M:4954:MET:HE2	1:M:4954:MET:HA	1.62	0.80
1:S:2624:ARG:O	1:S:2627:VAL:HG12	1.80	0.80
1:S:1299:GLN:HG2	2:T:32:GLN:NE2	1.96	0.80
1:A:1299:GLN:HG2	2:B:32:GLN:NE2	1.96	0.80
1:G:2624:ARG:O	1:G:2627:VAL:HG12	1.80	0.80
1:S:2101:MET:HE2	1:S:2101:MET:HA	1.65	0.79
1:M:2101:MET:HE2	1:M:2101:MET:HA	1.65	0.79
1:G:2101:MET:HA	1:G:2101:MET:HE2	1.65	0.77
1:A:4107:GLU:O	1:A:4111:LEU:HD23	1.85	0.77
1:A:2101:MET:HE2	1:A:2101:MET:HA	1.65	0.77
1:M:4107:GLU:O	1:M:4111:LEU:HD23	1.84	0.77
1:G:4107:GLU:O	1:G:4111:LEU:HD23	1.85	0.77
1:S:4107:GLU:O	1:S:4111:LEU:HD23	1.84	0.77
1:G:4242:ILE:CD1	1:G:4993:MET:HE3	2.15	0.77
1:S:1183:GLU:N	1:S:1183:GLU:OE2	2.18	0.76
1:M:1024:TYR:CE1	1:M:1032:LYS:HG2	2.20	0.76
1:S:1024:TYR:CE1	1:S:1032:LYS:HG2	2.20	0.76
1:G:1024:TYR:CE1	1:G:1032:LYS:HG2	2.20	0.76
1:G:1183:GLU:N	1:G:1183:GLU:OE2	2.18	0.76
1:S:4242:ILE:CD1	1:S:4993:MET:HE3	2.15	0.76
1:M:4242:ILE:CD1	1:M:4993:MET:HE3	2.15	0.75
1:A:1183:GLU:N	1:A:1183:GLU:OE2	2.18	0.75
1:M:1183:GLU:N	1:M:1183:GLU:OE2	2.18	0.75
1:A:1024:TYR:CE1	1:A:1032:LYS:HG2	2.20	0.75
1:A:4242:ILE:CD1	1:A:4993:MET:HE3	2.15	0.75
1:M:453:GLU:N	1:M:453:GLU:OE2	2.20	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:21:VAL:HG13	1:S:205:ILE:HD11	1.69	0.75
1:A:21:VAL:HG13	1:A:205:ILE:HD11	1.69	0.75
1:G:1933:GLU:N	1:G:1933:GLU:OE1	2.20	0.75
1:M:3248:ARG:NH2	1:M:3252:ASP:OD1	2.20	0.74
1:M:4839:MET:CE	1:S:4822:THR:HG21	2.17	0.74
1:S:1933:GLU:OE1	1:S:1933:GLU:N	2.20	0.74
1:S:3248:ARG:NH2	1:S:3252:ASP:OD1	2.20	0.74
1:A:453:GLU:N	1:A:453:GLU:OE2	2.20	0.74
1:M:1933:GLU:OE1	1:M:1933:GLU:N	2.19	0.74
1:A:4822:THR:HG21	1:S:4839:MET:CE	2.17	0.74
1:A:1933:GLU:OE1	1:A:1933:GLU:N	2.19	0.74
1:G:3248:ARG:NH2	1:G:3252:ASP:OD1	2.20	0.73
1:G:4839:MET:CE	1:M:4822:THR:HG21	2.17	0.73
1:A:3248:ARG:NH2	1:A:3252:ASP:OD1	2.20	0.73
1:A:4839:MET:CE	1:G:4822:THR:HG21	2.17	0.73
1:S:3333:THR:OG1	1:S:3336:LYS:NZ	2.22	0.73
1:G:21:VAL:HG13	1:G:205:ILE:HD11	1.69	0.73
1:G:453:GLU:N	1:G:453:GLU:OE2	2.20	0.73
1:M:21:VAL:HG13	1:M:205:ILE:HD11	1.69	0.73
1:G:275:ARG:NH2	1:G:338:GLU:OE2	2.22	0.73
1:M:3333:THR:OG1	1:M:3336:LYS:NZ	2.22	0.73
1:S:453:GLU:N	1:S:453:GLU:OE2	2.20	0.73
1:A:275:ARG:NH2	1:A:338:GLU:OE2	2.22	0.73
1:G:3333:THR:OG1	1:G:3336:LYS:NZ	2.22	0.73
1:S:275:ARG:NH2	1:S:338:GLU:OE2	2.22	0.73
1:A:4634:GLU:OE1	1:A:4634:GLU:N	2.23	0.72
1:M:275:ARG:NH2	1:M:338:GLU:OE2	2.22	0.72
1:M:1027:LEU:HD23	1:M:1032:LYS:HG2	1.72	0.72
1:A:3333:THR:OG1	1:A:3336:LYS:NZ	2.22	0.72
1:G:1027:LEU:HD23	1:G:1032:LYS:HG2	1.72	0.72
1:S:1027:LEU:HD23	1:S:1032:LYS:HG2	1.72	0.72
1:G:4634:GLU:OE1	1:G:4634:GLU:N	2.23	0.71
1:S:4634:GLU:N	1:S:4634:GLU:OE1	2.23	0.71
1:A:110:ARG:NH2	1:A:117:TYR:OH	2.24	0.71
1:G:3549:VAL:O	1:G:3553:LEU:HD12	1.90	0.71
1:G:4820:VAL:HG21	4:G:5103:117:C85	2.20	0.71
1:M:4634:GLU:OE1	1:M:4634:GLU:N	2.23	0.71
1:S:3549:VAL:O	1:S:3553:LEU:HD12	1.90	0.71
1:S:4910:GLU:O	1:S:4914:VAL:HG13	1.91	0.71
1:G:73:LEU:HD11	1:G:78:LEU:HB2	1.73	0.71
1:G:110:ARG:NH2	1:G:117:TYR:OH	2.24	0.71

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:3549:VAL:O	1:M:3553:LEU:HD12	1.90	0.71
1:A:3549:VAL:O	1:A:3553:LEU:HD12	1.90	0.71
1:G:4910:GLU:O	1:G:4914:VAL:HG13	1.91	0.71
1:M:4910:GLU:O	1:M:4914:VAL:HG13	1.91	0.71
1:S:73:LEU:HD11	1:S:78:LEU:HB2	1.73	0.70
1:G:19:GLU:OE1	1:G:19:GLU:N	2.23	0.70
1:M:526:LEU:O	1:M:530:ILE:HG22	1.92	0.70
1:S:19:GLU:OE1	1:S:19:GLU:N	2.23	0.70
1:S:110:ARG:NH2	1:S:117:TYR:OH	2.24	0.70
1:A:73:LEU:HD11	1:A:78:LEU:HB2	1.73	0.70
1:G:980:ALA:O	1:G:984:LEU:HD13	1.92	0.70
1:M:4820:VAL:HG21	4:M:5103:117:C85	2.20	0.70
1:M:4839:MET:HE1	1:S:4822:THR:CG2	2.22	0.70
1:A:19:GLU:N	1:A:19:GLU:OE1	2.23	0.70
1:M:110:ARG:NH2	1:M:117:TYR:OH	2.24	0.70
1:S:526:LEU:O	1:S:530:ILE:HG22	1.92	0.70
1:A:980:ALA:O	1:A:984:LEU:HD13	1.92	0.70
1:A:4910:GLU:O	1:A:4914:VAL:HG13	1.91	0.70
1:M:19:GLU:OE1	1:M:19:GLU:N	2.23	0.70
1:G:526:LEU:O	1:G:530:ILE:HG22	1.92	0.70
1:A:2523:ASP:OD2	1:A:2575:ARG:NH2	2.25	0.70
1:M:73:LEU:HD11	1:M:78:LEU:HB2	1.73	0.70
1:S:980:ALA:O	1:S:984:LEU:HD13	1.92	0.70
1:A:4820:VAL:HG21	4:A:5103:117:C85	2.20	0.70
1:A:4822:THR:CG2	1:S:4839:MET:HE1	2.22	0.69
1:G:2523:ASP:OD2	1:G:2575:ARG:NH2	2.25	0.69
1:G:4839:MET:HE1	1:M:4822:THR:CG2	2.22	0.69
1:A:526:LEU:O	1:A:530:ILE:HG22	1.92	0.69
1:A:1027:LEU:HD23	1:A:1032:LYS:HG2	1.72	0.69
1:S:1157:GLU:OE1	1:S:1157:GLU:N	2.26	0.69
1:A:1157:GLU:OE1	1:A:1157:GLU:N	2.26	0.69
1:M:980:ALA:O	1:M:984:LEU:HD13	1.92	0.69
1:S:2523:ASP:OD2	1:S:2575:ARG:NH2	2.25	0.69
1:M:2523:ASP:OD2	1:M:2575:ARG:NH2	2.25	0.69
1:M:4242:ILE:HD13	1:M:4993:MET:HE2	1.75	0.69
1:G:2196:ASN:OD1	1:G:2199:ARG:NH2	2.26	0.69
1:M:2196:ASN:OD1	1:M:2199:ARG:NH2	2.26	0.69
1:S:1228:ILE:O	1:S:1827:ARG:NH1	2.26	0.69
1:G:1228:ILE:O	1:G:1827:ARG:NH1	2.26	0.69
1:M:1228:ILE:O	1:M:1827:ARG:NH1	2.26	0.69
1:A:1228:ILE:O	1:A:1827:ARG:NH1	2.26	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:2196:ASN:OD1	1:S:2199:ARG:NH2	2.26	0.68
1:A:2196:ASN:OD1	1:A:2199:ARG:NH2	2.26	0.68
1:M:1157:GLU:N	1:M:1157:GLU:OE1	2.26	0.68
1:A:4839:MET:HE1	1:G:4822:THR:CG2	2.22	0.68
1:G:1157:GLU:OE1	1:G:1157:GLU:N	2.25	0.68
1:S:4820:VAL:HG21	4:S:5103:117:C85	2.20	0.68
1:G:4242:ILE:HD13	1:G:4993:MET:HE2	1.75	0.67
1:S:3930:ILE:HD11	1:S:3954:ALA:HB1	1.77	0.67
1:A:2629:ASP:O	1:A:2632:ILE:HD12	1.95	0.67
1:A:2670:GLU:OE1	1:A:2670:GLU:N	2.28	0.66
1:A:3930:ILE:HD11	1:A:3954:ALA:HB1	1.77	0.66
1:G:3443:ILE:HG23	1:G:3447:LYS:HE2	1.78	0.66
1:A:3443:ILE:HG23	1:A:3447:LYS:HE2	1.78	0.66
1:M:667:MET:SD	1:M:790:ARG:NH2	2.69	0.66
1:M:2629:ASP:O	1:M:2632:ILE:HD12	1.95	0.66
1:M:2670:GLU:OE1	1:M:2670:GLU:N	2.28	0.66
1:S:4822:THR:HG23	1:S:4823:LEU:HD12	1.78	0.66
1:G:2629:ASP:O	1:G:2632:ILE:HD12	1.95	0.66
1:A:4242:ILE:HD13	1:A:4993:MET:HE2	1.75	0.66
1:M:1535:GLU:N	1:M:1535:GLU:OE1	2.29	0.66
1:M:3930:ILE:HD11	1:M:3954:ALA:HB1	1.77	0.66
1:M:4822:THR:HG23	1:M:4823:LEU:HD12	1.78	0.66
1:G:2670:GLU:OE1	1:G:2670:GLU:N	2.28	0.66
1:S:1535:GLU:OE1	1:S:1535:GLU:N	2.29	0.66
1:S:2629:ASP:O	1:S:2632:ILE:HD12	1.95	0.65
1:S:4731:ILE:HG23	1:S:4732:PHE:HD1	1.61	0.65
1:A:4731:ILE:HG23	1:A:4732:PHE:HD1	1.61	0.65
1:G:293:LEU:HD13	1:G:378:LEU:HD12	1.78	0.65
1:M:3443:ILE:HG23	1:M:3447:LYS:HE2	1.78	0.65
1:S:2670:GLU:N	1:S:2670:GLU:OE1	2.28	0.65
1:G:4836:GLN:OE1	1:G:4836:GLN:N	2.29	0.65
1:M:4836:GLN:N	1:M:4836:GLN:OE1	2.30	0.65
1:G:1096:THR:HG22	1:G:1097:THR:H	1.62	0.65
1:M:4731:ILE:HG23	1:M:4732:PHE:HD1	1.61	0.65
1:G:667:MET:SD	1:G:790:ARG:NH2	2.69	0.65
1:S:667:MET:SD	1:S:790:ARG:NH2	2.69	0.65
1:S:3443:ILE:HG23	1:S:3447:LYS:HE2	1.78	0.65
1:A:667:MET:SD	1:A:790:ARG:NH2	2.69	0.65
1:A:4822:THR:HG23	1:A:4823:LEU:HD12	1.78	0.65
1:G:3930:ILE:HD11	1:G:3954:ALA:HB1	1.77	0.65
1:G:4731:ILE:HG23	1:G:4732:PHE:HD1	1.61	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:4822:THR:HG23	1:G:4823:LEU:HD12	1.78	0.65
1:S:73:LEU:CD1	1:S:74:SER:O	2.45	0.65
1:S:4242:ILE:HD13	1:S:4993:MET:HE2	1.75	0.65
1:A:4836:GLN:OE1	1:A:4836:GLN:N	2.29	0.65
1:M:937:CYS:SG	1:M:984:LEU:HG	2.37	0.65
1:S:1096:THR:HG22	1:S:1097:THR:H	1.62	0.64
1:A:293:LEU:HD13	1:A:378:LEU:HD12	1.78	0.64
1:G:73:LEU:CD1	1:G:74:SER:O	2.45	0.64
1:S:984:LEU:HD12	1:S:987:ARG:HH11	1.63	0.64
1:S:4836:GLN:OE1	1:S:4836:GLN:N	2.30	0.64
1:A:3777:GLU:OE1	1:A:3777:GLU:N	2.30	0.64
1:S:3777:GLU:OE1	1:S:3777:GLU:N	2.30	0.64
2:T:4:GLU:OE1	2:T:4:GLU:N	2.31	0.64
1:A:545:ASP:HA	1:A:548:VAL:HG22	1.80	0.64
1:G:984:LEU:HD12	1:G:987:ARG:HH11	1.62	0.64
1:G:1299:GLN:HG3	2:H:32:GLN:HE22	1.63	0.64
1:A:1299:GLN:HG3	2:B:32:GLN:HE22	1.63	0.64
1:A:4569:LEU:CD2	1:A:4646:LEU:HD22	2.28	0.64
1:G:937:CYS:SG	1:G:984:LEU:HG	2.37	0.64
1:M:545:ASP:HA	1:M:548:VAL:HG22	1.80	0.64
1:S:293:LEU:HD13	1:S:378:LEU:HD12	1.78	0.64
1:S:937:CYS:SG	1:S:984:LEU:HG	2.37	0.64
1:S:4569:LEU:CD2	1:S:4646:LEU:HD22	2.28	0.64
1:G:545:ASP:HA	1:G:548:VAL:HG22	1.80	0.64
2:H:4:GLU:OE1	2:H:4:GLU:N	2.31	0.64
1:M:2150:GLU:OE1	1:M:2150:GLU:N	2.30	0.64
1:G:3777:GLU:N	1:G:3777:GLU:OE1	2.30	0.64
1:M:984:LEU:HD12	1:M:987:ARG:HH11	1.62	0.64
1:M:3777:GLU:OE1	1:M:3777:GLU:N	2.30	0.64
2:N:4:GLU:OE1	2:N:4:GLU:N	2.31	0.64
1:A:937:CYS:SG	1:A:984:LEU:HG	2.37	0.63
1:A:1096:THR:HG22	1:A:1097:THR:H	1.62	0.63
1:G:4569:LEU:CD2	1:G:4646:LEU:HD22	2.28	0.63
1:G:1535:GLU:OE1	1:G:1535:GLU:N	2.29	0.63
1:G:3530:GLN:OE1	1:G:3530:GLN:N	2.32	0.63
1:A:3530:GLN:N	1:A:3530:GLN:OE1	2.32	0.63
1:M:1096:THR:HG22	1:M:1097:THR:H	1.62	0.63
2:B:4:GLU:N	2:B:4:GLU:OE1	2.31	0.63
1:M:2272:PRO:HA	1:M:2275:VAL:HG12	1.81	0.63
1:M:3530:GLN:OE1	1:M:3530:GLN:N	2.32	0.63
1:A:73:LEU:CD1	1:A:74:SER:O	2.45	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:293:LEU:HD13	1:M:378:LEU:HD12	1.78	0.63
1:M:4569:LEU:CD2	1:M:4646:LEU:HD22	2.28	0.63
1:M:4938:ASP:OD1	1:S:4944:ARG:NH1	2.32	0.63
1:A:984:LEU:HD12	1:A:987:ARG:HH11	1.63	0.63
1:A:2272:PRO:HA	1:A:2275:VAL:HG12	1.80	0.63
1:A:3212:GLU:OE1	1:A:3212:GLU:N	2.30	0.62
1:M:674:PHE:CE2	2:N:72:ARG:NH1	2.67	0.62
1:S:545:ASP:HA	1:S:548:VAL:HG22	1.80	0.62
1:S:2272:PRO:HA	1:S:2275:VAL:HG12	1.81	0.62
1:M:3560:GLN:OE1	1:M:3560:GLN:N	2.32	0.62
2:N:58:LYS:O	2:N:62:GLU:HG2	1.99	0.62
1:S:2211:MET:CE	1:S:2232:CYS:HB2	2.29	0.62
1:A:674:PHE:CE2	2:B:72:ARG:NH1	2.67	0.62
1:A:1535:GLU:OE1	1:A:1535:GLU:N	2.29	0.62
1:A:4938:ASP:OD1	1:G:4944:ARG:NH1	2.32	0.62
1:G:674:PHE:CE2	2:H:72:ARG:NH1	2.67	0.62
1:S:2150:GLU:OE1	1:S:2150:GLU:N	2.30	0.62
1:S:3530:GLN:OE1	1:S:3530:GLN:N	2.32	0.62
1:S:3560:GLN:N	1:S:3560:GLN:OE1	2.33	0.62
2:B:58:LYS:O	2:B:62:GLU:HG2	1.99	0.62
1:G:3212:GLU:OE1	1:G:3212:GLU:N	2.30	0.62
1:G:4938:ASP:OD1	1:M:4944:ARG:NH1	2.32	0.62
1:G:2272:PRO:HA	1:G:2275:VAL:HG12	1.80	0.62
1:A:4944:ARG:NH1	1:S:4938:ASP:OD1	2.32	0.62
1:M:73:LEU:CD1	1:M:74:SER:O	2.45	0.62
1:A:2025:GLU:OE1	1:A:2025:GLU:N	2.33	0.62
1:G:2226:PRO:HA	1:G:2229:VAL:HG22	1.82	0.62
1:A:3560:GLN:OE1	1:A:3560:GLN:N	2.33	0.62
1:M:2862:LEU:CD1	1:M:2932:MET:HE1	2.30	0.62
1:A:2150:GLU:OE1	1:A:2150:GLU:N	2.30	0.62
1:S:3175:LEU:HD23	1:S:3175:LEU:O	2.00	0.62
1:G:3020:THR:HG23	1:G:3023:LYS:H	1.65	0.62
1:G:3175:LEU:O	1:G:3175:LEU:HD23	2.00	0.62
1:M:1299:GLN:HG3	2:N:32:GLN:HE22	1.63	0.62
1:M:2211:MET:CE	1:M:2232:CYS:HB2	2.29	0.62
1:M:3020:THR:HG23	1:M:3023:LYS:H	1.65	0.62
1:M:3175:LEU:O	1:M:3175:LEU:HD23	2.00	0.62
1:S:3020:THR:HG23	1:S:3023:LYS:H	1.65	0.62
1:A:177:GLU:OE1	1:A:177:GLU:N	2.33	0.61
1:S:674:PHE:CE2	2:T:72:ARG:NH1	2.67	0.61
2:H:58:LYS:O	2:H:62:GLU:HG2	2.00	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3020:THR:HG23	1:A:3023:LYS:H	1.65	0.61
1:A:3175:LEU:O	1:A:3175:LEU:HD23	2.00	0.61
1:G:2211:MET:CE	1:G:2232:CYS:HB2	2.29	0.61
1:G:4126:GLU:OE1	1:G:4127:GLU:N	2.34	0.61
1:A:2211:MET:CE	1:A:2232:CYS:HB2	2.29	0.61
1:M:4126:GLU:OE1	1:M:4127:GLU:N	2.33	0.61
2:T:58:LYS:O	2:T:62:GLU:HG2	1.99	0.61
1:A:2862:LEU:CD1	1:A:2932:MET:HE1	2.30	0.61
1:A:1924:GLU:OE1	1:A:1924:GLU:N	2.34	0.61
1:M:177:GLU:N	1:M:177:GLU:OE1	2.33	0.61
1:G:177:GLU:OE1	1:G:177:GLU:N	2.33	0.61
1:G:2862:LEU:CD1	1:G:2932:MET:HE1	2.30	0.61
1:M:1924:GLU:N	1:M:1924:GLU:OE1	2.34	0.61
1:S:2862:LEU:CD1	1:S:2932:MET:HE1	2.30	0.61
1:S:4126:GLU:OE1	1:S:4127:GLU:N	2.34	0.61
1:M:674:PHE:CZ	2:N:72:ARG:NH2	2.69	0.61
1:S:1924:GLU:OE1	1:S:1924:GLU:N	2.34	0.61
1:A:4126:GLU:OE1	1:A:4127:GLU:N	2.34	0.61
1:G:674:PHE:CZ	2:H:72:ARG:NH2	2.69	0.61
1:A:2226:PRO:HA	1:A:2229:VAL:HG22	1.82	0.61
1:A:3535:LEU:HD21	1:A:3552:PHE:HE2	1.66	0.61
1:G:1924:GLU:N	1:G:1924:GLU:OE1	2.34	0.61
1:M:73:LEU:HD12	1:M:73:LEU:C	2.26	0.61
1:S:177:GLU:N	1:S:177:GLU:OE1	2.33	0.61
1:G:2150:GLU:OE1	1:G:2150:GLU:N	2.30	0.60
1:A:674:PHE:CZ	2:B:72:ARG:NH2	2.69	0.60
1:S:674:PHE:CZ	2:T:72:ARG:NH2	2.69	0.60
1:G:73:LEU:HD12	1:G:73:LEU:C	2.26	0.60
1:M:2025:GLU:OE1	1:M:2025:GLU:N	2.33	0.60
1:M:2226:PRO:HA	1:M:2229:VAL:HG22	1.82	0.60
1:G:3560:GLN:OE1	1:G:3560:GLN:N	2.33	0.60
1:S:2226:PRO:HA	1:S:2229:VAL:HG22	1.82	0.60
1:S:2598:ALA:O	1:S:2602:VAL:HG23	2.02	0.60
1:A:2598:ALA:O	1:A:2602:VAL:HG23	2.02	0.60
1:S:3212:GLU:OE1	1:S:3212:GLU:N	2.30	0.60
1:M:1114:GLU:OE1	1:M:1114:GLU:N	2.34	0.60
1:M:2710:LEU:HD12	1:M:2711:PRO:HD2	1.84	0.60
1:M:3535:LEU:HD21	1:M:3552:PHE:HE2	1.66	0.60
1:A:73:LEU:HD12	1:A:73:LEU:C	2.26	0.60
1:G:2598:ALA:O	1:G:2602:VAL:HG23	2.02	0.59
1:S:1299:GLN:HG3	2:T:32:GLN:HE22	1.63	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3535:LEU:HD21	1:G:3552:PHE:HE2	1.66	0.59
1:M:2598:ALA:O	1:M:2602:VAL:HG23	2.02	0.59
1:S:3535:LEU:HD21	1:S:3552:PHE:HE2	1.66	0.59
1:A:2710:LEU:HD12	1:A:2711:PRO:HD2	1.84	0.59
1:G:2025:GLU:OE1	1:G:2025:GLU:N	2.33	0.59
1:G:4569:LEU:HD23	1:G:4646:LEU:HD22	1.84	0.59
1:S:2710:LEU:HD12	1:S:2711:PRO:HD2	1.84	0.59
1:A:2313:LEU:HD22	1:A:2318:TYR:CD1	2.38	0.59
1:S:73:LEU:HD12	1:S:73:LEU:C	2.26	0.59
1:S:2025:GLU:N	1:S:2025:GLU:OE1	2.33	0.59
1:S:4569:LEU:HD23	1:S:4646:LEU:HD22	1.84	0.59
1:A:4658:ILE:HD12	1:A:4796:MET:HE2	1.84	0.59
1:S:4658:ILE:HD12	1:S:4796:MET:HE2	1.84	0.59
1:G:2313:LEU:HD22	1:G:2318:TYR:CD1	2.38	0.59
1:G:2710:LEU:HD12	1:G:2711:PRO:HD2	1.84	0.59
1:G:4658:ILE:HD12	1:G:4796:MET:HE2	1.84	0.59
1:S:2313:LEU:HD22	1:S:2318:TYR:CD1	2.38	0.59
1:A:1027:LEU:CD2	1:A:1032:LYS:HG3	2.33	0.58
1:M:2313:LEU:HD22	1:M:2318:TYR:CD1	2.38	0.58
1:S:1114:GLU:OE1	1:S:1114:GLU:N	2.34	0.58
1:M:4658:ILE:HD12	1:M:4796:MET:HE2	1.84	0.58
1:A:2302:LEU:HD23	1:A:2302:LEU:C	2.28	0.58
1:G:2302:LEU:HD23	1:G:2302:LEU:C	2.28	0.58
1:M:1008:SER:HB3	1:M:1017:ARG:HB3	1.86	0.58
1:S:1008:SER:HB3	1:S:1017:ARG:HB3	1.86	0.58
1:M:2302:LEU:C	1:M:2302:LEU:HD23	2.28	0.58
1:S:4680:LYS:HE3	1:S:4686:LEU:HD22	1.86	0.58
1:A:2527:LEU:HD12	1:A:2530:MET:HE2	1.86	0.57
1:A:4569:LEU:HD23	1:A:4646:LEU:HD22	1.84	0.57
1:G:989:ALA:HB2	1:G:1039:LEU:HD12	1.86	0.57
1:G:4740:LEU:HD23	1:G:4741:LEU:HD12	1.86	0.57
1:M:4569:LEU:HD23	1:M:4646:LEU:HD22	1.84	0.57
1:M:4740:LEU:HD23	1:M:4741:LEU:HD12	1.86	0.57
1:M:2109:ASP:OD1	1:M:2109:ASP:N	2.37	0.57
1:M:2527:LEU:HD12	1:M:2530:MET:HE2	1.86	0.57
1:M:3212:GLU:OE1	1:M:3212:GLU:N	2.30	0.57
1:S:864:PRO:HG2	1:S:867:LEU:HB2	1.86	0.57
1:A:989:ALA:HB2	1:A:1039:LEU:HD12	1.86	0.57
1:S:1156:THR:OG1	1:S:1157:GLU:OE1	2.11	0.57
1:S:4740:LEU:HD23	1:S:4741:LEU:HD12	1.86	0.57
1:S:2302:LEU:C	1:S:2302:LEU:HD23	2.28	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3604:TYR:O	1:A:3608:GLN:HG2	2.05	0.57
1:G:864:PRO:HG2	1:G:867:LEU:HB2	1.86	0.57
1:G:3604:TYR:O	1:G:3608:GLN:HG2	2.05	0.57
1:G:4680:LYS:HE3	1:G:4686:LEU:HD22	1.86	0.57
1:M:989:ALA:HB2	1:M:1039:LEU:HD12	1.86	0.57
1:A:4740:LEU:HD23	1:A:4741:LEU:HD12	1.86	0.57
1:M:544:LEU:O	1:M:548:VAL:HG13	2.05	0.57
1:A:1008:SER:HB3	1:A:1017:ARG:HB3	1.86	0.57
1:A:3078:ARG:NH1	1:A:3155:ASP:OD2	2.38	0.57
1:G:1008:SER:HB3	1:G:1017:ARG:HB3	1.86	0.57
1:G:544:LEU:O	1:G:548:VAL:HG13	2.05	0.57
1:G:2109:ASP:OD1	1:G:2109:ASP:N	2.37	0.57
1:M:3078:ARG:NH1	1:M:3155:ASP:OD2	2.38	0.57
1:S:544:LEU:O	1:S:548:VAL:HG13	2.05	0.56
1:A:989:ALA:HA	1:A:1039:LEU:CD1	2.35	0.56
1:A:4680:LYS:HE3	1:A:4686:LEU:HD22	1.86	0.56
1:G:2622:LEU:O	1:G:2626:LEU:HD22	2.06	0.56
1:M:674:PHE:HZ	2:N:72:ARG:NH2	2.03	0.56
1:M:989:ALA:HA	1:M:1039:LEU:CD1	2.35	0.56
1:A:864:PRO:HG2	1:A:867:LEU:HB2	1.86	0.56
1:G:3078:ARG:NH1	1:G:3155:ASP:OD2	2.38	0.56
1:S:989:ALA:HA	1:S:1039:LEU:CD1	2.35	0.56
1:S:1027:LEU:CD2	1:S:1032:LYS:HG3	2.33	0.56
1:S:2807:TRP:HB3	1:S:2808:PRO:HD3	1.88	0.56
1:A:674:PHE:HZ	2:B:72:ARG:NH2	2.03	0.56
1:G:1114:GLU:OE1	1:G:1114:GLU:N	2.34	0.56
1:A:2807:TRP:HB3	1:A:2808:PRO:HD3	1.88	0.56
1:S:2527:LEU:HD12	1:S:2530:MET:HE2	1.86	0.56
1:S:3078:ARG:NH1	1:S:3155:ASP:OD2	2.38	0.56
1:A:2622:LEU:O	1:A:2626:LEU:HD22	2.06	0.56
1:S:674:PHE:HZ	2:T:72:ARG:NH2	2.03	0.56
1:S:989:ALA:HB2	1:S:1039:LEU:HD12	1.86	0.56
1:A:81:MET:HA	1:A:81:MET:HE3	1.88	0.56
1:G:674:PHE:HZ	2:H:72:ARG:NH2	2.03	0.56
1:S:3606:LEU:O	1:S:3609:THR:HG22	2.06	0.56
1:G:2527:LEU:HD12	1:G:2530:MET:HE2	1.86	0.56
1:G:4661:TYR:OH	1:G:4788:SER:OG	2.22	0.56
1:M:4680:LYS:HE3	1:M:4686:LEU:HD22	1.86	0.56
1:A:544:LEU:O	1:A:548:VAL:HG13	2.05	0.56
1:M:1027:LEU:CD2	1:M:1032:LYS:HG3	2.33	0.56
1:M:2622:LEU:O	1:M:2626:LEU:HD22	2.06	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:4661:TYR:OH	1:M:4788:SER:OG	2.22	0.56
1:S:3604:TYR:O	1:S:3608:GLN:HG2	2.05	0.56
1:G:3606:LEU:O	1:G:3609:THR:HG22	2.06	0.56
1:M:2302:LEU:HD22	1:M:2363:CYS:HB3	1.87	0.56
1:M:2807:TRP:HB3	1:M:2808:PRO:HD3	1.88	0.56
1:G:81:MET:HA	1:G:81:MET:HE3	1.88	0.55
1:G:989:ALA:HB2	1:G:1039:LEU:CD1	2.36	0.55
1:A:509:GLU:O	1:A:513:GLU:CD	2.49	0.55
1:M:168:ASP:C	1:M:169:LEU:HD12	2.31	0.55
1:S:2622:LEU:O	1:S:2626:LEU:HD22	2.06	0.55
1:G:864:PRO:HG3	1:G:867:LEU:HD12	1.89	0.55
1:S:989:ALA:HB2	1:S:1039:LEU:CD1	2.36	0.55
1:G:3211:ASN:OD1	1:G:3211:ASN:O	2.25	0.55
1:M:864:PRO:HG2	1:M:867:LEU:HB2	1.86	0.55
1:M:989:ALA:HB2	1:M:1039:LEU:CD1	2.36	0.55
1:M:1156:THR:OG1	1:M:1157:GLU:OE1	2.11	0.55
1:M:3522:LEU:O	1:M:3525:CYS:SG	2.56	0.55
1:M:3604:TYR:O	1:M:3608:GLN:HG2	2.05	0.55
1:S:3330:ASP:OD1	1:S:3331:GLU:N	2.40	0.55
1:G:509:GLU:O	1:G:513:GLU:CD	2.50	0.55
1:G:989:ALA:HA	1:G:1039:LEU:CD1	2.36	0.55
1:M:2211:MET:HE3	1:M:2232:CYS:HB2	1.89	0.55
1:M:3606:LEU:O	1:M:3609:THR:HG22	2.06	0.55
1:A:168:ASP:C	1:A:169:LEU:HD12	2.31	0.55
1:A:2302:LEU:HD22	1:A:2363:CYS:HB3	1.87	0.55
1:A:3330:ASP:OD1	1:A:3331:GLU:N	2.40	0.55
1:G:1454:THR:OG1	1:G:1456:ASP:OD1	2.23	0.55
1:M:757:PHE:HB2	1:M:764:VAL:HG21	1.89	0.55
1:S:757:PHE:HB2	1:S:764:VAL:HG21	1.89	0.55
1:S:2499:LYS:O	1:S:2503:VAL:HG23	2.07	0.55
1:A:2109:ASP:N	1:A:2109:ASP:OD1	2.37	0.55
1:G:2302:LEU:HD22	1:G:2363:CYS:HB3	1.87	0.55
1:M:157:ARG:NH1	1:M:167:ASP:OD2	2.40	0.55
1:M:3517:MET:O	1:M:3520:ILE:HG22	2.07	0.55
1:S:509:GLU:O	1:S:513:GLU:CD	2.49	0.55
1:S:3517:MET:O	1:S:3520:ILE:HG22	2.07	0.55
1:A:864:PRO:HG3	1:A:867:LEU:HD12	1.88	0.55
1:G:2807:TRP:HB3	1:G:2808:PRO:HD3	1.88	0.55
1:G:3522:LEU:O	1:G:3525:CYS:SG	2.56	0.55
1:G:4089:SER:HA	1:G:4121:GLU:HA	1.89	0.55
1:S:168:ASP:C	1:S:169:LEU:HD12	2.31	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:509:GLU:O	1:M:513:GLU:CD	2.50	0.55
1:S:49:LEU:HD21	1:S:191:VAL:HG21	1.89	0.55
1:S:2109:ASP:N	1:S:2109:ASP:OD1	2.37	0.55
1:G:168:ASP:C	1:G:169:LEU:HD12	2.31	0.54
1:M:3330:ASP:OD1	1:M:3331:GLU:N	2.40	0.54
1:A:2499:LYS:O	1:A:2503:VAL:HG23	2.07	0.54
1:G:1027:LEU:CD2	1:G:1032:LYS:HG3	2.33	0.54
1:S:81:MET:HA	1:S:81:MET:HE3	1.88	0.54
1:M:78:LEU:HD22	1:M:106:ALA:CB	2.38	0.54
1:M:2778:GLY:HA3	1:M:2787:THR:HB	1.89	0.54
1:S:2302:LEU:HD22	1:S:2363:CYS:HB3	1.87	0.54
1:S:3211:ASN:OD1	1:S:3211:ASN:O	2.25	0.54
1:S:4089:SER:HA	1:S:4121:GLU:HA	1.89	0.54
1:A:4661:TYR:OH	1:A:4788:SER:OG	2.22	0.54
1:G:2211:MET:HE3	1:G:2232:CYS:HB2	1.89	0.54
1:A:989:ALA:HB2	1:A:1039:LEU:CD1	2.36	0.54
1:A:3606:LEU:O	1:A:3609:THR:HG22	2.06	0.54
1:M:184:THR:HG22	1:M:189:LEU:HD22	1.90	0.54
1:S:4661:TYR:OH	1:S:4788:SER:OG	2.22	0.54
1:G:2778:GLY:HA3	1:G:2787:THR:HB	1.89	0.54
1:M:81:MET:HA	1:M:81:MET:HE3	1.88	0.54
1:M:2499:LYS:O	1:M:2503:VAL:HG23	2.07	0.54
1:S:864:PRO:HG3	1:S:867:LEU:HD12	1.88	0.54
1:S:2211:MET:HE3	1:S:2232:CYS:HB2	1.89	0.54
1:S:4661:TYR:OH	1:S:4786:ASP:OD2	2.26	0.54
1:G:78:LEU:HD22	1:G:106:ALA:CB	2.38	0.54
1:G:3330:ASP:OD1	1:G:3331:GLU:N	2.40	0.54
1:M:864:PRO:HG3	1:M:867:LEU:HD12	1.89	0.54
1:S:184:THR:HG22	1:S:189:LEU:HD22	1.90	0.54
1:S:1454:THR:OG1	1:S:1456:ASP:OD1	2.23	0.54
1:A:157:ARG:NH1	1:A:167:ASP:OD2	2.40	0.54
1:A:1454:THR:OG1	1:A:1456:ASP:OD1	2.23	0.54
2:N:30:MET:CE	2:N:34:GLY:HA2	2.38	0.54
1:A:2211:MET:HE3	1:A:2232:CYS:HB2	1.89	0.54
1:A:3573:MET:O	1:A:3577:ARG:HD3	2.08	0.54
1:G:3517:MET:O	1:G:3520:ILE:HG22	2.07	0.54
1:S:78:LEU:HD22	1:S:106:ALA:CB	2.38	0.54
2:H:30:MET:CE	2:H:34:GLY:HA2	2.38	0.54
1:M:3211:ASN:OD1	1:M:3211:ASN:O	2.25	0.54
1:M:4661:TYR:OH	1:M:4786:ASP:OD2	2.26	0.54
1:A:49:LEU:HD21	1:A:191:VAL:HG21	1.89	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:LEU:HD22	1:A:106:ALA:CB	2.37	0.53
1:A:757:PHE:HB2	1:A:764:VAL:HG21	1.89	0.53
1:A:3211:ASN:O	1:A:3211:ASN:OD1	2.25	0.53
1:A:4089:SER:HA	1:A:4121:GLU:HA	1.89	0.53
1:M:49:LEU:HD21	1:M:191:VAL:HG21	1.89	0.53
1:M:4089:SER:HA	1:M:4121:GLU:HA	1.89	0.53
1:A:1114:GLU:OE1	1:A:1114:GLU:N	2.34	0.53
1:A:2778:GLY:HA3	1:A:2787:THR:HB	1.89	0.53
1:G:757:PHE:HB2	1:G:764:VAL:HG21	1.89	0.53
1:G:4106:PRO:HA	1:G:4109:GLN:OE1	2.09	0.53
2:T:30:MET:CE	2:T:34:GLY:HA2	2.38	0.53
1:G:2660:GLY:HA3	1:G:2666:VAL:HG12	1.91	0.53
1:A:184:THR:HG22	1:A:189:LEU:CD2	2.39	0.53
1:A:2660:GLY:HA3	1:A:2666:VAL:HG12	1.91	0.53
1:G:2499:LYS:O	1:G:2503:VAL:HG23	2.07	0.53
1:G:4202:ARG:O	1:G:4206:GLU:OE1	2.26	0.53
1:A:4106:PRO:HA	1:A:4109:GLN:OE1	2.08	0.53
1:G:184:THR:HG22	1:G:189:LEU:CD2	2.39	0.53
1:G:4661:TYR:OH	1:G:4786:ASP:OD2	2.26	0.53
1:S:184:THR:HG22	1:S:189:LEU:CD2	2.39	0.53
1:S:4202:ARG:O	1:S:4206:GLU:OE1	2.26	0.53
1:A:184:THR:HG22	1:A:189:LEU:HD22	1.90	0.53
1:A:3522:LEU:O	1:A:3525:CYS:SG	2.56	0.53
1:G:49:LEU:HD21	1:G:191:VAL:HG21	1.89	0.53
1:G:5001:THR:OG1	1:G:5002:GLU:OE1	2.20	0.53
1:A:3840:SER:OG	1:A:3877:ASP:OD1	2.27	0.53
2:B:80:ASP:OD2	2:B:81:VAL:HG23	2.09	0.53
1:M:184:THR:HG22	1:M:189:LEU:CD2	2.39	0.53
1:M:4202:ARG:O	1:M:4206:GLU:OE1	2.26	0.53
2:N:80:ASP:OD2	2:N:81:VAL:HG23	2.09	0.53
1:G:3573:MET:O	1:G:3577:ARG:HD3	2.08	0.53
1:G:4060:LYS:O	1:G:4063:ASP:OD1	2.27	0.53
1:M:757:PHE:O	1:M:764:VAL:HG22	2.09	0.53
2:T:80:ASP:OD2	2:T:81:VAL:HG23	2.09	0.53
1:G:157:ARG:NH1	1:G:167:ASP:OD2	2.40	0.53
1:S:3169:LEU:C	1:S:3169:LEU:HD23	2.34	0.53
1:G:3840:SER:OG	1:G:3877:ASP:OD1	2.27	0.53
2:H:80:ASP:OD2	2:H:81:VAL:HG23	2.09	0.53
1:S:2778:GLY:HA3	1:S:2787:THR:HB	1.89	0.53
1:S:3573:MET:O	1:S:3577:ARG:HD3	2.08	0.53
1:S:4060:LYS:O	1:S:4063:ASP:OD1	2.27	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2211:MET:HE3	1:A:2232:CYS:CB	2.39	0.52
1:A:3517:MET:O	1:A:3520:ILE:HG22	2.07	0.52
1:A:5001:THR:OG1	1:A:5002:GLU:OE1	2.20	0.52
1:M:4060:LYS:O	1:M:4063:ASP:OD1	2.27	0.52
1:M:4106:PRO:HA	1:M:4109:GLN:OE1	2.08	0.52
1:S:157:ARG:NH1	1:S:167:ASP:OD2	2.40	0.52
2:B:30:MET:CE	2:B:34:GLY:HA2	2.38	0.52
1:M:3573:MET:O	1:M:3577:ARG:HD3	2.08	0.52
1:S:4106:PRO:HA	1:S:4109:GLN:OE1	2.08	0.52
1:A:3169:LEU:HD23	1:A:3169:LEU:C	2.34	0.52
1:A:3527:PRO:O	1:A:3530:GLN:OE1	2.27	0.52
1:G:184:THR:HG22	1:G:189:LEU:HD22	1.90	0.52
1:M:3132:THR:HG23	1:M:3136:LEU:HD23	1.92	0.52
1:S:3522:LEU:O	1:S:3525:CYS:SG	2.56	0.52
1:A:757:PHE:O	1:A:764:VAL:HG22	2.09	0.52
1:S:757:PHE:O	1:S:764:VAL:HG22	2.09	0.52
1:S:1944:GLU:HG3	1:S:2126:ARG:HH12	1.75	0.52
1:S:3132:THR:HG23	1:S:3136:LEU:HD23	1.92	0.52
1:S:3527:PRO:O	1:S:3530:GLN:OE1	2.27	0.52
1:A:3132:THR:HG23	1:A:3136:LEU:HD23	1.92	0.52
1:A:4060:LYS:O	1:A:4063:ASP:OD1	2.27	0.52
1:M:2211:MET:HE3	1:M:2232:CYS:CB	2.39	0.52
1:M:3169:LEU:HD23	1:M:3169:LEU:C	2.34	0.52
1:M:3527:PRO:O	1:M:3530:GLN:OE1	2.27	0.52
1:M:4911:LEU:O	1:M:4914:VAL:HG22	2.10	0.52
1:S:2211:MET:HE3	1:S:2232:CYS:CB	2.39	0.52
1:S:2660:GLY:HA3	1:S:2666:VAL:HG12	1.91	0.52
1:S:4827:LEU:O	1:S:4830:VAL:HG12	2.10	0.52
1:A:1944:GLU:HG3	1:A:2126:ARG:HH12	1.75	0.52
1:M:3264:THR:OG1	1:M:3265:GLU:OE1	2.27	0.52
1:M:2660:GLY:HA3	1:M:2666:VAL:HG12	1.91	0.52
1:A:4202:ARG:O	1:A:4206:GLU:OE1	2.26	0.52
1:A:4661:TYR:OH	1:A:4786:ASP:OD2	2.26	0.52
1:G:2211:MET:HE3	1:G:2232:CYS:CB	2.39	0.52
2:H:58:LYS:NZ	2:H:62:GLU:OE1	2.43	0.52
1:S:3129:LEU:O	1:S:3133:THR:HG22	2.10	0.52
1:G:4911:LEU:O	1:G:4914:VAL:HG22	2.10	0.52
1:M:4827:LEU:O	1:M:4830:VAL:HG12	2.10	0.52
2:N:58:LYS:NZ	2:N:62:GLU:OE1	2.43	0.52
1:S:3264:THR:OG1	1:S:3265:GLU:OE1	2.27	0.52
1:A:3264:THR:OG1	1:A:3265:GLU:OE1	2.27	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:58:LYS:NZ	2:B:62:GLU:OE1	2.43	0.51
1:G:757:PHE:O	1:G:764:VAL:HG22	2.09	0.51
1:G:1944:GLU:HG3	1:G:2126:ARG:HH12	1.75	0.51
1:G:3129:LEU:O	1:G:3133:THR:HG22	2.10	0.51
1:S:2966:TRP:HA	1:S:2969:ILE:HD12	1.92	0.51
2:T:58:LYS:NZ	2:T:62:GLU:OE1	2.43	0.51
1:G:3132:THR:HG23	1:G:3136:LEU:HD23	1.92	0.51
1:A:3129:LEU:O	1:A:3133:THR:HG22	2.10	0.51
1:A:4072:VAL:O	1:A:4076:ALA:HB2	2.10	0.51
1:G:2966:TRP:HA	1:G:2969:ILE:HD12	1.92	0.51
1:G:4207:MET:O	1:G:4210:VAL:HG22	2.10	0.51
1:G:3527:PRO:O	1:G:3530:GLN:OE1	2.27	0.51
1:M:2490:MET:HE1	1:M:2546:MET:HE1	1.92	0.51
1:M:2966:TRP:HA	1:M:2969:ILE:HD12	1.92	0.51
1:G:3169:LEU:HD23	1:G:3169:LEU:C	2.34	0.51
2:N:24:VAL:HG22	2:N:106:ASN:HB3	1.92	0.51
1:S:4207:MET:HA	1:S:4207:MET:HE3	1.93	0.51
1:A:1089:TYR:HD2	1:A:1152:MET:HG2	1.76	0.51
1:S:1272:LEU:HD23	1:S:1561:VAL:HG21	1.92	0.51
1:S:4911:LEU:O	1:S:4914:VAL:HG22	2.10	0.51
1:A:4207:MET:HA	1:A:4207:MET:HE3	1.93	0.51
2:H:24:VAL:HG22	2:H:106:ASN:HB3	1.92	0.51
1:M:3175:LEU:HD21	1:M:3183:VAL:CG1	2.41	0.51
1:A:4911:LEU:O	1:A:4914:VAL:HG22	2.10	0.51
1:G:3989:VAL:CG1	1:G:4047:MET:HE2	2.41	0.51
1:G:4207:MET:HA	1:G:4207:MET:HE3	1.93	0.51
1:M:3989:VAL:CG1	1:M:4047:MET:HE2	2.41	0.51
1:G:1089:TYR:HD2	1:G:1152:MET:HG2	1.76	0.51
1:A:4827:LEU:O	1:A:4830:VAL:HG12	2.10	0.51
1:M:4072:VAL:O	1:M:4076:ALA:HB2	2.11	0.51
1:G:2490:MET:HE1	1:G:2546:MET:HE1	1.92	0.50
1:G:4072:VAL:O	1:G:4076:ALA:HB2	2.10	0.50
1:G:4853:VAL:O	1:G:4857:ASN:ND2	2.44	0.50
1:M:1944:GLU:HG3	1:M:2126:ARG:HH12	1.75	0.50
1:M:2116:LEU:O	1:M:2120:MET:HG2	2.11	0.50
1:S:1089:TYR:HD2	1:S:1152:MET:HG2	1.76	0.50
1:A:3989:VAL:CG1	1:A:4047:MET:HE2	2.41	0.50
1:G:4242:ILE:CD1	1:G:4993:MET:CE	2.79	0.50
1:M:2588:ARG:NH2	1:M:2901:THR:HG21	2.27	0.50
1:M:4207:MET:O	1:M:4210:VAL:HG22	2.10	0.50
1:S:3590:GLU:O	1:S:3594:ARG:HG2	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:4207:MET:O	1:S:4210:VAL:HG22	2.11	0.50
1:A:2490:MET:HE1	1:A:2546:MET:HE1	1.92	0.50
1:A:3590:GLU:O	1:A:3594:ARG:HG2	2.12	0.50
1:A:3969:ILE:HG21	1:A:3980:LEU:HD12	1.94	0.50
1:A:4839:MET:HE1	1:G:4822:THR:CB	2.42	0.50
1:A:4853:VAL:O	1:A:4857:ASN:ND2	2.44	0.50
1:G:2116:LEU:O	1:G:2120:MET:HG2	2.11	0.50
1:G:3264:THR:OG1	1:G:3265:GLU:OE1	2.27	0.50
1:M:1089:TYR:HD2	1:M:1152:MET:HG2	1.76	0.50
1:S:2116:LEU:O	1:S:2120:MET:HG2	2.11	0.50
1:S:3175:LEU:HD21	1:S:3183:VAL:CG1	2.41	0.50
1:S:3840:SER:OG	1:S:3877:ASP:OD1	2.27	0.50
1:S:4072:VAL:O	1:S:4076:ALA:HB2	2.10	0.50
2:T:24:VAL:HG22	2:T:106:ASN:HB3	1.93	0.50
1:A:3445:TRP:HA	1:A:3451:PHE:CD2	2.47	0.50
1:G:3969:ILE:HG21	1:G:3980:LEU:HD12	1.94	0.50
1:G:4827:LEU:O	1:G:4830:VAL:HG12	2.10	0.50
1:M:3324:VAL:HA	1:M:3327:LEU:CD2	2.42	0.50
1:M:4078:GLN:O	1:M:4079:ASP:OD1	2.30	0.50
1:S:3445:TRP:HA	1:S:3451:PHE:CD2	2.47	0.50
1:A:2966:TRP:HA	1:A:2969:ILE:HD12	1.92	0.50
1:G:1272:LEU:HD23	1:G:1561:VAL:HG21	1.92	0.50
1:G:3106:MET:HE3	1:G:3132:THR:HG21	1.93	0.50
1:M:1272:LEU:HD23	1:M:1561:VAL:HG21	1.92	0.50
1:S:2490:MET:HE1	1:S:2546:MET:HE1	1.92	0.50
1:A:2116:LEU:O	1:A:2120:MET:HG2	2.11	0.50
1:A:4207:MET:O	1:A:4210:VAL:HG22	2.11	0.50
1:M:4853:VAL:O	1:M:4857:ASN:ND2	2.44	0.50
1:S:3106:MET:HE3	1:S:3132:THR:HG21	1.93	0.50
1:S:3324:VAL:HA	1:S:3327:LEU:CD2	2.42	0.50
1:S:4078:GLN:O	1:S:4079:ASP:OD1	2.30	0.50
2:B:24:VAL:HG22	2:B:106:ASN:HB3	1.92	0.50
1:G:3590:GLU:O	1:G:3594:ARG:HG2	2.12	0.50
1:M:3969:ILE:HG21	1:M:3980:LEU:HD12	1.94	0.50
1:S:3989:VAL:CG1	1:S:4047:MET:HE2	2.41	0.50
1:A:2018:GLU:OE2	1:A:2028:ARG:NE	2.45	0.50
1:A:2588:ARG:NH2	1:A:2901:THR:HG21	2.27	0.50
1:A:2974:ILE:HD12	1:A:3057:PHE:CE1	2.47	0.50
1:A:4078:GLN:O	1:A:4079:ASP:OD1	2.30	0.50
1:G:3175:LEU:HD21	1:G:3183:VAL:CG1	2.41	0.50
1:M:2018:GLU:OE2	1:M:2028:ARG:NE	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:3445:TRP:HA	1:M:3451:PHE:CD2	2.47	0.50
1:S:2668:SER:OG	1:S:2671:GLU:OE1	2.27	0.50
1:A:2313:LEU:HD22	1:A:2318:TYR:CG	2.47	0.50
1:A:4242:ILE:CD1	1:A:4993:MET:CE	2.79	0.50
1:G:2018:GLU:OE2	1:G:2028:ARG:NE	2.45	0.50
1:M:3129:LEU:O	1:M:3133:THR:HG22	2.10	0.50
1:A:2123:LEU:O	1:A:2127:GLN:HG2	2.12	0.49
1:G:3324:VAL:HA	1:G:3327:LEU:CD2	2.42	0.49
1:M:1868:PRO:O	1:M:1872:THR:OG1	2.30	0.49
1:M:2313:LEU:HD22	1:M:2318:TYR:CG	2.47	0.49
1:S:2124:LEU:HD11	1:S:2128:TYR:HE1	1.77	0.49
1:A:3324:VAL:HA	1:A:3327:LEU:CD2	2.42	0.49
1:G:2123:LEU:O	1:G:2127:GLN:HG2	2.12	0.49
1:M:2974:ILE:HD12	1:M:3057:PHE:CE1	2.47	0.49
1:M:3540:TYR:CE1	1:M:3549:VAL:HG21	2.48	0.49
1:S:2588:ARG:NH2	1:S:2901:THR:HG21	2.27	0.49
1:S:3969:ILE:HG21	1:S:3980:LEU:HD12	1.94	0.49
1:A:1272:LEU:HD23	1:A:1561:VAL:HG21	1.92	0.49
1:G:2627:VAL:HG11	1:G:2674:LEU:CD1	2.43	0.49
1:G:3320:LEU:O	1:G:3323:ILE:HG22	2.13	0.49
1:M:4207:MET:HA	1:M:4207:MET:HE3	1.93	0.49
1:S:3320:LEU:O	1:S:3323:ILE:HG22	2.13	0.49
1:A:3175:LEU:HD21	1:A:3183:VAL:CG1	2.41	0.49
1:G:2313:LEU:HD22	1:G:2318:TYR:CG	2.47	0.49
1:G:3445:TRP:HA	1:G:3451:PHE:CD2	2.47	0.49
1:M:1454:THR:OG1	1:M:1456:ASP:OD1	2.23	0.49
1:M:2627:VAL:HG11	1:M:2674:LEU:CD1	2.43	0.49
1:M:3590:GLU:O	1:M:3594:ARG:HG2	2.11	0.49
1:S:3757:GLU:HA	1:S:3760:LYS:NZ	2.27	0.49
1:A:4088:ILE:HG21	1:A:4125:PHE:CZ	2.48	0.49
1:G:4740:LEU:HD23	1:G:4741:LEU:CD1	2.43	0.49
1:M:2123:LEU:O	1:M:2127:GLN:HG2	2.12	0.49
1:M:2265:LEU:CD1	1:M:2330:ARG:HD2	2.43	0.49
1:M:4839:MET:HE1	1:S:4822:THR:CB	2.42	0.49
1:S:2123:LEU:O	1:S:2127:GLN:HG2	2.12	0.49
1:A:3757:GLU:HA	1:A:3760:LYS:NZ	2.27	0.49
1:M:4160:LEU:O	1:M:4164:LEU:HD22	2.13	0.49
1:S:2313:LEU:HD22	1:S:2318:TYR:CG	2.47	0.49
1:A:752:VAL:O	1:A:752:VAL:HG13	2.13	0.49
1:A:1868:PRO:O	1:A:1872:THR:OG1	2.30	0.49
1:G:3540:TYR:CE1	1:G:3549:VAL:HG21	2.48	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:3320:LEU:O	1:M:3323:ILE:HG22	2.13	0.49
1:M:3435:PHE:HA	1:M:3517:MET:HE2	1.95	0.49
1:S:1024:TYR:HE1	1:S:1032:LYS:HG2	1.74	0.49
1:S:2974:ILE:HD12	1:S:3057:PHE:CE1	2.47	0.49
1:S:3540:TYR:CE1	1:S:3549:VAL:HG21	2.47	0.49
1:A:4822:THR:CB	1:S:4839:MET:HE1	2.42	0.49
1:G:577:ILE:O	1:G:577:ILE:HG22	2.13	0.49
1:M:3735:LEU:HD22	1:M:3735:LEU:N	2.28	0.49
1:S:73:LEU:HD12	1:S:73:LEU:O	2.12	0.49
1:S:4981:GLU:N	1:S:4981:GLU:OE1	2.46	0.49
1:A:4731:ILE:HG23	1:A:4732:PHE:CD1	2.46	0.49
1:G:2265:LEU:CD1	1:G:2330:ARG:HD2	2.43	0.49
1:G:2588:ARG:NH2	1:G:2901:THR:HG21	2.27	0.49
1:G:2628:PHE:CD1	1:G:2907:PRO:HD3	2.48	0.49
1:G:4078:GLN:O	1:G:4079:ASP:OD1	2.30	0.49
1:G:4160:LEU:O	1:G:4164:LEU:HD22	2.13	0.49
1:M:2124:LEU:HD11	1:M:2128:TYR:HE1	1.77	0.49
1:S:1439:VAL:CG1	1:S:1514:LEU:HB3	2.43	0.49
1:S:1868:PRO:O	1:S:1872:THR:OG1	2.30	0.49
1:S:3735:LEU:N	1:S:3735:LEU:HD22	2.28	0.49
1:S:4160:LEU:O	1:S:4164:LEU:HD22	2.13	0.49
1:A:1439:VAL:CG1	1:A:1514:LEU:HB3	2.43	0.49
1:G:2124:LEU:HD11	1:G:2128:TYR:HE1	1.77	0.49
1:G:3757:GLU:HA	1:G:3760:LYS:NZ	2.27	0.49
1:M:2668:SER:OG	1:M:2671:GLU:OE1	2.27	0.49
1:S:2650:ARG:NH1	1:S:2651:CYS:SG	2.86	0.49
1:S:4853:VAL:O	1:S:4857:ASN:ND2	2.44	0.49
2:T:25:VAL:HG12	2:T:104:LEU:HA	1.95	0.49
1:A:2124:LEU:HD11	1:A:2128:TYR:HE1	1.77	0.48
1:A:2265:LEU:CD1	1:A:2330:ARG:HD2	2.43	0.48
1:A:2628:PHE:CD1	1:A:2907:PRO:HD3	2.48	0.48
1:A:3320:LEU:O	1:A:3323:ILE:HG22	2.13	0.48
1:A:3540:TYR:CE1	1:A:3549:VAL:HG21	2.48	0.48
2:B:25:VAL:HG12	2:B:104:LEU:HA	1.95	0.48
1:G:4981:GLU:OE1	1:G:4981:GLU:N	2.46	0.48
1:M:937:CYS:SG	1:M:984:LEU:CG	3.01	0.48
1:M:3106:MET:HE3	1:M:3132:THR:HG21	1.93	0.48
1:M:3757:GLU:HA	1:M:3760:LYS:NZ	2.27	0.48
1:M:4088:ILE:HG21	1:M:4125:PHE:CZ	2.48	0.48
1:M:4138:ASP:O	1:M:4142:ASN:ND2	2.43	0.48
1:M:4731:ILE:HG23	1:M:4732:PHE:CD1	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:2018:GLU:OE2	1:S:2028:ARG:NE	2.45	0.48
1:S:2627:VAL:HG11	1:S:2674:LEU:CD1	2.43	0.48
1:S:3435:PHE:HA	1:S:3517:MET:HE2	1.95	0.48
1:A:2650:ARG:NH1	1:A:2651:CYS:SG	2.86	0.48
1:A:4160:LEU:O	1:A:4164:LEU:HD22	2.13	0.48
1:G:73:LEU:HD12	1:G:73:LEU:O	2.12	0.48
1:G:1868:PRO:O	1:G:1872:THR:OG1	2.30	0.48
1:G:4731:ILE:HG23	1:G:4732:PHE:CD1	2.46	0.48
1:G:4839:MET:HE1	1:M:4822:THR:CB	2.42	0.48
1:S:1966:VAL:HG11	1:S:3650:CYS:SG	2.53	0.48
1:S:4088:ILE:HG21	1:S:4125:PHE:CZ	2.48	0.48
1:A:3062:PRO:HA	1:A:3065:VAL:HG22	1.95	0.48
1:A:3735:LEU:HD22	1:A:3735:LEU:N	2.28	0.48
1:G:752:VAL:HG13	1:G:752:VAL:O	2.13	0.48
1:G:937:CYS:SG	1:G:984:LEU:CG	3.01	0.48
1:M:752:VAL:HG13	1:M:752:VAL:O	2.13	0.48
1:M:2650:ARG:NH1	1:M:2651:CYS:SG	2.86	0.48
1:A:2627:VAL:HG11	1:A:2674:LEU:CD1	2.43	0.48
1:A:4740:LEU:HD23	1:A:4741:LEU:CD1	2.43	0.48
1:G:2974:ILE:HD12	1:G:3057:PHE:CE1	2.47	0.48
1:M:1439:VAL:CG1	1:M:1514:LEU:HB3	2.43	0.48
1:M:3534:MET:HE2	1:M:3534:MET:HA	1.95	0.48
2:N:25:VAL:HG12	2:N:104:LEU:HA	1.95	0.48
1:S:4740:LEU:HD23	1:S:4741:LEU:CD1	2.43	0.48
1:A:4954:MET:HA	1:A:4954:MET:CE	2.41	0.48
1:G:73:LEU:HD13	1:G:77:ALA:HB3	1.96	0.48
1:G:1966:VAL:HG11	1:G:3650:CYS:SG	2.53	0.48
1:G:3735:LEU:HD22	1:G:3735:LEU:N	2.28	0.48
1:G:4088:ILE:HG21	1:G:4125:PHE:CZ	2.48	0.48
1:M:1966:VAL:HG11	1:M:3650:CYS:SG	2.53	0.48
1:S:1478:ASP:OD1	1:S:1481:GLY:N	2.46	0.48
1:S:3457:ASN:OD1	1:S:3457:ASN:C	2.57	0.48
1:A:73:LEU:HD12	1:A:73:LEU:O	2.12	0.48
1:A:937:CYS:SG	1:A:984:LEU:CG	3.01	0.48
1:A:3106:MET:HE3	1:A:3132:THR:HG21	1.93	0.48
1:A:3230:LEU:HD23	1:A:3230:LEU:H	1.78	0.48
1:G:1478:ASP:OD1	1:G:1481:GLY:N	2.46	0.48
1:M:1478:ASP:OD1	1:M:1481:GLY:N	2.47	0.48
1:M:2628:PHE:CD1	1:M:2907:PRO:HD3	2.48	0.48
1:M:4740:LEU:HD23	1:M:4741:LEU:CD1	2.43	0.48
1:S:73:LEU:HD13	1:S:77:ALA:HB3	1.96	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:2265:LEU:CD1	1:S:2330:ARG:HD2	2.43	0.48
1:G:3230:LEU:HD23	1:G:3230:LEU:H	1.78	0.48
1:G:3534:MET:HA	1:G:3534:MET:HE2	1.95	0.48
1:M:73:LEU:HD12	1:M:73:LEU:O	2.12	0.48
1:M:3840:SER:OG	1:M:3877:ASP:OD1	2.27	0.48
1:S:2628:PHE:CD1	1:S:2907:PRO:HD3	2.48	0.48
1:A:2023:LEU:O	1:A:2028:ARG:NH1	2.47	0.48
1:G:1439:VAL:CG1	1:G:1514:LEU:HB3	2.43	0.48
1:G:2650:ARG:NH1	1:G:2651:CYS:SG	2.86	0.48
1:G:3062:PRO:HA	1:G:3065:VAL:HG22	1.95	0.48
1:M:577:ILE:O	1:M:577:ILE:HG22	2.13	0.48
1:M:2023:LEU:O	1:M:2028:ARG:NH1	2.47	0.48
1:M:3768:SER:HA	1:M:3771:HIS:CD2	2.49	0.48
1:S:3230:LEU:HD23	1:S:3230:LEU:H	1.78	0.48
1:S:3455:GLU:C	1:S:3455:GLU:OE1	2.56	0.48
1:S:4041:ALA:O	1:S:4045:VAL:HG23	2.14	0.48
1:A:3768:SER:HA	1:A:3771:HIS:CD2	2.49	0.48
1:G:1024:TYR:HE1	1:G:1032:LYS:HG2	1.74	0.48
2:H:79:PRO:HB3	2:H:95:ASN:HA	1.96	0.48
1:M:73:LEU:HD13	1:M:77:ALA:HB3	1.96	0.48
2:N:79:PRO:HB3	2:N:95:ASN:HA	1.96	0.48
1:S:752:VAL:O	1:S:752:VAL:HG13	2.13	0.48
1:A:3455:GLU:C	1:A:3455:GLU:OE1	2.56	0.48
1:A:3457:ASN:OD1	1:A:3457:ASN:C	2.57	0.48
1:A:4104:THR:OG1	1:A:4105:GLY:N	2.47	0.48
1:M:4104:THR:OG1	1:M:4105:GLY:N	2.47	0.48
1:A:577:ILE:HG22	1:A:577:ILE:O	2.13	0.47
1:A:4041:ALA:O	1:A:4045:VAL:HG23	2.14	0.47
1:G:3165:CYS:HB3	1:G:3201:MET:HE1	1.97	0.47
1:G:3455:GLU:C	1:G:3455:GLU:OE1	2.57	0.47
1:G:4090:LYS:HE3	1:G:4117:ALA:HB3	1.96	0.47
1:S:3534:MET:HE2	1:S:3534:MET:HA	1.95	0.47
1:A:1966:VAL:HG11	1:A:3650:CYS:SG	2.53	0.47
1:A:2668:SER:OG	1:A:2671:GLU:OE1	2.27	0.47
1:A:3435:PHE:HA	1:A:3517:MET:HE2	1.95	0.47
1:A:4658:ILE:HD12	1:A:4796:MET:CE	2.44	0.47
1:G:82:LEU:HD11	1:G:144:GLU:HB3	1.96	0.47
2:T:79:PRO:HB3	2:T:95:ASN:HA	1.96	0.47
1:G:4689:THR:HG22	1:G:4732:PHE:CZ	2.49	0.47
2:H:25:VAL:HG12	2:H:104:LEU:HA	1.95	0.47
1:M:2598:ALA:HA	1:M:2601:ASP:OD2	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:577:ILE:O	1:S:577:ILE:HG22	2.13	0.47
1:S:4689:THR:HG22	1:S:4732:PHE:CZ	2.49	0.47
1:A:2598:ALA:HA	1:A:2601:ASP:OD2	2.14	0.47
1:A:3324:VAL:O	1:A:3327:LEU:HD23	2.15	0.47
1:A:4981:GLU:OE1	1:A:4981:GLU:N	2.46	0.47
2:B:79:PRO:HB3	2:B:95:ASN:HA	1.96	0.47
1:G:3539:ARG:O	1:G:3542:LEU:O	2.33	0.47
1:G:3768:SER:HA	1:G:3771:HIS:CD2	2.49	0.47
1:M:4090:LYS:HE3	1:M:4117:ALA:HB3	1.96	0.47
1:M:4658:ILE:HD12	1:M:4796:MET:CE	2.44	0.47
1:M:4981:GLU:OE1	1:M:4981:GLU:N	2.46	0.47
1:S:937:CYS:SG	1:S:984:LEU:CD2	3.03	0.47
1:A:1096:THR:HG22	1:A:1097:THR:N	2.29	0.47
1:G:1739:THR:HG23	1:G:1742:THR:H	1.80	0.47
1:G:2023:LEU:O	1:G:2028:ARG:NH1	2.47	0.47
1:G:2598:ALA:HA	1:G:2601:ASP:OD2	2.14	0.47
1:G:3457:ASN:C	1:G:3457:ASN:OD1	2.57	0.47
1:M:3230:LEU:HD23	1:M:3230:LEU:H	1.78	0.47
1:M:3455:GLU:OE1	1:M:3455:GLU:C	2.57	0.47
1:S:937:CYS:SG	1:S:984:LEU:CG	3.01	0.47
1:S:2023:LEU:O	1:S:2028:ARG:NH1	2.47	0.47
1:S:2598:ALA:HA	1:S:2601:ASP:OD2	2.14	0.47
1:S:4138:ASP:O	1:S:4142:ASN:ND2	2.43	0.47
1:A:73:LEU:HD13	1:A:77:ALA:HB3	1.96	0.47
1:A:1478:ASP:OD1	1:A:1481:GLY:N	2.46	0.47
1:G:3989:VAL:HG11	1:G:4047:MET:HE2	1.97	0.47
1:G:4658:ILE:HD12	1:G:4796:MET:CE	2.44	0.47
1:M:3553:LEU:HD22	1:M:3596:VAL:HG11	1.97	0.47
1:S:82:LEU:HD11	1:S:144:GLU:HB3	1.96	0.47
1:S:3108:GLU:HA	1:S:3111:ARG:HG2	1.97	0.47
1:S:3539:ARG:O	1:S:3542:LEU:O	2.33	0.47
1:S:3768:SER:HA	1:S:3771:HIS:CD2	2.49	0.47
1:A:2302:LEU:HD23	1:A:2302:LEU:O	2.15	0.47
1:A:3165:CYS:HB3	1:A:3201:MET:HE1	1.97	0.47
1:A:4689:THR:HG22	1:A:4732:PHE:CZ	2.49	0.47
1:G:4041:ALA:O	1:G:4045:VAL:HG23	2.14	0.47
1:G:4104:THR:OG1	1:G:4105:GLY:N	2.47	0.47
1:M:3062:PRO:HA	1:M:3065:VAL:HG22	1.95	0.47
1:M:3989:VAL:HG11	1:M:4047:MET:HE2	1.97	0.47
1:S:2382:GLU:OE2	1:S:2392:ARG:NH2	2.48	0.47
1:S:3062:PRO:HA	1:S:3065:VAL:HG22	1.95	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:600:LEU:CD2	1:A:1669:LEU:HD22	2.45	0.47
1:A:989:ALA:CB	1:A:1039:LEU:CD1	2.93	0.47
1:M:1739:THR:HG23	1:M:1742:THR:H	1.80	0.47
1:M:1963:GLU:O	1:M:1966:VAL:HG12	2.15	0.47
1:M:2348:GLU:OE1	1:M:2348:GLU:N	2.31	0.47
1:M:3165:CYS:HB3	1:M:3201:MET:HE1	1.96	0.47
1:M:4050:GLU:HA	1:M:4050:GLU:OE1	2.15	0.47
1:S:1739:THR:HG23	1:S:1742:THR:H	1.80	0.47
1:S:3324:VAL:O	1:S:3327:LEU:HD23	2.15	0.47
1:S:4104:THR:OG1	1:S:4105:GLY:N	2.47	0.47
1:G:1963:GLU:O	1:G:1966:VAL:HG12	2.15	0.47
1:G:3324:VAL:O	1:G:3327:LEU:HD23	2.15	0.47
1:G:3435:PHE:HA	1:G:3517:MET:HE2	1.95	0.47
1:M:989:ALA:CB	1:M:1039:LEU:CD1	2.93	0.47
1:M:3377:GLU:HA	1:M:3377:GLU:OE1	2.15	0.47
1:S:171:LEU:HD22	1:S:171:LEU:N	2.30	0.47
1:S:2668:SER:N	1:S:2671:GLU:OE1	2.41	0.47
1:S:3553:LEU:HD22	1:S:3596:VAL:HG11	1.97	0.47
1:S:4658:ILE:HD12	1:S:4796:MET:CE	2.44	0.47
1:A:2382:GLU:OE2	1:A:2392:ARG:NH2	2.48	0.47
1:A:3534:MET:HE2	1:A:3534:MET:HA	1.95	0.47
1:G:600:LEU:CD2	1:G:1669:LEU:HD22	2.45	0.47
1:G:937:CYS:SG	1:G:984:LEU:CD2	3.02	0.47
1:M:82:LEU:HD11	1:M:144:GLU:HB3	1.96	0.47
1:M:4689:THR:HG22	1:M:4732:PHE:CZ	2.49	0.47
1:A:176:SER:C	1:A:177:GLU:OE1	2.58	0.46
1:A:937:CYS:SG	1:A:984:LEU:CD2	3.03	0.46
1:A:3416:VAL:HG23	1:A:3423:TRP:HZ3	1.80	0.46
1:G:3108:GLU:HA	1:G:3111:ARG:HG2	1.97	0.46
1:M:2382:GLU:OE2	1:M:2392:ARG:NH2	2.48	0.46
1:M:3324:VAL:O	1:M:3327:LEU:HD23	2.15	0.46
1:M:4041:ALA:O	1:M:4045:VAL:HG23	2.14	0.46
1:S:684:VAL:HG22	1:S:781:VAL:HG12	1.98	0.46
1:A:1024:TYR:HE1	1:A:1032:LYS:HG2	1.74	0.46
1:A:2254:LEU:HD23	1:A:2254:LEU:C	2.41	0.46
1:G:2302:LEU:HD23	1:G:2302:LEU:O	2.15	0.46
1:M:171:LEU:HD22	1:M:171:LEU:N	2.30	0.46
1:M:684:VAL:HG22	1:M:781:VAL:HG12	1.97	0.46
1:M:937:CYS:SG	1:M:984:LEU:CD2	3.03	0.46
1:M:3457:ASN:C	1:M:3457:ASN:OD1	2.57	0.46
1:A:280:LEU:C	1:A:280:LEU:HD12	2.41	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4075:GLU:HA	1:A:4078:GLN:HB3	1.97	0.46
1:G:171:LEU:N	1:G:171:LEU:HD22	2.30	0.46
1:G:176:SER:C	1:G:177:GLU:OE1	2.58	0.46
1:G:280:LEU:C	1:G:280:LEU:HD12	2.41	0.46
1:G:2622:LEU:O	1:G:2626:LEU:CD2	2.64	0.46
1:G:2862:LEU:HD11	1:G:2932:MET:HE1	1.97	0.46
1:M:2271:THR:OG1	1:M:2272:PRO:HD2	2.16	0.46
1:M:2339:VAL:O	1:M:2339:VAL:HG12	2.15	0.46
1:M:4160:LEU:O	1:M:4164:LEU:CD2	2.64	0.46
1:S:176:SER:C	1:S:177:GLU:OE1	2.58	0.46
1:S:1963:GLU:O	1:S:1966:VAL:HG12	2.15	0.46
1:S:3592:ILE:O	1:S:3596:VAL:HG12	2.16	0.46
1:S:4075:GLU:HA	1:S:4078:GLN:HB3	1.97	0.46
1:A:171:LEU:HD22	1:A:171:LEU:N	2.30	0.46
1:A:992:GLY:O	1:A:995:VAL:HG12	2.16	0.46
1:A:3108:GLU:HA	1:A:3111:ARG:HG2	1.97	0.46
1:A:3352:GLU:OE2	1:A:3356:SER:HB3	2.16	0.46
1:A:3553:LEU:HD22	1:A:3596:VAL:HG11	1.97	0.46
1:G:2897:LYS:O	1:G:2897:LYS:HG2	2.16	0.46
1:G:3553:LEU:HD22	1:G:3596:VAL:HG11	1.97	0.46
1:M:2254:LEU:HD23	1:M:2254:LEU:C	2.41	0.46
1:M:3352:GLU:OE2	1:M:3356:SER:HB3	2.15	0.46
1:M:3416:VAL:HG23	1:M:3423:TRP:HZ3	1.80	0.46
1:S:3539:ARG:NH1	1:S:3542:LEU:HD21	2.30	0.46
1:S:4050:GLU:OE1	1:S:4050:GLU:HA	2.15	0.46
2:B:24:VAL:CG1	2:B:48:LYS:HG2	2.41	0.46
1:G:989:ALA:CB	1:G:1039:LEU:CD1	2.93	0.46
1:G:2254:LEU:C	1:G:2254:LEU:HD23	2.41	0.46
1:G:2382:GLU:OE2	1:G:2392:ARG:NH2	2.48	0.46
1:G:3416:VAL:HG23	1:G:3423:TRP:HZ3	1.80	0.46
4:G:5103:117:H932	4:G:5103:117:C18	2.46	0.46
1:S:2339:VAL:O	1:S:2339:VAL:HG12	2.15	0.46
1:S:3165:CYS:HB3	1:S:3201:MET:HE1	1.97	0.46
1:S:4160:LEU:O	1:S:4164:LEU:CD2	2.64	0.46
4:S:5103:117:C18	4:S:5103:117:H932	2.46	0.46
1:A:100:THR:O	1:A:102:LEU:HD22	2.16	0.46
1:A:674:PHE:CZ	2:B:72:ARG:CZ	2.99	0.46
1:A:2271:THR:HG23	1:A:2274:ASP:H	1.81	0.46
1:A:4090:LYS:HE3	1:A:4117:ALA:HB3	1.96	0.46
1:G:4075:GLU:HA	1:G:4078:GLN:HB3	1.97	0.46
1:M:2862:LEU:HD11	1:M:2932:MET:HE1	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:4075:GLU:HA	1:M:4078:GLN:HB3	1.97	0.46
1:A:1739:THR:HG23	1:A:1742:THR:H	1.80	0.46
1:A:2271:THR:OG1	1:A:2272:PRO:HD2	2.16	0.46
1:A:2825:LYS:HE3	1:A:2827:ARG:O	2.16	0.46
4:A:5103:117:H932	4:A:5103:117:C18	2.46	0.46
1:G:2339:VAL:O	1:G:2339:VAL:HG12	2.15	0.46
1:G:3539:ARG:NH1	1:G:3542:LEU:HD21	2.30	0.46
1:G:4954:MET:HA	1:G:4954:MET:CE	2.41	0.46
1:M:3539:ARG:O	1:M:3542:LEU:O	2.33	0.46
1:M:3539:ARG:NH1	1:M:3542:LEU:HD21	2.30	0.46
1:S:280:LEU:C	1:S:280:LEU:HD12	2.41	0.46
1:S:2271:THR:HG23	1:S:2274:ASP:H	1.81	0.46
1:A:3539:ARG:O	1:A:3542:LEU:O	2.33	0.46
1:A:5013:MET:HE2	1:A:5018:CYS:HB3	1.98	0.46
1:G:2271:THR:HG23	1:G:2274:ASP:H	1.81	0.46
1:G:3286:GLU:OE2	1:G:3287:ARG:NH1	2.49	0.46
1:G:4160:LEU:O	1:G:4164:LEU:CD2	2.64	0.46
1:M:176:SER:C	1:M:177:GLU:OE1	2.58	0.46
1:M:2897:LYS:O	1:M:2897:LYS:HG2	2.16	0.46
1:S:1275:ARG:HG3	1:S:1276:THR:HG23	1.98	0.46
1:S:2271:THR:OG1	1:S:2272:PRO:HD2	2.16	0.46
1:S:2622:LEU:O	1:S:2626:LEU:CD2	2.64	0.46
1:S:2897:LYS:O	1:S:2897:LYS:HG2	2.16	0.46
1:S:3352:GLU:OE2	1:S:3356:SER:HB3	2.15	0.46
1:S:3377:GLU:OE1	1:S:3377:GLU:HA	2.15	0.46
1:S:3989:VAL:HG11	1:S:4047:MET:HE2	1.97	0.46
1:A:82:LEU:HD11	1:A:144:GLU:HB3	1.96	0.46
1:A:2897:LYS:HG2	1:A:2897:LYS:O	2.16	0.46
1:A:3592:ILE:O	1:A:3596:VAL:HG12	2.16	0.46
1:A:4160:LEU:O	1:A:4164:LEU:CD2	2.64	0.46
1:G:5013:MET:HE2	1:G:5018:CYS:HB3	1.98	0.46
1:M:280:LEU:C	1:M:280:LEU:HD12	2.41	0.46
1:M:2302:LEU:HD23	1:M:2302:LEU:O	2.15	0.46
1:M:2519:LEU:HD13	1:M:2575:ARG:HD3	1.98	0.46
1:M:3003:LEU:HB2	1:M:3004:PRO:HD3	1.98	0.46
1:S:2862:LEU:HD11	1:S:2932:MET:HE1	1.97	0.46
1:S:3049:LEU:O	1:S:3049:LEU:HD23	2.16	0.46
1:A:2862:LEU:HD11	1:A:2932:MET:HE1	1.97	0.46
1:A:3539:ARG:NH1	1:A:3542:LEU:HD21	2.30	0.46
1:A:3610:GLU:OE1	1:A:3610:GLU:N	2.49	0.46
1:G:2668:SER:OG	1:G:2671:GLU:OE1	2.27	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3352:GLU:OE2	1:G:3356:SER:HB3	2.16	0.46
1:G:4050:GLU:OE1	1:G:4050:GLU:HA	2.15	0.46
1:G:4094:GLN:NE2	1:G:4098:ASP:OD2	2.49	0.46
1:M:3286:GLU:OE2	1:M:3287:ARG:NH1	2.49	0.46
1:M:3610:GLU:N	1:M:3610:GLU:OE1	2.49	0.46
1:M:4088:ILE:C	1:M:4121:GLU:HA	2.41	0.46
1:S:600:LEU:CD2	1:S:1669:LEU:HD22	2.45	0.46
1:S:4090:LYS:HE3	1:S:4117:ALA:HB3	1.96	0.46
1:M:3568:SER:HA	1:M:3571:TRP:NE1	2.32	0.45
1:S:674:PHE:CZ	2:T:72:ARG:CZ	2.99	0.45
1:S:992:GLY:O	1:S:995:VAL:HG12	2.16	0.45
1:S:2302:LEU:HD23	1:S:2302:LEU:O	2.15	0.45
1:S:3416:VAL:HG23	1:S:3423:TRP:HZ3	1.80	0.45
1:A:989:ALA:CB	1:A:1039:LEU:HD12	2.47	0.45
1:A:2272:PRO:O	1:A:2275:VAL:HG12	2.16	0.45
1:G:684:VAL:HG22	1:G:781:VAL:HG12	1.98	0.45
1:G:1275:ARG:HG3	1:G:1276:THR:HG23	1.98	0.45
1:G:3592:ILE:O	1:G:3596:VAL:HG12	2.16	0.45
1:M:3592:ILE:O	1:M:3596:VAL:HG12	2.16	0.45
1:S:2825:LYS:HE3	1:S:2827:ARG:O	2.16	0.45
1:S:3599:VAL:HG12	1:S:3603:LEU:HD12	1.99	0.45
1:A:2822:THR:OG1	1:A:2938:THR:OG1	2.34	0.45
1:G:100:THR:O	1:G:102:LEU:HD22	2.16	0.45
1:G:992:GLY:O	1:G:995:VAL:HG12	2.16	0.45
1:G:3377:GLU:OE1	1:G:3377:GLU:HA	2.15	0.45
1:M:600:LEU:CD2	1:M:1669:LEU:HD22	2.45	0.45
1:M:674:PHE:CZ	2:N:72:ARG:CZ	2.99	0.45
1:M:992:GLY:O	1:M:995:VAL:HG12	2.16	0.45
1:M:1275:ARG:HG3	1:M:1276:THR:HG23	1.98	0.45
1:M:3049:LEU:HD23	1:M:3049:LEU:O	2.16	0.45
1:M:3599:VAL:HG12	1:M:3603:LEU:HD12	1.99	0.45
1:S:2272:PRO:O	1:S:2275:VAL:HG12	2.17	0.45
1:A:1727:ARG:O	1:A:1731:LEU:HG	2.17	0.45
1:A:3049:LEU:O	1:A:3049:LEU:HD23	2.16	0.45
1:A:3240:CYS:HB3	1:A:3243:ILE:HD12	1.99	0.45
1:A:3377:GLU:OE1	1:A:3377:GLU:HA	2.15	0.45
1:G:2211:MET:O	1:G:2214:VAL:HG12	2.17	0.45
1:G:2271:THR:OG1	1:G:2272:PRO:HD2	2.16	0.45
1:G:3413:ILE:O	1:G:3416:VAL:HG12	2.17	0.45
1:G:4715:TYR:CZ	1:G:4717:ASP:OD2	2.70	0.45
1:M:2271:THR:HG23	1:M:2274:ASP:H	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:2622:LEU:O	1:M:2626:LEU:CD2	2.64	0.45
1:M:2822:THR:OG1	1:M:2938:THR:OG1	2.35	0.45
1:M:3108:GLU:HA	1:M:3111:ARG:HG2	1.97	0.45
1:S:989:ALA:CB	1:S:1039:LEU:CD1	2.93	0.45
1:S:2254:LEU:HD23	1:S:2254:LEU:C	2.41	0.45
1:S:3003:LEU:HB2	1:S:3004:PRO:HD3	1.98	0.45
1:S:3568:SER:HA	1:S:3571:TRP:NE1	2.32	0.45
1:A:1963:GLU:O	1:A:1966:VAL:HG12	2.15	0.45
1:A:3286:GLU:OE2	1:A:3287:ARG:NH1	2.49	0.45
1:A:4715:TYR:CZ	1:A:4717:ASP:OD2	2.69	0.45
1:G:674:PHE:CZ	2:H:72:ARG:CZ	2.99	0.45
1:G:3049:LEU:HD23	1:G:3049:LEU:O	2.16	0.45
1:G:3568:SER:HA	1:G:3571:TRP:NE1	2.32	0.45
1:G:4088:ILE:C	1:G:4121:GLU:HA	2.41	0.45
1:M:1727:ARG:O	1:M:1731:LEU:HG	2.17	0.45
1:M:2825:LYS:HE3	1:M:2827:ARG:O	2.16	0.45
1:M:4715:TYR:CZ	1:M:4717:ASP:OD2	2.70	0.45
4:M:5103:117:H932	4:M:5103:117:C18	2.46	0.45
1:S:1299:GLN:CD	2:T:32:GLN:HE21	2.24	0.45
1:S:3286:GLU:OE2	1:S:3287:ARG:NH1	2.49	0.45
1:S:4715:TYR:CZ	1:S:4717:ASP:OD2	2.70	0.45
1:A:2498:HIS:O	1:A:2502:MET:HG2	2.17	0.45
1:A:3406:TYR:CE2	1:A:3509:LEU:HD23	2.52	0.45
1:A:4088:ILE:C	1:A:4121:GLU:HA	2.41	0.45
1:G:3003:LEU:HB2	1:G:3004:PRO:HD3	1.98	0.45
1:M:2272:PRO:O	1:M:2275:VAL:HG12	2.16	0.45
1:M:4094:GLN:NE2	1:M:4098:ASP:OD2	2.49	0.45
1:S:4088:ILE:C	1:S:4121:GLU:HA	2.41	0.45
1:S:4731:ILE:HG23	1:S:4732:PHE:CD1	2.46	0.45
1:A:684:VAL:HG22	1:A:781:VAL:HG12	1.98	0.45
1:G:1856:ASP:O	1:G:1859:VAL:HG12	2.17	0.45
1:G:2514:ASN:OD1	1:G:2514:ASN:N	2.50	0.45
1:G:2825:LYS:HE3	1:G:2827:ARG:O	2.16	0.45
1:G:4231:MET:HE2	1:G:5022:PHE:CG	2.52	0.45
1:S:2211:MET:O	1:S:2214:VAL:HG12	2.17	0.45
1:S:3406:TYR:CE2	1:S:3509:LEU:HD23	2.52	0.45
1:A:2211:MET:O	1:A:2214:VAL:HG12	2.17	0.45
1:A:2622:LEU:O	1:A:2626:LEU:CD2	2.64	0.45
1:A:3989:VAL:HG11	1:A:4047:MET:HE2	1.97	0.45
1:A:4050:GLU:OE1	1:A:4050:GLU:HA	2.15	0.45
1:G:3130:THR:HA	1:G:3133:THR:HG22	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:1299:GLN:CD	2:N:32:GLN:HE21	2.24	0.45
1:M:1856:ASP:O	1:M:1859:VAL:HG12	2.17	0.45
1:M:2498:HIS:O	1:M:2502:MET:HG2	2.17	0.45
1:S:1928:GLN:OE1	1:S:1928:GLN:O	2.35	0.45
1:S:2514:ASN:N	1:S:2514:ASN:OD1	2.50	0.45
1:S:2519:LEU:HD13	1:S:2575:ARG:HD3	1.98	0.45
1:A:1299:GLN:CD	2:B:32:GLN:NE2	2.75	0.45
1:A:1810:LYS:HG2	1:A:1814:MET:SD	2.57	0.45
1:A:3852:LYS:O	1:A:3856:LEU:HD23	2.17	0.45
1:G:984:LEU:CD2	1:G:1053:ILE:HG22	2.47	0.45
1:G:1299:GLN:CD	2:H:32:GLN:NE2	2.75	0.45
1:G:1299:GLN:CD	2:H:32:GLN:HE21	2.25	0.45
1:G:2498:HIS:O	1:G:2502:MET:HG2	2.17	0.45
1:G:2822:THR:OG1	1:G:2938:THR:OG1	2.35	0.45
1:M:100:THR:O	1:M:102:LEU:HD22	2.16	0.45
1:M:2211:MET:O	1:M:2214:VAL:HG12	2.17	0.45
1:M:3413:ILE:O	1:M:3416:VAL:HG12	2.16	0.45
1:M:4231:MET:HE2	1:M:5022:PHE:CG	2.52	0.45
1:S:1299:GLN:CD	2:T:32:GLN:NE2	2.75	0.45
1:S:3046:LEU:O	1:S:3050:VAL:HG23	2.17	0.45
1:S:3413:ILE:O	1:S:3416:VAL:HG12	2.17	0.45
1:A:1275:ARG:HG3	1:A:1276:THR:HG23	1.98	0.45
1:A:1928:GLN:OE1	1:A:1928:GLN:O	2.35	0.45
1:A:2339:VAL:O	1:A:2339:VAL:HG12	2.15	0.45
1:G:1727:ARG:O	1:G:1731:LEU:HG	2.17	0.45
1:G:2272:PRO:O	1:G:2275:VAL:HG12	2.17	0.45
1:G:3852:LYS:O	1:G:3856:LEU:HD23	2.17	0.45
1:M:984:LEU:CD2	1:M:1053:ILE:HG22	2.47	0.45
1:M:1810:LYS:HG2	1:M:1814:MET:SD	2.57	0.45
1:M:3240:CYS:HB3	1:M:3243:ILE:HD12	1.99	0.45
1:S:1096:THR:HG22	1:S:1097:THR:N	2.29	0.45
1:S:1856:ASP:O	1:S:1859:VAL:HG12	2.17	0.45
1:S:2624:ARG:NE	1:S:2910:THR:O	2.48	0.45
1:S:3852:LYS:O	1:S:3856:LEU:HD23	2.17	0.45
1:A:2519:LEU:HD13	1:A:2575:ARG:HD3	1.98	0.44
1:A:3046:LEU:O	1:A:3050:VAL:HG23	2.17	0.44
1:A:3989:VAL:HG11	1:A:4047:MET:CE	2.48	0.44
1:A:4094:GLN:NE2	1:A:4098:ASP:OD2	2.49	0.44
1:G:1928:GLN:OE1	1:G:1928:GLN:O	2.35	0.44
1:G:3046:LEU:O	1:G:3050:VAL:HG23	2.17	0.44
1:G:3610:GLU:OE1	1:G:3610:GLU:N	2.49	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:622:THR:HG23	1:M:626:LEU:HD12	1.99	0.44
1:M:2226:PRO:O	1:M:2229:VAL:HG22	2.17	0.44
1:M:3046:LEU:O	1:M:3050:VAL:HG23	2.18	0.44
1:S:984:LEU:CD2	1:S:1053:ILE:HG22	2.47	0.44
1:S:2626:LEU:HD12	1:S:2640:PRO:HB3	1.99	0.44
1:S:3753:PHE:HA	1:S:3756:LYS:HG2	1.99	0.44
1:S:3989:VAL:HG11	1:S:4047:MET:CE	2.48	0.44
1:A:572:PRO:HA	1:A:575:LEU:HD13	2.00	0.44
1:A:1856:ASP:O	1:A:1859:VAL:HG12	2.17	0.44
1:A:2668:SER:N	1:A:2671:GLU:OE1	2.42	0.44
1:G:78:LEU:HD21	1:G:147:TRP:CB	2.47	0.44
1:G:2226:PRO:O	1:G:2229:VAL:HG22	2.17	0.44
1:G:3406:TYR:CE2	1:G:3509:LEU:HD23	2.52	0.44
1:M:78:LEU:HD21	1:M:147:TRP:CB	2.47	0.44
1:M:572:PRO:HA	1:M:575:LEU:HD13	1.99	0.44
1:M:1096:THR:HG22	1:M:1097:THR:N	2.29	0.44
1:S:100:THR:O	1:S:102:LEU:HD22	2.16	0.44
1:S:4231:MET:HE2	1:S:5022:PHE:CG	2.52	0.44
1:A:1299:GLN:CD	2:B:32:GLN:HE21	2.24	0.44
1:A:1820:ARG:O	1:A:1824:GLN:HG2	2.17	0.44
1:A:3753:PHE:HA	1:A:3756:LYS:HG2	1.99	0.44
1:G:2768:PHE:O	1:G:2772:GLN:HG2	2.17	0.44
1:G:4088:ILE:HG23	1:G:4123:ILE:HB	1.99	0.44
1:M:5013:MET:HE2	1:M:5018:CYS:HB3	1.98	0.44
1:S:989:ALA:CB	1:S:1039:LEU:HD12	2.47	0.44
1:S:2348:GLU:OE1	1:S:2348:GLU:N	2.31	0.44
1:S:2822:THR:OG1	1:S:2938:THR:OG1	2.35	0.44
1:S:3610:GLU:OE1	1:S:3610:GLU:N	2.49	0.44
1:S:4094:GLN:NE2	1:S:4098:ASP:OD2	2.49	0.44
1:A:2768:PHE:O	1:A:2772:GLN:HG2	2.17	0.44
1:A:3413:ILE:O	1:A:3416:VAL:HG12	2.16	0.44
1:G:1820:ARG:O	1:G:1824:GLN:HG2	2.17	0.44
1:M:4088:ILE:HG23	1:M:4123:ILE:HB	2.00	0.44
1:S:1727:ARG:O	1:S:1731:LEU:HG	2.16	0.44
1:S:1820:ARG:O	1:S:1824:GLN:HG2	2.17	0.44
1:S:1995:THR:O	1:S:1995:THR:HG22	2.18	0.44
1:S:2376:LEU:O	1:S:2380:ILE:HG12	2.18	0.44
1:S:2768:PHE:O	1:S:2772:GLN:HG2	2.18	0.44
1:S:3365:LEU:CD2	1:S:3405:LEU:HD12	2.48	0.44
1:M:728:ARG:NH2	1:M:1489:CYS:SG	2.91	0.44
1:S:280:LEU:HD12	1:S:280:LEU:O	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:572:PRO:HA	1:S:575:LEU:HD13	2.00	0.44
1:S:989:ALA:CA	1:S:1039:LEU:CD1	2.96	0.44
1:S:2498:HIS:O	1:S:2502:MET:HG2	2.17	0.44
1:S:2874:MET:HE1	1:S:2937:VAL:HG12	2.00	0.44
1:A:49:LEU:HD21	1:A:191:VAL:CG2	2.48	0.44
1:A:984:LEU:CD2	1:A:1053:ILE:HG22	2.47	0.44
1:A:2376:LEU:O	1:A:2380:ILE:HG12	2.18	0.44
1:A:3568:SER:HA	1:A:3571:TRP:NE1	2.32	0.44
1:A:4640:GLU:HB3	1:A:4641:PRO:HD3	2.00	0.44
1:G:280:LEU:HD12	1:G:280:LEU:O	2.17	0.44
1:G:1096:THR:HG22	1:G:1097:THR:N	2.29	0.44
1:G:2763:HIS:HE1	1:G:2790:MET:O	2.01	0.44
1:G:3240:CYS:HB3	1:G:3243:ILE:HD12	1.99	0.44
1:G:3753:PHE:HA	1:G:3756:LYS:HG2	1.99	0.44
1:M:1995:THR:HG22	1:M:1995:THR:O	2.18	0.44
1:M:3130:THR:HA	1:M:3133:THR:HG22	1.99	0.44
1:M:4118:ASP:O	1:M:4122:MET:CB	2.66	0.44
1:S:78:LEU:HD21	1:S:147:TRP:CB	2.47	0.44
1:S:728:ARG:NH2	1:S:1489:CYS:SG	2.91	0.44
1:S:3240:CYS:HB3	1:S:3243:ILE:HD12	1.99	0.44
1:A:78:LEU:HD21	1:A:147:TRP:CB	2.47	0.44
1:A:280:LEU:HD12	1:A:280:LEU:O	2.17	0.44
1:A:2226:PRO:O	1:A:2229:VAL:HG22	2.17	0.44
1:A:2302:LEU:CD2	1:A:2363:CYS:HB3	2.48	0.44
1:G:3989:VAL:HG11	1:G:4047:MET:CE	2.48	0.44
1:G:4640:GLU:HB3	1:G:4641:PRO:HD3	2.00	0.44
1:M:280:LEU:HD12	1:M:280:LEU:O	2.17	0.44
1:M:492:ASP:OD1	1:M:546:TRP:NE1	2.51	0.44
1:M:989:ALA:CB	1:M:1039:LEU:HD12	2.47	0.44
1:M:1928:GLN:OE1	1:M:1928:GLN:O	2.35	0.44
1:M:2763:HIS:HE1	1:M:2790:MET:O	2.01	0.44
1:M:2768:PHE:O	1:M:2772:GLN:HG2	2.17	0.44
1:M:3852:LYS:O	1:M:3856:LEU:HD23	2.17	0.44
1:S:1861:GLN:O	1:S:1865:MET:HG3	2.18	0.44
1:S:3850:GLN:O	1:S:3854:GLU:HG2	2.18	0.44
1:S:5013:MET:HE2	1:S:5018:CYS:HB3	1.98	0.44
1:A:530:ILE:HD12	1:A:530:ILE:O	2.18	0.44
1:A:2874:MET:HE1	1:A:2937:VAL:HG12	2.00	0.44
1:A:3850:GLN:O	1:A:3854:GLU:HG2	2.18	0.44
1:G:728:ARG:NH2	1:G:1489:CYS:SG	2.91	0.44
1:S:2763:HIS:HE1	1:S:2790:MET:O	2.01	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:4118:ASP:O	1:S:4122:MET:CB	2.66	0.44
1:A:728:ARG:NH2	1:A:1489:CYS:SG	2.91	0.44
1:A:2045:GLN:NE2	1:A:2046:LEU:O	2.51	0.44
1:A:2514:ASN:OD1	1:A:2514:ASN:N	2.50	0.44
1:A:3003:LEU:HB2	1:A:3004:PRO:HD3	1.98	0.44
1:G:1810:LYS:HG2	1:G:1814:MET:SD	2.57	0.44
1:G:2624:ARG:NE	1:G:2910:THR:O	2.48	0.44
1:G:2626:LEU:HD12	1:G:2640:PRO:HB3	1.99	0.44
1:G:3365:LEU:CD2	1:G:3405:LEU:HD12	2.48	0.44
1:M:989:ALA:CA	1:M:1039:LEU:CD1	2.96	0.44
1:M:1024:TYR:HE1	1:M:1032:LYS:HG2	1.74	0.44
1:M:2514:ASN:OD1	1:M:2514:ASN:N	2.50	0.44
1:M:3850:GLN:O	1:M:3854:GLU:HG2	2.18	0.44
2:N:58:LYS:HB2	2:N:81:VAL:HG13	2.00	0.44
1:S:530:ILE:HD12	1:S:530:ILE:O	2.18	0.44
1:S:622:THR:HG23	1:S:626:LEU:HD12	1.99	0.44
1:S:1810:LYS:HG2	1:S:1814:MET:SD	2.57	0.44
1:S:2045:GLN:NE2	1:S:2046:LEU:O	2.51	0.44
1:S:3551:GLU:OE1	1:S:3551:GLU:HA	2.18	0.44
1:A:1861:GLN:O	1:A:1865:MET:HG3	2.18	0.43
1:G:572:PRO:HA	1:G:575:LEU:HD13	2.00	0.43
1:G:622:THR:HG23	1:G:626:LEU:HD12	1.99	0.43
1:G:1861:GLN:O	1:G:1865:MET:HG3	2.18	0.43
1:G:3542:LEU:C	1:G:3542:LEU:HD12	2.43	0.43
1:M:3365:LEU:CD2	1:M:3405:LEU:HD12	2.48	0.43
1:M:3542:LEU:C	1:M:3542:LEU:HD12	2.43	0.43
1:M:3753:PHE:HA	1:M:3756:LYS:HG2	1.99	0.43
1:M:4885:PHE:O	1:M:4889:VAL:HG22	2.18	0.43
1:S:3085:PRO:O	1:S:3088:VAL:HG22	2.18	0.43
1:S:3130:THR:HA	1:S:3133:THR:HG22	1.99	0.43
1:A:622:THR:HG23	1:A:626:LEU:HD12	1.99	0.43
1:A:1464:PHE:O	1:A:1465:ASP:OD1	2.36	0.43
1:G:49:LEU:HD21	1:G:191:VAL:CG2	2.48	0.43
1:G:2519:LEU:HD13	1:G:2575:ARG:HD3	1.98	0.43
1:G:3518:LEU:O	1:G:3522:LEU:HD13	2.18	0.43
1:M:530:ILE:HD13	1:M:536:ASN:HB3	2.01	0.43
1:M:1820:ARG:O	1:M:1824:GLN:HG2	2.17	0.43
1:M:2302:LEU:CD2	1:M:2363:CYS:HB3	2.48	0.43
1:M:3406:TYR:CE2	1:M:3509:LEU:HD23	2.52	0.43
1:M:3593:VAL:HA	1:M:3596:VAL:HG12	2.00	0.43
2:T:58:LYS:HB2	2:T:81:VAL:HG13	2.00	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:168:ASP:HB3	1:A:199:LEU:HD12	2.00	0.43
1:A:3085:PRO:O	1:A:3088:VAL:HG22	2.18	0.43
1:A:3365:LEU:CD2	1:A:3405:LEU:HD12	2.48	0.43
1:A:4231:MET:HE2	1:A:5022:PHE:CG	2.52	0.43
1:A:4885:PHE:O	1:A:4889:VAL:HG22	2.18	0.43
1:G:530:ILE:HD12	1:G:530:ILE:O	2.18	0.43
1:G:1995:THR:O	1:G:1995:THR:HG22	2.18	0.43
1:G:2668:SER:N	1:G:2671:GLU:OE1	2.41	0.43
1:G:3850:GLN:O	1:G:3854:GLU:HG2	2.18	0.43
1:G:4075:GLU:O	1:G:4076:ALA:C	2.62	0.43
1:G:4885:PHE:O	1:G:4889:VAL:HG22	2.18	0.43
1:M:989:ALA:CA	1:M:1039:LEU:HD13	2.48	0.43
1:M:1464:PHE:O	1:M:1465:ASP:OD1	2.36	0.43
1:M:1861:GLN:O	1:M:1865:MET:HG3	2.18	0.43
1:S:2226:PRO:O	1:S:2229:VAL:HG22	2.17	0.43
1:S:2302:LEU:CD2	1:S:2363:CYS:HB3	2.48	0.43
1:S:3593:VAL:HA	1:S:3596:VAL:HG12	2.00	0.43
1:S:4640:GLU:HB3	1:S:4641:PRO:HD3	2.00	0.43
1:A:530:ILE:HD13	1:A:536:ASN:HB3	2.01	0.43
1:A:3542:LEU:C	1:A:3542:LEU:HD12	2.43	0.43
1:A:3599:VAL:HG12	1:A:3603:LEU:HD12	1.99	0.43
1:A:4118:ASP:O	1:A:4122:MET:CB	2.66	0.43
1:G:989:ALA:CA	1:G:1039:LEU:CD1	2.96	0.43
1:M:49:LEU:HD21	1:M:191:VAL:CG2	2.48	0.43
1:M:1299:GLN:CD	2:N:32:GLN:NE2	2.75	0.43
1:M:2045:GLN:NE2	1:M:2046:LEU:O	2.51	0.43
1:M:3989:VAL:HG11	1:M:4047:MET:CE	2.48	0.43
1:S:2669:GLU:HG2	1:S:2669:GLU:O	2.18	0.43
1:S:3542:LEU:HD12	1:S:3542:LEU:C	2.43	0.43
2:T:58:LYS:NZ	2:T:58:LYS:HB3	2.34	0.43
1:A:3130:THR:HA	1:A:3133:THR:HG22	1.99	0.43
1:A:3518:LEU:O	1:A:3522:LEU:HD13	2.18	0.43
2:B:16:PHE:O	2:B:18:LYS:NZ	2.52	0.43
1:G:168:ASP:HB3	1:G:199:LEU:HD12	2.00	0.43
1:G:1464:PHE:O	1:G:1465:ASP:OD1	2.36	0.43
1:G:2045:GLN:NE2	1:G:2046:LEU:O	2.51	0.43
2:H:58:LYS:NZ	2:H:58:LYS:HB3	2.34	0.43
1:M:1690:ASP:OD1	1:M:1693:GLN:NE2	2.52	0.43
1:M:3085:PRO:O	1:M:3088:VAL:HG22	2.18	0.43
1:M:4075:GLU:O	1:M:4076:ALA:C	2.62	0.43
1:M:4649:LEU:O	1:M:4653:VAL:HG23	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:492:ASP:OD1	1:S:546:TRP:NE1	2.51	0.43
1:S:3825:GLU:OE1	1:S:3825:GLU:N	2.41	0.43
1:A:989:ALA:CA	1:A:1039:LEU:CD1	2.96	0.43
1:A:3343:GLN:O	1:A:3346:VAL:HG12	2.19	0.43
1:A:4655:PHE:HA	1:A:4796:MET:HE1	2.01	0.43
1:A:4992:LEU:O	1:A:4996:ILE:HG13	2.19	0.43
1:G:3593:VAL:HA	1:G:3596:VAL:HG12	2.00	0.43
1:G:3599:VAL:HG12	1:G:3603:LEU:HD12	1.99	0.43
1:M:2376:LEU:O	1:M:2380:ILE:HG12	2.18	0.43
1:M:4655:PHE:HA	1:M:4796:MET:HE1	2.01	0.43
1:S:1690:ASP:OD1	1:S:1693:GLN:NE2	2.52	0.43
1:S:3343:GLN:O	1:S:3346:VAL:HG12	2.19	0.43
1:A:989:ALA:CA	1:A:1039:LEU:HD13	2.48	0.43
1:G:530:ILE:HD13	1:G:536:ASN:HB3	2.01	0.43
1:G:2302:LEU:CD2	1:G:2363:CYS:HB3	2.48	0.43
1:M:530:ILE:O	1:M:530:ILE:HD12	2.18	0.43
1:M:2874:MET:HE1	1:M:2937:VAL:HG12	2.00	0.43
1:M:3517:MET:O	1:M:3520:ILE:CG2	2.67	0.43
1:M:4089:SER:CA	1:M:4121:GLU:HA	2.49	0.43
1:M:4234:PHE:CE1	1:M:4985:LEU:HD23	2.53	0.43
1:M:4901:ILE:HG22	1:M:4902:GLU:N	2.34	0.43
1:M:4992:LEU:O	1:M:4996:ILE:HG13	2.19	0.43
2:N:16:PHE:O	2:N:18:LYS:NZ	2.52	0.43
1:S:989:ALA:CA	1:S:1039:LEU:HD13	2.48	0.43
1:S:1236:THR:OG1	1:S:1608:MET:SD	2.77	0.43
1:S:3518:LEU:O	1:S:3522:LEU:HD13	2.19	0.43
1:A:2763:HIS:HE1	1:A:2790:MET:O	2.01	0.43
1:A:3509:LEU:HD22	1:A:3509:LEU:N	2.34	0.43
1:G:492:ASP:OD1	1:G:546:TRP:NE1	2.51	0.43
1:G:989:ALA:CA	1:G:1039:LEU:HD13	2.48	0.43
1:G:2669:GLU:O	1:G:2669:GLU:HG2	2.18	0.43
1:G:3085:PRO:O	1:G:3088:VAL:HG22	2.18	0.43
1:G:3551:GLU:HA	1:G:3551:GLU:OE1	2.18	0.43
1:G:3652:MET:O	1:G:3655:GLU:HG2	2.19	0.43
1:M:2626:LEU:HD12	1:M:2640:PRO:HB3	1.99	0.43
1:S:49:LEU:HD21	1:S:191:VAL:CG2	2.48	0.43
1:S:3509:LEU:HD22	1:S:3509:LEU:N	2.34	0.43
1:S:4075:GLU:O	1:S:4076:ALA:C	2.62	0.43
1:S:4088:ILE:HG23	1:S:4123:ILE:HB	2.00	0.43
1:S:4234:PHE:CE1	1:S:4985:LEU:HD23	2.53	0.43
1:S:4885:PHE:O	1:S:4889:VAL:HG22	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3593:VAL:HA	1:A:3596:VAL:HG12	2.00	0.43
1:A:4088:ILE:HG23	1:A:4123:ILE:HB	2.00	0.43
1:G:2348:GLU:H	1:G:2348:GLU:CD	2.23	0.43
1:G:4089:SER:CA	1:G:4121:GLU:HA	2.49	0.43
1:G:4649:LEU:O	1:G:4653:VAL:HG23	2.19	0.43
1:G:4655:PHE:HA	1:G:4796:MET:HE1	2.01	0.43
1:M:168:ASP:HB3	1:M:199:LEU:HD12	2.00	0.43
1:M:4242:ILE:CD1	1:M:4993:MET:CE	2.79	0.43
1:S:14:LEU:HD12	1:S:14:LEU:N	2.34	0.43
1:S:3652:MET:O	1:S:3655:GLU:HG2	2.19	0.43
1:S:4901:ILE:HG22	1:S:4902:GLU:N	2.34	0.43
1:A:2669:GLU:HG2	1:A:2669:GLU:O	2.18	0.43
1:A:4649:LEU:O	1:A:4653:VAL:HG23	2.19	0.43
1:G:1690:ASP:OD1	1:G:1693:GLN:NE2	2.52	0.43
1:G:2614:ILE:HD13	1:G:2614:ILE:HA	1.93	0.43
1:G:2874:MET:HE1	1:G:2937:VAL:HG12	2.00	0.43
1:G:3770:LEU:HB3	1:G:3804:ILE:HD11	2.01	0.43
1:G:4118:ASP:O	1:G:4122:MET:CB	2.66	0.43
1:G:4234:PHE:CE1	1:G:4985:LEU:HD23	2.53	0.43
2:H:16:PHE:O	2:H:18:LYS:NZ	2.52	0.43
1:M:2668:SER:N	1:M:2671:GLU:OE1	2.41	0.43
1:M:3551:GLU:OE1	1:M:3551:GLU:HA	2.18	0.43
1:S:3517:MET:O	1:S:3520:ILE:CG2	2.67	0.43
1:S:4655:PHE:HA	1:S:4796:MET:HE1	2.01	0.43
1:S:4992:LEU:O	1:S:4996:ILE:HG13	2.19	0.43
1:A:937:CYS:SG	1:A:984:LEU:HD21	2.60	0.42
1:A:2974:ILE:HD13	1:A:3049:LEU:HD23	2.00	0.42
1:A:4234:PHE:CE1	1:A:4985:LEU:HD23	2.53	0.42
1:G:2974:ILE:HD13	1:G:3049:LEU:HD23	2.00	0.42
1:G:4992:LEU:O	1:G:4996:ILE:HG13	2.19	0.42
2:H:58:LYS:HB2	2:H:81:VAL:HG13	2.00	0.42
1:M:575:LEU:HD12	1:M:575:LEU:N	2.34	0.42
1:M:2669:GLU:O	1:M:2669:GLU:HG2	2.18	0.42
1:S:530:ILE:HD13	1:S:536:ASN:HB3	2.01	0.42
1:S:2974:ILE:HD13	1:S:3049:LEU:HD23	2.00	0.42
1:S:3106:MET:CE	1:S:3132:THR:HB	2.49	0.42
1:A:2206:THR:O	1:A:2210:VAL:HG23	2.20	0.42
2:B:58:LYS:NZ	2:B:58:LYS:HB3	2.34	0.42
1:G:2376:LEU:O	1:G:2380:ILE:HG12	2.18	0.42
1:G:3652:MET:HA	1:G:3655:GLU:HG2	2.01	0.42
1:G:4018:ASP:OD2	1:G:4019:LEU:N	2.53	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:3106:MET:CE	1:M:3132:THR:HB	2.50	0.42
1:M:3652:MET:O	1:M:3655:GLU:HG2	2.19	0.42
1:M:4018:ASP:OD2	1:M:4019:LEU:N	2.53	0.42
1:M:4640:GLU:HB3	1:M:4641:PRO:HD3	2.00	0.42
1:S:575:LEU:N	1:S:575:LEU:HD12	2.34	0.42
1:A:1690:ASP:OD1	1:A:1693:GLN:NE2	2.52	0.42
1:A:3336:LYS:O	1:A:3340:VAL:HG13	2.19	0.42
1:A:3652:MET:O	1:A:3655:GLU:HG2	2.19	0.42
1:A:4018:ASP:OD2	1:A:4019:LEU:N	2.53	0.42
1:A:4075:GLU:O	1:A:4076:ALA:C	2.62	0.42
1:A:4089:SER:CA	1:A:4121:GLU:HA	2.49	0.42
1:G:3343:GLN:O	1:G:3346:VAL:HG12	2.19	0.42
1:G:3509:LEU:HD22	1:G:3509:LEU:N	2.34	0.42
1:M:797:HIS:CE1	1:M:821:LEU:HD23	2.54	0.42
1:M:1221:GLU:N	1:M:1221:GLU:OE1	2.53	0.42
1:M:3509:LEU:N	1:M:3509:LEU:HD22	2.34	0.42
1:S:937:CYS:SG	1:S:984:LEU:HD21	2.60	0.42
1:S:3652:MET:HA	1:S:3655:GLU:HG2	2.00	0.42
1:A:1995:THR:O	1:A:1995:THR:HG22	2.18	0.42
1:A:2348:GLU:H	1:A:2348:GLU:CD	2.22	0.42
1:A:2626:LEU:HD12	1:A:2640:PRO:HB3	1.99	0.42
1:G:989:ALA:CB	1:G:1039:LEU:HD12	2.47	0.42
1:M:14:LEU:HD12	1:M:14:LEU:N	2.34	0.42
1:M:2515:GLN:O	1:M:2519:LEU:HG	2.20	0.42
1:M:2599:GLN:O	1:M:2603:ILE:HG13	2.20	0.42
1:M:3175:LEU:HD11	1:M:3183:VAL:HG13	2.02	0.42
1:S:3175:LEU:HD11	1:S:3183:VAL:HG13	2.02	0.42
1:A:2599:GLN:O	1:A:2603:ILE:HG13	2.20	0.42
1:G:864:PRO:CG	1:G:867:LEU:HD12	2.50	0.42
1:G:2515:GLN:O	1:G:2519:LEU:HG	2.20	0.42
1:G:2628:PHE:HD1	1:G:2907:PRO:HD3	1.85	0.42
1:M:2974:ILE:HD13	1:M:3049:LEU:HD23	2.00	0.42
1:M:3157:ILE:HA	1:M:3161:VAL:HG23	2.01	0.42
1:M:3355:HIS:HD1	1:M:3355:HIS:C	2.28	0.42
2:N:51:ILE:HD12	2:N:51:ILE:HA	1.84	0.42
1:S:74:SER:HA	1:S:105:HIS:CD2	2.55	0.42
1:S:1464:PHE:O	1:S:1465:ASP:OD1	2.36	0.42
1:S:3336:LYS:O	1:S:3340:VAL:HG13	2.19	0.42
1:S:3355:HIS:C	1:S:3355:HIS:HD1	2.28	0.42
1:S:3770:LEU:HB3	1:S:3804:ILE:HD11	2.01	0.42
2:T:24:VAL:CG1	2:T:48:LYS:HG2	2.41	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3157:ILE:HA	1:A:3161:VAL:HG23	2.01	0.42
1:A:3517:MET:O	1:A:3520:ILE:CG2	2.67	0.42
1:A:3599:VAL:HG12	1:A:3603:LEU:CD1	2.50	0.42
1:A:4093:PHE:CE1	1:A:4097:MET:HE2	2.54	0.42
1:G:73:LEU:HD11	1:G:78:LEU:CB	2.47	0.42
1:G:575:LEU:HD12	1:G:575:LEU:N	2.34	0.42
1:G:3517:MET:O	1:G:3520:ILE:CG2	2.67	0.42
1:G:4093:PHE:CE1	1:G:4097:MET:HE2	2.54	0.42
1:M:864:PRO:CG	1:M:867:LEU:HD12	2.50	0.42
1:M:2639:MET:HB3	1:M:2640:PRO:HD3	2.02	0.42
1:M:2750:LYS:O	1:M:2750:LYS:HG2	2.19	0.42
1:M:3050:VAL:O	1:M:3050:VAL:HG12	2.20	0.42
1:S:2206:THR:O	1:S:2210:VAL:HG23	2.20	0.42
1:S:2639:MET:HB3	1:S:2640:PRO:HD3	2.02	0.42
1:S:4018:ASP:OD2	1:S:4019:LEU:N	2.53	0.42
1:S:4093:PHE:CE1	1:S:4097:MET:HE2	2.54	0.42
1:A:797:HIS:CE1	1:A:821:LEU:HD23	2.54	0.42
1:A:3106:MET:CE	1:A:3132:THR:HB	2.50	0.42
1:A:3567:PRO:O	1:A:3570:ARG:HB3	2.20	0.42
1:A:3770:LEU:HB3	1:A:3804:ILE:HD11	2.01	0.42
1:G:2639:MET:HB3	1:G:2640:PRO:HD3	2.02	0.42
1:G:3157:ILE:HA	1:G:3161:VAL:HG23	2.01	0.42
2:H:24:VAL:CG1	2:H:48:LYS:HG2	2.41	0.42
1:M:1119:GLU:OE1	1:M:1119:GLU:N	2.39	0.42
1:M:2206:THR:O	1:M:2210:VAL:HG23	2.20	0.42
1:M:3343:GLN:O	1:M:3346:VAL:HG12	2.19	0.42
1:M:3518:LEU:O	1:M:3522:LEU:HD13	2.19	0.42
1:M:4901:ILE:CG2	1:M:4902:GLU:N	2.83	0.42
1:S:797:HIS:CE1	1:S:821:LEU:HD23	2.54	0.42
1:S:1221:GLU:OE1	1:S:1221:GLU:N	2.53	0.42
1:S:3696:ASP:OD1	1:S:3699:HIS:HB2	2.20	0.42
1:S:4954:MET:HA	1:S:4954:MET:CE	2.41	0.42
1:A:196:MET:SD	1:A:196:MET:N	2.93	0.42
1:A:2750:LYS:HG2	1:A:2750:LYS:O	2.19	0.42
1:A:3551:GLU:OE1	1:A:3551:GLU:HA	2.18	0.42
1:A:4063:ASP:OD1	1:A:4064:MET:N	2.53	0.42
1:A:4901:ILE:CG2	1:A:4902:GLU:N	2.83	0.42
2:B:58:LYS:HB2	2:B:81:VAL:HG13	2.00	0.42
1:G:14:LEU:HD12	1:G:14:LEU:N	2.34	0.42
1:G:71:GLN:HE21	1:G:108:LEU:CD2	2.33	0.42
1:G:2599:GLN:O	1:G:2603:ILE:HG13	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:3753:PHE:O	1:G:3756:LYS:HG2	2.20	0.42
1:G:4138:ASP:O	1:G:4142:ASN:ND2	2.43	0.42
1:M:71:GLN:HE21	1:M:108:LEU:CD2	2.33	0.42
1:M:937:CYS:SG	1:M:984:LEU:HD21	2.60	0.42
1:S:3157:ILE:HA	1:S:3161:VAL:HG23	2.01	0.42
1:S:3599:VAL:HG12	1:S:3603:LEU:CD1	2.50	0.42
1:S:3854:GLU:OE1	1:S:3854:GLU:HA	2.20	0.42
1:S:4063:ASP:OD1	1:S:4064:MET:N	2.52	0.42
1:A:575:LEU:HD12	1:A:575:LEU:N	2.34	0.42
1:A:2515:GLN:O	1:A:2519:LEU:HG	2.20	0.42
1:G:196:MET:N	1:G:196:MET:SD	2.93	0.42
1:G:483:MET:HA	1:G:483:MET:HE3	2.02	0.42
1:G:3599:VAL:HG12	1:G:3603:LEU:CD1	2.50	0.42
1:M:3456:GLN:HA	1:M:3459:VAL:HG12	2.02	0.42
1:A:121:LEU:N	1:A:134:ASP:O	2.53	0.42
1:A:864:PRO:CG	1:A:867:LEU:HD12	2.50	0.42
1:A:3133:THR:HG23	1:A:3134:VAL:HG23	2.02	0.42
1:G:121:LEU:N	1:G:134:ASP:O	2.53	0.42
1:G:645:ARG:HG2	1:G:826:ILE:HG12	2.02	0.42
1:G:797:HIS:CE1	1:G:821:LEU:HD23	2.54	0.42
1:M:1024:TYR:O	1:M:1025:ARG:C	2.63	0.42
1:M:3567:PRO:O	1:M:3570:ARG:HB3	2.20	0.42
1:M:3854:GLU:OE1	1:M:3854:GLU:HA	2.20	0.42
2:N:24:VAL:CG1	2:N:48:LYS:HG2	2.41	0.42
1:S:803:LEU:HD12	1:S:803:LEU:HA	1.95	0.42
1:S:2515:GLN:O	1:S:2519:LEU:HG	2.20	0.42
1:S:3753:PHE:O	1:S:3756:LYS:HG2	2.20	0.42
1:S:4649:LEU:O	1:S:4653:VAL:HG23	2.19	0.42
1:A:74:SER:HA	1:A:105:HIS:CD2	2.55	0.41
1:A:483:MET:HA	1:A:483:MET:HE3	2.02	0.41
1:A:1024:TYR:O	1:A:1025:ARG:C	2.63	0.41
1:A:1474:VAL:HG13	1:A:1474:VAL:O	2.20	0.41
1:A:2198:MET:CE	1:A:2203:MET:SD	3.08	0.41
1:A:3854:GLU:OE1	1:A:3854:GLU:HA	2.20	0.41
1:A:4073:GLY:O	1:A:4074:SER:HB3	2.20	0.41
1:G:904:HIS:HE1	1:G:906:CYS:SG	2.43	0.41
1:G:2206:THR:O	1:G:2210:VAL:HG23	2.20	0.41
1:G:3106:MET:HE3	1:G:3132:THR:CG2	2.50	0.41
1:G:3106:MET:CE	1:G:3132:THR:HB	2.49	0.41
1:G:3133:THR:HG23	1:G:3134:VAL:HG23	2.02	0.41
1:G:4021:LYS:HA	1:G:4024:VAL:HG22	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:121:LEU:N	1:M:134:ASP:O	2.53	0.41
1:M:3336:LYS:O	1:M:3340:VAL:HG13	2.19	0.41
2:N:58:LYS:NZ	2:N:58:LYS:HB3	2.34	0.41
1:S:1815:LEU:HD23	1:S:1865:MET:HE1	2.02	0.41
1:S:2166:LEU:HD11	1:S:2206:THR:HG23	2.02	0.41
1:S:4901:ILE:CG2	1:S:4902:GLU:N	2.83	0.41
1:A:904:HIS:HE1	1:A:906:CYS:SG	2.43	0.41
1:A:3652:MET:HA	1:A:3655:GLU:HG2	2.01	0.41
1:G:1255:TYR:CZ	1:G:1287:LEU:HD11	2.55	0.41
1:G:2166:LEU:HD11	1:G:2206:THR:HG23	2.02	0.41
1:G:4063:ASP:OD1	1:G:4064:MET:N	2.53	0.41
1:G:4901:ILE:HG22	1:G:4902:GLU:N	2.34	0.41
1:M:196:MET:N	1:M:196:MET:SD	2.93	0.41
1:M:4063:ASP:OD1	1:M:4064:MET:N	2.53	0.41
1:M:4093:PHE:CE1	1:M:4097:MET:HE2	2.54	0.41
1:S:71:GLN:HE21	1:S:108:LEU:CD2	2.33	0.41
1:S:168:ASP:HB3	1:S:199:LEU:HD12	2.00	0.41
1:S:196:MET:N	1:S:196:MET:SD	2.93	0.41
1:S:864:PRO:CG	1:S:867:LEU:HD12	2.50	0.41
1:S:1010:VAL:O	1:S:1010:VAL:HG23	2.21	0.41
1:S:2198:MET:CE	1:S:2203:MET:SD	3.08	0.41
1:S:2750:LYS:O	1:S:2750:LYS:HG2	2.20	0.41
1:S:4582:VAL:HG22	1:S:4630:TYR:CE2	2.55	0.41
1:A:3106:MET:HE3	1:A:3132:THR:CG2	2.50	0.41
1:A:4138:ASP:O	1:A:4142:ASN:ND2	2.43	0.41
1:A:4835:LYS:O	1:A:4839:MET:HG3	2.20	0.41
1:G:2750:LYS:O	1:G:2750:LYS:HG2	2.19	0.41
1:G:3336:LYS:O	1:G:3340:VAL:HG13	2.19	0.41
1:G:3567:PRO:O	1:G:3570:ARG:HB3	2.20	0.41
1:G:3696:ASP:OD1	1:G:3699:HIS:HB2	2.20	0.41
1:G:3705:PHE:HA	1:G:3708:THR:HG22	2.03	0.41
1:M:74:SER:HA	1:M:105:HIS:CD2	2.55	0.41
1:M:645:ARG:HG2	1:M:826:ILE:HG12	2.02	0.41
1:M:1167:GLU:OE1	1:M:1167:GLU:C	2.63	0.41
1:M:2198:MET:CE	1:M:2203:MET:SD	3.08	0.41
1:M:3531:ASP:OD1	1:M:3531:ASP:N	2.53	0.41
1:M:3535:LEU:O	1:M:3539:ARG:HG2	2.21	0.41
1:M:3569:LEU:HD12	1:M:3569:LEU:C	2.45	0.41
1:M:3599:VAL:HG12	1:M:3603:LEU:CD1	2.50	0.41
1:M:4073:GLY:O	1:M:4074:SER:HB3	2.21	0.41
1:M:4582:VAL:HG22	1:M:4630:TYR:CE2	2.55	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:544:LEU:HD22	1:S:574:VAL:HG13	2.02	0.41
1:S:1255:TYR:CZ	1:S:1287:LEU:HD11	2.55	0.41
1:S:3535:LEU:O	1:S:3539:ARG:HG2	2.21	0.41
1:A:14:LEU:N	1:A:14:LEU:HD12	2.34	0.41
1:A:140:ASP:OD1	1:A:140:ASP:N	2.53	0.41
1:A:1221:GLU:OE1	1:A:1221:GLU:N	2.53	0.41
1:A:1236:THR:OG1	1:A:1608:MET:SD	2.77	0.41
1:A:2639:MET:HB3	1:A:2640:PRO:HD3	2.02	0.41
1:G:544:LEU:HD22	1:G:574:VAL:HG13	2.02	0.41
1:G:1221:GLU:N	1:G:1221:GLU:OE1	2.53	0.41
1:G:4835:LYS:O	1:G:4839:MET:HG3	2.20	0.41
1:M:3652:MET:HA	1:M:3655:GLU:HG2	2.01	0.41
1:M:3770:LEU:HB3	1:M:3804:ILE:HD11	2.01	0.41
1:S:121:LEU:N	1:S:134:ASP:O	2.53	0.41
1:S:400:ALA:HA	1:S:403:MET:HE2	2.03	0.41
1:S:645:ARG:HG2	1:S:826:ILE:HG12	2.02	0.41
1:S:1167:GLU:C	1:S:1167:GLU:OE1	2.63	0.41
1:S:2230:THR:HG23	1:S:2270:SER:H	1.86	0.41
1:S:2527:LEU:HD23	1:S:2531:ARG:NH2	2.36	0.41
1:S:2599:GLN:O	1:S:2603:ILE:HG13	2.20	0.41
1:S:3050:VAL:O	1:S:3050:VAL:HG12	2.20	0.41
1:S:3567:PRO:O	1:S:3570:ARG:HB3	2.20	0.41
1:A:2527:LEU:HD23	1:A:2531:ARG:NH2	2.36	0.41
1:A:3753:PHE:O	1:A:3756:LYS:HG2	2.20	0.41
1:A:4582:VAL:HG22	1:A:4630:TYR:CE2	2.55	0.41
1:G:3050:VAL:O	1:G:3050:VAL:HG12	2.20	0.41
1:M:544:LEU:HD22	1:M:574:VAL:HG13	2.02	0.41
1:M:1474:VAL:O	1:M:1474:VAL:HG13	2.20	0.41
1:M:2166:LEU:HD11	1:M:2206:THR:HG23	2.02	0.41
1:M:3696:ASP:OD1	1:M:3699:HIS:HB2	2.20	0.41
1:M:4021:LYS:HA	1:M:4024:VAL:HG22	2.02	0.41
1:S:347:PHE:N	1:S:347:PHE:CD1	2.89	0.41
1:S:483:MET:HA	1:S:483:MET:HE3	2.02	0.41
1:S:789:VAL:CG1	1:S:790:ARG:N	2.84	0.41
1:S:3409:TYR:N	1:S:3410:PRO:HD2	2.36	0.41
1:S:4021:LYS:HA	1:S:4024:VAL:HG22	2.03	0.41
1:A:1815:LEU:HD23	1:A:1865:MET:HE1	2.02	0.41
1:A:2230:THR:HG23	1:A:2270:SER:H	1.86	0.41
1:A:2348:GLU:OE1	1:A:2348:GLU:N	2.31	0.41
1:A:3456:GLN:HA	1:A:3459:VAL:HG12	2.02	0.41
1:A:3569:LEU:HD12	1:A:3569:LEU:C	2.45	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1773:PRO:HA	1:G:1774:PRO:HD3	1.96	0.41
1:M:1255:TYR:CZ	1:M:1287:LEU:HD11	2.55	0.41
1:M:2348:GLU:H	1:M:2348:GLU:CD	2.22	0.41
1:S:904:HIS:HE1	1:S:906:CYS:SG	2.43	0.41
1:S:3106:MET:HE3	1:S:3132:THR:CG2	2.50	0.41
1:A:1255:TYR:CZ	1:A:1287:LEU:HD11	2.55	0.41
1:A:1299:GLN:NE2	2:B:32:GLN:HE21	2.19	0.41
1:A:2628:PHE:HD1	1:A:2907:PRO:HD3	1.85	0.41
1:A:3531:ASP:N	1:A:3531:ASP:OD1	2.53	0.41
1:A:3705:PHE:HA	1:A:3708:THR:HG22	2.02	0.41
1:A:4079:ASP:HB2	1:A:4096:ALA:HA	2.03	0.41
1:G:501:ALA:O	1:G:505:GLU:HG3	2.21	0.41
1:G:3916:ILE:CG2	1:G:3980:LEU:HD21	2.51	0.41
1:M:2012:PHE:CZ	1:M:2031:LEU:HD23	2.56	0.41
1:S:1474:VAL:O	1:S:1474:VAL:HG13	2.20	0.41
1:S:2005:GLN:O	1:S:2009:LEU:HG	2.21	0.41
1:S:3549:VAL:O	1:S:3553:LEU:CD1	2.67	0.41
1:S:4073:GLY:O	1:S:4074:SER:HB3	2.21	0.41
1:S:4079:ASP:HB2	1:S:4096:ALA:HA	2.03	0.41
1:A:71:GLN:HE21	1:A:108:LEU:CD2	2.33	0.41
1:A:789:VAL:CG1	1:A:790:ARG:N	2.84	0.41
1:A:1167:GLU:C	1:A:1167:GLU:OE1	2.63	0.41
1:A:2624:ARG:NE	1:A:2910:THR:O	2.48	0.41
1:A:4021:LYS:HA	1:A:4024:VAL:HG22	2.02	0.41
1:A:4052:SER:O	1:A:4055:VAL:HG12	2.21	0.41
1:A:4839:MET:CE	1:G:4822:THR:CG2	2.91	0.41
1:G:347:PHE:N	1:G:347:PHE:CD1	2.89	0.41
1:G:1474:VAL:O	1:G:1474:VAL:HG13	2.20	0.41
1:G:2348:GLU:OE1	1:G:2348:GLU:N	2.31	0.41
1:G:3187:ARG:N	1:G:3188:PRO:HD2	2.36	0.41
1:G:3355:HIS:HD1	1:G:3355:HIS:C	2.28	0.41
1:G:3409:TYR:N	1:G:3410:PRO:HD2	2.35	0.41
1:G:3569:LEU:HD12	1:G:3569:LEU:C	2.46	0.41
1:G:3804:ILE:O	1:G:3804:ILE:CG2	2.69	0.41
1:G:4582:VAL:HG22	1:G:4630:TYR:CE2	2.55	0.41
1:G:4901:ILE:CG2	1:G:4902:GLU:N	2.83	0.41
1:M:1010:VAL:HG23	1:M:1010:VAL:O	2.21	0.41
1:S:3456:GLN:O	1:S:3460:VAL:HG22	2.21	0.41
1:S:3510:ILE:O	1:S:3513:THR:HG22	2.21	0.41
1:S:3916:ILE:CG2	1:S:3980:LEU:HD21	2.51	0.41
1:S:4175:ARG:N	1:S:4176:PRO:HD2	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:347:PHE:N	1:A:347:PHE:CD1	2.89	0.41
1:A:501:ALA:O	1:A:505:GLU:HG3	2.21	0.41
1:A:645:ARG:HG2	1:A:826:ILE:HG12	2.02	0.41
1:A:1441:ALA:N	1:A:1513:ASP:OD1	2.49	0.41
1:A:2005:GLN:O	1:A:2009:LEU:HG	2.21	0.41
1:A:2419:GLY:O	1:A:2423:MET:SD	2.79	0.41
1:A:3050:VAL:O	1:A:3050:VAL:HG12	2.20	0.41
1:A:3183:VAL:O	1:A:3187:ARG:HG3	2.21	0.41
1:A:3355:HIS:C	1:A:3355:HIS:HD1	2.28	0.41
1:A:3409:TYR:N	1:A:3410:PRO:HD2	2.36	0.41
1:A:3959:LYS:NZ	1:A:4022:ASP:OD2	2.49	0.41
1:A:4175:ARG:N	1:A:4176:PRO:HD2	2.36	0.41
1:A:4822:THR:CG2	1:S:4839:MET:CE	2.91	0.41
1:A:4901:ILE:HG22	1:A:4902:GLU:N	2.34	0.41
2:B:69:LEU:HD13	2:B:107:LEU:HD12	2.03	0.41
1:G:74:SER:HA	1:G:105:HIS:CD2	2.55	0.41
1:G:937:CYS:SG	1:G:984:LEU:HD21	2.59	0.41
1:G:1007:TYR:CD1	1:G:1008:SER:N	2.89	0.41
1:G:1167:GLU:C	1:G:1167:GLU:OE1	2.63	0.41
1:G:1820:ARG:HH11	1:G:1820:ARG:HG3	1.86	0.41
1:G:3510:ILE:O	1:G:3513:THR:HG22	2.21	0.41
1:M:347:PHE:N	1:M:347:PHE:CD1	2.89	0.41
1:M:400:ALA:HA	1:M:403:MET:HE2	2.03	0.41
1:M:789:VAL:CG1	1:M:790:ARG:N	2.84	0.41
1:M:3133:THR:HG23	1:M:3134:VAL:HG23	2.02	0.41
1:M:3705:PHE:HA	1:M:3708:THR:HG22	2.02	0.41
1:M:4184:MET:HE3	1:M:4188:ARG:HA	2.03	0.41
1:S:3456:GLN:HA	1:S:3459:VAL:HG12	2.02	0.41
1:S:3529:ASP:O	1:S:3533:ILE:HG12	2.21	0.41
1:S:3531:ASP:N	1:S:3531:ASP:OD1	2.53	0.41
1:S:3569:LEU:C	1:S:3569:LEU:HD12	2.45	0.41
1:S:4052:SER:O	1:S:4055:VAL:HG12	2.21	0.41
1:S:4114:CYS:SG	1:S:4131:ARG:NH2	2.94	0.41
1:S:4835:LYS:O	1:S:4839:MET:HG3	2.20	0.41
2:T:16:PHE:O	2:T:18:LYS:NZ	2.52	0.41
1:A:544:LEU:HD22	1:A:574:VAL:HG13	2.02	0.41
1:A:2166:LEU:HD11	1:A:2206:THR:HG23	2.02	0.41
1:A:2351:ASN:HA	1:A:2354:VAL:HG12	2.03	0.41
2:B:53:LYS:C	2:B:54:GLN:OE1	2.64	0.41
1:G:35:LEU:HD11	1:G:189:LEU:HD13	2.03	0.41
1:G:140:ASP:OD1	1:G:140:ASP:N	2.53	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:1815:LEU:HD23	1:G:1865:MET:HE1	2.03	0.41
1:M:3409:TYR:N	1:M:3410:PRO:HD2	2.36	0.41
1:M:3916:ILE:O	1:M:3920:VAL:HG23	2.21	0.41
1:S:984:LEU:HD12	1:S:987:ARG:NH1	2.34	0.41
1:S:1269:CYS:HA	1:S:1564:PHE:O	2.21	0.41
1:S:2419:GLY:O	1:S:2423:MET:SD	2.79	0.41
1:S:3183:VAL:O	1:S:3187:ARG:HG3	2.21	0.41
1:A:73:LEU:HD11	1:A:78:LEU:CB	2.47	0.40
1:A:1167:GLU:OE1	1:A:1167:GLU:O	2.39	0.40
1:A:2377:LEU:HB2	1:A:2465:ASP:OD1	2.22	0.40
1:A:3696:ASP:OD1	1:A:3699:HIS:HB2	2.20	0.40
1:A:3754:GLU:HG2	1:A:3755:GLU:OE1	2.21	0.40
1:G:530:ILE:HD11	1:G:537:CYS:SG	2.61	0.40
1:G:789:VAL:CG1	1:G:790:ARG:N	2.84	0.40
1:G:1299:GLN:NE2	2:H:32:GLN:HE21	2.19	0.40
1:G:2005:GLN:O	1:G:2009:LEU:HG	2.21	0.40
1:G:2198:MET:CE	1:G:2203:MET:SD	3.08	0.40
1:G:2440:MET:C	1:G:2440:MET:HE3	2.46	0.40
1:G:3754:GLU:HG2	1:G:3755:GLU:OE1	2.21	0.40
1:G:4114:CYS:SG	1:G:4131:ARG:NH2	2.94	0.40
1:G:4184:MET:HE3	1:G:4188:ARG:HA	2.03	0.40
1:M:1658:ASP:N	1:M:1658:ASP:OD1	2.54	0.40
1:M:3753:PHE:O	1:M:3756:LYS:HG2	2.20	0.40
1:M:3754:GLU:HG2	1:M:3755:GLU:OE1	2.21	0.40
1:M:4052:SER:O	1:M:4055:VAL:HG12	2.21	0.40
1:M:4771:ILE:HD13	1:M:4771:ILE:N	2.37	0.40
1:S:35:LEU:HD11	1:S:189:LEU:HD13	2.03	0.40
1:S:1007:TYR:CD1	1:S:1008:SER:N	2.89	0.40
1:S:1024:TYR:O	1:S:1025:ARG:C	2.63	0.40
1:S:2348:GLU:H	1:S:2348:GLU:CD	2.22	0.40
1:A:1007:TYR:CD1	1:A:1008:SER:N	2.89	0.40
1:A:1658:ASP:N	1:A:1658:ASP:OD1	2.54	0.40
1:A:4114:CYS:SG	1:A:4131:ARG:NH2	2.94	0.40
1:A:4945:ASP:O	1:A:4945:ASP:OD1	2.39	0.40
1:G:1024:TYR:O	1:G:1025:ARG:C	2.63	0.40
1:G:1269:CYS:HA	1:G:1564:PHE:O	2.21	0.40
2:H:53:LYS:C	2:H:54:GLN:OE1	2.64	0.40
1:M:202:MET:HE3	1:M:202:MET:HB2	2.00	0.40
1:M:3163:VAL:O	1:M:3167:ARG:HG3	2.22	0.40
1:M:4835:LYS:O	1:M:4839:MET:HG3	2.20	0.40
1:S:1943:LEU:HD13	1:S:2098:VAL:HG22	2.04	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:3187:ARG:N	1:S:3188:PRO:HD2	2.36	0.40
1:S:3916:ILE:O	1:S:3920:VAL:HG23	2.21	0.40
1:A:2012:PHE:CZ	1:A:2031:LEU:HD23	2.56	0.40
1:A:3175:LEU:HD11	1:A:3183:VAL:HG13	2.02	0.40
1:A:3187:ARG:N	1:A:3188:PRO:HD2	2.36	0.40
1:A:3529:ASP:O	1:A:3533:ILE:HG12	2.21	0.40
1:G:400:ALA:HA	1:G:403:MET:HE2	2.03	0.40
1:G:1010:VAL:O	1:G:1010:VAL:HG23	2.21	0.40
1:G:2012:PHE:CZ	1:G:2031:LEU:HD23	2.56	0.40
1:G:3175:LEU:HD11	1:G:3183:VAL:HG13	2.02	0.40
2:H:69:LEU:HD13	2:H:107:LEU:HD12	2.03	0.40
1:M:1815:LEU:HD23	1:M:1865:MET:HE1	2.02	0.40
1:M:2305:CYS:SG	1:M:2324:ASN:HB3	2.62	0.40
1:M:2419:GLY:O	1:M:2423:MET:SD	2.79	0.40
1:M:2440:MET:C	1:M:2440:MET:HE3	2.46	0.40
1:M:2527:LEU:HD23	1:M:2531:ARG:NH2	2.36	0.40
1:M:3183:VAL:O	1:M:3187:ARG:HG3	2.21	0.40
1:M:3804:ILE:O	1:M:3804:ILE:CG2	2.69	0.40
1:S:2012:PHE:CZ	1:S:2031:LEU:HD23	2.56	0.40
1:S:3754:GLU:HG2	1:S:3755:GLU:OE1	2.21	0.40
1:A:2440:MET:HE3	1:A:2440:MET:C	2.46	0.40
1:A:3456:GLN:O	1:A:3460:VAL:HG22	2.21	0.40
1:G:1167:GLU:OE1	1:G:1167:GLU:O	2.39	0.40
1:G:3456:GLN:HA	1:G:3459:VAL:HG12	2.02	0.40
1:G:3854:GLU:OE1	1:G:3854:GLU:HA	2.20	0.40
1:G:4079:ASP:HB2	1:G:4096:ALA:HA	2.03	0.40
1:G:4839:MET:CE	1:M:4822:THR:CG2	2.91	0.40
1:G:4897:ILE:HD12	1:G:4897:ILE:HA	1.99	0.40
1:M:904:HIS:HE1	1:M:906:CYS:SG	2.43	0.40
1:M:1007:TYR:CD1	1:M:1008:SER:N	2.89	0.40
1:M:2628:PHE:HD1	1:M:2907:PRO:HD3	1.85	0.40
1:M:3388:GLU:O	1:M:3392:LEU:CD2	2.70	0.40
1:S:347:PHE:N	1:S:347:PHE:HD1	2.20	0.40
1:S:1820:ARG:HH11	1:S:1820:ARG:HG3	1.86	0.40
1:S:1828:ASP:N	1:S:1828:ASP:OD1	2.55	0.40
1:A:400:ALA:HA	1:A:403:MET:HE2	2.03	0.40
1:A:492:ASP:OD1	1:A:546:TRP:NE1	2.51	0.40
1:A:1010:VAL:HG23	1:A:1010:VAL:O	2.21	0.40
1:A:3163:VAL:O	1:A:3167:ARG:HG3	2.22	0.40
1:A:3916:ILE:O	1:A:3920:VAL:HG23	2.21	0.40
1:G:2351:ASN:HA	1:G:2354:VAL:HG12	2.03	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:2527:LEU:HD23	1:G:2531:ARG:NH2	2.36	0.40
1:G:2716:ASP:OD1	1:G:2716:ASP:N	2.55	0.40
1:G:3945:GLU:HG2	1:G:3946:GLN:N	2.36	0.40
1:G:4052:SER:O	1:G:4055:VAL:HG12	2.21	0.40
1:M:483:MET:HE3	1:M:483:MET:HA	2.02	0.40
1:M:2005:GLN:O	1:M:2009:LEU:HG	2.21	0.40
1:M:2230:THR:HG23	1:M:2270:SER:H	1.86	0.40
1:M:3235:SER:O	1:M:3238:GLU:HG2	2.22	0.40
1:M:3510:ILE:O	1:M:3513:THR:HG22	2.21	0.40
1:M:3945:GLU:HG2	1:M:3946:GLN:N	2.36	0.40
2:N:53:LYS:C	2:N:54:GLN:OE1	2.64	0.40
1:S:530:ILE:HD11	1:S:537:CYS:SG	2.61	0.40
1:S:2305:CYS:SG	1:S:2324:ASN:HB3	2.62	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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	4128/5037 (82%)	4047 (98%)	81 (2%)	0	100	100
1	G	4128/5037 (82%)	4047 (98%)	81 (2%)	0	100	100
1	M	4128/5037 (82%)	4047 (98%)	81 (2%)	0	100	100
1	S	4128/5037 (82%)	4047 (98%)	81 (2%)	0	100	100
2	B	105/111 (95%)	100 (95%)	5 (5%)	0	100	100
2	H	105/111 (95%)	100 (95%)	5 (5%)	0	100	100
2	N	105/111 (95%)	100 (95%)	5 (5%)	0	100	100
2	T	105/111 (95%)	100 (95%)	5 (5%)	0	100	100
All	All	16932/20592 (82%)	16588 (98%)	344 (2%)	0	100	100

There are no Ramachandran outliers to report.

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 PDB entries followed by that with respect to all EM entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	3492/4276 (82%)	3491 (100%)	1 (0%)	100	100
1	G	3492/4276 (82%)	3491 (100%)	1 (0%)	100	100
1	M	3492/4276 (82%)	3491 (100%)	1 (0%)	100	100
1	S	3492/4276 (82%)	3491 (100%)	1 (0%)	100	100
2	B	86/91 (94%)	86 (100%)	0	100	100
2	H	86/91 (94%)	86 (100%)	0	100	100
2	N	86/91 (94%)	86 (100%)	0	100	100
2	T	86/91 (94%)	86 (100%)	0	100	100
All	All	14312/17468 (82%)	14308 (100%)	4 (0%)	100	100

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	272	SER
1	G	272	SER
1	M	272	SER
1	S	272	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (145) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	GLN
1	A	79	GLN
1	A	105	HIS
1	A	151	HIS
1	A	181	HIS
1	A	495	ASN
1	A	533	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	797	HIS
1	A	866	HIS
1	A	909	ASN
1	A	911	HIS
1	A	1158	ASN
1	A	1299	GLN
1	A	1463	ASN
1	A	1484	HIS
1	A	1598	GLN
1	A	1640	HIS
1	A	1702	HIS
1	A	1953	HIS
1	A	2308	GLN
1	A	2515	GLN
1	A	2520	HIS
1	A	2773	ASN
1	A	2780	ASN
1	A	2856	ASN
1	A	2858	GLN
1	A	2877	GLN
1	A	2962	GLN
1	A	3127	GLN
1	A	3146	HIS
1	A	3809	ASN
1	A	3960	GLN
1	A	3970	GLN
1	A	4100	GLN
1	A	4812	HIS
2	B	32	GLN
1	G	71	GLN
1	G	79	GLN
1	G	105	HIS
1	G	151	HIS
1	G	181	HIS
1	G	461	HIS
1	G	495	ASN
1	G	533	ASN
1	G	797	HIS
1	G	866	HIS
1	G	909	ASN
1	G	911	HIS
1	G	1158	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	G	1165	ASN
1	G	1299	GLN
1	G	1463	ASN
1	G	1484	HIS
1	G	1558	HIS
1	G	1598	GLN
1	G	1640	HIS
1	G	1702	HIS
1	G	1953	HIS
1	G	2253	HIS
1	G	2308	GLN
1	G	2515	GLN
1	G	2520	HIS
1	G	2773	ASN
1	G	2780	ASN
1	G	2877	GLN
1	G	2931	GLN
1	G	2962	GLN
1	G	3127	GLN
1	G	3146	HIS
1	G	3268	HIS
1	G	3960	GLN
1	G	3970	GLN
1	G	4100	GLN
1	G	4812	HIS
1	G	4864	ASN
2	H	32	GLN
1	M	71	GLN
1	M	79	GLN
1	M	105	HIS
1	M	151	HIS
1	M	181	HIS
1	M	495	ASN
1	M	533	ASN
1	M	866	HIS
1	M	909	ASN
1	M	911	HIS
1	M	1158	ASN
1	M	1299	GLN
1	M	1484	HIS
1	M	1558	HIS
1	M	1598	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	M	1640	HIS
1	M	1702	HIS
1	M	1953	HIS
1	M	2253	HIS
1	M	2308	GLN
1	M	2515	GLN
1	M	2520	HIS
1	M	2773	ASN
1	M	2780	ASN
1	M	2877	GLN
1	M	2962	GLN
1	M	3127	GLN
1	M	3146	HIS
1	M	3268	HIS
1	M	3809	ASN
1	M	3960	GLN
1	M	3970	GLN
1	M	4100	GLN
1	M	4201	ASN
1	M	4864	ASN
2	N	32	GLN
1	S	71	GLN
1	S	79	GLN
1	S	105	HIS
1	S	181	HIS
1	S	495	ASN
1	S	533	ASN
1	S	797	HIS
1	S	866	HIS
1	S	909	ASN
1	S	911	HIS
1	S	1158	ASN
1	S	1299	GLN
1	S	1484	HIS
1	S	1598	GLN
1	S	1640	HIS
1	S	1702	HIS
1	S	1953	HIS
1	S	2253	HIS
1	S	2308	GLN
1	S	2515	GLN
1	S	2520	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	S	2773	ASN
1	S	2780	ASN
1	S	2877	GLN
1	S	2931	GLN
1	S	2962	GLN
1	S	3127	GLN
1	S	3146	HIS
1	S	3809	ASN
1	S	3970	GLN
1	S	4100	GLN
1	S	4201	ASN
2	T	32	GLN

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](#)

Of 12 ligands modelled in this entry, 8 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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 $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	117	A	5103	-	44,44,44	0.78	1 (2%)	55,61,61	1.06	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	117	G	5103	-	44,44,44	0.78	1 (2%)	55,61,61	1.06	4 (7%)
4	117	M	5103	-	44,44,44	0.78	1 (2%)	55,61,61	1.06	4 (7%)
4	117	S	5103	-	44,44,44	0.78	1 (2%)	55,61,61	1.07	4 (7%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	117	A	5103	-	-	1/33/33/33	0/4/4/4
4	117	G	5103	-	-	1/33/33/33	0/4/4/4
4	117	M	5103	-	-	1/33/33/33	0/4/4/4
4	117	S	5103	-	-	1/33/33/33	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	5103	117	C12-C10	-2.06	1.45	1.49
4	G	5103	117	C12-C10	-2.05	1.45	1.49
4	M	5103	117	C12-C10	-2.04	1.45	1.49
4	S	5103	117	C12-C10	-2.03	1.45	1.49

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	S	5103	117	C6-C7-N1	3.06	117.50	112.16
4	G	5103	117	C6-C7-N1	3.03	117.46	112.16
4	A	5103	117	C6-C7-N1	3.02	117.43	112.16
4	M	5103	117	C6-C7-N1	3.02	117.43	112.16
4	G	5103	117	C11-C18-N2	-2.60	111.38	115.81
4	M	5103	117	C11-C18-N2	-2.58	111.40	115.81
4	S	5103	117	C11-C18-N2	-2.58	111.41	115.81
4	M	5103	117	O1B-C1-O1A	2.56	129.91	123.33
4	M	5103	117	O1A-C1-C2	-2.56	114.99	122.84
4	A	5103	117	C11-C18-N2	-2.55	111.46	115.81
4	A	5103	117	O1A-C1-C2	-2.54	115.05	122.84
4	A	5103	117	O1B-C1-O1A	2.54	129.86	123.33
4	G	5103	117	O1B-C1-O1A	2.53	129.84	123.33
4	S	5103	117	O1A-C1-C2	-2.53	115.07	122.84
4	G	5103	117	O1A-C1-C2	-2.53	115.07	122.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	S	5103	117	O1B-C1-O1A	2.52	129.81	123.33

There are no chirality outliers.

All (4) torsion outliers are listed below:

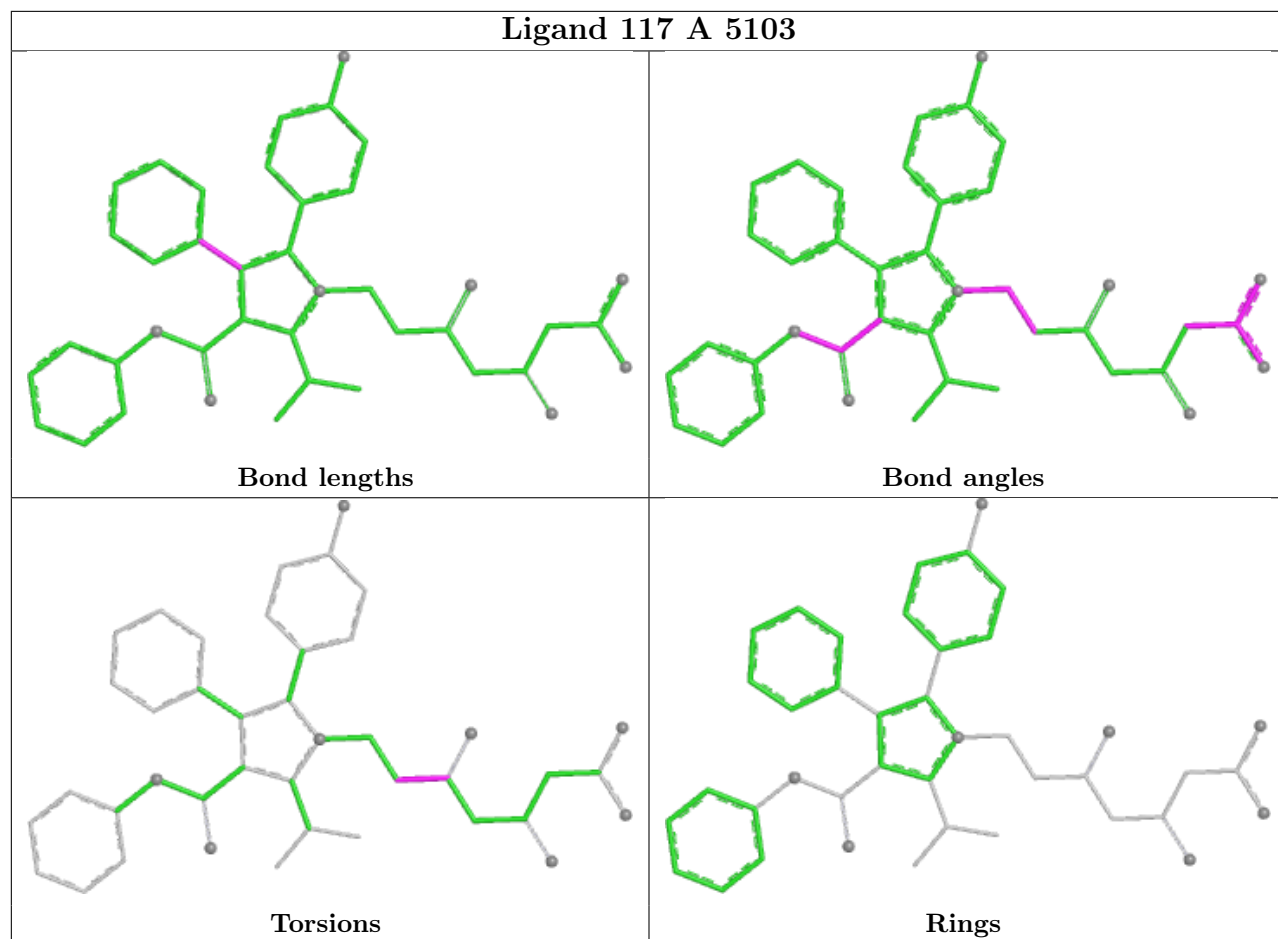
Mol	Chain	Res	Type	Atoms
4	A	5103	117	O5-C5-C6-C7
4	G	5103	117	O5-C5-C6-C7
4	M	5103	117	O5-C5-C6-C7
4	S	5103	117	O5-C5-C6-C7

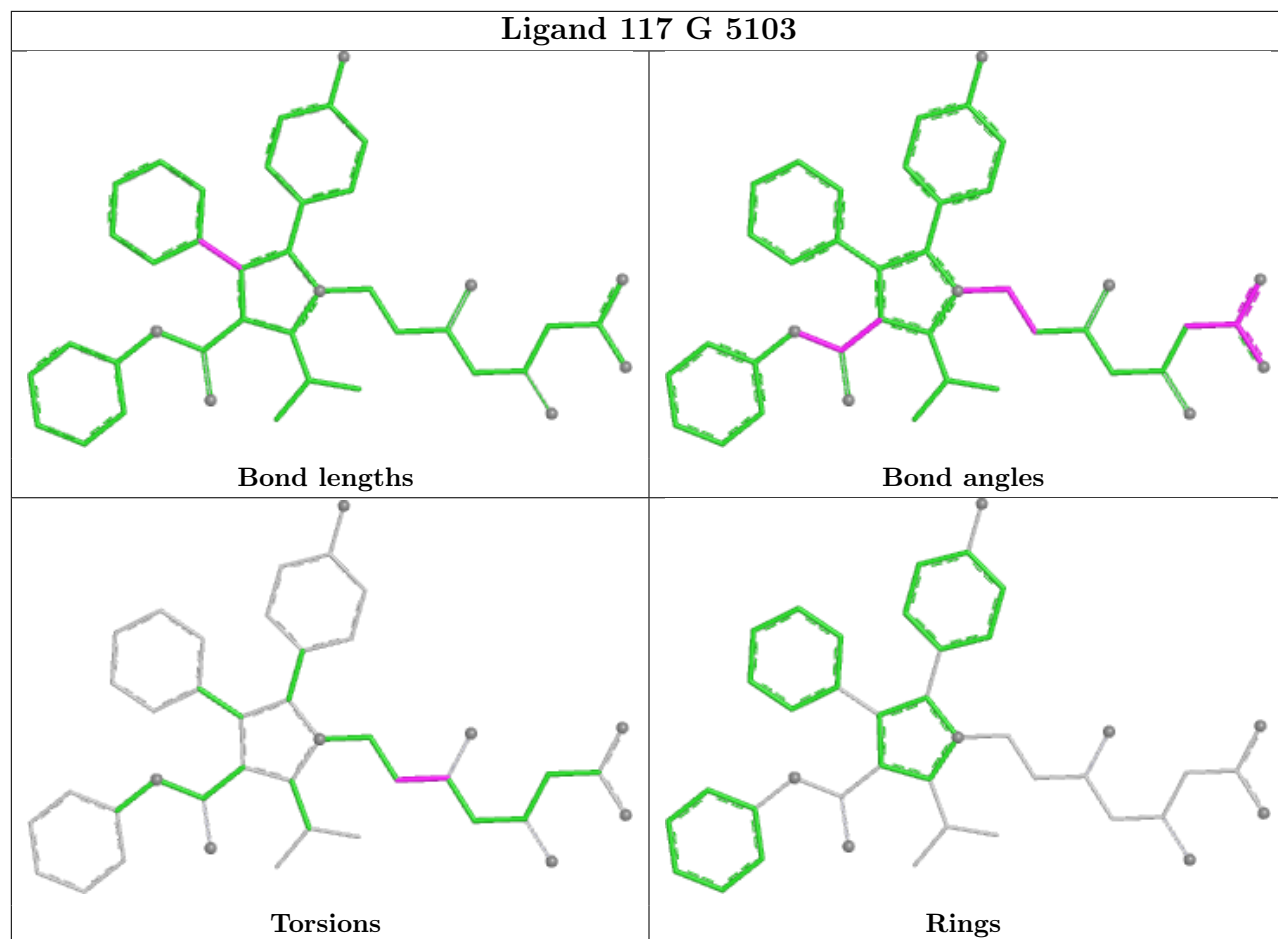
There are no ring outliers.

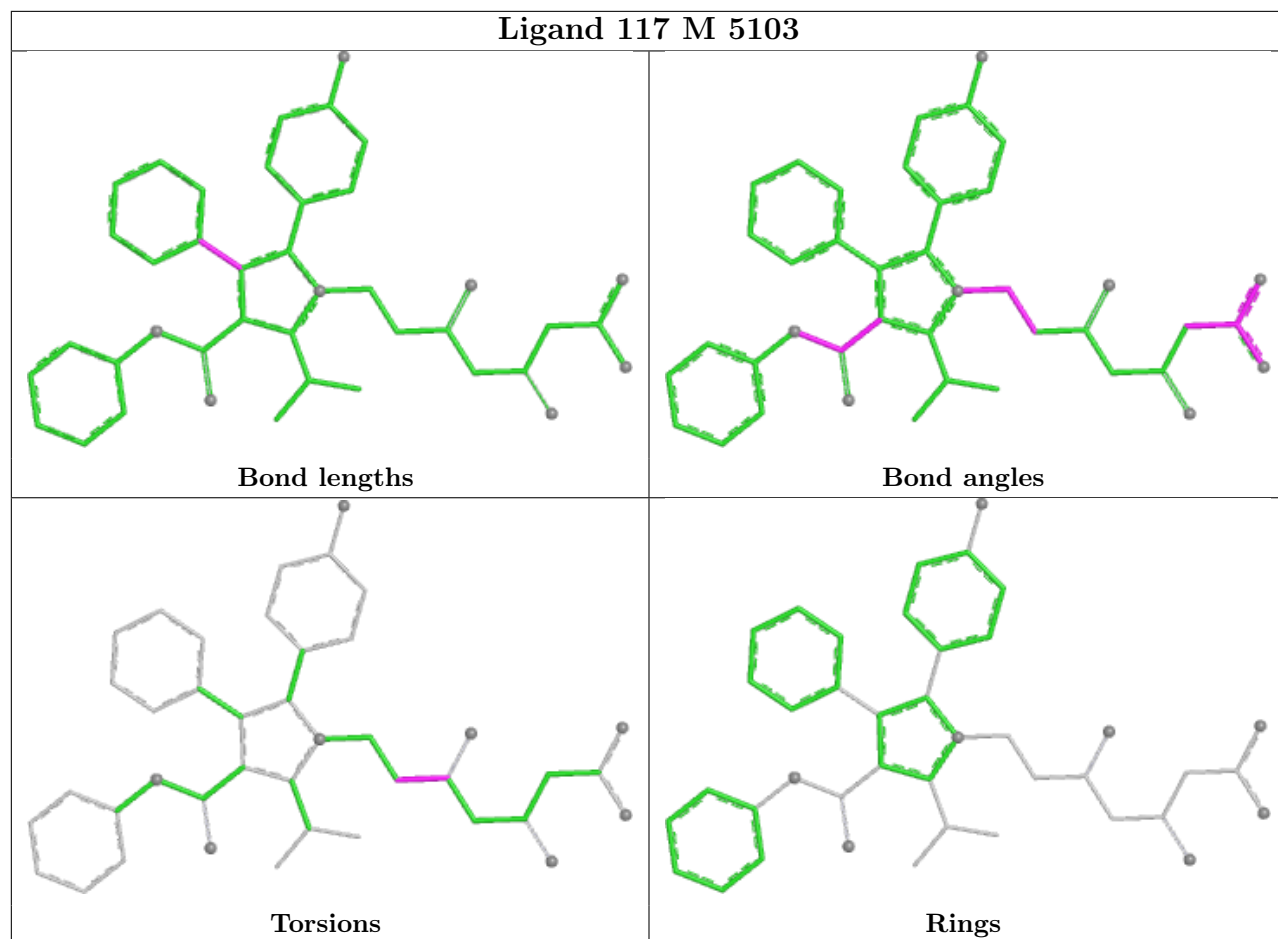
4 monomers are involved in 12 short contacts:

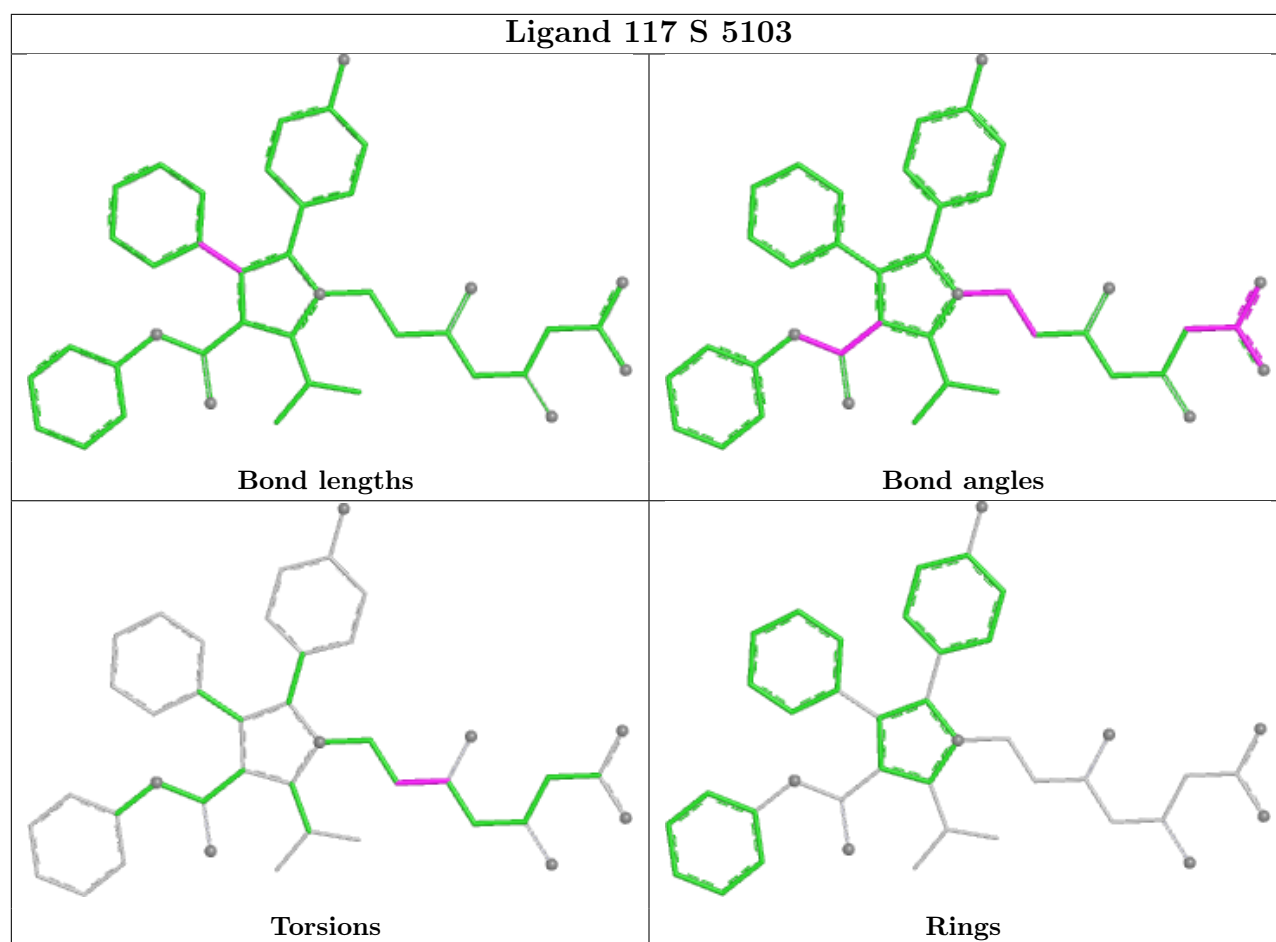
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	5103	117	3	0
4	G	5103	117	3	0
4	M	5103	117	3	0
4	S	5103	117	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

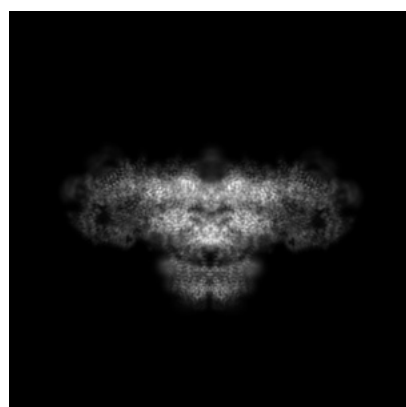
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-70590. These allow visual inspection of the internal detail of the map and identification of artifacts.

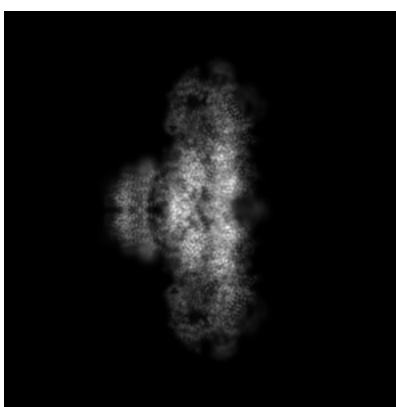
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

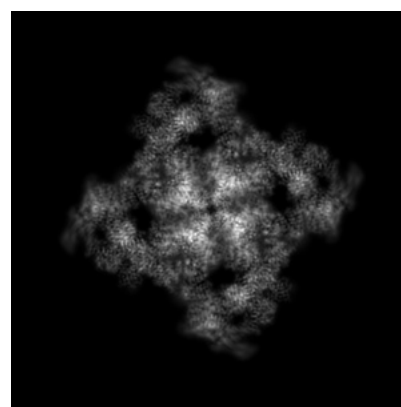
6.1.1 Primary map



X



Y



Z

The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

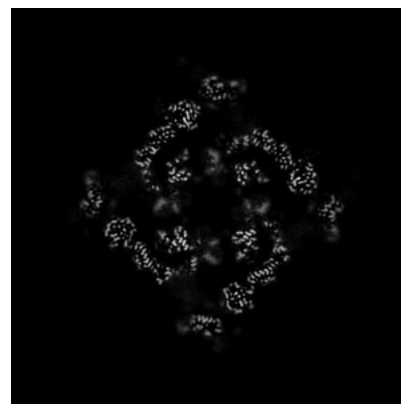
6.2.1 Primary map



X Index: 256



Y Index: 256



Z Index: 256

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

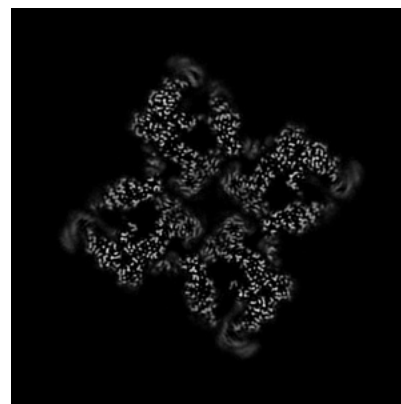
6.3.1 Primary map



X Index: 224



Y Index: 236

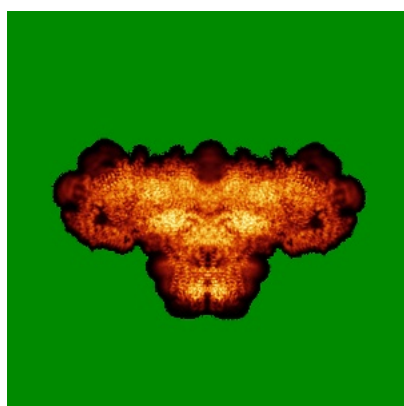


Z Index: 284

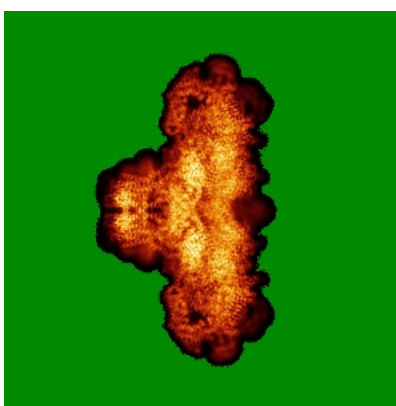
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

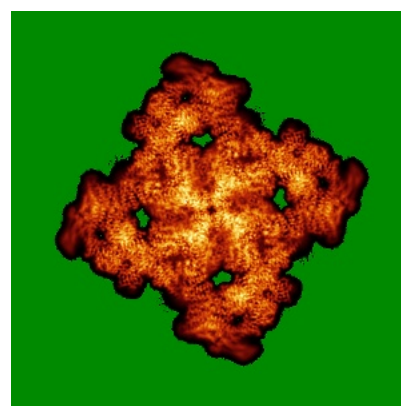
6.4.1 Primary map



X



Y

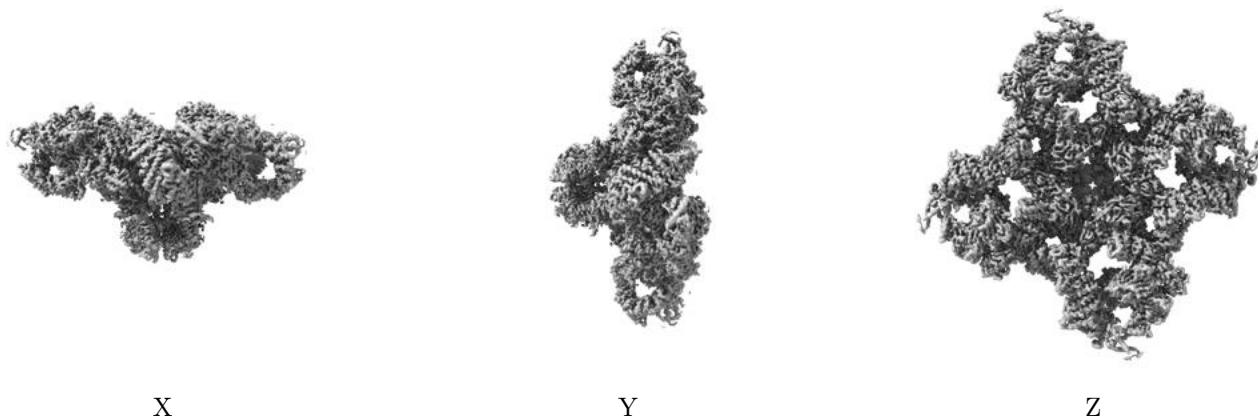


Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.123. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

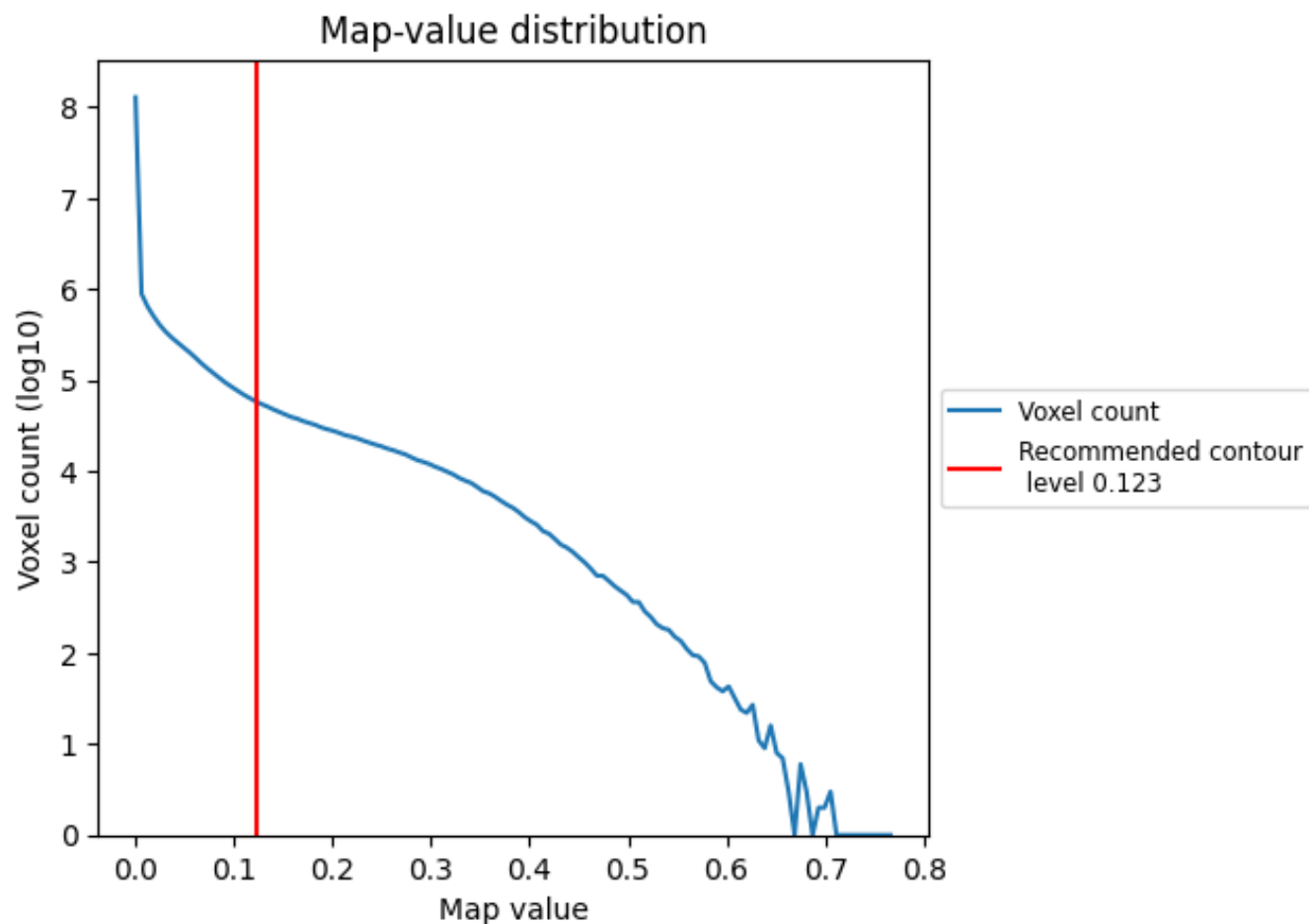
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

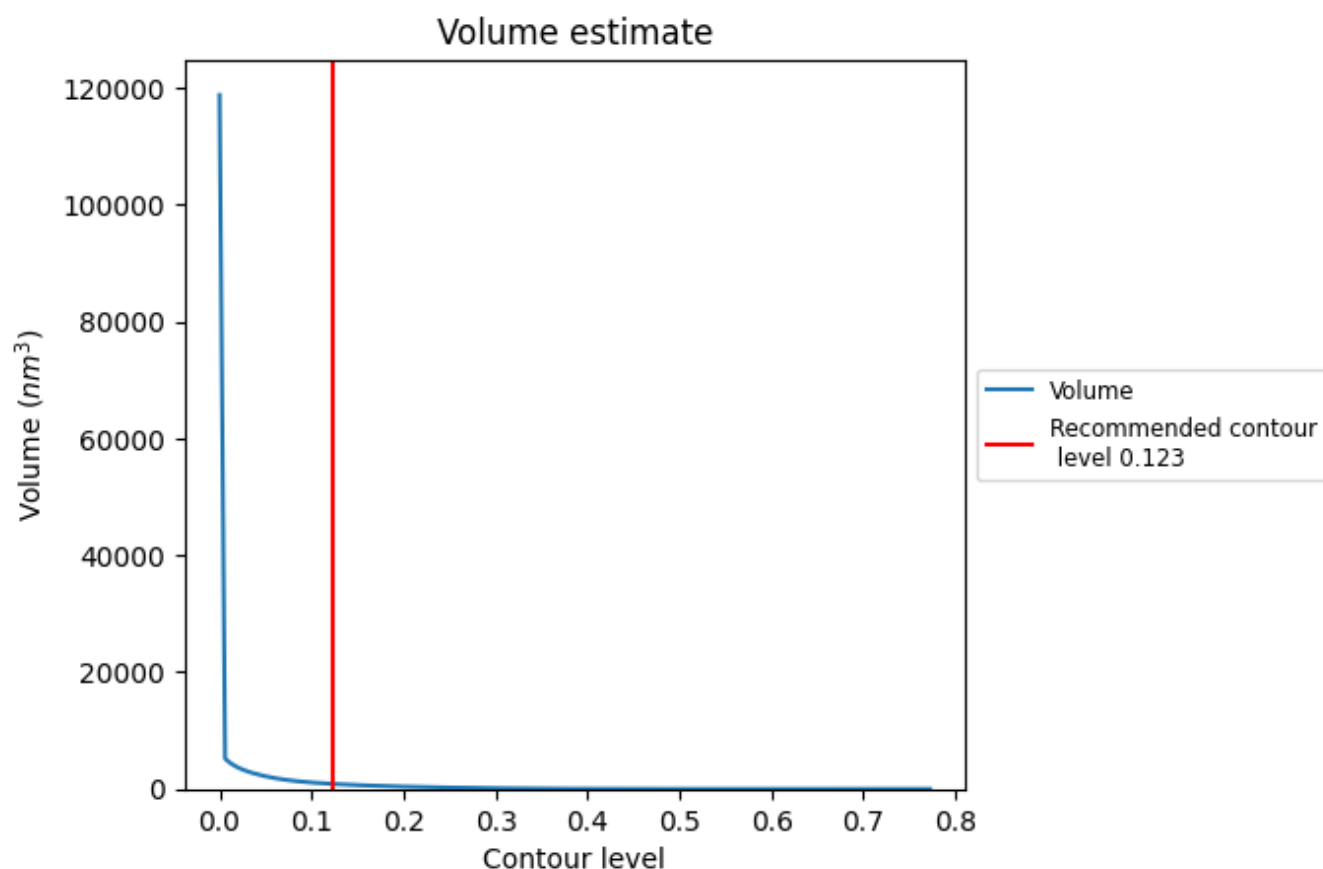
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

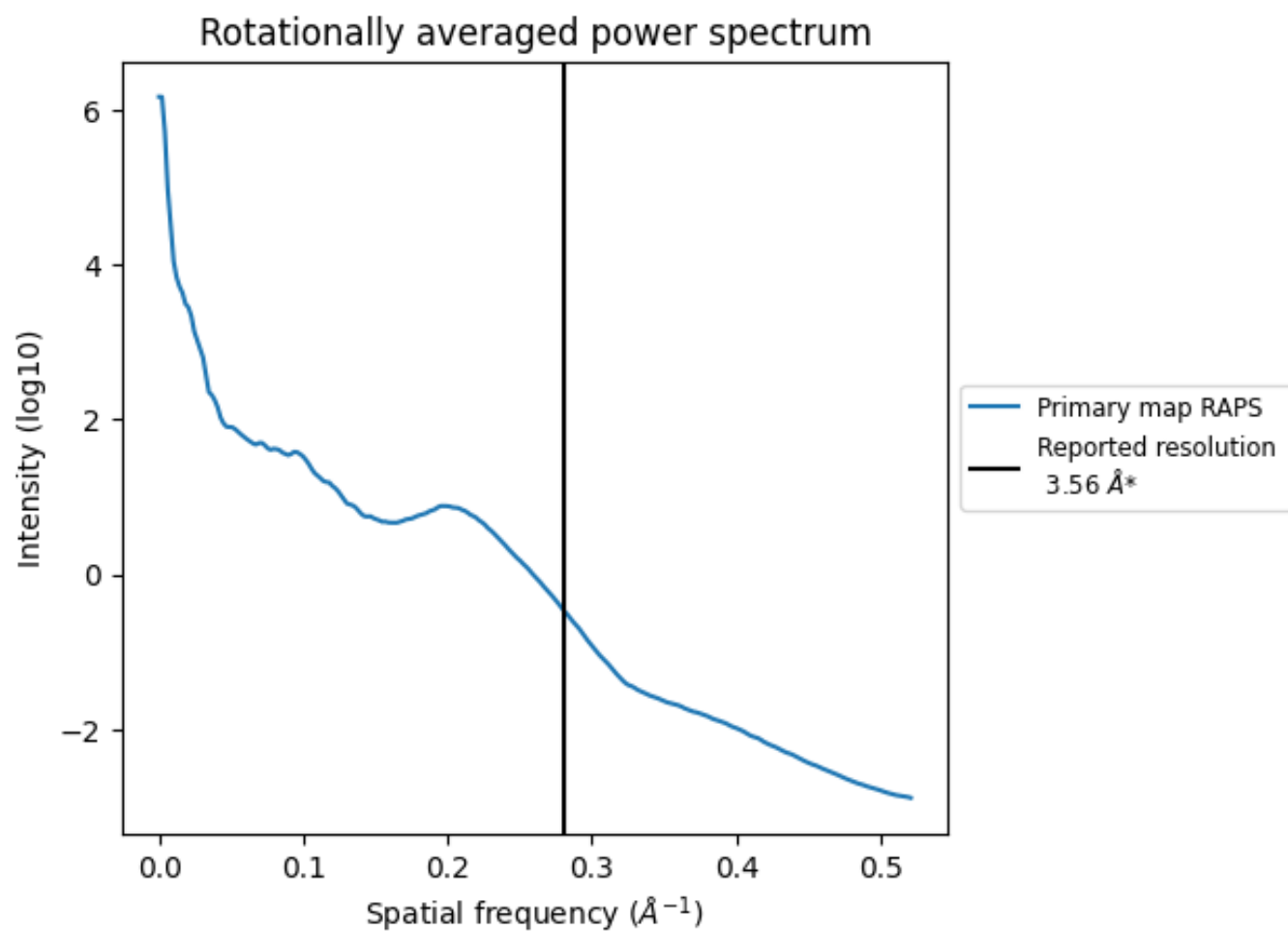
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 867 nm³; this corresponds to an approximate mass of 783 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ



*Reported resolution corresponds to spatial frequency of 0.281 Å⁻¹

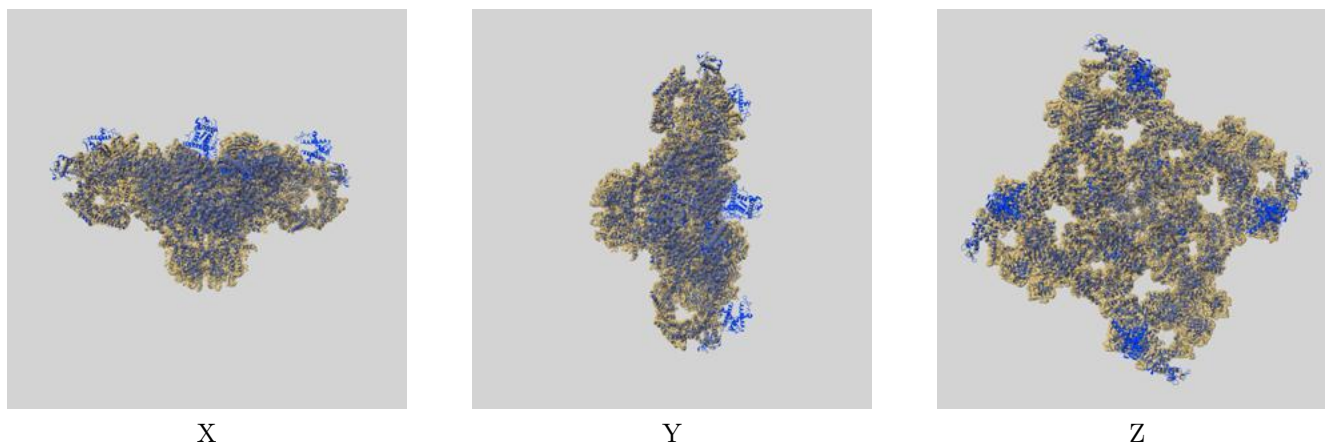
8 Fourier-Shell correlation ⓘ

This section was not generated. No FSC curve or half-maps provided.

9 Map-model fit [i](#)

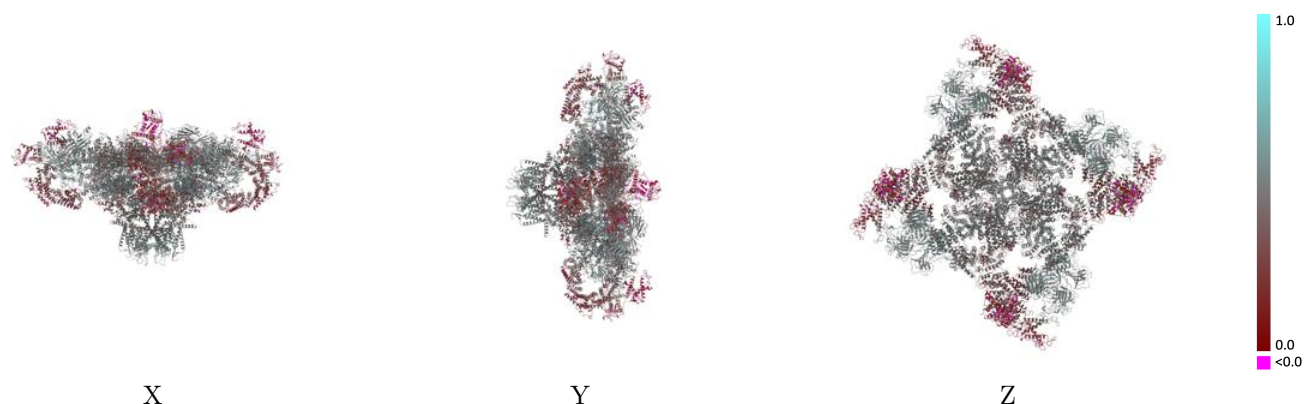
This section contains information regarding the fit between EMDB map EMD-70590 and PDB model 9OL5. Per-residue inclusion information can be found in section [3](#) on page [7](#).

9.1 Map-model overlay [i](#)



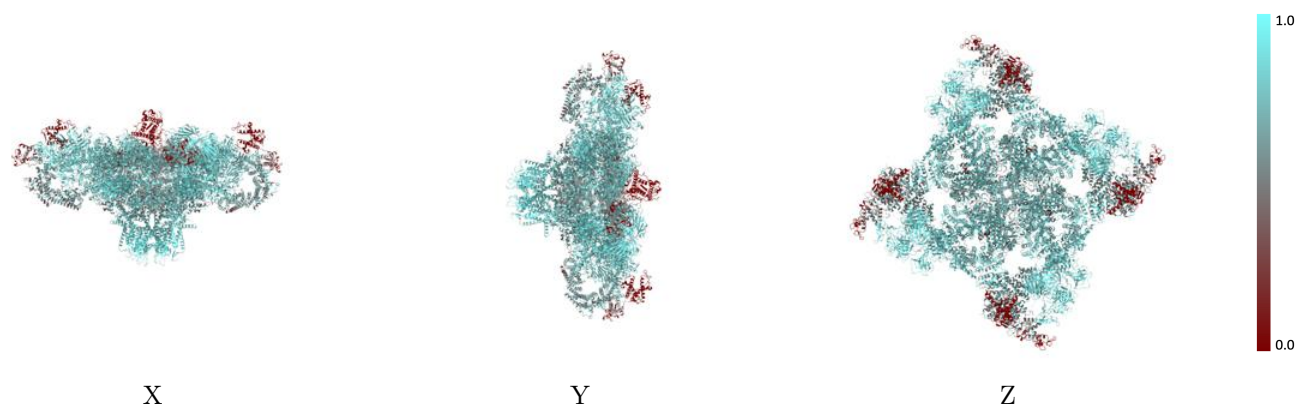
The images above show the 3D surface view of the map at the recommended contour level 0.123 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



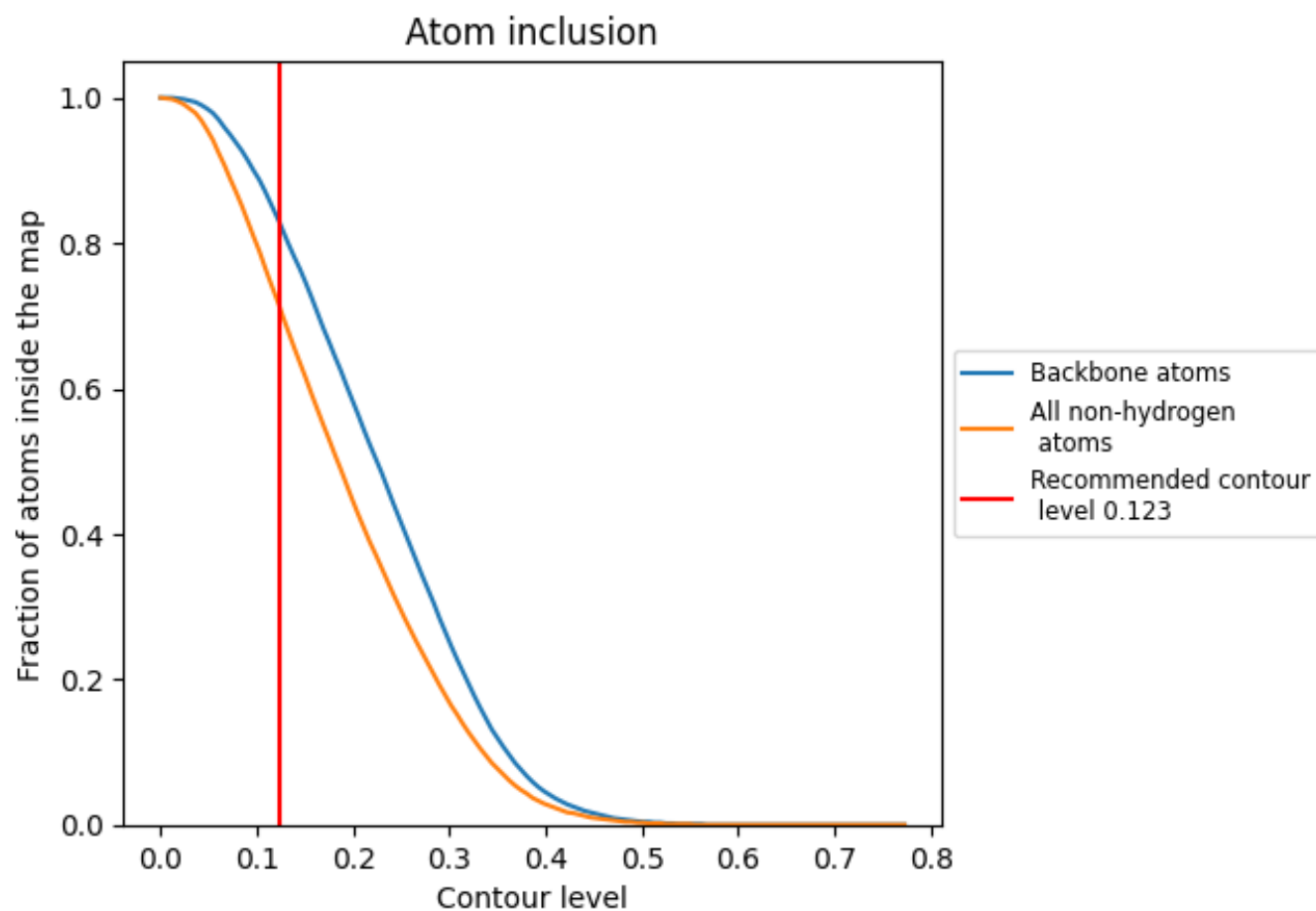
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.123).

9.4 Atom inclusion ⓘ



At the recommended contour level, 83% of all backbone atoms, 72% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

The table lists the average atom inclusion at the recommended contour level (0.123) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7150	0.4160
A	0.7120	0.4130
B	0.8330	0.5070
G	0.7120	0.4150
H	0.8230	0.5070
M	0.7120	0.4160
N	0.8400	0.5120
S	0.7120	0.4130
T	0.8230	0.5060

1.0

0.0

<0.0