



Full wwPDB EM Validation Report ⓘ

Mar 25, 2026 – 02:49 AM UTC

PDB ID : 6JII / pdb_00006jii
EMDB ID : EMD-9834
Title : Structure of RyR2 (F/A/C/L-Ca2+/apo-CaM-M dataset)
Authors : Gong, D.S.; Chi, X.M.; Zhou, G.W.; Huang, G.X.Y.; Lei, J.L.; Yan, N.
Deposited on : 2019-02-21
Resolution : 4.20 Å(reported)

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:

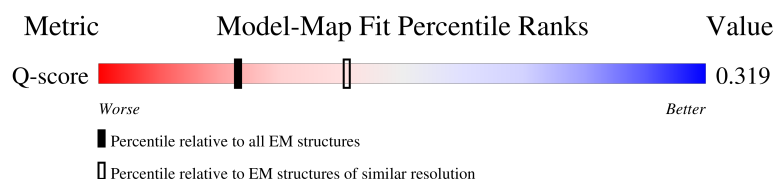
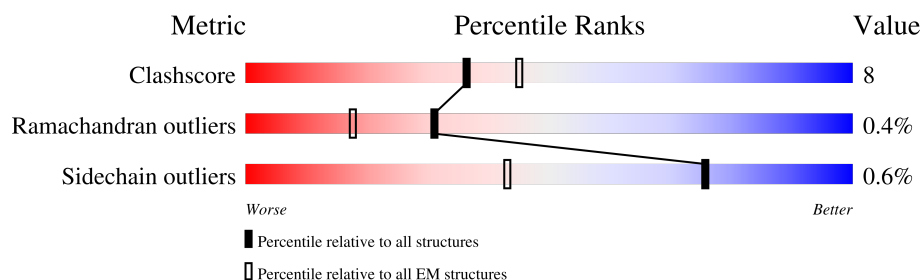
EMDB validation analysis : 0.0.1.dev132
Mogul : 2022.3.0, CSD as543be (2022)
MolProbity : 4-5-2 with Phenix2.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics : 202505.v01 (Using data in the EMDb 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 4.20 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	5410 (3.70 - 4.70)

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	108	 79% 20% .
1	D	108	 77% 22% .
1	G	108	 76% 23% .
1	J	108	 76% 23% .

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	B	4968	
2	E	4968	
2	H	4968	
2	K	4968	
3	C	149	
3	F	149	
3	I	149	
3	L	149	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	CFF	B	6002	-	X	-	-
6	CFF	E	6002	-	X	-	-
6	CFF	H	6002	-	X	-	-
6	CFF	K	6002	-	X	-	-

2 Entry composition [i](#)

There are 7 unique types of molecules in this entry. The entry contains 115028 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 Peptidyl-prolyl cis-trans isomerase FKBP1B.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
1	D	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
1	G	107	Total	C	N	O	S	0	0
			819	516	144	155	4		
1	J	107	Total	C	N	O	S	0	0
			819	516	144	155	4		

- Molecule 2 is a protein called Ryr2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	3508	Total	C	N	O	S	0	0
			26813	17078	4599	4977	159		
2	E	3508	Total	C	N	O	S	0	0
			26813	17078	4599	4977	159		
2	H	3508	Total	C	N	O	S	0	0
			26813	17078	4599	4977	159		
2	K	3508	Total	C	N	O	S	0	0
			26813	17078	4599	4977	159		

- Molecule 3 is a protein called Calmodulin-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	138	Total	C	N	O	S	0	0
			1078	668	176	225	9		
3	F	138	Total	C	N	O	S	0	0
			1078	668	176	225	9		
3	I	138	Total	C	N	O	S	0	0
			1078	668	176	225	9		
3	L	138	Total	C	N	O	S	0	0
			1078	668	176	225	9		

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	32	ALA	GLU	engineered mutation	UNP P0DP23
C	68	ALA	GLU	engineered mutation	UNP P0DP23
C	105	ALA	GLU	engineered mutation	UNP P0DP23
C	141	ALA	GLU	engineered mutation	UNP P0DP23
F	32	ALA	GLU	engineered mutation	UNP P0DP23
F	68	ALA	GLU	engineered mutation	UNP P0DP23
F	105	ALA	GLU	engineered mutation	UNP P0DP23
F	141	ALA	GLU	engineered mutation	UNP P0DP23
I	32	ALA	GLU	engineered mutation	UNP P0DP23
I	68	ALA	GLU	engineered mutation	UNP P0DP23
I	105	ALA	GLU	engineered mutation	UNP P0DP23
I	141	ALA	GLU	engineered mutation	UNP P0DP23
L	32	ALA	GLU	engineered mutation	UNP P0DP23
L	68	ALA	GLU	engineered mutation	UNP P0DP23
L	105	ALA	GLU	engineered mutation	UNP P0DP23
L	141	ALA	GLU	engineered mutation	UNP P0DP23

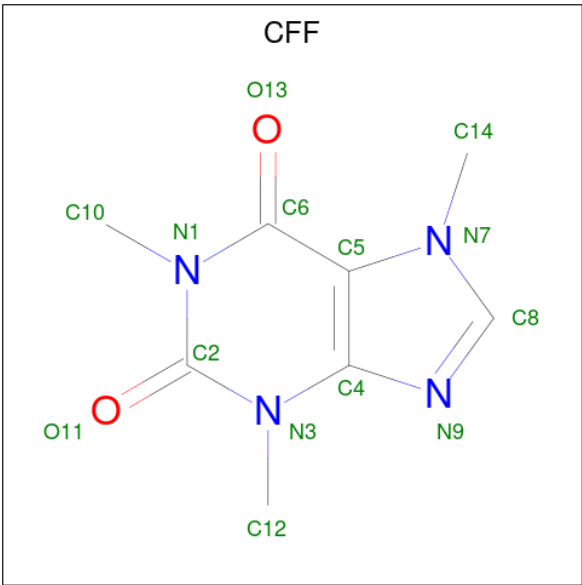
- Molecule 4 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	AltConf
4	B	1	Total Zn 1 1	0
4	E	1	Total Zn 1 1	0
4	H	1	Total Zn 1 1	0
4	K	1	Total Zn 1 1	0

- Molecule 5 is CALCIUM ION (CCD ID: CA) (formula: Ca).

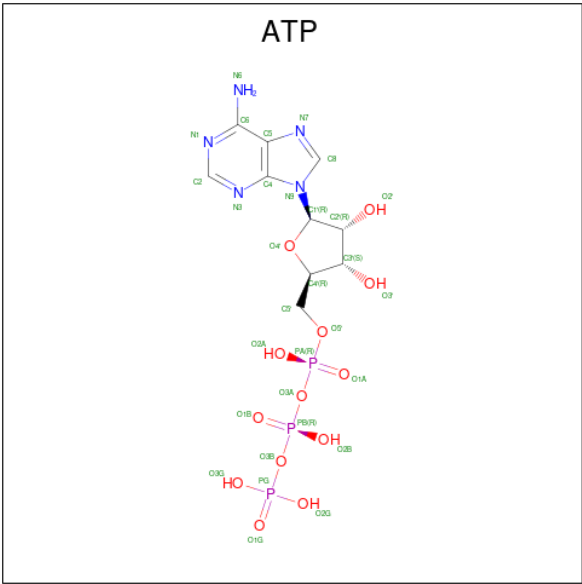
Mol	Chain	Residues	Atoms	AltConf
5	B	1	Total Ca 1 1	0
5	E	1	Total Ca 1 1	0
5	H	1	Total Ca 1 1	0
5	K	1	Total Ca 1 1	0

- Molecule 6 is CAFFEINE (CCD ID: CFF) (formula: C₈H₁₀N₄O₂).



Mol	Chain	Residues	Atoms				AltConf
6	B	1	Total	C	N	O	0
			14	8	4	2	
6	E	1	Total	C	N	O	0
			14	8	4	2	
6	H	1	Total	C	N	O	0
			14	8	4	2	
6	K	1	Total	C	N	O	0
			14	8	4	2	

- Molecule 7 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
7	B	1	Total 31	C 10	N 5	O 13	P 3	0
7	E	1	Total 31	C 10	N 5	O 13	P 3	0
7	H	1	Total 31	C 10	N 5	O 13	P 3	0
7	K	1	Total 31	C 10	N 5	O 13	P 3	0

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: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain A: 



- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain D: 



- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain G: 



- Molecule 1: Peptidyl-prolyl cis-trans isomerase FKBP1B

Chain J: 



- Molecule 2: Ryr2

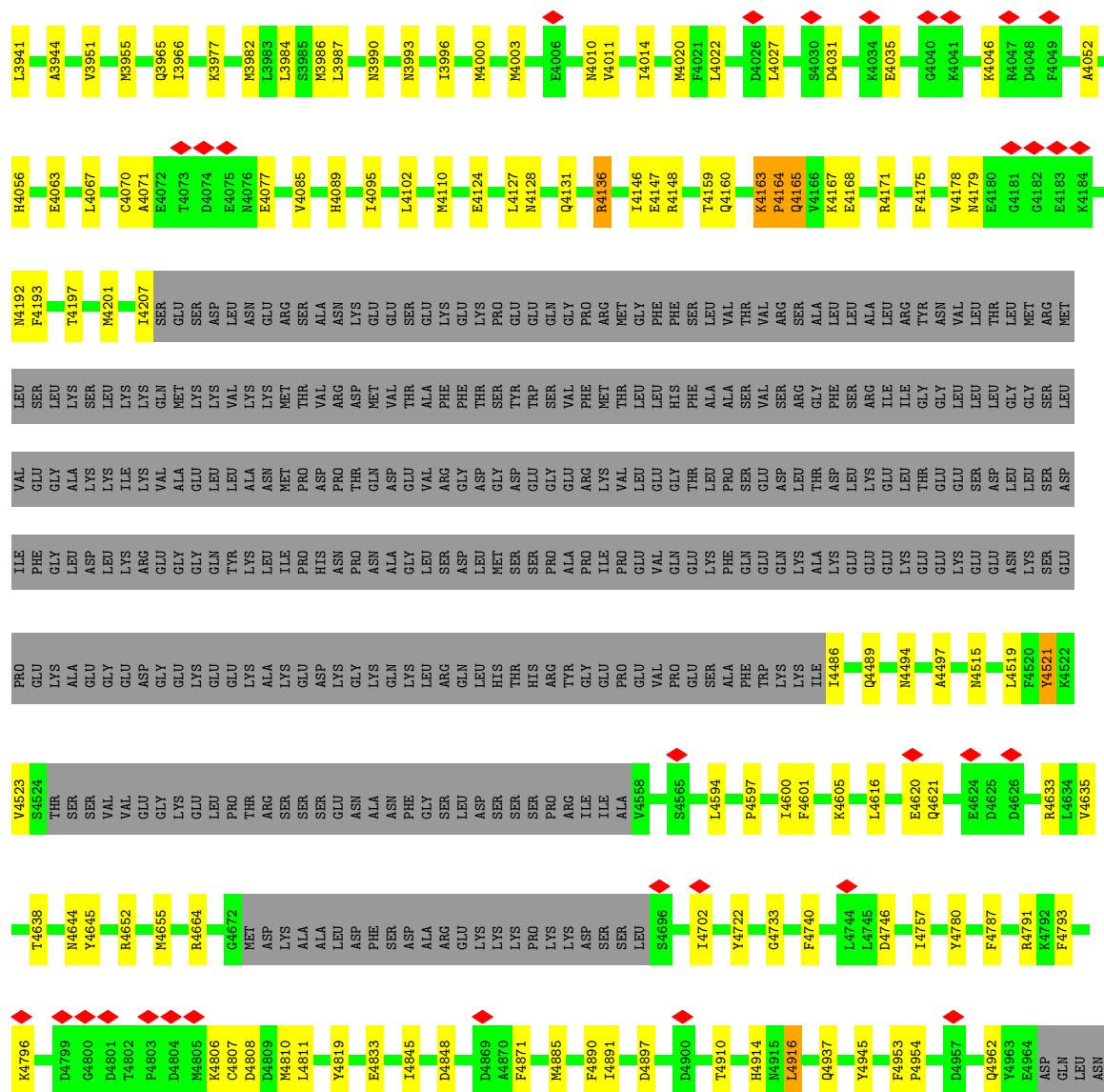
Chain B: 



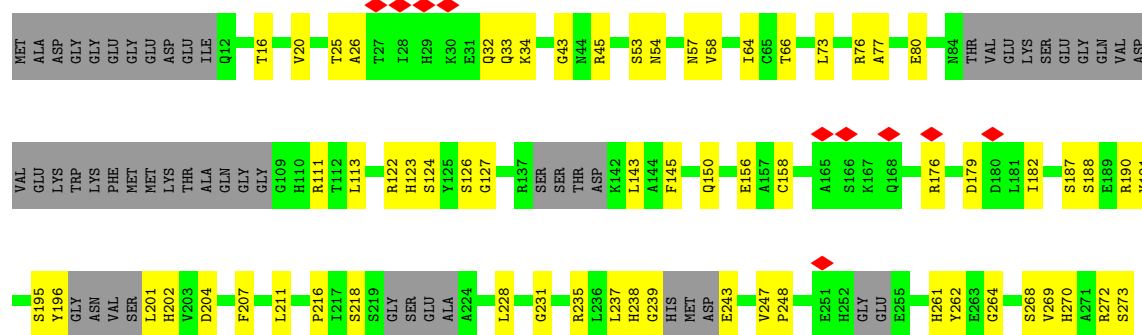








• Molecule 2: Ryr2

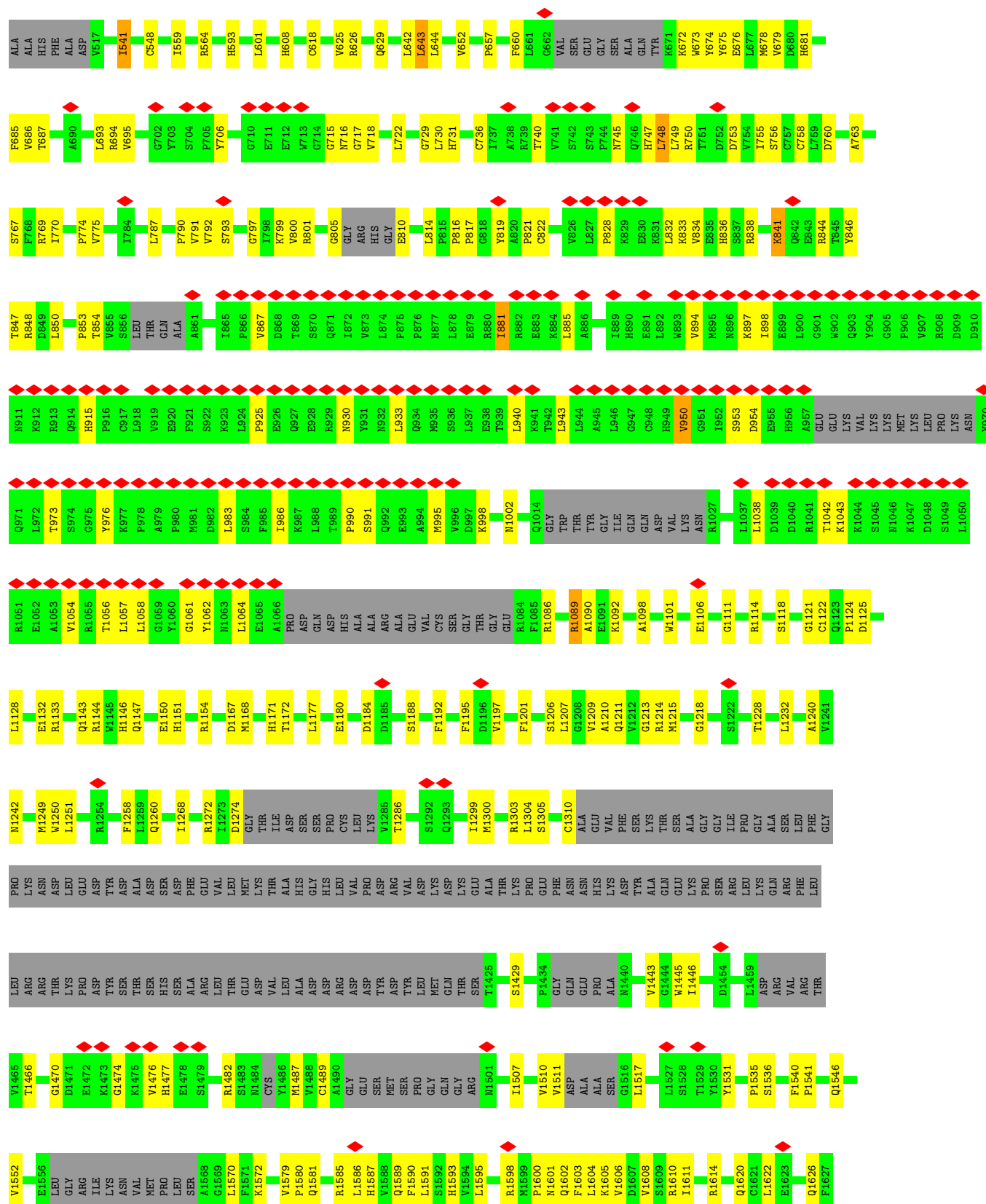






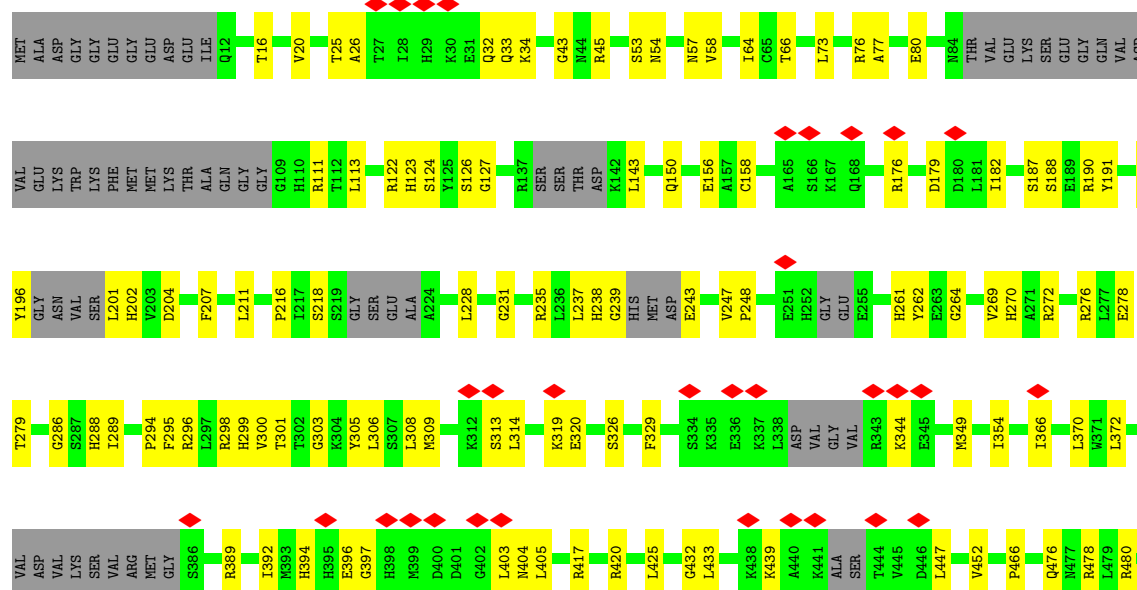






M1628	S1629	I1630	H1631	I1632	P1633	E1634	N1772	N1773	E1781	D1785	K1788	L1642	E1643	L1644	L1651	H1656	L1667	G1668	H1669	L1676	E1847	P1848	S1849	V1680	P1683	L1686	Y1687	A1688	I1689	Y1703	H1710	L1711	Y1714	I1726	E1732	T1733	K1734	S1735	L1748	G1752	L1753	S1754	T1755	S1756	L1757	R1758	M1761	Q1762	F1763	L1771									
GLY	LYS	ARG	PRO	LYS	GLU	G1893	L1894	Q1912	D1931	L1953	MET	GLN	SER	ALA	ALA	LYS	LEU	THR	ALA	VAL	GLU	ARG	LYS	THR	LYS	GLU	PHE	LYS	SER	ALA	PRO	PRO	GLN	GLU	ASN	MET	LEU	ASN	PHE	LYS	PRO	CYS	ASP	LYS	SER	GLU	ASP	GLU	GLY	SER	GLY	GLY							
ASN	SER	ASP	L2024	R2029	S2032	Y2039	LEU	LYS	LYS	LYS	L1953	GLN	SER	ALA	GLU	LYS	LEU	VAL	GLU	ASP	SER	SER	LYS	LYS	LYS	GLU	PHE	SER	SER	SER	T2068	Q2072	V2075	I2076	L2081	L2088	V2114	E2115	D2116	T2117	V2133	ARG	MET	GLY	LYS	E2138	N2153	K2154	V2155	G2181	GLY	GLY	GLU	SER					
LYS	GLU	ILE	THR	PHE	P2191	L2201	Q2212	K2213	L2241	S2247	V2248	N2262	F2263	L2264	L2275	GLN	SER	CYS	GLN	MET	LEU	VAL	SER	SER	LYS	GLY	TYR	PRO	ASP	ASP	ILE	ILE	GLY	TRP	ASN	P2293	R2298	F2308	C2309	N2310	N2319	R2323	T2326	K2327	E2330	CYS	PHE	GLY	PRO	ALA									
LEU	ARG	GLY	GLY	GLY	ASN	G2343	E2349	L2352	K2353	I2354	ALA	ASP	PRO	SER	ARG	GLY	PRO	PRO	THR	SER	GLY	SER	SER	LYS	MET	PRO	THR	THR	GLY	GLU	GLU	ASP	THR	ILE	ILE	HIS	MET	G2386	I2397	D2398	R2402	E2406	I2410	A2413	E2416	A2417													
I2418	R2419	I2420	R2425	S2426	L2427	G2431	L2432	L2433	V2436	I2439	A2440	F2441	Q2442	MET	PRO	THR	ILE	ALA	LYS	ASP	GLY	ASN	VAL	VAL	GLU	PRO	ASP	ASP	F2461	C2462	D2464	H2465	K2466	Y2477	GLY	ILE	V2481	L2488	L2489	VAL	G2492	L2503	ASP	THR	ALA	ALA													
LEU	SER	ALA	T2511	A2516	L2521	L2526	L2529	THR	ARG	CYS	ALA	PRO	LEU	PHE	A2537	V2563	TYR	ARG	LEU	SER	K2568	A2565	S2569	S2576	ILE	CYS	GLY	GLN	R2582	N2601	HIS	ALA	K2605	T2612	Y2615	G2627	TRP	GLY	ASN	PHE	GLY	ALA	A2634	S2635															
L2653	SER	GLN	LYS	Y2658	K2664	L2665	A2666	C2669	V2673	A2674	G2675	P2678	P2679	ASP	TYR	MET	GLU	SER	ASN	VAL	SER	MET	GLU	GLY	LYS	GLN	SER	MET	ASP	GLU	GLY	N2701	F2702	N2703	P2704	Q2705	P2706	V2707	D2708	T2709	S2710	N2711	I2712	T2713	I2714	P2715	E2716	K2717	L2718	E2719	Y2720								
F2721	I2722	N2723	K2724	A2725	V2726	E2727	H2728	S2729	H2730	D2731	K2732	W2733	S2734	M2735	D2736	K2737	L2738	A2739	N2740	G2741	I2743	Y2744	G2745	E2746	I2747	Y2748	Y2749	D2750	S2751	S2752	K2753	V2754	Q2755	P2756	L2757	M2758	K2759	P2760	Y2761	K2762	L2763	T2764	S2765	E2766	K2767	E2768	K2769	I2770	I2771	Y2772	R2773	W2774	P2775	I2776	K2777	S2779	L2780		
K2781	T2782	M2783	L2784	A2785	V2786	G2787	W2788	R2789	I2790	E2791	R2792	L2793	R2794	E2795	G2796	D2797	SER	MET	ALA	LEU	TYR	ASN	THR	ARG	ARG	ARG	ILE	SER	GLN	THR	GLN	VAL	SER	ASP	A2818	A2819	H2820	G2821	Y2822	S2823	P2824	R2825	A2826	I2827	D2828	M2829	S2830	N2831	V2832	T2833	L2834	S2835	R2836	D2837	L2838	H2839	A2840		
M2841	A2842	E2843	M2844	A2845	A2846	E2847	Y2848	Y2849	H2850	M2851	L2852	A2853	A2854	K2855	K2856	K2857	K2858	L2859	E2860	L2861	E2862	S2863	K2864	G2865	G2866	G2867	N2868	H2869	P2870	L2871	L2872	V2873	P2874	Y2875	D2876	T2877	L2878	T2879	A2880	K2881	E2882	K2883	A2884	K2885	D2886	R2887	E2888	K2889	A2890	Q2891	D2892	L2893	L2894	K2895	F2896	L2897	Q2898	L2899	N2900
G2901	Y2902	A2903	V2904	S2905	R2906	G2907	PHE	LYS	ASP	LEU	GLU	LEU	ASP	THR	PRO	SER	ILE	GLU	ARG	PHE	ALA	ALA	TYR	SER	PHE	PHE	GLN	LEU	GLN	VAL	ASP	GLU	ALA	HIS	GLN	TYR	ILE	LEU	GLU	PHE	ASP	GLY	GLY	SER	ARG	SER	LYS	GLY	GLU	HIS	PHE	PRO	TYR	GLU	GLN	GLU			

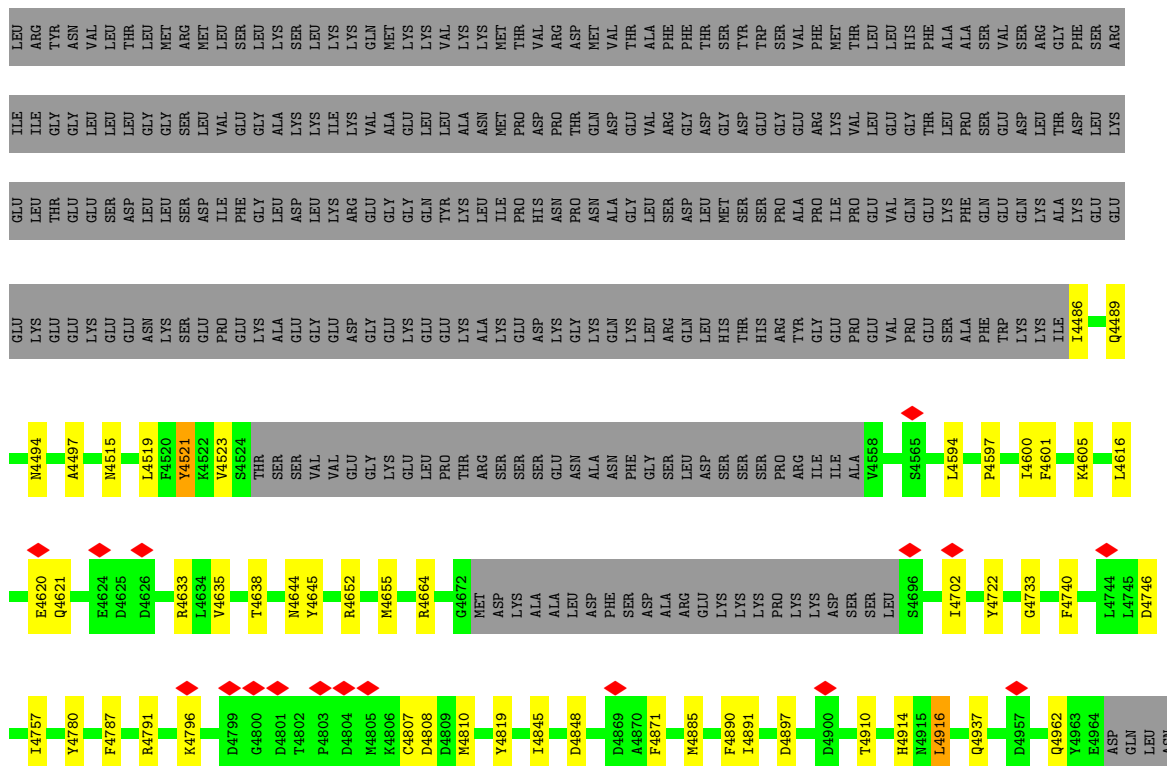




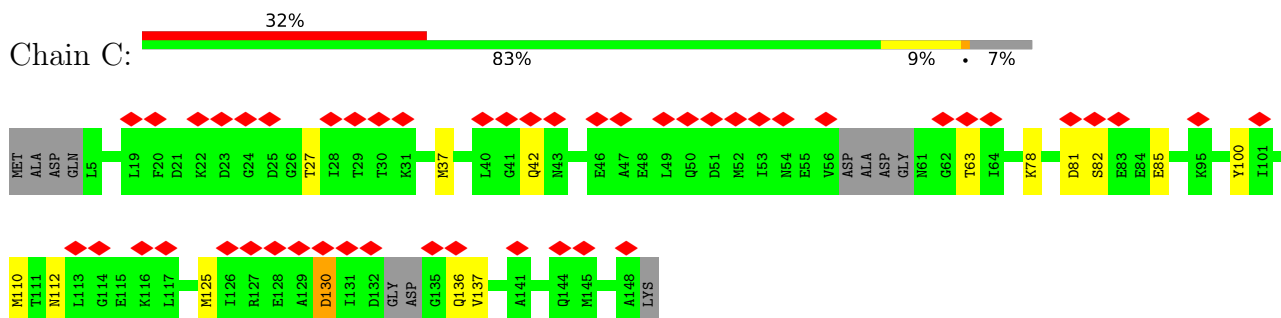




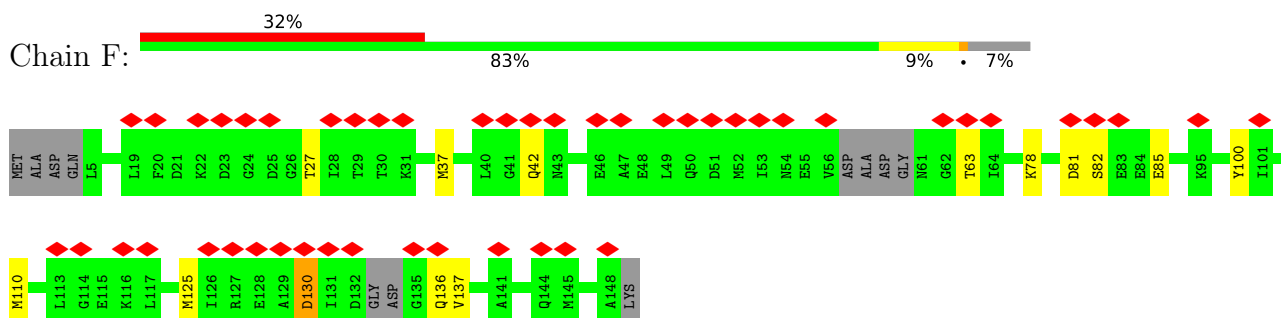




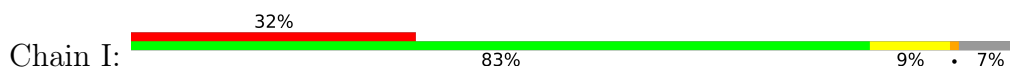
- Molecule 3: Calmodulin-1

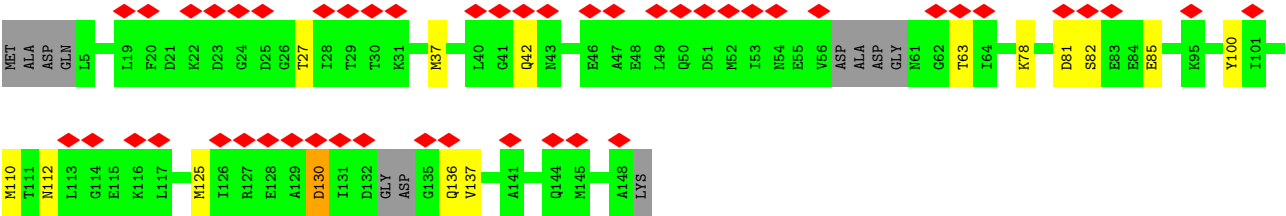


- Molecule 3: Calmodulin-1

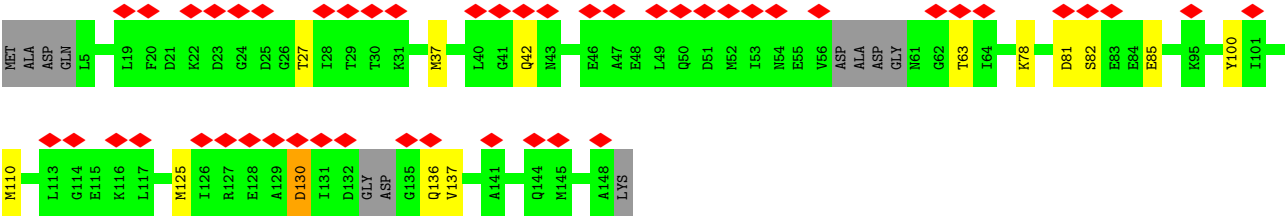
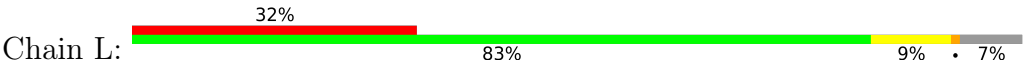


- Molecule 3: Calmodulin-1





• Molecule 3: Calmodulin-1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	69556	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	50	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.096	Depositor
Minimum map value	-0.036	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.022	Depositor
Map size (Å)	436.4, 436.4, 436.4	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.091, 1.091, 1.091	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.30	0/835	0.54	0/1123
1	D	0.30	0/835	0.54	0/1123
1	G	0.30	0/835	0.54	0/1123
1	J	0.30	0/835	0.54	0/1123
2	B	0.36	0/27315	0.64	12/36936 (0.0%)
2	E	0.36	0/27315	0.64	12/36936 (0.0%)
2	H	0.36	0/27315	0.64	10/36936 (0.0%)
2	K	0.36	0/27315	0.64	12/36936 (0.0%)
3	C	0.28	0/1088	0.60	0/1459
3	F	0.28	0/1088	0.60	0/1459
3	I	0.28	0/1088	0.60	0/1459
3	L	0.28	0/1088	0.60	0/1459
All	All	0.36	0/116952	0.64	46/158072 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
2	B	0	24
2	E	0	24
2	H	0	24
2	K	0	24
All	All	0	96

There are no bond length outliers.

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	4165	GLN	N-CA-C	-6.15	107.01	114.75
2	B	4165	GLN	N-CA-C	-6.14	107.02	114.75
2	K	4165	GLN	N-CA-C	-6.14	107.02	114.75
2	E	4165	GLN	N-CA-C	-6.11	107.05	114.75
2	B	2431	GLY	CA-C-N	5.67	128.66	120.38
2	B	2431	GLY	C-N-CA	5.67	128.66	120.38
2	E	2431	GLY	CA-C-N	5.66	128.65	120.38
2	E	2431	GLY	C-N-CA	5.66	128.65	120.38
2	H	2431	GLY	CA-C-N	5.66	128.65	120.38
2	H	2431	GLY	C-N-CA	5.66	128.65	120.38
2	K	2431	GLY	CA-C-N	5.64	128.62	120.38
2	K	2431	GLY	C-N-CA	5.64	128.62	120.38
2	B	1604	LEU	CA-C-N	5.37	127.73	120.38
2	B	1604	LEU	C-N-CA	5.37	127.73	120.38
2	E	1604	LEU	CA-C-N	5.37	127.73	120.38
2	E	1604	LEU	C-N-CA	5.37	127.73	120.38
2	H	1604	LEU	CA-C-N	5.37	127.73	120.38
2	H	1604	LEU	C-N-CA	5.37	127.73	120.38
2	K	686	VAL	CA-C-N	5.35	131.75	121.54
2	K	686	VAL	C-N-CA	5.35	131.75	121.54
2	K	1604	LEU	CA-C-N	5.34	127.70	120.38
2	K	1604	LEU	C-N-CA	5.34	127.70	120.38
2	E	686	VAL	CA-C-N	5.34	131.73	121.54
2	E	686	VAL	C-N-CA	5.34	131.73	121.54
2	B	686	VAL	CA-C-N	5.32	131.70	121.54
2	B	686	VAL	C-N-CA	5.32	131.70	121.54
2	H	686	VAL	CA-C-N	5.32	131.70	121.54
2	H	686	VAL	C-N-CA	5.32	131.70	121.54
2	B	3803	VAL	N-CA-C	-5.31	98.30	109.34
2	E	3803	VAL	N-CA-C	-5.29	98.33	109.34
2	H	3803	VAL	N-CA-C	-5.29	98.33	109.34
2	K	3803	VAL	N-CA-C	-5.28	98.37	109.34
2	H	2248	VAL	CA-C-N	5.14	128.53	120.82
2	H	2248	VAL	C-N-CA	5.14	128.53	120.82
2	K	2248	VAL	CA-C-N	5.14	128.53	120.82
2	K	2248	VAL	C-N-CA	5.14	128.53	120.82
2	E	2248	VAL	CA-C-N	5.12	128.50	120.82
2	E	2248	VAL	C-N-CA	5.12	128.50	120.82
2	B	2248	VAL	CA-C-N	5.10	128.47	120.82
2	B	2248	VAL	C-N-CA	5.10	128.47	120.82
2	E	1580	PRO	CA-C-N	5.02	131.13	121.54
2	E	1580	PRO	C-N-CA	5.02	131.13	121.54
2	B	1580	PRO	CA-C-N	5.01	131.11	121.54

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1580	PRO	C-N-CA	5.01	131.11	121.54
2	K	1580	PRO	CA-C-N	5.01	131.11	121.54
2	K	1580	PRO	C-N-CA	5.01	131.11	121.54

There are no chirality outliers.

All (96) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	1476	VAL	Peptide
2	B	1570	LEU	Peptide
2	B	1579	VAL	Peptide
2	B	1748	LEU	Peptide
2	B	1808	ASP	Peptide
2	B	1809	PRO	Peptide
2	B	1847	GLU	Peptide
2	B	2075	VAL	Peptide
2	B	2308	PHE	Peptide
2	B	3612	LEU	Peptide
2	B	3802	SER	Peptide
2	B	3805	ASP	Peptide
2	B	4070	CYS	Peptide
2	B	4163	LYS	Peptide
2	B	685	PHE	Peptide
2	B	729	GLY	Peptide
2	B	748	LEU	Peptide
2	B	791	VAL	Peptide
2	B	816	PRO	Peptide
2	B	817	PRO	Peptide
2	B	819	TYR	Peptide
2	B	838	ARG	Peptide
2	B	841	LYS	Peptide
2	B	854	THR	Peptide
2	E	1476	VAL	Peptide
2	E	1570	LEU	Peptide
2	E	1579	VAL	Peptide
2	E	1748	LEU	Peptide
2	E	1808	ASP	Peptide
2	E	1809	PRO	Peptide
2	E	1847	GLU	Peptide
2	E	2075	VAL	Peptide
2	E	2308	PHE	Peptide
2	E	3612	LEU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	E	3802	SER	Peptide
2	E	3805	ASP	Peptide
2	E	4070	CYS	Peptide
2	E	4163	LYS	Peptide
2	E	685	PHE	Peptide
2	E	729	GLY	Peptide
2	E	748	LEU	Peptide
2	E	791	VAL	Peptide
2	E	816	PRO	Peptide
2	E	817	PRO	Peptide
2	E	819	TYR	Peptide
2	E	838	ARG	Peptide
2	E	841	LYS	Peptide
2	E	854	THR	Peptide
2	H	1476	VAL	Peptide
2	H	1570	LEU	Peptide
2	H	1579	VAL	Peptide
2	H	1748	LEU	Peptide
2	H	1808	ASP	Peptide
2	H	1809	PRO	Peptide
2	H	1847	GLU	Peptide
2	H	2075	VAL	Peptide
2	H	2308	PHE	Peptide
2	H	3612	LEU	Peptide
2	H	3802	SER	Peptide
2	H	3805	ASP	Peptide
2	H	4070	CYS	Peptide
2	H	4163	LYS	Peptide
2	H	685	PHE	Peptide
2	H	729	GLY	Peptide
2	H	748	LEU	Peptide
2	H	791	VAL	Peptide
2	H	816	PRO	Peptide
2	H	817	PRO	Peptide
2	H	819	TYR	Peptide
2	H	838	ARG	Peptide
2	H	841	LYS	Peptide
2	H	854	THR	Peptide
2	K	1476	VAL	Peptide
2	K	1570	LEU	Peptide
2	K	1579	VAL	Peptide
2	K	1748	LEU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
2	K	1808	ASP	Peptide
2	K	1809	PRO	Peptide
2	K	1847	GLU	Peptide
2	K	2075	VAL	Peptide
2	K	2308	PHE	Peptide
2	K	3612	LEU	Peptide
2	K	3802	SER	Peptide
2	K	3805	ASP	Peptide
2	K	4070	CYS	Peptide
2	K	4163	LYS	Peptide
2	K	685	PHE	Peptide
2	K	729	GLY	Peptide
2	K	748	LEU	Peptide
2	K	791	VAL	Peptide
2	K	816	PRO	Peptide
2	K	817	PRO	Peptide
2	K	819	TYR	Peptide
2	K	838	ARG	Peptide
2	K	841	LYS	Peptide
2	K	854	THR	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	819	0	824	13	0
1	D	819	0	824	14	0
1	G	819	0	824	15	0
1	J	819	0	824	15	0
2	B	26813	0	25339	463	0
2	E	26813	0	25339	454	0
2	H	26813	0	25339	454	0
2	K	26813	0	25339	451	0
3	C	1078	0	1032	9	0
3	F	1078	0	1032	8	0
3	I	1078	0	1032	9	0
3	L	1078	0	1032	8	0
4	B	1	0	0	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	E	1	0	0	0	0
4	H	1	0	0	0	0
4	K	1	0	0	0	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
5	H	1	0	0	0	0
5	K	1	0	0	0	0
6	B	14	0	10	1	0
6	E	14	0	10	1	0
6	H	14	0	10	0	0
6	K	14	0	10	0	0
7	B	31	0	12	4	0
7	E	31	0	12	4	0
7	H	31	0	12	5	0
7	K	31	0	12	4	0
All	All	115028	0	108868	1732	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 8.

All (1732) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:1986:GLU:N	2:K:1989:CYS:HG	1.54	1.05
2:B:1986:GLU:N	2:B:1989:CYS:HG	1.54	1.05
2:H:1986:GLU:N	2:H:1989:CYS:HG	1.55	1.03
2:B:4811:LEU:HD13	2:E:4519:LEU:HD21	1.39	1.03
2:E:1986:GLU:N	2:E:1989:CYS:HG	1.56	1.02
2:E:4848:ASP:CG	2:H:4819:TYR:HE1	1.67	1.01
2:B:76:ARG:NH2	2:E:3806:LEU:HD11	1.77	1.00
2:B:4848:ASP:CG	2:E:4819:TYR:HE1	1.68	1.00
2:B:4819:TYR:HE1	2:K:4848:ASP:CG	1.69	1.00
2:H:4848:ASP:CG	2:K:4819:TYR:HE1	1.70	0.99
2:E:76:ARG:NH2	2:H:3806:LEU:HD11	1.78	0.98
2:B:3806:LEU:HD11	2:K:76:ARG:NH2	1.77	0.98
2:H:76:ARG:NH2	2:K:3806:LEU:HD11	1.78	0.96
2:B:207:PHE:CZ	2:E:2326:ILE:HG23	2.00	0.96
2:E:207:PHE:CZ	2:H:2326:ILE:HG23	2.00	0.96
2:B:2326:ILE:HG23	2:K:207:PHE:CZ	2.01	0.95
2:H:207:PHE:CZ	2:K:2326:ILE:HG23	2.01	0.93
2:E:4848:ASP:CG	2:H:4819:TYR:CE1	2.48	0.91

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1843:LEU:O	2:B:1847:GLU:HB2	1.71	0.91
2:E:76:ARG:HH21	2:H:3806:LEU:HD21	1.36	0.91
2:E:1843:LEU:O	2:E:1847:GLU:HB2	1.71	0.91
2:B:4848:ASP:CG	2:E:4819:TYR:CE1	2.50	0.90
2:K:1843:LEU:O	2:K:1847:GLU:HB2	1.71	0.90
2:H:1843:LEU:O	2:H:1847:GLU:HB2	1.71	0.90
2:B:4796:LYS:NZ	2:B:4807:CYS:SG	2.45	0.90
2:H:143:LEU:HD11	2:K:2426:SER:O	1.72	0.90
2:K:4020:MET:HE2	2:K:4063:GLU:HB3	1.54	0.90
2:E:143:LEU:HD11	2:H:2426:SER:O	1.72	0.89
2:H:76:ARG:HH21	2:K:3806:LEU:HD21	1.38	0.89
2:E:4020:MET:HE2	2:E:4063:GLU:HB3	1.54	0.89
2:B:4819:TYR:CE1	2:K:4848:ASP:CG	2.50	0.88
2:H:4848:ASP:CG	2:K:4819:TYR:CE1	2.51	0.88
2:B:2426:SER:O	2:K:143:LEU:HD11	1.72	0.88
2:B:3806:LEU:HD21	2:K:76:ARG:HH21	1.38	0.88
2:B:76:ARG:HH21	2:E:3806:LEU:HD21	1.38	0.88
2:B:4020:MET:HE2	2:B:4063:GLU:HB3	1.54	0.87
2:B:76:ARG:HH21	2:E:3806:LEU:HD11	1.36	0.87
2:B:143:LEU:HD11	2:E:2426:SER:O	1.73	0.86
2:H:4020:MET:HE2	2:H:4063:GLU:HB3	1.54	0.86
2:E:76:ARG:HH21	2:H:3806:LEU:HD11	1.38	0.86
2:B:4811:LEU:HD13	2:E:4519:LEU:CD2	2.04	0.85
2:E:76:ARG:NH2	2:H:3806:LEU:HD21	1.91	0.84
2:H:76:ARG:NH2	2:K:3806:LEU:HD21	1.93	0.84
2:B:3806:LEU:HD21	2:K:76:ARG:NH2	1.92	0.84
2:B:3806:LEU:HD11	2:K:76:ARG:HH21	1.37	0.83
2:H:76:ARG:HH21	2:K:3806:LEU:HD11	1.37	0.83
2:B:76:ARG:NH2	2:E:3806:LEU:HD21	1.92	0.82
2:H:143:LEU:CD1	2:K:2426:SER:O	2.28	0.81
2:B:2426:SER:O	2:K:143:LEU:CD1	2.28	0.81
2:E:143:LEU:CD1	2:H:2426:SER:O	2.29	0.80
2:B:4848:ASP:OD2	2:E:4819:TYR:CE1	2.35	0.80
2:E:4848:ASP:OD2	2:H:4819:TYR:CE1	2.34	0.80
2:E:143:LEU:HD13	2:H:2426:SER:OG	1.81	0.80
2:B:4819:TYR:CE1	2:K:4848:ASP:OD2	2.35	0.80
2:B:143:LEU:CD1	2:E:2426:SER:O	2.29	0.80
2:H:4848:ASP:OD2	2:K:4819:TYR:CE1	2.36	0.79
2:H:143:LEU:HD13	2:K:2426:SER:OG	1.82	0.78
2:B:143:LEU:HD13	2:E:2426:SER:OG	1.84	0.78
2:B:2426:SER:OG	2:K:143:LEU:HD13	1.83	0.78

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:4787:PHE:HD1	2:B:4808:ASP:O	1.66	0.78
2:K:123:HIS:HD2	2:K:126:SER:H	1.32	0.77
2:H:123:HIS:HD2	2:H:126:SER:H	1.32	0.77
2:B:2419:ARG:HD3	2:K:156:GLU:OE1	1.86	0.76
2:B:156:GLU:OE1	2:E:2419:ARG:HD3	1.85	0.75
2:H:156:GLU:OE1	2:K:2419:ARG:HD3	1.86	0.75
2:B:123:HIS:HD2	2:B:126:SER:H	1.32	0.74
2:B:143:LEU:CD1	2:E:2427:LEU:HD13	2.18	0.74
2:E:123:HIS:HD2	2:E:126:SER:H	1.32	0.74
2:E:156:GLU:OE1	2:H:2419:ARG:HD3	1.88	0.74
2:B:143:LEU:HD11	2:E:2427:LEU:HD13	1.69	0.74
2:B:2427:LEU:HD13	2:K:143:LEU:HD11	1.70	0.73
2:B:2427:LEU:HD13	2:K:143:LEU:CD1	2.19	0.73
2:H:143:LEU:CD1	2:K:2427:LEU:HD13	2.19	0.73
2:E:143:LEU:HD11	2:H:2427:LEU:HD13	1.71	0.72
2:H:143:LEU:HD11	2:K:2427:LEU:HD13	1.71	0.72
2:E:143:LEU:CD1	2:H:2427:LEU:HD13	2.20	0.72
2:B:4519:LEU:O	2:K:4810:MET:CB	2.39	0.71
2:E:207:PHE:CE2	2:H:2326:ILE:HG23	2.26	0.71
2:B:76:ARG:HH21	2:E:3806:LEU:CD1	2.04	0.70
3:F:100:TYR:HB3	3:F:136:GLN:HB3	1.72	0.70
2:H:4810:MET:CB	2:K:4519:LEU:O	2.38	0.70
2:B:207:PHE:CZ	2:E:2326:ILE:CG2	2.74	0.70
3:C:100:TYR:HB3	3:C:136:GLN:HB3	1.72	0.70
2:H:207:PHE:CZ	2:K:2326:ILE:CG2	2.75	0.70
2:E:207:PHE:CZ	2:H:2326:ILE:CG2	2.74	0.70
2:B:299:HIS:HE2	2:B:301:THR:HG1	1.40	0.69
2:H:1605:LYS:HD3	2:H:1606:VAL:HG23	1.74	0.69
3:L:100:TYR:HB3	3:L:136:GLN:HB3	1.72	0.69
2:E:299:HIS:HE2	2:E:301:THR:HG1	1.39	0.69
2:E:4848:ASP:CB	2:H:4819:TYR:HE1	2.04	0.69
3:I:100:TYR:HB3	3:I:136:GLN:HB3	1.72	0.69
2:B:2326:ILE:CG2	2:K:207:PHE:CZ	2.75	0.69
2:H:4046:LYS:H	2:H:4077:GLU:HB3	1.57	0.69
2:K:4046:LYS:H	2:K:4077:GLU:HB3	1.57	0.69
2:B:2326:ILE:HG23	2:K:207:PHE:CE2	2.27	0.69
2:B:207:PHE:CE2	2:E:2326:ILE:HG23	2.27	0.69
2:E:76:ARG:HH21	2:H:3806:LEU:CD1	2.06	0.69
2:E:76:ARG:HH21	2:H:3806:LEU:CD2	2.06	0.69
2:K:1605:LYS:HD3	2:K:1606:VAL:HG23	1.74	0.69
2:H:207:PHE:CE2	2:K:2326:ILE:HG23	2.27	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1089:ARG:HE	2:B:1600:PRO:HB3	1.59	0.68
2:B:3806:LEU:CD1	2:K:76:ARG:HH21	2.05	0.68
2:B:1605:LYS:HD3	2:B:1606:VAL:HG23	1.74	0.68
2:B:2327:ARG:HH21	2:K:191:TYR:HE2	1.42	0.68
2:E:4046:LYS:H	2:E:4077:GLU:HB3	1.57	0.68
2:B:3806:LEU:CD2	2:K:76:ARG:HH21	2.07	0.68
2:B:4046:LYS:H	2:B:4077:GLU:HB3	1.57	0.68
2:E:1089:ARG:HE	2:E:1600:PRO:HB3	1.59	0.68
2:E:1605:LYS:HD3	2:E:1606:VAL:HG23	1.74	0.68
2:E:4810:MET:CB	2:H:4519:LEU:O	2.42	0.68
2:H:191:TYR:HE2	2:K:2327:ARG:HH21	1.42	0.68
2:H:4848:ASP:CB	2:K:4819:TYR:HE1	2.06	0.68
2:K:657:PRO:HA	2:K:834:VAL:HA	1.76	0.67
2:B:4848:ASP:CB	2:E:4819:TYR:HE1	2.07	0.67
2:H:1089:ARG:HE	2:H:1600:PRO:HB3	1.59	0.67
2:K:1089:ARG:HE	2:K:1600:PRO:HB3	1.59	0.67
2:B:4819:TYR:HE1	2:K:4848:ASP:CB	2.07	0.67
2:B:850:LEU:HB3	2:B:1207:LEU:HD11	1.77	0.67
2:H:657:PRO:HA	2:H:834:VAL:HA	1.76	0.67
2:K:3951:VAL:O	2:K:3955:MET:HB2	1.95	0.67
2:E:191:TYR:HE2	2:H:2327:ARG:HH21	1.42	0.67
2:B:3951:VAL:O	2:B:3955:MET:HB2	1.95	0.66
2:E:758:CYS:HB3	2:E:767:SER:HB2	1.78	0.66
2:H:758:CYS:HB3	2:H:767:SER:HB2	1.78	0.66
2:E:3951:VAL:O	2:E:3955:MET:HB2	1.95	0.66
2:H:3951:VAL:O	2:H:3955:MET:HB2	1.96	0.66
2:E:657:PRO:HA	2:E:834:VAL:HA	1.76	0.66
2:H:76:ARG:HH21	2:K:3806:LEU:CD2	2.08	0.66
2:B:191:TYR:HE2	2:E:2327:ARG:HH21	1.42	0.66
2:H:76:ARG:HH21	2:K:3806:LEU:CD1	2.06	0.66
2:B:207:PHE:CE1	2:E:2326:ILE:CG2	2.79	0.66
2:E:850:LEU:HB3	2:E:1207:LEU:HD11	1.77	0.66
2:B:657:PRO:HA	2:B:834:VAL:HA	1.76	0.65
2:K:758:CYS:HB3	2:K:767:SER:HB2	1.78	0.65
2:B:758:CYS:HB3	2:B:767:SER:HB2	1.78	0.65
2:H:207:PHE:CE1	2:K:2326:ILE:CG2	2.80	0.65
2:K:850:LEU:HB3	2:K:1207:LEU:HD11	1.77	0.65
2:B:2326:ILE:CG2	2:K:207:PHE:CE1	2.79	0.65
2:E:207:PHE:CE1	2:H:2326:ILE:CG2	2.80	0.65
2:K:797:GLY:HA2	2:K:1622:LEU:HA	1.79	0.65
2:B:76:ARG:HH21	2:E:3806:LEU:CD2	2.07	0.65

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:850:LEU:HB2	2:B:1213:GLY:H	1.62	0.65
2:H:850:LEU:HB3	2:H:1207:LEU:HD11	1.77	0.65
2:H:299:HIS:HE2	2:H:301:THR:HG1	1.39	0.64
2:B:797:GLY:HA2	2:B:1622:LEU:HA	1.79	0.64
2:E:26:ALA:HB3	2:E:33:GLN:HB3	1.80	0.64
2:H:26:ALA:HB3	2:H:33:GLN:HB3	1.80	0.64
2:H:1303:ARG:HH12	2:H:1595:LEU:HB2	1.62	0.64
2:K:1303:ARG:HH12	2:K:1595:LEU:HB2	1.62	0.64
2:E:1303:ARG:HH12	2:E:1595:LEU:HB2	1.62	0.63
2:E:4796:LYS:NZ	2:E:4807:CYS:SG	2.71	0.63
2:K:26:ALA:HB3	2:K:33:GLN:HB3	1.80	0.63
2:E:850:LEU:HB2	2:E:1213:GLY:H	1.62	0.63
2:K:4796:LYS:NZ	2:K:4807:CYS:SG	2.71	0.63
2:B:26:ALA:HB3	2:B:33:GLN:HB3	1.80	0.63
2:H:797:GLY:HA2	2:H:1622:LEU:HA	1.79	0.63
2:H:4146:ILE:HD12	2:H:4962:GLN:HB2	1.81	0.63
2:H:4796:LYS:NZ	2:H:4807:CYS:SG	2.71	0.63
2:H:850:LEU:HB2	2:H:1213:GLY:H	1.62	0.63
2:K:850:LEU:HB2	2:K:1213:GLY:H	1.62	0.63
2:B:1303:ARG:HH12	2:B:1595:LEU:HB2	1.62	0.63
2:E:247:VAL:O	2:E:272:ARG:NH1	2.30	0.63
2:E:797:GLY:HA2	2:E:1622:LEU:HA	1.79	0.63
2:E:4146:ILE:HD12	2:E:4962:GLN:HB2	1.81	0.63
2:H:1299:ILE:HG12	2:H:1546:GLN:HG2	1.81	0.63
2:K:299:HIS:HE2	2:K:301:THR:HG1	1.40	0.63
2:B:1299:ILE:HG12	2:B:1546:GLN:HG2	1.81	0.62
2:K:4146:ILE:HD12	2:K:4962:GLN:HB2	1.81	0.62
2:B:3806:LEU:CD1	2:K:76:ARG:NH2	2.59	0.62
1:G:77:THR:HG22	1:G:79:ASP:H	1.63	0.62
2:K:476:GLN:HE22	2:K:3678:THR:HG22	1.65	0.62
2:B:247:VAL:O	2:B:272:ARG:NH1	2.30	0.62
2:B:80:GLU:HG3	2:E:3891:TRP:HZ3	1.63	0.62
2:B:4811:LEU:HD22	2:E:4520:PHE:CE1	2.35	0.62
1:J:77:THR:HG22	1:J:79:ASP:H	1.63	0.62
2:B:476:GLN:HE22	2:B:3678:THR:HG22	1.65	0.62
1:D:77:THR:HG22	1:D:79:ASP:H	1.63	0.62
2:B:143:LEU:HD12	2:E:2427:LEU:CD1	2.30	0.62
2:B:4146:ILE:HD12	2:B:4962:GLN:HB2	1.81	0.62
2:B:4808:ASP:OD2	2:E:4523:VAL:HG21	1.99	0.62
2:E:80:GLU:HG3	2:H:3891:TRP:HZ3	1.63	0.62
1:A:77:THR:HG22	1:A:79:ASP:H	1.63	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:476:GLN:HE22	2:E:3678:THR:HG22	1.65	0.62
2:H:76:ARG:NH2	2:K:3806:LEU:CD1	2.60	0.61
2:H:476:GLN:HE22	2:H:3678:THR:HG22	1.65	0.61
2:K:4031:ASP:HB3	2:K:4035:GLU:HB2	1.83	0.61
2:B:3891:TRP:HZ3	2:K:80:GLU:HG3	1.64	0.61
2:E:1299:ILE:HG12	2:E:1546:GLN:HG2	1.81	0.61
2:H:4031:ASP:HB3	2:H:4035:GLU:HB2	1.83	0.61
2:K:247:VAL:O	2:K:272:ARG:NH1	2.30	0.61
2:B:694:ARG:HB2	2:B:793:SER:HB2	1.83	0.61
2:B:1114:ARG:HB3	2:B:1128:LEU:HD22	1.83	0.61
2:K:195:SER:HB3	2:K:202:HIS:HB2	1.82	0.61
2:E:694:ARG:HB2	2:E:793:SER:HB2	1.83	0.61
2:K:930:ASN:HA	2:K:933:LEU:HB2	1.83	0.61
2:B:4810:MET:CB	2:E:4519:LEU:O	2.49	0.61
2:E:4022:LEU:HA	2:E:4089:HIS:HE1	1.66	0.61
2:H:195:SER:HB3	2:H:202:HIS:HB2	1.82	0.61
2:H:80:GLU:HG3	2:K:3891:TRP:HZ3	1.65	0.60
2:K:1114:ARG:HB3	2:K:1128:LEU:HD22	1.83	0.60
2:B:4022:LEU:HA	2:B:4089:HIS:HE1	1.66	0.60
2:B:4031:ASP:HB3	2:B:4035:GLU:HB2	1.83	0.60
2:K:1272:ARG:NH1	2:K:1587:HIS:O	2.34	0.60
2:E:4031:ASP:HB3	2:E:4035:GLU:HB2	1.83	0.60
2:H:694:ARG:HB2	2:H:793:SER:HB2	1.83	0.60
2:H:930:ASN:HA	2:H:933:LEU:HB2	1.83	0.60
2:B:195:SER:HB3	2:B:202:HIS:HB2	1.82	0.60
2:E:1114:ARG:HB3	2:E:1128:LEU:HD22	1.83	0.60
2:E:1272:ARG:NH1	2:E:1587:HIS:O	2.34	0.60
2:H:247:VAL:O	2:H:272:ARG:NH1	2.30	0.60
2:K:1299:ILE:HG12	2:K:1546:GLN:HG2	1.81	0.60
2:H:1272:ARG:NH1	2:H:1587:HIS:O	2.34	0.60
2:K:1249:MET:H	2:K:1603:PHE:HB2	1.67	0.60
2:B:2427:LEU:CD1	2:K:143:LEU:HD12	2.31	0.60
2:E:195:SER:HB3	2:E:202:HIS:HB2	1.82	0.60
2:E:3663:ASP:OD2	2:E:3735:ARG:NH2	2.35	0.60
2:H:1249:MET:H	2:H:1603:PHE:HB2	1.67	0.60
2:B:3663:ASP:OD2	2:B:3735:ARG:NH2	2.35	0.60
2:E:674:TYR:HB3	2:E:821:PRO:HA	1.84	0.60
2:K:3663:ASP:OD2	2:K:3735:ARG:NH2	2.35	0.60
2:H:3663:ASP:OD2	2:H:3735:ARG:NH2	2.35	0.60
2:K:4022:LEU:HA	2:K:4089:HIS:HE1	1.66	0.60
2:E:143:LEU:HD12	2:H:2427:LEU:CD1	2.32	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:191:TYR:CE2	2:K:2327:ARG:NH2	2.70	0.60
2:B:1272:ARG:NH1	2:B:1587:HIS:O	2.34	0.60
2:H:4020:MET:CE	2:H:4063:GLU:HB3	2.31	0.60
2:K:694:ARG:HB2	2:K:793:SER:HB2	1.83	0.60
2:B:930:ASN:HA	2:B:933:LEU:HB2	1.83	0.59
2:E:4020:MET:CE	2:E:4063:GLU:HB3	2.30	0.59
2:H:674:TYR:HB3	2:H:821:PRO:HA	1.84	0.59
2:E:1249:MET:H	2:E:1603:PHE:HB2	1.67	0.59
2:H:143:LEU:HD12	2:K:2427:LEU:CD1	2.32	0.59
2:H:1114:ARG:HB3	2:H:1128:LEU:HD22	1.83	0.59
2:H:4022:LEU:HA	2:H:4089:HIS:HE1	1.66	0.59
2:B:1171:HIS:ND1	2:B:1195:PHE:O	2.36	0.59
2:B:2327:ARG:NH2	2:K:191:TYR:CE2	2.70	0.59
2:E:191:TYR:CE2	2:H:2327:ARG:NH2	2.71	0.59
2:B:674:TYR:HB3	2:B:821:PRO:HA	1.84	0.59
2:B:1249:MET:H	2:B:1603:PHE:HB2	1.67	0.59
2:K:1090:ALA:HA	2:K:1249:MET:HG2	1.85	0.59
2:B:626:ARG:HD2	2:B:1669:ASN:HD21	1.68	0.59
2:B:1090:ALA:HA	2:B:1249:MET:HG2	1.85	0.59
2:B:4020:MET:CE	2:B:4063:GLU:HB3	2.30	0.59
2:E:930:ASN:HA	2:E:933:LEU:HB2	1.83	0.59
2:K:674:TYR:HB3	2:K:821:PRO:HA	1.84	0.59
2:K:3799:GLN:O	2:K:3881:ARG:NH1	2.35	0.59
2:B:76:ARG:NH2	2:E:3806:LEU:CD1	2.58	0.59
2:B:4791:ARG:HB3	2:B:4808:ASP:HB2	1.83	0.59
2:E:1090:ALA:HA	2:E:1249:MET:HG2	1.85	0.59
2:H:1754:SER:HB2	2:H:1758:ARG:HH12	1.68	0.58
2:B:3799:GLN:O	2:B:3881:ARG:NH1	2.35	0.58
2:E:76:ARG:NH2	2:H:3806:LEU:CD1	2.59	0.58
2:H:1090:ALA:HA	2:H:1249:MET:HG2	1.85	0.58
2:K:25:THR:HG22	2:K:34:LYS:HG2	1.85	0.58
2:B:25:THR:HG22	2:B:34:LYS:HG2	1.85	0.58
2:B:4020:MET:HE3	2:B:4067:LEU:CD1	2.34	0.58
2:E:1154:ARG:HH21	2:E:1177:LEU:HD23	1.68	0.58
2:K:1171:HIS:ND1	2:K:1195:PHE:O	2.36	0.58
2:K:1754:SER:HB2	2:K:1758:ARG:HH12	1.69	0.58
2:K:2770:GLU:HA	2:K:2773:ARG:HB2	1.85	0.58
2:B:4124:GLU:HG3	2:B:4128:ASN:HD21	1.69	0.58
2:E:480:ARG:NH2	2:E:3679:GLU:OE2	2.36	0.58
2:H:25:THR:HG22	2:H:34:LYS:HG2	1.85	0.58
2:B:191:TYR:CE2	2:E:2327:ARG:NH2	2.70	0.58

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:21:THR:HG1	1:D:49:ARG:HH21	1.48	0.58
2:H:4124:GLU:HG3	2:H:4128:ASN:HD21	1.69	0.58
2:K:4020:MET:HE3	2:K:4067:LEU:CD1	2.34	0.58
2:B:1754:SER:HB2	2:B:1758:ARG:HH12	1.69	0.58
2:E:1754:SER:HB2	2:E:1758:ARG:HH12	1.69	0.58
2:E:2770:GLU:HA	2:E:2773:ARG:HB2	1.85	0.58
2:E:4020:MET:HE3	2:E:4067:LEU:CD1	2.34	0.58
2:H:2770:GLU:HA	2:H:2773:ARG:HB2	1.85	0.58
2:K:1154:ARG:HH21	2:K:1177:LEU:HD23	1.68	0.58
2:E:943:LEU:HB3	2:E:950:VAL:HG21	1.86	0.58
2:E:4124:GLU:HG3	2:E:4128:ASN:HD21	1.69	0.58
2:H:1154:ARG:HH21	2:H:1177:LEU:HD23	1.68	0.58
2:H:270:HIS:ND1	2:H:491:GLU:OE1	2.37	0.58
2:H:480:ARG:NH2	2:H:3679:GLU:OE2	2.36	0.58
2:K:480:ARG:NH2	2:K:3679:GLU:OE2	2.36	0.58
2:K:626:ARG:HD2	2:K:1669:ASN:HD21	1.68	0.58
2:B:4159:THR:O	2:B:4163:LYS:NZ	2.37	0.58
2:E:626:ARG:HD2	2:E:1669:ASN:HD21	1.68	0.58
2:K:4124:GLU:HG3	2:K:4128:ASN:HD21	1.69	0.58
2:K:706:TYR:OH	2:K:1086:ARG:NH2	2.37	0.58
2:B:270:HIS:ND1	2:B:491:GLU:OE1	2.37	0.57
2:B:943:LEU:HB3	2:B:950:VAL:HG21	1.86	0.57
2:B:2275:LEU:H	2:B:2293:PRO:HD3	1.69	0.57
2:E:3799:GLN:O	2:E:3881:ARG:NH1	2.35	0.57
2:E:3805:ASP:OD2	2:E:3809:PHE:N	2.37	0.57
2:H:943:LEU:HB3	2:H:950:VAL:HG11	1.86	0.57
2:K:248:PRO:HD3	2:K:261:HIS:HD2	1.69	0.57
2:B:1146:HIS:HB2	2:B:1192:PHE:HE1	1.70	0.57
2:E:270:HIS:ND1	2:E:491:GLU:OE1	2.37	0.57
2:E:1171:HIS:ND1	2:E:1195:PHE:O	2.36	0.57
2:H:626:ARG:HD2	2:H:1669:ASN:HD21	1.68	0.57
2:K:300:VAL:O	2:K:420:ARG:NH2	2.37	0.57
2:B:2770:GLU:HA	2:B:2773:ARG:HB2	1.85	0.57
2:K:375:GLN:HE21	2:K:392:ILE:HD13	1.69	0.57
2:B:3921:LEU:HB3	2:B:3982:MET:HE3	1.87	0.57
2:E:706:TYR:OH	2:E:1086:ARG:NH2	2.37	0.57
2:H:2436:VAL:O	2:H:2466:LYS:NZ	2.38	0.57
2:E:1628:MET:HB2	2:E:1687:TYR:HE2	1.70	0.57
2:H:300:VAL:O	2:H:420:ARG:NH2	2.37	0.57
2:B:300:VAL:O	2:B:420:ARG:NH2	2.37	0.57
2:B:375:GLN:HE21	2:B:392:ILE:HD13	1.69	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:248:PRO:HD3	2:E:261:HIS:HD2	1.69	0.57
2:E:375:GLN:HE21	2:E:392:ILE:HD13	1.69	0.57
2:E:2436:VAL:O	2:E:2466:LYS:NZ	2.38	0.57
2:B:2436:VAL:O	2:B:2466:LYS:NZ	2.38	0.57
2:E:867:VAL:O	2:E:1002:ASN:ND2	2.38	0.57
2:H:1171:HIS:ND1	2:H:1195:PHE:O	2.36	0.57
2:H:1628:MET:HB2	2:H:1687:TYR:HE2	1.70	0.57
2:H:3799:GLN:O	2:H:3881:ARG:NH1	2.35	0.57
2:H:4020:MET:HE3	2:H:4067:LEU:CD1	2.34	0.57
2:K:1146:HIS:HB2	2:K:1192:PHE:HE1	1.70	0.57
2:B:248:PRO:HD3	2:B:261:HIS:HD2	1.69	0.57
2:E:25:THR:HG22	2:E:34:LYS:HG2	1.85	0.57
2:E:2275:LEU:H	2:E:2293:PRO:HD3	1.69	0.57
2:K:270:HIS:ND1	2:K:491:GLU:OE1	2.37	0.57
2:K:3805:ASP:OD2	2:K:3809:PHE:N	2.37	0.57
2:K:3921:LEU:HB3	2:K:3982:MET:HE3	1.87	0.57
2:E:300:VAL:O	2:E:420:ARG:NH2	2.37	0.57
2:E:954:ASP:HB2	2:E:1061:GLY:HA3	1.87	0.57
2:E:4020:MET:HE3	2:E:4067:LEU:HD13	1.87	0.57
2:H:706:TYR:OH	2:H:1086:ARG:NH2	2.37	0.57
2:K:4192:ASN:OD1	2:K:4605:LYS:NZ	2.29	0.57
2:K:4890:PHE:H	7:K:6003:ATP:HN61	1.53	0.57
2:B:278:GLU:HB2	2:B:296:ARG:HB2	1.87	0.56
2:B:480:ARG:NH2	2:B:3679:GLU:OE2	2.36	0.56
2:B:1154:ARG:HH21	2:B:1177:LEU:HD23	1.68	0.56
2:E:3921:LEU:HB3	2:E:3982:MET:HE3	1.87	0.56
2:H:375:GLN:HE21	2:H:392:ILE:HD13	1.69	0.56
1:J:23:VAL:HB	1:J:105:ASN:H	1.70	0.56
2:B:867:VAL:O	2:B:1002:ASN:ND2	2.38	0.56
2:B:3901:GLU:OE1	2:B:3902:GLN:NE2	2.39	0.56
2:B:3919:ASN:O	2:B:3922:THR:OG1	2.23	0.56
2:H:3805:ASP:OD2	2:H:3809:PHE:N	2.37	0.56
2:K:1628:MET:HB2	2:K:1687:TYR:HE2	1.70	0.56
2:K:2275:LEU:H	2:K:2293:PRO:HD3	1.69	0.56
2:B:954:ASP:HB2	2:B:1061:GLY:HA3	1.87	0.56
2:B:3805:ASP:OD2	2:B:3809:PHE:N	2.37	0.56
2:B:4020:MET:HE3	2:B:4067:LEU:HD13	1.87	0.56
2:E:1146:HIS:HB2	2:E:1192:PHE:HE1	1.70	0.56
2:E:2834:LEU:HD11	2:E:2894:LEU:HB3	1.88	0.56
2:E:4159:THR:O	2:E:4163:LYS:NZ	2.37	0.56
1:G:23:VAL:HB	1:G:105:ASN:H	1.70	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:248:PRO:HD3	2:H:261:HIS:HD2	1.69	0.56
2:H:867:VAL:O	2:H:1002:ASN:ND2	2.38	0.56
2:H:4890:PHE:H	7:H:6003:ATP:HN61	1.53	0.56
2:K:867:VAL:O	2:K:1002:ASN:ND2	2.38	0.56
2:K:3901:GLU:OE1	2:K:3902:GLN:NE2	2.39	0.56
2:B:2464:ASP:OD1	2:B:2464:ASP:N	2.36	0.56
2:E:2521:LEU:HD22	2:E:2565:ALA:HB2	1.88	0.56
2:E:2707:VAL:HG21	2:E:2786:TRP:HE1	1.71	0.56
2:H:954:ASP:HB2	2:H:1061:GLY:HA3	1.87	0.56
2:H:3901:GLU:OE1	2:H:3902:GLN:NE2	2.39	0.56
2:H:4159:THR:O	2:H:4163:LYS:NZ	2.37	0.56
2:K:943:LEU:HB3	2:K:950:VAL:HG11	1.86	0.56
2:B:4791:ARG:CB	2:B:4808:ASP:CB	2.84	0.56
2:B:4890:PHE:H	7:B:6003:ATP:HN61	1.53	0.56
2:E:3901:GLU:OE1	2:E:3902:GLN:NE2	2.39	0.56
2:H:2275:LEU:H	2:H:2293:PRO:HD3	1.69	0.56
2:H:2707:VAL:HG21	2:H:2786:TRP:HE1	1.71	0.56
2:H:3921:LEU:HB3	2:H:3982:MET:HE3	1.87	0.56
2:K:954:ASP:HB2	2:K:1061:GLY:HA3	1.87	0.56
1:D:23:VAL:HB	1:D:105:ASN:H	1.70	0.56
2:E:1144:ARG:NH2	2:E:1150:GLU:OE1	2.39	0.56
2:K:2436:VAL:O	2:K:2466:LYS:NZ	2.38	0.56
2:K:4020:MET:HE3	2:K:4067:LEU:HD13	1.87	0.56
2:B:4168:GLU:HB2	2:B:4171:ARG:NH1	2.20	0.56
2:E:278:GLU:HB2	2:E:296:ARG:HB2	1.87	0.56
2:H:2521:LEU:HD22	2:H:2565:ALA:HB2	1.87	0.56
2:K:1144:ARG:NH2	2:K:1150:GLU:OE1	2.39	0.56
1:A:23:VAL:HB	1:A:105:ASN:H	1.70	0.56
2:B:1628:MET:HB2	2:B:1687:TYR:HE2	1.70	0.56
2:B:2834:LEU:HD11	2:B:2894:LEU:HB3	1.88	0.56
2:H:1303:ARG:HH22	2:H:1595:LEU:HD13	1.71	0.56
2:K:833:LYS:HA	2:K:1614:ARG:HH12	1.71	0.56
2:K:3919:ASN:O	2:K:3922:THR:OG1	2.23	0.56
2:H:1144:ARG:NH2	2:H:1150:GLU:OE1	2.39	0.56
2:B:706:TYR:OH	2:B:1086:ARG:NH2	2.37	0.56
2:B:1303:ARG:HH22	2:B:1595:LEU:HD13	1.71	0.56
2:H:278:GLU:HB2	2:H:296:ARG:HB2	1.87	0.56
2:H:1146:HIS:HB2	2:H:1192:PHE:HE1	1.70	0.56
2:B:2426:SER:HG	2:K:143:LEU:HD13	1.70	0.55
2:H:4020:MET:HE3	2:H:4067:LEU:HD13	1.88	0.55
2:K:278:GLU:HB2	2:K:296:ARG:HB2	1.87	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:4085:VAL:O	2:K:4089:HIS:N	2.40	0.55
2:B:1144:ARG:NH2	2:B:1150:GLU:OE1	2.39	0.55
2:B:2521:LEU:HD22	2:B:2565:ALA:HB2	1.87	0.55
2:E:4890:PHE:H	7:E:6003:ATP:HN61	1.54	0.55
2:K:417:ARG:HH11	2:K:420:ARG:HH11	1.55	0.55
2:B:289:ILE:HG22	2:B:354:ILE:HD12	1.88	0.55
2:H:3919:ASN:O	2:H:3922:THR:OG1	2.23	0.55
2:B:417:ARG:HH11	2:B:420:ARG:HH11	1.54	0.55
2:H:2834:LEU:HD11	2:H:2894:LEU:HB3	1.88	0.55
2:H:289:ILE:HG22	2:H:354:ILE:HD12	1.88	0.55
2:H:298:ARG:HE	2:H:303:GLY:HA2	1.72	0.55
2:K:1303:ARG:HH22	2:K:1595:LEU:HD13	1.71	0.55
2:E:833:LYS:HA	2:E:1614:ARG:HH12	1.71	0.55
2:H:231:GLY:O	2:H:276:ARG:NH1	2.40	0.55
2:K:289:ILE:HG22	2:K:354:ILE:HD12	1.88	0.55
2:K:2521:LEU:HD22	2:K:2565:ALA:HB2	1.87	0.55
2:B:833:LYS:HA	2:B:1614:ARG:HH12	1.71	0.55
2:E:1303:ARG:HH22	2:E:1595:LEU:HD13	1.71	0.55
2:E:3919:ASN:O	2:E:3922:THR:OG1	2.23	0.55
2:B:2707:VAL:HG21	2:B:2786:TRP:HE1	1.71	0.54
2:E:289:ILE:HG22	2:E:354:ILE:HD12	1.88	0.54
2:H:833:LYS:HA	2:H:1614:ARG:HH12	1.71	0.54
2:K:231:GLY:O	2:K:276:ARG:NH1	2.40	0.54
2:K:4020:MET:CE	2:K:4063:GLU:HB3	2.31	0.54
2:K:298:ARG:HE	2:K:303:GLY:HA2	1.72	0.54
2:K:2834:LEU:HD11	2:K:2894:LEU:HB3	1.88	0.54
2:B:841:LYS:HB2	2:B:848:ARG:HD3	1.90	0.54
2:E:1572:LYS:HE2	2:E:1585:ARG:HB3	1.90	0.54
2:K:288:HIS:ND1	2:K:349:MET:O	2.40	0.54
2:K:841:LYS:HB2	2:K:848:ARG:HD3	1.90	0.54
2:B:1572:LYS:HE2	2:B:1585:ARG:HB3	1.90	0.54
2:H:1242:ASN:HB2	2:H:1807:ARG:HG2	1.90	0.54
2:K:2707:VAL:HG21	2:K:2786:TRP:HE1	1.71	0.54
2:H:1303:ARG:HB2	2:H:1593:HIS:HB2	1.90	0.54
2:B:288:HIS:ND1	2:B:349:MET:O	2.40	0.54
2:B:3800:SER:OG	2:B:3801:CYS:N	2.41	0.54
2:B:4791:ARG:HB2	2:B:4808:ASP:CB	2.38	0.54
2:E:231:GLY:O	2:E:276:ARG:NH1	2.40	0.54
2:B:626:ARG:NH2	2:B:1667:LEU:O	2.41	0.54
2:H:143:LEU:CD1	2:K:2427:LEU:CD1	2.86	0.54
2:H:841:LYS:HB2	2:H:848:ARG:HD3	1.90	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:626:ARG:NH2	2:K:1667:LEU:O	2.41	0.54
2:K:1242:ASN:HB2	2:K:1807:ARG:HG2	1.90	0.54
2:E:674:TYR:OH	2:E:676:GLU:OE2	2.21	0.54
2:H:288:HIS:ND1	2:H:349:MET:O	2.40	0.54
2:K:674:TYR:OH	2:K:676:GLU:OE2	2.21	0.54
2:B:231:GLY:O	2:B:276:ARG:NH1	2.40	0.54
2:H:417:ARG:HH11	2:H:420:ARG:HH11	1.55	0.54
2:H:1272:ARG:HG3	2:H:1586:LEU:HD13	1.90	0.54
2:B:756:SER:HB3	2:B:769:ARG:H	1.73	0.54
2:B:2413:ALA:HB1	2:B:2418:ILE:HD11	1.90	0.54
2:E:841:LYS:HB2	2:E:848:ARG:HD3	1.90	0.54
2:E:4497:ALA:HB1	2:E:4594:LEU:HD13	1.90	0.54
2:H:626:ARG:NH2	2:H:1667:LEU:O	2.41	0.54
2:H:681:HIS:HB2	2:H:799:LYS:HG2	1.90	0.54
2:B:4085:VAL:O	2:B:4089:HIS:N	2.40	0.53
2:B:156:GLU:OE1	2:E:2419:ARG:NH1	2.41	0.53
2:E:417:ARG:HH11	2:E:420:ARG:HH11	1.55	0.53
2:E:844:ARG:HG2	2:E:846:TYR:H	1.74	0.53
2:H:207:PHE:CE1	2:K:2326:ILE:HG23	2.43	0.53
2:K:1572:LYS:HE2	2:K:1585:ARG:HB3	1.90	0.53
2:K:2464:ASP:N	2:K:2464:ASP:OD1	2.36	0.53
2:B:1429:SER:HA	2:B:1507:ILE:HG12	1.90	0.53
2:E:288:HIS:ND1	2:E:349:MET:O	2.40	0.53
2:K:309:MET:O	2:K:313:SER:N	2.42	0.53
2:E:298:ARG:HE	2:E:303:GLY:HA2	1.72	0.53
2:E:626:ARG:NH2	2:E:1667:LEU:O	2.41	0.53
2:E:2413:ALA:HB1	2:E:2418:ILE:HD11	1.91	0.53
2:E:1242:ASN:HB2	2:E:1807:ARG:HG2	1.90	0.53
2:E:1303:ARG:HB2	2:E:1593:HIS:HB2	1.90	0.53
2:H:1572:LYS:HE2	2:H:1585:ARG:HB3	1.90	0.53
2:K:1429:SER:HA	2:K:1507:ILE:HG12	1.91	0.53
2:B:681:HIS:HB2	2:B:799:LYS:HG2	1.90	0.53
2:E:1272:ARG:HG3	2:E:1586:LEU:HD13	1.90	0.53
2:K:1272:ARG:NH2	2:K:1590:PHE:O	2.42	0.53
2:B:1242:ASN:HB2	2:B:1807:ARG:HG2	1.90	0.53
2:B:4020:MET:CE	2:B:4067:LEU:HD13	2.39	0.53
2:B:4193:PHE:O	2:B:4197:THR:OG1	2.25	0.53
2:B:4497:ALA:HB1	2:B:4594:LEU:HD13	1.90	0.53
2:E:66:THR:HG1	2:E:124:SER:HG	1.53	0.53
2:E:143:LEU:CD1	2:H:2427:LEU:CD1	2.86	0.53
2:H:309:MET:O	2:H:313:SER:N	2.42	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:756:SER:HB3	2:H:769:ARG:H	1.73	0.53
2:H:1272:ARG:NH2	2:H:1590:PHE:O	2.42	0.53
2:K:681:HIS:HB2	2:K:799:LYS:HG2	1.90	0.53
2:K:844:ARG:HG2	2:K:846:TYR:H	1.74	0.53
2:B:844:ARG:HG2	2:B:846:TYR:H	1.74	0.53
2:E:4193:PHE:O	2:E:4197:THR:OG1	2.25	0.53
2:K:1272:ARG:HG3	2:K:1586:LEU:HD13	1.90	0.53
2:K:2413:ALA:HB1	2:K:2418:ILE:HD11	1.90	0.53
2:K:4020:MET:CE	2:K:4067:LEU:HD13	2.39	0.53
2:B:4787:PHE:CD1	2:B:4808:ASP:O	2.56	0.53
2:E:156:GLU:OE1	2:H:2419:ARG:NH1	2.42	0.53
2:E:681:HIS:HB2	2:E:799:LYS:HG2	1.90	0.53
2:B:309:MET:O	2:B:313:SER:N	2.42	0.53
2:B:1303:ARG:HB2	2:B:1593:HIS:HB2	1.90	0.53
2:E:1429:SER:HA	2:E:1507:ILE:HG12	1.91	0.53
2:E:1487:MET:HE1	2:E:1531:TYR:H	1.74	0.53
2:H:2413:ALA:HB1	2:H:2418:ILE:HD11	1.90	0.53
2:K:466:PRO:HB3	2:K:478:ARG:HD2	1.91	0.53
2:K:2406:GLU:O	2:K:2410:ILE:N	2.42	0.53
2:E:309:MET:O	2:E:313:SER:N	2.42	0.52
2:E:716:ASN:HA	2:E:722:LEU:HD13	1.91	0.52
2:E:4020:MET:CE	2:E:4067:LEU:HD13	2.39	0.52
2:E:4085:VAL:O	2:E:4089:HIS:N	2.40	0.52
2:E:4605:LYS:HG3	2:E:4645:TYR:HE1	1.73	0.52
2:H:466:PRO:HB3	2:H:478:ARG:HD2	1.91	0.52
2:H:1250:TRP:HB3	2:H:1600:PRO:HB2	1.91	0.52
2:H:4020:MET:CE	2:H:4067:LEU:HD13	2.39	0.52
2:K:2116:ASP:OD1	2:K:2153:ASN:ND2	2.43	0.52
2:K:4159:THR:O	2:K:4163:LYS:NZ	2.37	0.52
2:B:298:ARG:HE	2:B:303:GLY:HA2	1.72	0.52
2:B:1272:ARG:HG3	2:B:1586:LEU:HD13	1.90	0.52
2:B:4605:LYS:HG3	2:B:4645:TYR:HE1	1.73	0.52
2:E:756:SER:HB3	2:E:769:ARG:H	1.74	0.52
2:K:1250:TRP:HB3	2:K:1600:PRO:HB2	1.91	0.52
2:E:308:LEU:HD21	2:E:370:LEU:HD12	1.91	0.52
2:H:1487:MET:HE1	2:H:1531:TYR:H	1.74	0.52
2:K:66:THR:OG1	2:K:124:SER:OG	2.25	0.52
2:K:756:SER:HB3	2:K:769:ARG:H	1.74	0.52
2:K:3800:SER:OG	2:K:3801:CYS:N	2.41	0.52
2:B:1272:ARG:NH2	2:B:1590:PHE:O	2.42	0.52
2:H:308:LEU:HD21	2:H:370:LEU:HD12	1.91	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:844:ARG:HG2	2:H:846:TYR:H	1.74	0.52
2:H:1114:ARG:NH1	2:H:1128:LEU:O	2.43	0.52
2:H:4085:VAL:O	2:H:4089:HIS:N	2.40	0.52
2:K:4605:LYS:HG3	2:K:4645:TYR:HE1	1.73	0.52
2:B:716:ASN:HA	2:B:722:LEU:HD13	1.91	0.52
2:B:2419:ARG:NH1	2:K:156:GLU:OE1	2.42	0.52
2:E:1250:TRP:HB3	2:E:1600:PRO:HB2	1.91	0.52
2:H:1429:SER:HA	2:H:1507:ILE:HG12	1.91	0.52
2:K:3729:GLN:O	2:K:3733:HIS:ND1	2.43	0.52
2:E:943:LEU:HA	2:E:995:MET:HE1	1.92	0.52
2:H:716:ASN:HA	2:H:722:LEU:HD13	1.91	0.52
2:H:2116:ASP:OD1	2:H:2153:ASN:ND2	2.43	0.52
2:K:1114:ARG:NH1	2:K:1128:LEU:O	2.43	0.52
1:G:21:THR:HG1	1:G:49:ARG:HH21	1.54	0.52
2:H:943:LEU:HA	2:H:995:MET:HE1	1.92	0.52
2:B:1487:MET:HE1	2:B:1531:TYR:H	1.74	0.52
2:H:4605:LYS:HG3	2:H:4645:TYR:HE1	1.73	0.52
2:K:644:LEU:HD22	2:K:1632:ILE:HG22	1.92	0.52
2:K:4497:ALA:HB1	2:K:4594:LEU:HD13	1.90	0.52
2:B:4192:ASN:OD1	2:B:4605:LYS:NZ	2.29	0.52
2:H:687:THR:HG23	2:H:1626:GLN:HE21	1.75	0.52
2:H:4722:TYR:OH	2:H:4746:ASP:OD1	2.23	0.52
2:K:1303:ARG:HB2	2:K:1593:HIS:HB2	1.90	0.52
2:B:1114:ARG:NH1	2:B:1128:LEU:O	2.43	0.51
2:B:2406:GLU:O	2:B:2410:ILE:N	2.42	0.51
2:E:466:PRO:HB3	2:E:478:ARG:HD2	1.91	0.51
2:E:1114:ARG:NH1	2:E:1128:LEU:O	2.43	0.51
2:E:2116:ASP:OD1	2:E:2153:ASN:ND2	2.43	0.51
2:E:2730:HIS:NE2	2:E:2759:LYS:O	2.43	0.51
2:K:1260:GLN:HG2	2:K:1591:LEU:HD13	1.92	0.51
2:B:1250:TRP:HB3	2:B:1600:PRO:HB2	1.92	0.51
2:B:2427:LEU:CD1	2:K:143:LEU:CD1	2.86	0.51
2:E:279:THR:O	2:E:296:ARG:NH2	2.43	0.51
2:E:805:GLY:HA2	2:E:810:GLU:HB2	1.92	0.51
2:E:1272:ARG:NH2	2:E:1590:PHE:O	2.42	0.51
2:E:2406:GLU:O	2:E:2410:ILE:N	2.42	0.51
2:H:4497:ALA:HB1	2:H:4594:LEU:HD13	1.90	0.51
2:B:279:THR:O	2:B:296:ARG:NH2	2.43	0.51
2:K:559:ILE:HD13	2:K:593:HIS:HB3	1.93	0.51
2:B:176:ARG:N	2:B:179:ASP:OD2	2.44	0.51
2:B:559:ILE:HD13	2:B:593:HIS:HB3	1.93	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:2730:HIS:NE2	2:B:2759:LYS:O	2.43	0.51
2:E:559:ILE:HD13	2:E:593:HIS:HB3	1.93	0.51
2:K:1209:VAL:N	2:K:1211:GLN:OE1	2.44	0.51
2:B:687:THR:HG23	2:B:1626:GLN:HE21	1.75	0.51
2:B:1209:VAL:N	2:B:1211:GLN:OE1	2.44	0.51
2:K:1111:GLY:HA3	2:K:1211:GLN:HE21	1.76	0.51
2:K:1487:MET:HE1	2:K:1531:TYR:H	1.74	0.51
2:K:2734:SER:HB2	2:K:2758:MET:HE1	1.93	0.51
2:B:466:PRO:HB3	2:B:478:ARG:HD2	1.91	0.51
2:E:20:VAL:HG12	2:E:216:PRO:HA	1.93	0.51
2:E:644:LEU:HD22	2:E:1632:ILE:HG22	1.92	0.51
2:H:20:VAL:HG12	2:H:216:PRO:HA	1.93	0.51
2:H:182:ILE:HD11	2:H:211:LEU:HD23	1.92	0.51
2:H:279:THR:O	2:H:296:ARG:NH2	2.43	0.51
2:H:559:ILE:HD13	2:H:593:HIS:HB3	1.93	0.51
2:K:308:LEU:HD21	2:K:370:LEU:HD12	1.91	0.51
2:B:644:LEU:HD22	2:B:1632:ILE:HG22	1.92	0.51
2:B:2116:ASP:OD1	2:B:2153:ASN:ND2	2.43	0.51
1:D:27:THR:HA	1:D:38:SER:HA	1.93	0.51
2:K:176:ARG:N	2:K:179:ASP:OD2	2.44	0.51
2:B:308:LEU:HD21	2:B:370:LEU:HD12	1.91	0.51
2:B:760:ASP:HB2	2:B:763:ALA:HB3	1.93	0.51
2:B:943:LEU:HA	2:B:995:MET:HE1	1.92	0.51
2:E:196:TYR:HA	2:E:201:LEU:HD23	1.92	0.51
2:E:4192:ASN:OD1	2:E:4605:LYS:NZ	2.29	0.51
2:H:176:ARG:N	2:H:179:ASP:OD2	2.44	0.51
2:H:196:TYR:HA	2:H:201:LEU:HD23	1.92	0.51
2:H:2734:SER:HB2	2:H:2758:MET:HE1	1.93	0.51
1:J:9:PRO:HA	1:J:70:GLN:HG3	1.92	0.51
2:K:805:GLY:HA2	2:K:810:GLU:HB2	1.92	0.51
2:K:943:LEU:HA	2:K:995:MET:HE1	1.92	0.51
1:D:9:PRO:HA	1:D:70:GLN:HG3	1.92	0.51
2:E:1209:VAL:N	2:E:1211:GLN:OE1	2.44	0.51
2:H:1209:VAL:N	2:H:1211:GLN:OE1	2.44	0.51
2:K:687:THR:HG23	2:K:1626:GLN:HE21	1.75	0.51
2:K:2730:HIS:NE2	2:K:2759:LYS:O	2.43	0.51
2:B:3729:GLN:O	2:B:3733:HIS:ND1	2.43	0.51
2:E:182:ILE:HD11	2:E:211:LEU:HD23	1.92	0.51
2:E:672:LYS:HA	2:E:760:ASP:HA	1.93	0.51
2:E:760:ASP:HB2	2:E:763:ALA:HB3	1.93	0.51
2:H:1098:ALA:O	2:H:1101:TRP:NE1	2.38	0.51

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1114:ARG:HB2	2:H:1206:SER:HB3	1.92	0.51
2:K:196:TYR:HA	2:K:201:LEU:HD23	1.92	0.51
2:K:672:LYS:HA	2:K:760:ASP:HA	1.93	0.51
2:K:716:ASN:HA	2:K:722:LEU:HD13	1.91	0.51
1:A:9:PRO:HA	1:A:70:GLN:HG3	1.92	0.50
2:B:143:LEU:CD1	2:E:2427:LEU:CD1	2.85	0.50
2:B:672:LYS:HA	2:B:760:ASP:HA	1.93	0.50
2:B:1114:ARG:HB2	2:B:1206:SER:HB3	1.92	0.50
3:C:27:THR:HA	3:C:63:THR:HB	1.94	0.50
2:E:4486:ILE:HG22	2:E:4489:GLN:H	1.77	0.50
2:H:156:GLU:OE1	2:K:2419:ARG:NH1	2.43	0.50
2:K:644:LEU:HB3	2:K:1630:LEU:HD12	1.94	0.50
2:K:1114:ARG:HB2	2:K:1206:SER:HB3	1.92	0.50
2:B:196:TYR:HA	2:B:201:LEU:HD23	1.92	0.50
2:B:1038:LEU:HD12	2:B:1043:LYS:HE3	1.94	0.50
2:E:43:GLY:H	2:E:45:ARG:HH12	1.59	0.50
2:E:1038:LEU:HD12	2:E:1043:LYS:HE3	1.94	0.50
2:E:2029:ARG:O	2:E:2032:SER:OG	2.28	0.50
2:H:2114:VAL:O	2:H:2117:THR:OG1	2.28	0.50
2:K:4616:LEU:HA	2:K:4620:GLU:HB2	1.93	0.50
3:L:27:THR:HA	3:L:63:THR:HB	1.94	0.50
2:B:1303:ARG:O	2:B:1593:HIS:N	2.45	0.50
2:E:687:THR:HG23	2:E:1626:GLN:HE21	1.75	0.50
2:E:1771:ILE:HG22	2:E:1773:ASN:H	1.76	0.50
2:H:1111:GLY:HA3	2:H:1211:GLN:HE21	1.76	0.50
1:J:27:THR:HA	1:J:38:SER:HA	1.93	0.50
2:B:43:GLY:H	2:B:45:ARG:HH12	1.59	0.50
2:E:644:LEU:HB3	2:E:1630:LEU:HD12	1.94	0.50
2:E:1114:ARG:HB2	2:E:1206:SER:HB3	1.92	0.50
2:H:43:GLY:H	2:H:45:ARG:HH12	1.59	0.50
2:H:805:GLY:HA2	2:H:810:GLU:HB2	1.92	0.50
2:K:279:THR:O	2:K:296:ARG:NH2	2.43	0.50
2:K:678:MET:HE2	2:K:801:ARG:HD3	1.93	0.50
2:B:295:PHE:N	2:B:329:PHE:O	2.44	0.50
2:B:1111:GLY:HA3	2:B:1211:GLN:HE21	1.76	0.50
2:E:1260:GLN:HG2	2:E:1591:LEU:HD13	1.92	0.50
2:E:4167:LYS:NZ	7:E:6003:ATP:O2B	2.44	0.50
1:G:27:THR:HA	1:G:38:SER:HA	1.93	0.50
2:H:644:LEU:HD22	2:H:1632:ILE:HG22	1.92	0.50
2:H:672:LYS:HA	2:H:760:ASP:HA	1.92	0.50
2:H:1303:ARG:O	2:H:1593:HIS:N	2.45	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:4486:ILE:HG22	2:H:4489:GLN:H	1.77	0.50
2:K:182:ILE:HD11	2:K:211:LEU:HD23	1.92	0.50
2:K:295:PHE:N	2:K:329:PHE:O	2.44	0.50
2:K:760:ASP:HB2	2:K:763:ALA:HB3	1.93	0.50
2:K:1303:ARG:O	2:K:1593:HIS:N	2.45	0.50
2:B:805:GLY:HA2	2:B:810:GLU:HB2	1.92	0.50
2:E:176:ARG:N	2:E:179:ASP:OD2	2.44	0.50
3:F:27:THR:HA	3:F:63:THR:HB	1.94	0.50
1:G:9:PRO:HA	1:G:70:GLN:HG3	1.92	0.50
2:H:1038:LEU:HD12	2:H:1043:LYS:HE3	1.94	0.50
2:H:4616:LEU:HA	2:H:4620:GLU:HB2	1.93	0.50
2:K:20:VAL:HG12	2:K:216:PRO:HA	1.93	0.50
2:B:678:MET:HE2	2:B:801:ARG:HD3	1.93	0.50
2:H:1171:HIS:HE1	2:H:1197:VAL:H	1.60	0.50
2:B:20:VAL:HG12	2:B:216:PRO:HA	1.93	0.50
2:B:182:ILE:HD11	2:B:211:LEU:HD23	1.92	0.50
2:B:1260:GLN:HG2	2:B:1591:LEU:HD13	1.92	0.50
2:B:2832:VAL:O	2:B:2895:LYS:NZ	2.38	0.50
2:B:3803:VAL:HG22	2:B:3881:ARG:HH21	1.77	0.50
2:E:1611:ILE:HB	2:E:1620:GLN:HB3	1.94	0.50
2:E:4616:LEU:HA	2:E:4620:GLU:HB2	1.93	0.50
2:H:1304:LEU:HB3	2:H:1541:PRO:HG2	1.94	0.50
2:H:2730:HIS:NE2	2:H:2759:LYS:O	2.43	0.50
2:K:1171:HIS:HE1	2:K:1197:VAL:H	1.60	0.50
2:B:693:LEU:HD13	2:B:749:LEU:HD22	1.94	0.50
2:B:1304:LEU:HB3	2:B:1541:PRO:HG2	1.94	0.50
2:B:2734:SER:HB2	2:B:2758:MET:HE1	1.93	0.50
2:E:1111:GLY:HA3	2:E:1211:GLN:HE21	1.76	0.50
2:H:1847:GLU:OE1	2:H:1849:SER:OG	2.25	0.50
3:I:27:THR:HA	3:I:63:THR:HB	1.94	0.50
2:B:1184:ASP:OD2	2:B:1188:SER:OG	2.30	0.49
2:B:1611:ILE:HB	2:B:1620:GLN:HB3	1.94	0.49
2:B:1771:ILE:HG22	2:B:1773:ASN:H	1.76	0.49
2:B:4486:ILE:HG22	2:B:4489:GLN:H	1.77	0.49
2:B:4521:TYR:HB3	2:K:4787:PHE:CZ	2.47	0.49
2:H:678:MET:HE2	2:H:801:ARG:HD3	1.93	0.49
2:H:1771:ILE:HG22	2:H:1773:ASN:H	1.76	0.49
2:K:3803:VAL:HG22	2:K:3881:ARG:HH21	1.77	0.49
2:E:2734:SER:HB2	2:E:2758:MET:HE1	1.93	0.49
2:H:693:LEU:HD13	2:H:749:LEU:HD22	1.94	0.49
2:H:4787:PHE:CZ	2:K:4521:TYR:HB3	2.46	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:4486:ILE:HG22	2:K:4489:GLN:H	1.77	0.49
2:B:1154:ARG:NH2	2:B:1180:GLU:OE1	2.46	0.49
2:B:4616:LEU:HA	2:B:4620:GLU:HB2	1.93	0.49
2:H:295:PHE:N	2:H:329:PHE:O	2.44	0.49
2:H:1443:VAL:HB	2:H:1489:CYS:HB2	1.94	0.49
2:K:693:LEU:HD13	2:K:749:LEU:HD22	1.94	0.49
2:K:748:LEU:HD22	2:K:750:ARG:HE	1.78	0.49
2:K:1038:LEU:HD12	2:K:1043:LYS:HE3	1.94	0.49
2:K:1304:LEU:HB3	2:K:1541:PRO:HG2	1.94	0.49
2:B:644:LEU:HB3	2:B:1630:LEU:HD12	1.94	0.49
2:B:4168:GLU:CB	2:B:4171:ARG:NH1	2.75	0.49
2:B:4722:TYR:OH	2:B:4746:ASP:OD1	2.23	0.49
2:H:760:ASP:HB2	2:H:763:ALA:HB3	1.93	0.49
2:K:2114:VAL:O	2:K:2117:THR:OG1	2.28	0.49
2:B:4167:LYS:NZ	7:B:6003:ATP:O2B	2.44	0.49
2:H:991:SER:OG	2:H:1064:LEU:O	2.30	0.49
2:H:1260:GLN:HG2	2:H:1591:LEU:HD13	1.92	0.49
2:H:1611:ILE:HB	2:H:1620:GLN:HB3	1.94	0.49
2:K:1443:VAL:HB	2:K:1489:CYS:HB2	1.94	0.49
2:K:1611:ILE:HB	2:K:1620:GLN:HB3	1.94	0.49
2:K:1771:ILE:HG22	2:K:1773:ASN:H	1.76	0.49
2:B:748:LEU:HD22	2:B:750:ARG:HE	1.78	0.49
2:B:1171:HIS:HE1	2:B:1197:VAL:H	1.60	0.49
2:E:1304:LEU:HB3	2:E:1541:PRO:HG2	1.94	0.49
2:H:1154:ARG:NH2	2:H:1180:GLU:OE1	2.46	0.49
2:B:991:SER:OG	2:B:1064:LEU:O	2.30	0.49
2:B:1242:ASN:HD22	2:B:1807:ARG:HD2	1.78	0.49
2:B:4787:PHE:CZ	2:E:4521:TYR:HB3	2.48	0.49
2:E:1184:ASP:N	2:E:1188:SER:O	2.45	0.49
2:H:1184:ASP:OD2	2:H:1188:SER:OG	2.30	0.49
2:H:3803:VAL:HG22	2:H:3881:ARG:HH21	1.77	0.49
2:K:1184:ASP:OD2	2:K:1188:SER:OG	2.30	0.49
2:K:1242:ASN:HD22	2:K:1807:ARG:HD2	1.78	0.49
2:K:1847:GLU:OE1	2:K:1849:SER:OG	2.25	0.49
1:A:27:THR:HA	1:A:38:SER:HA	1.93	0.49
2:E:678:MET:HE2	2:E:801:ARG:HD3	1.93	0.49
2:E:3803:VAL:HG22	2:E:3881:ARG:HH21	1.77	0.49
2:E:4164:PRO:HB2	2:E:4165:GLN:HG3	1.95	0.49
2:E:4207:ILE:HD12	2:E:4494:ASN:HD22	1.78	0.49
2:E:295:PHE:N	2:E:329:PHE:O	2.44	0.49
2:E:991:SER:OG	2:E:1064:LEU:O	2.30	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:748:LEU:HD22	2:H:750:ARG:HE	1.77	0.49
2:H:2832:VAL:O	2:H:2895:LYS:NZ	2.38	0.49
2:H:4164:PRO:HB2	2:H:4165:GLN:HG3	1.95	0.49
2:B:76:ARG:NH2	2:E:3806:LEU:CD2	2.71	0.49
2:B:4207:ILE:HD12	2:B:4494:ASN:HD22	1.78	0.49
2:B:4910:THR:HG21	7:B:6003:ATP:C5	2.48	0.49
2:E:1154:ARG:NH2	2:E:1180:GLU:OE1	2.46	0.49
2:E:1847:GLU:OE1	2:E:1849:SER:OG	2.25	0.49
2:H:1589:GLN:NE2	2:H:1634:GLU:OE1	2.46	0.49
2:H:3977:LYS:HB2	2:H:4095:ILE:HG13	1.95	0.49
2:K:16:THR:OG1	2:K:111:ARG:O	2.29	0.49
2:K:991:SER:OG	2:K:1064:LEU:O	2.30	0.49
2:B:1125:ASP:HA	2:B:1598:ARG:HH11	1.78	0.48
2:B:4791:ARG:HB2	2:B:4808:ASP:HB3	1.96	0.48
2:E:693:LEU:HD13	2:E:749:LEU:HD22	1.94	0.48
2:E:1171:HIS:HE1	2:E:1197:VAL:H	1.60	0.48
2:E:3729:GLN:O	2:E:3733:HIS:ND1	2.43	0.48
1:G:49:ARG:HB3	1:G:52:LYS:HE2	1.95	0.48
2:H:644:LEU:HB3	2:H:1630:LEU:HD12	1.94	0.48
2:H:1125:ASP:HA	2:H:1598:ARG:HH11	1.78	0.48
2:H:4207:ILE:HD12	2:H:4494:ASN:HD22	1.78	0.48
2:H:4655:MET:O	2:H:4664:ARG:NH1	2.46	0.48
2:K:43:GLY:H	2:K:45:ARG:HH12	1.59	0.48
2:K:2832:VAL:O	2:K:2895:LYS:NZ	2.38	0.48
1:A:49:ARG:HB3	1:A:52:LYS:HE2	1.95	0.48
2:B:674:TYR:OH	2:B:676:GLU:OE2	2.21	0.48
1:D:49:ARG:HB3	1:D:52:LYS:HE2	1.95	0.48
2:E:953:SER:OG	2:E:1061:GLY:O	2.32	0.48
2:E:1303:ARG:O	2:E:1593:HIS:N	2.45	0.48
2:E:3977:LYS:HB2	2:E:4095:ILE:HG13	1.95	0.48
2:H:4910:THR:HG21	7:H:6003:ATP:C5	2.48	0.48
1:J:49:ARG:HB3	1:J:52:LYS:HE2	1.95	0.48
2:B:218:SER:HB3	2:B:286:GLY:HA3	1.96	0.48
2:B:239:GLY:O	2:B:243:GLU:N	2.46	0.48
2:B:1589:GLN:NE2	2:B:1634:GLU:OE1	2.46	0.48
2:B:4164:PRO:HB2	2:B:4165:GLN:HG3	1.95	0.48
2:E:1251:LEU:O	2:E:1601:ASN:N	2.47	0.48
2:H:1242:ASN:HD22	2:H:1807:ARG:HD2	1.78	0.48
2:K:218:SER:HB3	2:K:286:GLY:HA3	1.96	0.48
2:K:1733:THR:HG22	2:K:1755:THR:HB	1.96	0.48
2:K:3593:SER:O	2:K:3597:LYS:NZ	2.42	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:4207:ILE:HD12	2:K:4494:ASN:HD22	1.78	0.48
2:E:1443:VAL:HB	2:E:1489:CYS:HB2	1.94	0.48
2:E:4910:THR:HG21	7:E:6003:ATP:C5	2.48	0.48
2:H:58:VAL:HG22	2:H:320:GLU:HA	1.96	0.48
2:H:673:TRP:HE3	2:H:822:CYS:HA	1.78	0.48
3:I:37:MET:HB3	3:I:42:GLN:HB2	1.96	0.48
2:H:218:SER:HB3	2:H:286:GLY:HA3	1.96	0.48
2:K:1154:ARG:NH2	2:K:1180:GLU:OE1	2.46	0.48
2:B:718:VAL:HA	2:B:736:CYS:N	2.29	0.48
2:B:4891:ILE:HD13	2:B:4914:HIS:HB3	1.95	0.48
2:E:1184:ASP:OD2	2:E:1188:SER:OG	2.30	0.48
2:H:799:LYS:HB3	2:H:1620:GLN:HG3	1.95	0.48
2:K:673:TRP:HE3	2:K:822:CYS:HA	1.78	0.48
2:K:4891:ILE:HD13	2:K:4914:HIS:HB3	1.95	0.48
2:K:4910:THR:HG21	7:K:6003:ATP:C5	2.48	0.48
2:B:1733:THR:HG22	2:B:1755:THR:HB	1.96	0.48
2:E:673:TRP:HE3	2:E:822:CYS:HA	1.78	0.48
2:E:748:LEU:HD22	2:E:750:ARG:HE	1.78	0.48
2:H:674:TYR:OH	2:H:676:GLU:OE2	2.21	0.48
2:H:1167:ASP:OD2	2:H:1172:THR:OG1	2.32	0.48
2:H:1733:THR:HG22	2:H:1755:THR:HB	1.96	0.48
1:J:62:GLY:HA3	1:J:74:LEU:HD21	1.96	0.48
2:K:239:GLY:O	2:K:243:GLU:N	2.47	0.48
2:E:1242:ASN:HD22	2:E:1807:ARG:HD2	1.78	0.48
2:E:1733:THR:HG22	2:E:1755:THR:HB	1.96	0.48
2:E:4022:LEU:HD12	2:E:4089:HIS:CE1	2.49	0.48
2:H:239:GLY:O	2:H:243:GLU:N	2.46	0.48
2:H:4891:ILE:HD13	2:H:4914:HIS:HB3	1.95	0.48
2:K:718:VAL:HA	2:K:736:CYS:N	2.29	0.48
2:K:1589:GLN:NE2	2:K:1634:GLU:OE1	2.46	0.48
2:K:4164:PRO:HB2	2:K:4165:GLN:HG3	1.95	0.48
2:B:58:VAL:HG22	2:B:320:GLU:HA	1.96	0.48
2:B:1443:VAL:HB	2:B:1489:CYS:HB2	1.94	0.48
2:E:218:SER:HB3	2:E:286:GLY:HA3	1.96	0.48
2:E:1589:GLN:NE2	2:E:1634:GLU:OE1	2.46	0.48
1:G:62:GLY:HA3	1:G:74:LEU:HD21	1.96	0.48
2:K:847:THR:OG1	2:K:1215:MET:O	2.32	0.48
2:K:3977:LYS:HB2	2:K:4095:ILE:HG13	1.95	0.48
2:B:1106:GLU:O	2:B:1214:ARG:N	2.47	0.48
2:B:4655:MET:O	2:B:4664:ARG:NH1	2.46	0.48
2:E:239:GLY:O	2:E:243:GLU:N	2.46	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:4722:TYR:OH	2:E:4746:ASP:OD1	2.23	0.48
2:K:799:LYS:HB3	2:K:1620:GLN:HG3	1.95	0.48
2:K:1445:TRP:H	2:K:1487:MET:HB2	1.79	0.48
2:K:4655:MET:O	2:K:4664:ARG:NH1	2.46	0.48
3:L:37:MET:HB3	3:L:42:GLN:HB2	1.96	0.48
2:B:799:LYS:HB3	2:B:1620:GLN:HG3	1.95	0.47
2:B:3977:LYS:HB2	2:B:4095:ILE:HG13	1.95	0.47
2:E:541:ILE:HG23	2:E:548:CYS:HB3	1.96	0.47
2:E:1106:GLU:O	2:E:1214:ARG:N	2.47	0.47
2:E:2114:VAL:O	2:E:2117:THR:OG1	2.28	0.47
3:F:37:MET:HB3	3:F:42:GLN:HB2	1.96	0.47
2:H:1251:LEU:O	2:H:1601:ASN:N	2.47	0.47
2:H:2464:ASP:OD1	2:H:2464:ASP:N	2.36	0.47
2:K:1106:GLU:O	2:K:1214:ARG:N	2.47	0.47
2:K:1143:GLN:HA	2:K:1151:HIS:HA	1.96	0.47
2:K:4167:LYS:NZ	7:K:6003:ATP:O2B	2.44	0.47
2:B:4791:ARG:HB3	2:B:4808:ASP:CB	2.43	0.47
1:D:62:GLY:HA3	1:D:74:LEU:HD21	1.96	0.47
2:H:143:LEU:HD12	2:K:2427:LEU:HD13	1.93	0.47
2:H:1106:GLU:O	2:H:1214:ARG:N	2.47	0.47
2:H:1143:GLN:HA	2:H:1151:HIS:HA	1.96	0.47
2:H:1184:ASP:N	2:H:1188:SER:O	2.45	0.47
2:B:235:ARG:NH2	2:B:269:VAL:O	2.39	0.47
2:E:433:LEU:HD12	2:E:447:LEU:HD11	1.97	0.47
2:H:847:THR:OG1	2:H:1215:MET:O	2.32	0.47
2:H:2072:GLN:NE2	2:H:3647:LYS:O	2.47	0.47
2:H:4621:GLN:HE22	2:H:4633:ARG:HH12	1.62	0.47
2:K:58:VAL:HG22	2:K:320:GLU:HA	1.96	0.47
2:K:953:SER:OG	2:K:1061:GLY:O	2.32	0.47
2:K:3936:LEU:HD21	2:K:3941:LEU:HD22	1.96	0.47
2:K:4621:GLN:HE22	2:K:4633:ARG:HH12	1.62	0.47
1:A:62:GLY:HA3	1:A:74:LEU:HD21	1.96	0.47
2:B:953:SER:OG	2:B:1061:GLY:O	2.32	0.47
2:B:1167:ASP:OD2	2:B:1172:THR:OG1	2.32	0.47
2:B:1445:TRP:H	2:B:1487:MET:HB2	1.79	0.47
2:B:2029:ARG:O	2:B:2032:SER:OG	2.27	0.47
2:E:4655:MET:O	2:E:4664:ARG:NH1	2.46	0.47
2:E:4845:ILE:HG23	2:H:4819:TYR:HB2	1.97	0.47
2:H:2029:ARG:O	2:H:2032:SER:OG	2.28	0.47
2:K:1125:ASP:HA	2:K:1598:ARG:HH11	1.78	0.47
2:K:2029:ARG:O	2:K:2032:SER:OG	2.28	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:3904:GLN:NE2	2:K:3965:GLN:OE1	2.48	0.47
2:B:731:HIS:CG	2:B:740:THR:HA	2.50	0.47
2:B:1218:GLY:HA3	2:B:1240:ALA:H	1.79	0.47
2:E:1218:GLY:HA3	2:E:1240:ALA:H	1.78	0.47
2:E:2832:VAL:O	2:E:2895:LYS:NZ	2.38	0.47
2:E:4891:ILE:HD13	2:E:4914:HIS:HB3	1.95	0.47
2:H:143:LEU:HD13	2:K:2426:SER:O	2.13	0.47
2:H:1218:GLY:HA3	2:H:1240:ALA:H	1.78	0.47
2:H:1445:TRP:H	2:H:1487:MET:HB2	1.79	0.47
2:H:4022:LEU:HD12	2:H:4089:HIS:CE1	2.49	0.47
2:B:433:LEU:HD12	2:B:447:LEU:HD11	1.97	0.47
2:B:673:TRP:HE3	2:B:822:CYS:HA	1.78	0.47
2:B:1143:GLN:HA	2:B:1151:HIS:HA	1.96	0.47
2:B:3904:GLN:NE2	2:B:3965:GLN:OE1	2.48	0.47
2:B:4621:GLN:HE22	2:B:4633:ARG:HH12	1.62	0.47
3:C:78:LYS:HA	3:C:81:ASP:HB2	1.97	0.47
2:E:188:SER:HB2	2:E:190:ARG:HH21	1.80	0.47
2:E:1125:ASP:HA	2:E:1598:ARG:HH11	1.78	0.47
2:E:1167:ASP:OD2	2:E:1172:THR:OG1	2.32	0.47
2:E:1445:TRP:H	2:E:1487:MET:HB2	1.79	0.47
2:E:3834:ASP:O	2:E:3837:THR:OG1	2.31	0.47
2:H:3729:GLN:O	2:H:3733:HIS:ND1	2.43	0.47
2:K:4010:ASN:OD1	2:K:4010:ASN:N	2.48	0.47
2:B:1184:ASP:N	2:B:1188:SER:O	2.45	0.47
2:B:1602:GLN:HE22	2:B:1642:LEU:HB3	1.80	0.47
2:B:2072:GLN:NE2	2:B:3647:LYS:O	2.47	0.47
2:B:4022:LEU:HD12	2:B:4089:HIS:CE1	2.49	0.47
3:C:37:MET:HB3	3:C:42:GLN:HB2	1.96	0.47
1:D:26:TYR:N	1:D:39:SER:OG	2.47	0.47
2:E:731:HIS:CG	2:E:740:THR:HA	2.50	0.47
2:E:1602:GLN:HE22	2:E:1642:LEU:HB3	1.80	0.47
2:E:4787:PHE:CZ	2:H:4521:TYR:HB3	2.49	0.47
1:G:26:TYR:N	1:G:39:SER:OG	2.47	0.47
2:H:1602:GLN:HE22	2:H:1642:LEU:HB3	1.80	0.47
2:K:731:HIS:CG	2:K:740:THR:HA	2.50	0.47
2:K:2072:GLN:NE2	2:K:3647:LYS:O	2.47	0.47
2:B:156:GLU:HB2	2:B:187:SER:HB3	1.97	0.47
2:B:1847:GLU:OE1	2:B:1849:SER:OG	2.25	0.47
2:E:306:LEU:HD11	2:E:314:LEU:HG	1.97	0.47
2:E:3904:GLN:NE2	2:E:3965:GLN:OE1	2.48	0.47
2:H:953:SER:OG	2:H:1061:GLY:O	2.32	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:995:MET:HG2	2:H:998:LYS:HD2	1.97	0.47
2:K:541:ILE:HG23	2:K:548:CYS:HB3	1.96	0.47
2:K:995:MET:HG2	2:K:998:LYS:HD2	1.97	0.47
2:K:1167:ASP:OD2	2:K:1172:THR:OG1	2.32	0.47
2:B:3936:LEU:HD21	2:B:3941:LEU:HD22	1.96	0.47
2:E:4621:GLN:HE22	2:E:4633:ARG:HH12	1.62	0.47
2:H:262:TYR:HB2	2:H:389:ARG:HB3	1.96	0.47
2:H:433:LEU:HD12	2:H:447:LEU:HD11	1.97	0.47
2:H:541:ILE:HG23	2:H:548:CYS:HB3	1.96	0.47
2:K:4022:LEU:HD12	2:K:4089:HIS:CE1	2.49	0.47
2:B:4010:ASN:OD1	2:B:4010:ASN:N	2.48	0.47
1:G:40:ARG:NH2	1:G:102:GLU:OE1	2.48	0.47
2:H:306:LEU:HD11	2:H:314:LEU:HG	1.97	0.47
2:H:4010:ASN:OD1	2:H:4010:ASN:N	2.48	0.47
2:E:799:LYS:HB3	2:E:1620:GLN:HG3	1.95	0.46
2:E:2072:GLN:NE2	2:E:3647:LYS:O	2.47	0.46
2:H:731:HIS:CG	2:H:740:THR:HA	2.50	0.46
2:H:2406:GLU:O	2:H:2410:ILE:N	2.42	0.46
2:K:1218:GLY:HA3	2:K:1240:ALA:H	1.79	0.46
2:B:541:ILE:HG23	2:B:548:CYS:HB3	1.96	0.46
2:B:995:MET:HG2	2:B:998:LYS:HD2	1.97	0.46
2:B:1132:GLU:HB3	2:B:1147:GLN:HE21	1.80	0.46
2:E:262:TYR:HB2	2:E:389:ARG:HB3	1.96	0.46
2:E:718:VAL:HA	2:E:736:CYS:N	2.29	0.46
2:E:836:HIS:CE1	2:E:1610:ARG:HD2	2.51	0.46
2:E:1608:VAL:HG12	2:E:1610:ARG:HB2	1.97	0.46
2:H:718:VAL:HA	2:H:736:CYS:N	2.29	0.46
2:K:188:SER:HB2	2:K:190:ARG:HH21	1.80	0.46
2:K:1602:GLN:HE22	2:K:1642:LEU:HB3	1.80	0.46
1:A:40:ARG:NH2	1:A:102:GLU:OE1	2.48	0.46
2:B:188:SER:HB2	2:B:190:ARG:HH21	1.80	0.46
2:E:204:ASP:N	2:E:204:ASP:OD1	2.48	0.46
2:E:1132:GLU:HB3	2:E:1147:GLN:HE21	1.80	0.46
3:F:78:LYS:HA	3:F:81:ASP:HB2	1.97	0.46
2:H:836:HIS:CE1	2:H:1610:ARG:HD2	2.51	0.46
1:A:26:TYR:N	1:A:39:SER:OG	2.47	0.46
2:B:1676:LEU:O	2:B:1680:VAL:N	2.47	0.46
2:B:3834:ASP:O	2:B:3837:THR:OG1	2.31	0.46
2:E:58:VAL:HG22	2:E:320:GLU:HA	1.96	0.46
2:E:156:GLU:HB2	2:E:187:SER:HB3	1.97	0.46
1:G:92:PRO:HG2	1:G:95:ALA:HB2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:679:VAL:HA	2:H:800:VAL:HG12	1.97	0.46
2:H:1676:LEU:O	2:H:1680:VAL:N	2.47	0.46
2:H:1912:GLN:HB2	2:H:2088:LEU:HD11	1.98	0.46
2:H:3680:LYS:NZ	2:H:3684:GLU:OE2	2.47	0.46
2:H:3904:GLN:NE2	2:H:3965:GLN:OE1	2.48	0.46
2:K:433:LEU:HD12	2:K:447:LEU:HD11	1.97	0.46
1:A:21:THR:HG1	1:A:49:ARG:HH21	1.59	0.46
1:D:92:PRO:HG2	1:D:95:ALA:HB2	1.98	0.46
2:E:1143:GLN:HA	2:E:1151:HIS:HA	1.96	0.46
2:E:2319:ASN:OD1	2:E:2323:ARG:NH2	2.49	0.46
2:E:3936:LEU:HD21	2:E:3941:LEU:HD22	1.96	0.46
2:E:4848:ASP:CB	2:H:4819:TYR:CE1	2.93	0.46
2:H:1608:VAL:HG12	2:H:1610:ARG:HB2	1.97	0.46
2:H:3683:LEU:HD12	2:H:3748:SER:HB3	1.98	0.46
2:K:4000:MET:HA	2:K:4003:MET:HG2	1.98	0.46
2:K:4808:ASP:OD1	2:K:4808:ASP:N	2.47	0.46
3:L:78:LYS:HA	3:L:81:ASP:HB2	1.97	0.46
2:B:1608:VAL:HG12	2:B:1610:ARG:HB2	1.96	0.46
2:B:2114:VAL:O	2:B:2117:THR:OG1	2.28	0.46
2:B:3607:ALA:HB3	3:C:85:GLU:HG2	1.98	0.46
2:B:3808:ALA:O	2:B:3812:GLN:HB2	2.16	0.46
2:E:995:MET:HG2	2:E:998:LYS:HD2	1.97	0.46
2:E:3683:LEU:HD12	2:E:3748:SER:HB3	1.98	0.46
2:H:122:ARG:HH21	2:H:127:GLY:HA2	1.81	0.46
2:H:288:HIS:N	2:H:349:MET:O	2.47	0.46
2:H:4167:LYS:NZ	7:H:6003:ATP:O2B	2.44	0.46
1:J:92:PRO:HG2	1:J:95:ALA:HB2	1.98	0.46
2:K:306:LEU:HD11	2:K:314:LEU:HG	1.97	0.46
2:K:3834:ASP:O	2:K:3837:THR:OG1	2.31	0.46
2:E:4757:ILE:HG23	2:E:4871:PHE:HZ	1.81	0.46
2:H:1470:GLY:HA2	2:H:1474:GLY:HA2	1.98	0.46
2:H:4000:MET:HA	2:H:4003:MET:HG2	1.98	0.46
2:H:4192:ASN:OD1	2:H:4605:LYS:NZ	2.29	0.46
2:K:3680:LYS:NZ	2:K:3684:GLU:OE2	2.47	0.46
2:B:1912:GLN:HB2	2:B:2088:LEU:HD11	1.97	0.46
2:B:2319:ASN:OD1	2:B:2323:ARG:NH2	2.49	0.46
2:E:394:HIS:HD2	2:E:397:GLY:H	1.63	0.46
2:E:1098:ALA:O	2:E:1101:TRP:NE1	2.38	0.46
2:E:1756:SER:OG	2:E:1757:LEU:N	2.49	0.46
2:E:1912:GLN:HB2	2:E:2088:LEU:HD11	1.98	0.46
2:E:3607:ALA:HB3	3:F:85:GLU:HG2	1.98	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:156:GLU:HB2	2:H:187:SER:HB3	1.97	0.46
2:H:204:ASP:N	2:H:204:ASP:OD1	2.48	0.46
2:H:2117:THR:HG22	2:H:2155:VAL:HG11	1.98	0.46
2:H:3607:ALA:HB3	3:I:85:GLU:HG2	1.98	0.46
2:K:288:HIS:N	2:K:349:MET:O	2.47	0.46
2:K:836:HIS:CE1	2:K:1610:ARG:HD2	2.51	0.46
2:K:1132:GLU:HB3	2:K:1147:GLN:HE21	1.80	0.46
2:K:3683:LEU:HD12	2:K:3748:SER:HB3	1.98	0.46
1:A:92:PRO:HG2	1:A:95:ALA:HB2	1.98	0.46
2:B:122:ARG:HH21	2:B:127:GLY:HA2	1.81	0.46
2:B:836:HIS:CE1	2:B:1610:ARG:HD2	2.51	0.46
2:E:1730:THR:O	2:E:1733:THR:OG1	2.28	0.46
2:H:188:SER:HB2	2:H:190:ARG:HH21	1.80	0.46
2:H:2252:ASN:HD22	2:H:3595:GLN:HG3	1.81	0.46
2:H:3936:LEU:HD21	2:H:3941:LEU:HD22	1.96	0.46
2:K:262:TYR:HB2	2:K:389:ARG:HB3	1.96	0.46
2:K:1098:ALA:O	2:K:1101:TRP:NE1	2.38	0.46
2:K:2252:ASN:HD22	2:K:3595:GLN:HG3	1.81	0.46
2:B:262:TYR:HB2	2:B:389:ARG:HB3	1.96	0.46
2:B:306:LEU:HD11	2:B:314:LEU:HG	1.97	0.46
2:K:235:ARG:NH2	2:K:269:VAL:O	2.39	0.46
2:K:894:VAL:HG11	2:K:976:TYR:HD2	1.81	0.46
2:K:897:LYS:HE2	2:K:915:HIS:CG	2.51	0.46
2:K:1608:VAL:HG12	2:K:1610:ARG:HB2	1.96	0.46
2:K:1912:GLN:HB2	2:K:2088:LEU:HD11	1.98	0.46
2:K:3607:ALA:HB3	3:L:85:GLU:HG2	1.98	0.46
2:B:204:ASP:OD1	2:B:204:ASP:N	2.48	0.45
2:B:986:ILE:HB	2:B:1058:LEU:HB3	1.98	0.45
2:B:3806:LEU:CD2	2:K:76:ARG:NH2	2.72	0.45
2:E:1690:GLU:OE2	2:E:1790:LYS:NZ	2.40	0.45
2:E:2252:ASN:HD22	2:E:3595:GLN:HG3	1.81	0.45
2:E:2425:ARG:HH12	2:E:2477:TYR:HA	1.81	0.45
2:E:3993:ASN:HD22	2:E:4110:MET:HG3	1.81	0.45
2:H:894:VAL:HG11	2:H:976:TYR:HD2	1.81	0.45
2:H:1132:GLU:HB3	2:H:1147:GLN:HE21	1.80	0.45
1:J:26:TYR:N	1:J:39:SER:OG	2.47	0.45
2:K:3993:ASN:HD22	2:K:4110:MET:HG3	1.81	0.45
2:K:4147:GLU:OE1	2:K:4937:GLN:NE2	2.49	0.45
2:B:894:VAL:HG11	2:B:976:TYR:HD2	1.81	0.45
2:B:2252:ASN:HD22	2:B:3595:GLN:HG3	1.81	0.45
2:E:288:HIS:N	2:E:349:MET:O	2.47	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:986:ILE:HB	2:E:1058:LEU:HB3	1.98	0.45
2:E:1511:VAL:HA	2:E:1517:LEU:H	1.81	0.45
2:E:2464:ASP:OD1	2:E:2464:ASP:N	2.36	0.45
2:H:1763:PHE:HB3	2:H:1781:GLU:HB3	1.98	0.45
3:I:78:LYS:HA	3:I:81:ASP:HB2	1.97	0.45
2:K:679:VAL:HA	2:K:800:VAL:HG12	1.97	0.45
2:K:769:ARG:HA	2:K:775:VAL:HG23	1.99	0.45
2:K:1251:LEU:O	2:K:1601:ASN:N	2.47	0.45
2:K:1763:PHE:HB3	2:K:1781:GLU:HB3	1.98	0.45
2:K:4757:ILE:HG23	2:K:4871:PHE:HZ	1.81	0.45
2:B:80:GLU:HG3	2:E:3891:TRP:CZ3	2.49	0.45
2:B:769:ARG:HA	2:B:775:VAL:HG23	1.99	0.45
2:B:4000:MET:HE3	2:B:4000:MET:HB2	1.88	0.45
2:B:4147:GLU:OE1	2:B:4937:GLN:NE2	2.49	0.45
1:D:11:ASP:OD2	1:D:14:THR:OG1	2.34	0.45
2:E:76:ARG:HH21	2:H:3806:LEU:CG	2.29	0.45
2:E:897:LYS:HE2	2:E:915:HIS:CG	2.52	0.45
2:E:2117:THR:HG22	2:E:2155:VAL:HG11	1.98	0.45
2:E:3808:ALA:O	2:E:3812:GLN:HB2	2.16	0.45
2:H:66:THR:OG1	2:H:124:SER:OG	2.25	0.45
2:H:4845:ILE:HG23	2:K:4819:TYR:HB2	1.99	0.45
2:K:156:GLU:HB2	2:K:187:SER:HB3	1.97	0.45
2:K:4722:TYR:OH	2:K:4746:ASP:OD1	2.23	0.45
2:K:4733:GLY:HA3	2:K:4740:PHE:HD1	1.82	0.45
2:B:394:HIS:HD2	2:B:397:GLY:H	1.63	0.45
2:E:76:ARG:HH22	2:H:3806:LEU:HD11	1.75	0.45
2:E:1763:PHE:HB3	2:E:1781:GLU:HB3	1.98	0.45
2:H:394:HIS:HD2	2:H:397:GLY:H	1.63	0.45
2:H:3984:LEU:HB2	2:H:4102:LEU:HD12	1.99	0.45
2:H:4147:GLU:OE1	2:H:4937:GLN:NE2	2.49	0.45
2:K:1710:HIS:HB2	2:K:1711:LEU:HD12	1.99	0.45
2:K:4160:GLN:HB3	2:K:4201:MET:HE1	1.99	0.45
2:B:268:SER:O	2:B:273:SER:OG	2.31	0.45
2:B:847:THR:OG1	2:B:1215:MET:O	2.32	0.45
2:B:1251:LEU:O	2:B:1601:ASN:N	2.47	0.45
2:B:1470:GLY:HA2	2:B:1474:GLY:HA2	1.98	0.45
2:B:1511:VAL:HA	2:B:1517:LEU:H	1.81	0.45
2:B:1726:ILE:HG13	2:B:1757:LEU:HD23	1.98	0.45
2:B:1763:PHE:HB3	2:B:1781:GLU:HB3	1.98	0.45
2:B:2425:ARG:HH12	2:B:2477:TYR:HA	1.81	0.45
2:B:3993:ASN:HD22	2:B:4110:MET:HG3	1.81	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:268:SER:O	2:E:273:SER:OG	2.31	0.45
2:E:770:ILE:HG12	2:E:775:VAL:HG21	1.99	0.45
2:E:847:THR:OG1	2:E:1215:MET:O	2.32	0.45
2:E:1710:HIS:HB2	2:E:1711:LEU:HD12	1.99	0.45
2:H:643:LEU:H	2:H:643:LEU:HG	1.60	0.45
2:K:3808:ALA:O	2:K:3812:GLN:HB2	2.16	0.45
2:B:897:LYS:HE2	2:B:915:HIS:CG	2.51	0.45
2:B:1710:HIS:HB2	2:B:1711:LEU:HD12	1.99	0.45
2:B:2117:THR:HG22	2:B:2155:VAL:HG11	1.98	0.45
2:B:2426:SER:O	2:K:143:LEU:HD13	2.13	0.45
2:B:3683:LEU:HD12	2:B:3748:SER:HB3	1.98	0.45
2:B:4819:TYR:CE1	2:K:4848:ASP:CB	2.95	0.45
2:E:1986:GLU:N	2:E:1989:CYS:SG	2.73	0.45
2:H:76:ARG:HH22	2:K:3806:LEU:HD11	1.76	0.45
2:H:1726:ILE:HG13	2:H:1757:LEU:HD23	1.98	0.45
2:H:3993:ASN:HD22	2:H:4110:MET:HG3	1.81	0.45
2:K:305:TYR:HE2	2:K:319:LYS:HG2	1.81	0.45
2:K:394:HIS:HD2	2:K:397:GLY:H	1.63	0.45
2:K:1470:GLY:HA2	2:K:1474:GLY:HA2	1.98	0.45
2:K:1756:SER:OG	2:K:1757:LEU:N	2.49	0.45
2:B:1756:SER:OG	2:B:1757:LEU:N	2.49	0.45
2:B:4897:ASP:OD1	2:B:4897:ASP:N	2.50	0.45
2:E:122:ARG:HH21	2:E:127:GLY:HA2	1.81	0.45
2:E:3844:LEU:HD23	2:E:3844:LEU:HA	1.79	0.45
2:H:1511:VAL:HA	2:H:1517:LEU:H	1.81	0.45
2:H:2425:ARG:HH12	2:H:2477:TYR:HA	1.81	0.45
2:H:4733:GLY:HA3	2:H:4740:PHE:HD1	1.82	0.45
2:K:308:LEU:N	2:K:326:SER:O	2.49	0.45
2:K:1184:ASP:N	2:K:1188:SER:O	2.45	0.45
2:K:1640:ASP:OD1	2:K:1640:ASP:N	2.44	0.45
2:B:16:THR:OG1	2:B:111:ARG:O	2.29	0.45
2:B:4000:MET:HA	2:B:4003:MET:HG2	1.98	0.45
2:B:4168:GLU:HA	2:B:4171:ARG:CZ	2.46	0.45
2:E:679:VAL:HA	2:E:800:VAL:HG12	1.97	0.45
2:E:769:ARG:HA	2:E:775:VAL:HG23	1.99	0.45
2:E:3984:LEU:HB2	2:E:4102:LEU:HD12	1.99	0.45
2:H:235:ARG:NH2	2:H:269:VAL:O	2.39	0.45
2:H:769:ARG:HA	2:H:775:VAL:HG23	1.99	0.45
2:H:1756:SER:OG	2:H:1757:LEU:N	2.49	0.45
2:H:3808:ALA:O	2:H:3812:GLN:HB2	2.16	0.45
2:H:3921:LEU:HD23	2:H:3921:LEU:HA	1.73	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:204:ASP:N	2:K:204:ASP:OD1	2.48	0.45
2:K:986:ILE:HB	2:K:1058:LEU:HB3	1.98	0.45
2:K:2319:ASN:OD1	2:K:2323:ARG:NH2	2.49	0.45
2:B:76:ARG:HH21	2:E:3806:LEU:CG	2.30	0.45
2:B:770:ILE:HG12	2:B:775:VAL:HG21	1.99	0.45
2:B:3680:LYS:NZ	2:B:3684:GLU:OE2	2.47	0.45
2:B:4733:GLY:HA3	2:B:4740:PHE:HD1	1.82	0.45
2:B:4757:ILE:HG23	2:B:4871:PHE:HZ	1.81	0.45
2:E:4897:ASP:N	2:E:4897:ASP:OD1	2.50	0.45
2:H:305:TYR:HE2	2:H:319:LYS:HG2	1.81	0.45
2:H:4022:LEU:HA	2:H:4089:HIS:CE1	2.50	0.45
2:K:122:ARG:HH21	2:K:127:GLY:HA2	1.81	0.45
2:K:4022:LEU:HA	2:K:4089:HIS:CE1	2.50	0.45
2:B:660:PHE:HB3	2:B:787:LEU:HD22	1.99	0.45
2:B:679:VAL:HA	2:B:800:VAL:HG12	1.97	0.45
2:B:695:VAL:HA	2:B:792:VAL:HG22	1.99	0.45
3:C:110:MET:HE3	3:C:125:MET:HG3	1.99	0.45
2:E:80:GLU:HG3	2:H:3891:TRP:CZ3	2.49	0.45
2:E:3970:LYS:HB3	2:E:3970:LYS:HE2	1.82	0.45
2:E:4733:GLY:HA3	2:E:4740:PHE:HD1	1.82	0.45
3:F:110:MET:HE3	3:F:125:MET:HG3	1.99	0.45
2:K:54:ASN:HB3	2:K:57:ASN:HB3	1.99	0.45
2:K:394:HIS:CD2	2:K:396:GLU:H	2.35	0.45
3:L:130:ASP:O	3:L:137:VAL:HG22	2.17	0.45
2:E:1470:GLY:HA2	2:E:1474:GLY:HA2	1.98	0.44
2:E:4000:MET:HA	2:E:4003:MET:HG2	1.98	0.44
2:E:4022:LEU:HA	2:E:4089:HIS:CE1	2.50	0.44
2:E:4147:GLU:OE1	2:E:4937:GLN:NE2	2.49	0.44
2:E:4808:ASP:N	2:E:4808:ASP:OD1	2.47	0.44
2:H:986:ILE:HB	2:H:1058:LEU:HB3	1.98	0.44
2:H:1710:HIS:HB2	2:H:1711:LEU:HD12	1.98	0.44
2:H:4897:ASP:N	2:H:4897:ASP:OD1	2.50	0.44
2:K:1726:ILE:HG13	2:K:1757:LEU:HD23	1.98	0.44
2:K:2117:THR:HG22	2:K:2155:VAL:HG11	1.98	0.44
2:B:54:ASN:HB3	2:B:57:ASN:HB3	1.99	0.44
2:B:143:LEU:HD12	2:E:2427:LEU:HD11	2.00	0.44
2:B:288:HIS:N	2:B:349:MET:O	2.47	0.44
2:B:643:LEU:H	2:B:643:LEU:HG	1.60	0.44
2:B:1210:ALA:N	2:B:1211:GLN:OE1	2.50	0.44
2:B:4022:LEU:HA	2:B:4089:HIS:CE1	2.50	0.44
3:C:130:ASP:O	3:C:137:VAL:HG22	2.17	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:305:TYR:HE2	2:E:319:LYS:HG2	1.81	0.44
2:E:660:PHE:HB3	2:E:787:LEU:HD22	2.00	0.44
2:E:894:VAL:HG11	2:E:976:TYR:HD2	1.81	0.44
2:E:1726:ILE:HG13	2:E:1757:LEU:HD23	1.98	0.44
2:E:2891:GLN:HG2	2:E:2894:LEU:HD12	1.99	0.44
2:H:695:VAL:HA	2:H:792:VAL:HG22	1.99	0.44
2:H:748:LEU:HB2	2:H:750:ARG:HG3	1.99	0.44
2:H:2319:ASN:OD1	2:H:2323:ARG:NH2	2.48	0.44
2:K:1258:PHE:HB3	2:K:1303:ARG:NH1	2.33	0.44
2:K:3642:ILE:HG22	2:K:3731:ARG:HD3	1.99	0.44
2:K:3844:LEU:HD23	2:K:3844:LEU:HA	1.79	0.44
2:B:76:ARG:HH22	2:E:3806:LEU:HD11	1.74	0.44
2:B:394:HIS:CD2	2:B:396:GLU:H	2.35	0.44
2:B:2760:PRO:HD2	2:B:2763:LEU:HD12	1.99	0.44
2:B:4160:GLN:HB3	2:B:4201:MET:HE1	1.99	0.44
2:E:750:ARG:N	2:E:753:ASP:OD2	2.46	0.44
2:E:4010:ASN:OD1	2:E:4010:ASN:N	2.48	0.44
3:F:130:ASP:O	3:F:137:VAL:HG22	2.17	0.44
2:H:191:TYR:OH	2:K:2327:ARG:CZ	2.66	0.44
2:H:2891:GLN:HG2	2:H:2894:LEU:HD12	1.99	0.44
3:I:130:ASP:O	3:I:137:VAL:HG22	2.17	0.44
2:K:1162:VAL:O	2:K:1176:THR:OG1	2.33	0.44
2:K:1511:VAL:HA	2:K:1517:LEU:H	1.81	0.44
2:K:2425:ARG:HH12	2:K:2477:TYR:HA	1.81	0.44
2:K:2760:PRO:HD2	2:K:2763:LEU:HD12	1.99	0.44
2:B:1640:ASP:OD1	2:B:1640:ASP:N	2.44	0.44
2:B:2891:GLN:HG2	2:B:2894:LEU:HD12	1.99	0.44
2:B:3806:LEU:HD11	2:K:76:ARG:HH22	1.75	0.44
2:B:4175:PHE:O	2:B:4179:ASN:ND2	2.51	0.44
2:E:294:PRO:HB3	2:E:366:ILE:HD11	1.99	0.44
2:E:3642:ILE:HG22	2:E:3731:ARG:HD3	1.99	0.44
2:H:308:LEU:N	2:H:326:SER:O	2.49	0.44
2:H:1601:ASN:ND2	2:H:1643:GLU:OE2	2.36	0.44
2:H:3760:LEU:HD23	2:H:3760:LEU:HA	1.81	0.44
2:H:4757:ILE:HG23	2:H:4871:PHE:HZ	1.81	0.44
2:K:3984:LEU:HB2	2:K:4102:LEU:HD12	1.99	0.44
3:L:110:MET:HE3	3:L:125:MET:HG3	1.99	0.44
2:B:674:TYR:HE2	2:B:814:LEU:HB2	1.83	0.44
2:B:2880:ALA:O	2:B:2884:ALA:N	2.49	0.44
2:E:394:HIS:CD2	2:E:396:GLU:H	2.35	0.44
2:E:2398:ASP:OD1	2:E:2402:ARG:NH2	2.50	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:394:HIS:CD2	2:H:396:GLU:H	2.35	0.44
2:H:660:PHE:HB3	2:H:787:LEU:HD22	1.99	0.44
2:H:3844:LEU:HD23	2:H:3844:LEU:HA	1.79	0.44
2:H:4160:GLN:HB3	2:H:4201:MET:HE1	1.99	0.44
2:H:4175:PHE:O	2:H:4179:ASN:ND2	2.51	0.44
1:J:40:ARG:NH2	1:J:102:GLU:OE1	2.48	0.44
2:K:1121:GLY:O	2:K:1133:ARG:NH1	2.51	0.44
2:B:305:TYR:HE2	2:B:319:LYS:HG2	1.82	0.44
2:B:1258:PHE:HB3	2:B:1303:ARG:NH1	2.33	0.44
2:B:2327:ARG:CZ	2:K:191:TYR:OH	2.66	0.44
2:E:238:HIS:N	2:E:243:GLU:O	2.43	0.44
2:E:674:TYR:HE2	2:E:814:LEU:HB2	1.83	0.44
2:E:4136:ARG:HH21	2:E:4148:ARG:CZ	2.31	0.44
2:H:2770:GLU:O	2:H:2774:TRP:HB2	2.18	0.44
2:H:4136:ARG:HH21	2:H:4148:ARG:CZ	2.31	0.44
2:K:4601:PHE:HD1	2:K:4644:ASN:HB3	1.83	0.44
2:B:506:HIS:NE2	2:B:564:ARG:HG2	2.33	0.44
2:B:1121:GLY:O	2:B:1133:ARG:NH1	2.51	0.44
2:E:76:ARG:NH2	2:H:3806:LEU:CD2	2.70	0.44
2:E:1121:GLY:O	2:E:1133:ARG:NH1	2.51	0.44
2:E:1258:PHE:HB3	2:E:1303:ARG:NH1	2.33	0.44
2:E:2880:ALA:O	2:E:2884:ALA:N	2.49	0.44
2:H:76:ARG:HH21	2:K:3806:LEU:CG	2.31	0.44
2:H:1305:SER:HB2	2:H:1591:LEU:HB2	2.00	0.44
2:K:4136:ARG:HH21	2:K:4148:ARG:CZ	2.31	0.44
2:K:4175:PHE:O	2:K:4179:ASN:ND2	2.51	0.44
2:B:308:LEU:N	2:B:326:SER:O	2.49	0.44
2:B:3806:LEU:CG	2:K:76:ARG:HH21	2.30	0.44
2:B:3984:LEU:HB2	2:B:4102:LEU:HD12	1.99	0.44
2:B:4791:ARG:CB	2:B:4808:ASP:HB3	2.47	0.44
1:D:30:LEU:HD12	1:D:34:LYS:HB2	2.00	0.44
1:D:40:ARG:NH2	1:D:102:GLU:OE1	2.48	0.44
2:E:4160:GLN:HB3	2:E:4201:MET:HE1	1.99	0.44
2:H:294:PRO:HB3	2:H:366:ILE:HD11	2.00	0.44
2:H:770:ILE:HG12	2:H:775:VAL:HG21	1.99	0.44
2:H:897:LYS:HE2	2:H:915:HIS:CG	2.52	0.44
2:K:660:PHE:HB3	2:K:787:LEU:HD22	1.99	0.44
2:K:770:ILE:HG12	2:K:775:VAL:HG21	1.99	0.44
2:K:3921:LEU:HD23	2:K:3921:LEU:HA	1.73	0.44
2:B:191:TYR:OH	2:E:2327:ARG:CZ	2.65	0.44
2:B:1274:ASP:HB2	2:B:1286:THR:HA	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:54:ASN:HB3	2:E:57:ASN:HB3	1.99	0.44
2:E:695:VAL:HA	2:E:792:VAL:HG22	1.99	0.44
2:E:3680:LYS:NZ	2:E:3684:GLU:OE2	2.47	0.44
2:H:3642:ILE:HG22	2:H:3731:ARG:HD3	1.99	0.44
2:H:4601:PHE:HD1	2:H:4644:ASN:HB3	1.83	0.44
2:K:748:LEU:HB2	2:K:750:ARG:HG3	1.99	0.44
2:K:2891:GLN:HG2	2:K:2894:LEU:HD12	1.99	0.44
2:E:228:LEU:HD11	2:E:405:LEU:HD13	2.00	0.43
2:E:769:ARG:HG2	2:E:774:PRO:HA	2.00	0.43
2:E:2856:LYS:O	2:E:2860:GLU:HB2	2.18	0.43
2:H:694:ARG:HG2	2:H:716:ASN:HB3	2.00	0.43
2:H:750:ARG:N	2:H:753:ASP:OD2	2.46	0.43
2:H:769:ARG:HG2	2:H:774:PRO:HA	2.00	0.43
2:H:4635:VAL:O	2:H:4638:THR:OG1	2.33	0.43
3:I:110:MET:HE3	3:I:125:MET:HG3	1.99	0.43
2:K:1305:SER:HB2	2:K:1591:LEU:HB2	2.00	0.43
2:K:2770:GLU:O	2:K:2774:TRP:HB2	2.18	0.43
2:K:3880:LEU:HD23	2:K:3944:ALA:HB2	2.00	0.43
2:K:4178:VAL:HG21	2:K:4885:MET:HE3	2.00	0.43
2:B:694:ARG:HG2	2:B:716:ASN:HB3	2.00	0.43
2:B:3593:SER:O	2:B:3597:LYS:NZ	2.42	0.43
2:B:4819:TYR:HB2	2:K:4845:ILE:HG23	2.00	0.43
2:E:506:HIS:NE2	2:E:564:ARG:HG2	2.33	0.43
2:E:748:LEU:HB2	2:E:750:ARG:HG3	1.99	0.43
2:E:3800:SER:OG	2:E:3801:CYS:N	2.41	0.43
1:J:30:LEU:HD12	1:J:34:LYS:HB2	2.00	0.43
2:K:1757:LEU:HD13	2:K:1757:LEU:HA	1.88	0.43
2:B:2241:LEU:HD12	2:B:2298:ARG:HG3	2.01	0.43
2:B:4845:ILE:HG23	2:E:4819:TYR:HB2	2.00	0.43
2:E:143:LEU:HD13	2:H:2426:SER:O	2.14	0.43
2:E:898:ILE:HD13	2:E:973:THR:HG22	2.00	0.43
2:H:2241:LEU:HD12	2:H:2298:ARG:HG3	2.00	0.43
2:H:2856:LYS:O	2:H:2860:GLU:HB2	2.18	0.43
2:K:694:ARG:HG2	2:K:716:ASN:HB3	2.00	0.43
2:K:2856:LYS:O	2:K:2860:GLU:HB2	2.18	0.43
2:B:769:ARG:HG2	2:B:774:PRO:HA	2.00	0.43
2:B:4601:PHE:HD1	2:B:4644:ASN:HB3	1.83	0.43
2:E:2241:LEU:HD12	2:E:2298:ARG:HG3	2.01	0.43
2:H:54:ASN:HB3	2:H:57:ASN:HB3	1.99	0.43
2:H:718:VAL:HA	2:H:736:CYS:H	1.83	0.43
2:H:1057:LEU:O	2:H:1062:TYR:N	2.51	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1121:GLY:O	2:H:1133:ARG:NH1	2.51	0.43
2:H:1258:PHE:HB3	2:H:1303:ARG:NH1	2.33	0.43
2:K:674:TYR:HE2	2:K:814:LEU:HB2	1.83	0.43
2:K:695:VAL:HA	2:K:792:VAL:HG22	1.99	0.43
2:K:2212:GLN:HE21	2:K:2247:SER:C	2.27	0.43
2:B:1098:ALA:O	2:B:1101:TRP:NE1	2.38	0.43
2:B:2212:GLN:HE21	2:B:2247:SER:C	2.27	0.43
2:B:4178:VAL:HG21	2:B:4885:MET:HE3	2.00	0.43
2:E:2212:GLN:HE21	2:E:2247:SER:C	2.27	0.43
2:E:4011:VAL:HA	2:E:4014:ILE:HG12	2.00	0.43
2:H:674:TYR:HE2	2:H:814:LEU:HB2	1.83	0.43
2:H:1734:LYS:HE2	2:H:1931:ASP:HB3	2.00	0.43
2:H:2212:GLN:HE21	2:H:2247:SER:C	2.27	0.43
2:H:2397:ILE:HD12	2:H:2397:ILE:HA	1.94	0.43
2:H:2760:PRO:HD2	2:H:2763:LEU:HD12	1.99	0.43
2:H:2880:ALA:O	2:H:2884:ALA:N	2.49	0.43
2:H:3800:SER:OG	2:H:3801:CYS:N	2.41	0.43
2:H:4178:VAL:HG21	2:H:4885:MET:HE3	2.00	0.43
2:H:4848:ASP:CB	2:K:4819:TYR:CE1	2.95	0.43
2:K:718:VAL:HA	2:K:736:CYS:H	1.83	0.43
2:K:2241:LEU:HD12	2:K:2298:ARG:HG3	2.00	0.43
2:K:2463:PRO:HB3	2:K:2516:ALA:HB2	2.01	0.43
2:B:4523:VAL:HG21	2:K:4791:ARG:HD2	2.00	0.43
2:B:4780:TYR:OH	2:E:4515:ASN:HB3	2.19	0.43
2:E:2760:PRO:HD2	2:E:2763:LEU:HD12	1.99	0.43
2:E:4175:PHE:O	2:E:4179:ASN:ND2	2.51	0.43
2:E:4601:PHE:HD1	2:E:4644:ASN:HB3	1.83	0.43
1:G:30:LEU:HD12	1:G:34:LYS:HB2	2.00	0.43
2:H:1274:ASP:HB2	2:H:1286:THR:HA	2.00	0.43
2:H:2252:ASN:HB2	2:H:2310:ASN:HD21	1.84	0.43
2:K:769:ARG:HG2	2:K:774:PRO:HA	2.00	0.43
2:K:1305:SER:HA	2:K:1593:HIS:HD2	1.84	0.43
2:K:2398:ASP:OD1	2:K:2402:ARG:NH2	2.50	0.43
2:K:2731:ASP:HB3	2:K:2826:ALA:HB2	2.01	0.43
2:B:294:PRO:HB3	2:B:366:ILE:HD11	1.99	0.43
2:B:601:LEU:HG	2:B:642:LEU:HD23	2.01	0.43
2:B:1734:LYS:HE2	2:B:1931:ASP:HB3	2.00	0.43
2:B:3921:LEU:HD23	2:B:3921:LEU:HA	1.73	0.43
2:E:601:LEU:HG	2:E:642:LEU:HD23	2.01	0.43
2:E:1057:LEU:O	2:E:1062:TYR:N	2.51	0.43
2:E:1305:SER:HA	2:E:1593:HIS:HD2	1.84	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:2252:ASN:HB2	2:E:2310:ASN:HD21	1.84	0.43
2:H:425:LEU:HD21	2:H:452:VAL:HG13	2.01	0.43
2:H:1228:THR:HA	2:H:1232:LEU:HD12	2.01	0.43
2:H:1785:ASP:OD1	2:H:1788:LYS:NZ	2.51	0.43
2:H:1986:GLU:N	2:H:1989:CYS:SG	2.73	0.43
2:K:652:VAL:HG11	2:K:715:GLY:HA2	2.01	0.43
2:K:1310:CYS:HB2	2:K:1536:SER:HA	2.01	0.43
2:K:1785:ASP:OD1	2:K:1788:LYS:NZ	2.50	0.43
2:B:228:LEU:HD11	2:B:405:LEU:HD13	2.00	0.43
2:B:1714:TYR:CD1	2:B:1761:MET:HB3	2.54	0.43
2:B:2463:PRO:HB3	2:B:2516:ALA:HB2	2.01	0.43
2:B:3642:ILE:HG22	2:B:3731:ARG:HD3	1.99	0.43
2:B:4136:ARG:HH21	2:B:4148:ARG:CZ	2.31	0.43
2:E:308:LEU:N	2:E:326:SER:O	2.49	0.43
2:E:1601:ASN:ND2	2:E:1643:GLU:OE2	2.36	0.43
2:H:2759:LYS:HA	2:H:2760:PRO:HD3	1.92	0.43
2:H:3665:LEU:HD11	2:H:3696:MET:HE2	2.01	0.43
2:H:3986:MET:HG2	2:H:3996:ILE:HD11	2.01	0.43
2:K:898:ILE:HD13	2:K:973:THR:HG22	2.00	0.43
2:K:1676:LEU:O	2:K:1680:VAL:N	2.47	0.43
2:K:4787:PHE:HD1	2:K:4808:ASP:O	2.02	0.43
2:B:898:ILE:HD13	2:B:973:THR:HG22	2.00	0.43
2:B:2770:GLU:O	2:B:2774:TRP:HB2	2.18	0.43
2:B:3891:TRP:CZ3	2:K:80:GLU:HG3	2.50	0.43
2:E:3612:LEU:HD23	2:E:3617:ALA:HB2	2.01	0.43
2:E:3665:LEU:HD11	2:E:3696:MET:HE2	2.01	0.43
2:H:228:LEU:HD11	2:H:405:LEU:HD13	2.00	0.43
2:H:506:HIS:NE2	2:H:564:ARG:HG2	2.33	0.43
2:H:898:ILE:HD13	2:H:973:THR:HG22	2.00	0.43
2:K:506:HIS:NE2	2:K:564:ARG:HG2	2.33	0.43
2:K:1274:ASP:HB2	2:K:1286:THR:HA	2.00	0.43
2:K:3612:LEU:HD23	2:K:3617:ALA:HB2	2.01	0.43
2:B:718:VAL:HA	2:B:736:CYS:H	1.83	0.43
2:B:1305:SER:HB2	2:B:1591:LEU:HB2	2.00	0.43
2:B:2252:ASN:HB2	2:B:2310:ASN:HD21	1.84	0.43
2:B:2427:LEU:HD11	2:K:143:LEU:HD12	2.01	0.43
2:B:3760:LEU:HD23	2:B:3760:LEU:HA	1.81	0.43
2:E:425:LEU:HD21	2:E:452:VAL:HG13	2.01	0.43
2:E:940:LEU:HD23	2:E:940:LEU:HA	1.89	0.43
2:E:1274:ASP:HB2	2:E:1286:THR:HA	2.00	0.43
2:E:2770:GLU:O	2:E:2774:TRP:HB2	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:601:LEU:HG	2:H:642:LEU:HD23	2.01	0.43
2:H:1305:SER:HA	2:H:1593:HIS:HD2	1.84	0.43
2:H:1310:CYS:HB2	2:H:1536:SER:HA	2.01	0.43
2:H:1836:ASN:HA	2:H:1839:LEU:HB2	2.01	0.43
2:H:2076:ILE:HG21	2:H:2081:LEU:HD22	2.00	0.43
2:H:2731:ASP:HB3	2:H:2826:ALA:HB2	2.01	0.43
2:K:601:LEU:HG	2:K:642:LEU:HD23	2.01	0.43
2:K:1601:ASN:ND2	2:K:1643:GLU:OE2	2.36	0.43
1:A:30:LEU:HD12	1:A:34:LYS:HB2	2.00	0.42
2:B:243:GLU:HA	2:B:264:GLY:HA2	2.01	0.42
2:B:2247:SER:O	2:B:2247:SER:OG	2.37	0.42
2:B:4011:VAL:HA	2:B:4014:ILE:HG12	2.00	0.42
2:B:4515:ASN:HB3	2:K:4780:TYR:OH	2.19	0.42
1:D:9:PRO:HD2	2:E:748:LEU:HD11	2.01	0.42
2:E:64:ILE:H	2:E:64:ILE:HG13	1.74	0.42
2:E:191:TYR:OH	2:H:2327:ARG:CZ	2.67	0.42
2:E:235:ARG:NH2	2:E:269:VAL:O	2.39	0.42
2:E:243:GLU:HA	2:E:264:GLY:HA2	2.00	0.42
2:E:1228:THR:HA	2:E:1232:LEU:HD12	2.01	0.42
2:E:1310:CYS:HB2	2:E:1536:SER:HA	2.01	0.42
2:E:1714:TYR:CD1	2:E:1761:MET:HB3	2.54	0.42
2:E:2076:ILE:HG21	2:E:2081:LEU:HD22	2.01	0.42
2:E:2716:GLU:HA	2:E:2719:GLU:HB2	2.01	0.42
2:E:2731:ASP:HB3	2:E:2826:ALA:HB2	2.01	0.42
2:E:3880:LEU:HD23	2:E:3944:ALA:HB2	2.00	0.42
2:E:4787:PHE:HD1	2:E:4808:ASP:O	2.02	0.42
2:H:1466:THR:HG22	2:H:1482:ARG:HG2	2.01	0.42
2:H:3777:LYS:HE3	2:H:3777:LYS:HB2	1.87	0.42
2:K:238:HIS:N	2:K:243:GLU:O	2.43	0.42
2:K:1210:ALA:N	2:K:1211:GLN:OE1	2.50	0.42
2:K:1836:ASN:HA	2:K:1839:LEU:HB2	2.01	0.42
2:K:4635:VAL:O	2:K:4638:THR:OG1	2.33	0.42
2:B:1057:LEU:O	2:B:1062:TYR:N	2.51	0.42
2:B:1305:SER:HA	2:B:1593:HIS:HD2	1.84	0.42
2:B:1310:CYS:HB2	2:B:1536:SER:HA	2.01	0.42
2:B:2759:LYS:HA	2:B:2760:PRO:HD3	1.92	0.42
2:B:4168:GLU:HB2	2:B:4171:ARG:HH12	1.84	0.42
1:D:77:THR:HB	1:D:80:VAL:HG23	2.01	0.42
2:E:32:GLN:O	2:E:53:SER:OG	2.28	0.42
2:E:694:ARG:HG2	2:E:716:ASN:HB3	2.00	0.42
2:E:2834:LEU:HD13	2:E:2838:LEU:HB3	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:243:GLU:HA	2:H:264:GLY:HA2	2.01	0.42
2:H:3605:ARG:HH12	3:I:82:SER:HB3	1.85	0.42
2:H:3612:LEU:HD23	2:H:3617:ALA:HB2	2.01	0.42
2:H:4787:PHE:HD1	2:H:4808:ASP:O	2.02	0.42
2:H:4890:PHE:H	7:H:6003:ATP:N6	2.17	0.42
1:J:11:ASP:OD2	1:J:14:THR:OG1	2.34	0.42
2:K:243:GLU:HA	2:K:264:GLY:HA2	2.01	0.42
2:K:425:LEU:HD21	2:K:452:VAL:HG13	2.01	0.42
2:K:1714:TYR:CD1	2:K:1761:MET:HB3	2.54	0.42
2:K:2252:ASN:HB2	2:K:2310:ASN:HD21	1.84	0.42
2:K:2834:LEU:HD13	2:K:2838:LEU:HB3	2.01	0.42
2:K:4011:VAL:HA	2:K:4014:ILE:HG12	2.00	0.42
2:B:143:LEU:HD13	2:E:2426:SER:O	2.13	0.42
2:B:237:LEU:HB2	2:B:404:ASN:HB3	2.02	0.42
2:B:675:TYR:CE1	2:B:790:PRO:HB3	2.54	0.42
2:B:676:GLU:HG3	2:B:814:LEU:HB3	2.01	0.42
2:B:748:LEU:HB2	2:B:750:ARG:HG3	1.99	0.42
2:B:2731:ASP:HB3	2:B:2826:ALA:HB2	2.01	0.42
2:B:2856:LYS:O	2:B:2860:GLU:HB2	2.18	0.42
2:B:3612:LEU:HD23	2:B:3617:ALA:HB2	2.01	0.42
2:E:2433:LEU:HD22	2:E:2488:LEU:HD22	2.01	0.42
2:E:4178:VAL:HG21	2:E:4885:MET:HE3	2.00	0.42
2:E:4597:PRO:HA	2:E:4600:ILE:HG22	2.01	0.42
1:G:77:THR:HB	1:G:80:VAL:HG23	2.01	0.42
2:H:652:VAL:HG11	2:H:715:GLY:HA2	2.01	0.42
2:H:1092:LYS:H	2:H:1250:TRP:HZ3	1.67	0.42
2:H:2463:PRO:HB3	2:H:2516:ALA:HB2	2.00	0.42
1:J:21:THR:HG1	1:J:49:ARG:HH21	1.59	0.42
2:K:1730:THR:O	2:K:1733:THR:OG1	2.28	0.42
2:K:1734:LYS:HE2	2:K:1931:ASP:HB3	2.00	0.42
2:K:3986:MET:HG2	2:K:3996:ILE:HD11	2.01	0.42
2:B:294:PRO:HD3	2:B:344:LYS:HE3	2.02	0.42
2:B:1228:THR:HA	2:B:1232:LEU:HD12	2.01	0.42
2:B:3605:ARG:HH12	3:C:82:SER:HB3	1.85	0.42
2:E:143:LEU:HD12	2:H:2427:LEU:HD11	2.01	0.42
2:E:294:PRO:HD3	2:E:344:LYS:HE3	2.02	0.42
2:E:652:VAL:HG11	2:E:715:GLY:HA2	2.01	0.42
2:E:1734:LYS:HE2	2:E:1931:ASP:HB3	2.00	0.42
2:E:3987:LEU:HG	2:E:3990:ASN:HD21	1.85	0.42
2:K:294:PRO:HB3	2:K:366:ILE:HD11	1.99	0.42
2:K:675:TYR:CE1	2:K:790:PRO:HB3	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:4897:ASP:OD1	2:K:4897:ASP:N	2.50	0.42
2:B:394:HIS:CD2	2:B:397:GLY:H	2.38	0.42
2:B:745:ASN:HB3	2:B:747:HIS:HB2	2.02	0.42
2:B:2076:ILE:HG21	2:B:2081:LEU:HD22	2.00	0.42
2:B:2433:LEU:HD22	2:B:2488:LEU:HD22	2.01	0.42
2:B:2716:GLU:HA	2:B:2719:GLU:HB2	2.01	0.42
2:B:3986:MET:HG2	2:B:3996:ILE:HD11	2.01	0.42
2:E:439:LYS:HE3	2:E:439:LYS:HB3	1.91	0.42
2:E:618:CYS:SG	2:E:629:GLN:NE2	2.93	0.42
2:E:718:VAL:HA	2:E:736:CYS:H	1.83	0.42
2:E:745:ASN:HB3	2:E:747:HIS:HB2	2.02	0.42
2:E:755:ILE:HA	2:E:770:ILE:HD13	2.02	0.42
2:E:1305:SER:HB2	2:E:1591:LEU:HB2	2.00	0.42
2:H:3880:LEU:HD23	2:H:3944:ALA:HB2	2.00	0.42
2:H:4791:ARG:HD2	2:K:4523:VAL:HG21	2.00	0.42
2:K:618:CYS:SG	2:K:629:GLN:NE2	2.93	0.42
2:K:1092:LYS:H	2:K:1250:TRP:HZ3	1.67	0.42
2:K:3605:ARG:HH12	3:L:82:SER:HB3	1.85	0.42
2:B:1168:MET:HE1	2:B:1201:PHE:HD2	1.85	0.42
2:B:1836:ASN:HA	2:B:1839:LEU:HB2	2.01	0.42
2:B:1986:GLU:N	2:B:1989:CYS:SG	2.73	0.42
2:B:3880:LEU:HD23	2:B:3944:ALA:HB2	2.00	0.42
2:B:4635:VAL:O	2:B:4638:THR:OG1	2.33	0.42
2:E:3921:LEU:HD23	2:E:3921:LEU:HA	1.73	0.42
2:H:268:SER:O	2:H:273:SER:OG	2.31	0.42
2:H:676:GLU:HG3	2:H:814:LEU:HB3	2.01	0.42
2:H:1124:PRO:HG2	2:H:1598:ARG:HG3	2.01	0.42
2:H:2433:LEU:HD22	2:H:2488:LEU:HD22	2.01	0.42
2:H:3987:LEU:HG	2:H:3990:ASN:HD21	1.85	0.42
2:K:228:LEU:HD11	2:K:405:LEU:HD13	2.00	0.42
2:K:1466:THR:HG22	2:K:1482:ARG:HG2	2.01	0.42
2:K:4020:MET:HE3	2:K:4067:LEU:HD11	2.02	0.42
2:B:73:LEU:HB3	2:B:77:ALA:HB3	2.02	0.42
2:B:675:TYR:CZ	2:B:790:PRO:HB3	2.55	0.42
2:B:983:LEU:HD23	2:B:1056:THR:HA	2.02	0.42
2:B:1124:PRO:HG2	2:B:1598:ARG:HG3	2.01	0.42
2:B:2834:LEU:HD13	2:B:2838:LEU:HB3	2.01	0.42
2:E:16:THR:OG1	2:E:111:ARG:O	2.29	0.42
2:E:675:TYR:CE1	2:E:790:PRO:HB3	2.54	0.42
2:E:1676:LEU:O	2:E:1680:VAL:N	2.47	0.42
2:E:2463:PRO:HB3	2:E:2516:ALA:HB2	2.01	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:618:CYS:SG	2:H:629:GLN:NE2	2.93	0.42
2:H:675:TYR:CE1	2:H:790:PRO:HB3	2.54	0.42
2:H:1210:ALA:N	2:H:1211:GLN:OE1	2.51	0.42
2:H:1676:LEU:HD23	2:H:1676:LEU:HA	1.89	0.42
2:K:237:LEU:HB2	2:K:404:ASN:HB3	2.02	0.42
2:K:294:PRO:HD3	2:K:344:LYS:HE3	2.02	0.42
2:K:394:HIS:CD2	2:K:397:GLY:H	2.38	0.42
2:K:676:GLU:HG3	2:K:814:LEU:HB3	2.01	0.42
2:K:745:ASN:HB3	2:K:747:HIS:HB2	2.02	0.42
2:K:755:ILE:HA	2:K:770:ILE:HD13	2.02	0.42
2:K:2076:ILE:HG21	2:K:2081:LEU:HD22	2.01	0.42
2:B:652:VAL:HG11	2:B:715:GLY:HA2	2.01	0.42
2:B:4020:MET:HE3	2:B:4067:LEU:HD11	2.02	0.42
2:B:4597:PRO:HA	2:B:4600:ILE:HG22	2.01	0.42
2:E:3986:MET:HG2	2:E:3996:ILE:HD11	2.01	0.42
2:H:294:PRO:HD3	2:H:344:LYS:HE3	2.02	0.42
2:H:1168:MET:HE1	2:H:1201:PHE:HD2	1.85	0.42
2:H:2398:ASP:OD1	2:H:2402:ARG:NH2	2.50	0.42
1:J:9:PRO:HD2	2:K:748:LEU:HD11	2.01	0.42
2:K:372:LEU:HD23	2:K:403:LEU:HD11	2.02	0.42
2:K:2716:GLU:HA	2:K:2719:GLU:HB2	2.01	0.42
2:B:3777:LYS:HB2	2:B:3777:LYS:HE3	1.87	0.42
2:B:3804:LEU:HB3	2:B:3885:SER:OG	2.20	0.42
2:E:237:LEU:HB2	2:E:404:ASN:HB3	2.02	0.42
2:E:675:TYR:CZ	2:E:790:PRO:HB3	2.55	0.42
2:E:676:GLU:HG3	2:E:814:LEU:HB3	2.01	0.42
2:E:3683:LEU:HD11	2:E:3747:ALA:HB3	2.02	0.42
2:H:675:TYR:CZ	2:H:790:PRO:HB3	2.55	0.42
2:H:940:LEU:HD23	2:H:940:LEU:HA	1.89	0.42
2:H:1714:TYR:CD1	2:H:1761:MET:HB3	2.54	0.42
2:H:4597:PRO:HA	2:H:4600:ILE:HG22	2.01	0.42
2:K:2880:ALA:O	2:K:2884:ALA:N	2.49	0.42
2:K:3925:ILE:HD11	2:K:3936:LEU:HD13	2.02	0.42
1:A:77:THR:HB	1:A:80:VAL:HG23	2.01	0.42
2:B:1846:ILE:HG23	2:B:1894:LEU:HB3	2.02	0.42
2:E:195:SER:OG	2:E:196:TYR:N	2.53	0.42
2:E:881:ILE:O	2:E:885:LEU:HB2	2.20	0.42
2:E:1210:ALA:N	2:E:1211:GLN:OE1	2.51	0.42
2:E:1466:THR:HG22	2:E:1482:ARG:HG2	2.01	0.42
2:E:3605:ARG:HH12	3:F:82:SER:HB3	1.85	0.42
2:H:32:GLN:O	2:H:53:SER:OG	2.28	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:372:LEU:HD23	2:H:403:LEU:HD11	2.02	0.42
2:H:2213:LYS:HA	2:H:2254:LEU:HD21	2.02	0.42
2:H:2716:GLU:HA	2:H:2719:GLU:HB2	2.01	0.42
2:H:3834:ASP:O	2:H:3837:THR:OG1	2.31	0.42
2:K:73:LEU:HB3	2:K:77:ALA:HB3	2.02	0.42
2:K:675:TYR:CZ	2:K:790:PRO:HB3	2.55	0.42
2:K:1118:SER:HB2	2:K:1122:CYS:SG	2.60	0.42
2:K:1168:MET:HE1	2:K:1201:PHE:HD2	1.85	0.42
2:K:3665:LEU:HD11	2:K:3696:MET:HE2	2.01	0.42
1:A:9:PRO:HD2	2:B:748:LEU:HD11	2.01	0.41
2:B:76:ARG:CZ	2:E:3806:LEU:HD21	2.50	0.41
2:B:425:LEU:HD21	2:B:452:VAL:HG13	2.01	0.41
2:B:755:ILE:HA	2:B:770:ILE:HD13	2.02	0.41
2:B:4521:TYR:HD1	2:B:4521:TYR:HA	1.72	0.41
2:E:394:HIS:CD2	2:E:397:GLY:H	2.38	0.41
2:E:4027:LEU:HD22	2:E:4056:HIS:HB3	2.02	0.41
2:H:73:LEU:HB3	2:H:77:ALA:HB3	2.02	0.41
2:H:195:SER:OG	2:H:196:TYR:N	2.53	0.41
2:H:1446:ILE:O	2:H:1540:PHE:N	2.42	0.41
2:H:4011:VAL:HA	2:H:4014:ILE:HG12	2.00	0.41
2:K:195:SER:OG	2:K:196:TYR:N	2.53	0.41
2:K:1683:PRO:HA	2:K:1686:LEU:HD12	2.02	0.41
2:K:1846:ILE:HG23	2:K:1894:LEU:HB3	2.02	0.41
2:K:3804:LEU:HB3	2:K:3885:SER:OG	2.20	0.41
2:K:3987:LEU:HG	2:K:3990:ASN:HD21	1.85	0.41
2:B:2773:ARG:HD3	2:B:2777:LYS:HE3	2.02	0.41
2:H:1683:PRO:HA	2:H:1686:LEU:HD12	2.02	0.41
2:H:3804:LEU:HB3	2:H:3885:SER:OG	2.20	0.41
2:H:3925:ILE:HD11	2:H:3936:LEU:HD13	2.02	0.41
2:H:4780:TYR:OH	2:K:4515:ASN:HB3	2.19	0.41
2:K:2433:LEU:HD22	2:K:2488:LEU:HD22	2.01	0.41
2:B:1683:PRO:HA	2:B:1686:LEU:HD12	2.02	0.41
2:E:983:LEU:HD23	2:E:1056:THR:HA	2.02	0.41
2:E:1168:MET:HE1	2:E:1201:PHE:HD2	1.85	0.41
2:E:1705:LEU:HD23	2:E:1705:LEU:HA	1.90	0.41
2:E:1836:ASN:HA	2:E:1839:LEU:HB2	2.01	0.41
2:E:2213:LYS:HA	2:E:2254:LEU:HD21	2.02	0.41
2:E:2773:ARG:HD3	2:E:2777:LYS:HE3	2.03	0.41
2:E:3683:LEU:HD23	2:E:3683:LEU:HA	1.92	0.41
2:E:3804:LEU:HB3	2:E:3885:SER:OG	2.20	0.41
2:H:394:HIS:CD2	2:H:397:GLY:H	2.38	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:745:ASN:HB3	2:H:747:HIS:HB2	2.02	0.41
2:H:3804:LEU:HD22	2:H:3886:ILE:HD13	2.02	0.41
2:K:1057:LEU:O	2:K:1062:TYR:N	2.51	0.41
2:K:1228:THR:HA	2:K:1232:LEU:HD12	2.01	0.41
2:K:4027:LEU:HD22	2:K:4056:HIS:HB3	2.02	0.41
2:B:195:SER:OG	2:B:196:TYR:N	2.53	0.41
2:B:881:ILE:O	2:B:885:LEU:HB2	2.20	0.41
2:B:1268:ILE:HD11	2:B:1300:MET:HG3	2.01	0.41
2:B:3831:LEU:HD13	2:B:3831:LEU:HA	1.97	0.41
2:E:1739:PHE:HA	2:E:1740:PRO:HD3	1.91	0.41
1:G:9:PRO:HD2	2:H:748:LEU:HD11	2.01	0.41
2:H:16:THR:OG1	2:H:111:ARG:O	2.29	0.41
2:H:1118:SER:HB2	2:H:1122:CYS:SG	2.60	0.41
2:K:750:ARG:N	2:K:753:ASP:OD2	2.46	0.41
2:B:1092:LYS:H	2:B:1250:TRP:HZ3	1.67	0.41
2:B:1466:THR:HG22	2:B:1482:ARG:HG2	2.02	0.41
2:B:1689:ILE:HA	2:B:1703:TYR:CE1	2.56	0.41
2:B:1730:THR:O	2:B:1733:THR:OG1	2.28	0.41
2:E:73:LEU:HB3	2:E:77:ALA:HB3	2.02	0.41
2:E:717:GLY:H	2:E:722:LEU:HB3	1.85	0.41
2:E:4891:ILE:HD11	2:E:4916:LEU:HD13	2.03	0.41
2:H:237:LEU:HB2	2:H:404:ASN:HB3	2.02	0.41
2:H:1510:VAL:HG12	2:H:1511:VAL:HG23	2.03	0.41
2:H:1689:ILE:HA	2:H:1703:TYR:CE1	2.56	0.41
2:H:2349:GLU:HA	2:H:2352:ILE:HD11	2.03	0.41
1:J:77:THR:HB	1:J:80:VAL:HG23	2.01	0.41
2:K:1091:GLU:HB3	2:K:1094:TYR:HD2	1.86	0.41
2:K:1268:ILE:HD11	2:K:1300:MET:HG3	2.02	0.41
2:K:3677:LEU:HD23	2:K:3677:LEU:HA	1.90	0.41
2:K:3973:MET:HE3	2:K:4095:ILE:HD13	2.02	0.41
2:B:1118:SER:HB2	2:B:1122:CYS:SG	2.60	0.41
2:B:3665:LEU:HD11	2:B:3696:MET:HE2	2.01	0.41
2:B:3683:LEU:HD11	2:B:3747:ALA:HB3	2.02	0.41
2:B:4910:THR:HG21	7:B:6003:ATP:C4	2.55	0.41
2:E:1124:PRO:HG2	2:E:1598:ARG:HG3	2.01	0.41
2:E:1640:ASP:OD1	2:E:1640:ASP:N	2.44	0.41
2:E:1683:PRO:HA	2:E:1686:LEU:HD12	2.02	0.41
2:E:1689:ILE:HA	2:E:1703:TYR:CE1	2.56	0.41
2:E:3925:ILE:HD11	2:E:3936:LEU:HD13	2.02	0.41
2:E:4052:ALA:O	2:E:4056:HIS:ND1	2.54	0.41
2:H:432:GLY:HA3	2:H:447:LEU:HG	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:755:ILE:HA	2:H:770:ILE:HD13	2.02	0.41
2:H:2834:LEU:HD13	2:H:2838:LEU:HB3	2.01	0.41
2:K:123:HIS:CD2	2:K:126:SER:H	2.23	0.41
2:K:983:LEU:HD23	2:K:1056:THR:HA	2.02	0.41
2:K:1732:GLU:O	2:K:1735:SER:OG	2.32	0.41
2:K:4597:PRO:HA	2:K:4600:ILE:HG22	2.01	0.41
2:B:1733:THR:HA	2:B:1755:THR:HG21	2.03	0.41
2:B:1757:LEU:HD13	2:B:1757:LEU:HA	1.88	0.41
2:B:3804:LEU:HD22	2:B:3886:ILE:HD13	2.02	0.41
2:B:4891:ILE:HD11	2:B:4916:LEU:HD13	2.03	0.41
2:E:150:GLN:NE2	2:E:158:CYS:SG	2.85	0.41
2:E:1091:GLU:HB3	2:E:1094:TYR:HD2	1.86	0.41
2:K:677:LEU:HD23	2:K:802:PHE:HA	2.03	0.41
2:K:1510:VAL:HG12	2:K:1511:VAL:HG23	2.03	0.41
2:B:372:LEU:HD23	2:B:403:LEU:HD11	2.02	0.41
2:B:1601:ASN:ND2	2:B:1643:GLU:OE2	2.36	0.41
2:B:4848:ASP:CB	2:E:4819:TYR:CE1	2.95	0.41
2:E:1092:LYS:H	2:E:1250:TRP:HZ3	1.66	0.41
2:E:1733:THR:HA	2:E:1755:THR:HG21	2.03	0.41
2:E:4793:PHE:HD1	2:E:4833:GLU:HB2	1.86	0.41
2:H:2416:GLU:HB3	2:H:2419:ARG:HH21	1.85	0.41
2:H:3911:ILE:HD13	2:H:3911:ILE:HA	1.94	0.41
2:K:643:LEU:H	2:K:643:LEU:HG	1.60	0.41
2:K:1124:PRO:HG2	2:K:1598:ARG:HG3	2.01	0.41
2:K:2213:LYS:HA	2:K:2254:LEU:HD21	2.02	0.41
2:K:4052:ALA:O	2:K:4056:HIS:ND1	2.54	0.41
2:K:4910:THR:HG21	7:K:6003:ATP:C4	2.56	0.41
2:B:227:TYR:HE1	2:B:355:LYS:HG2	1.86	0.41
2:B:750:ARG:N	2:B:753:ASP:OD2	2.46	0.41
2:B:2213:LYS:HA	2:B:2254:LEU:HD21	2.02	0.41
2:B:3806:LEU:HD21	2:K:76:ARG:CZ	2.50	0.41
2:B:3925:ILE:HD11	2:B:3936:LEU:HD13	2.02	0.41
2:B:3966:ILE:H	2:B:3966:ILE:HG13	1.70	0.41
2:B:3987:LEU:HG	2:B:3990:ASN:HD21	1.85	0.41
2:B:4806:LYS:O	2:B:4807:CYS:SG	2.73	0.41
2:B:4953:PHE:HA	2:B:4954:PRO:HD3	1.94	0.41
2:E:372:LEU:HD23	2:E:403:LEU:HD11	2.02	0.41
2:E:432:GLY:HA3	2:E:447:LEU:HG	2.03	0.41
2:E:530:LEU:HD23	2:E:530:LEU:HA	1.91	0.41
2:E:1268:ILE:HD11	2:E:1300:MET:HG3	2.01	0.41
2:E:1846:ILE:HG23	2:E:1894:LEU:HB3	2.02	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:3677:LEU:HD23	2:E:3677:LEU:HA	1.91	0.41
2:E:4809:ASP:HB2	2:E:4812:THR:CG2	2.51	0.41
2:H:80:GLU:HG3	2:K:3891:TRP:CZ3	2.51	0.41
2:H:143:LEU:HD12	2:K:2427:LEU:HD11	2.01	0.41
2:H:238:HIS:N	2:H:243:GLU:O	2.43	0.41
2:H:506:HIS:CE1	2:H:564:ARG:HG2	2.56	0.41
2:H:657:PRO:HB3	2:H:834:VAL:HG22	2.03	0.41
2:H:1732:GLU:O	2:H:1735:SER:OG	2.32	0.41
2:H:1733:THR:HA	2:H:1755:THR:HG21	2.03	0.41
2:H:4020:MET:HE3	2:H:4067:LEU:HD11	2.02	0.41
2:H:4027:LEU:HD22	2:H:4056:HIS:HB3	2.02	0.41
2:H:4910:THR:HG21	7:H:6003:ATP:C4	2.55	0.41
2:K:506:HIS:CE1	2:K:564:ARG:HG2	2.56	0.41
2:K:717:GLY:H	2:K:722:LEU:HB3	1.85	0.41
2:K:881:ILE:O	2:K:885:LEU:HB2	2.20	0.41
2:K:1689:ILE:HA	2:K:1703:TYR:CE1	2.56	0.41
2:K:1986:GLU:N	2:K:1989:CYS:SG	2.73	0.41
2:K:2349:GLU:HA	2:K:2352:ILE:HD11	2.03	0.41
2:K:3804:LEU:HD22	2:K:3886:ILE:HD13	2.02	0.41
2:K:4891:ILE:HD11	2:K:4916:LEU:HD13	2.03	0.41
2:B:618:CYS:SG	2:B:629:GLN:NE2	2.93	0.41
2:B:717:GLY:H	2:B:722:LEU:HB3	1.85	0.41
2:B:4027:LEU:HD22	2:B:4056:HIS:HB3	2.02	0.41
2:B:4127:LEU:O	2:B:4131:GLN:N	2.54	0.41
2:E:1118:SER:HB2	2:E:1122:CYS:SG	2.60	0.41
1:G:27:THR:HG23	1:G:100:ASP:HB3	2.03	0.41
2:H:717:GLY:H	2:H:722:LEU:HB3	1.85	0.41
2:H:881:ILE:O	2:H:885:LEU:HB2	2.20	0.41
2:H:1846:ILE:HG23	2:H:1894:LEU:HB3	2.02	0.41
2:K:1057:LEU:HB3	2:K:1062:TYR:HB2	2.03	0.41
2:K:4127:LEU:O	2:K:4131:GLN:N	2.54	0.41
2:B:432:GLY:HA3	2:B:447:LEU:HG	2.03	0.40
2:E:1644:LEU:HD21	2:E:1651:LEU:HA	2.03	0.40
2:E:3804:LEU:HD22	2:E:3886:ILE:HD13	2.02	0.40
2:E:3831:LEU:HD23	2:E:3906:ASN:HD21	1.86	0.40
2:H:227:TYR:HE1	2:H:355:LYS:HG2	1.86	0.40
2:H:983:LEU:HD23	2:H:1056:THR:HA	2.02	0.40
2:H:2201:LEU:HD23	2:H:2201:LEU:HA	1.92	0.40
2:H:2773:ARG:HD3	2:H:2777:LYS:HE3	2.02	0.40
2:H:3683:LEU:HD11	2:H:3747:ALA:HB3	2.02	0.40
2:H:4809:ASP:HB2	2:H:4812:THR:CG2	2.51	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:150:GLN:NE2	2:K:158:CYS:SG	2.85	0.40
2:K:228:LEU:HB3	2:K:289:ILE:HB	2.04	0.40
2:K:432:GLY:HA3	2:K:447:LEU:HG	2.03	0.40
2:K:1177:LEU:N	2:K:1180:GLU:O	2.55	0.40
2:K:1644:LEU:HD21	2:K:1651:LEU:HA	2.04	0.40
2:K:1733:THR:HA	2:K:1755:THR:HG21	2.03	0.40
2:K:2416:GLU:HB3	2:K:2419:ARG:HH21	1.85	0.40
2:K:2759:LYS:HA	2:K:2760:PRO:HD3	1.92	0.40
2:K:3683:LEU:HD11	2:K:3747:ALA:HB3	2.02	0.40
2:K:3777:LYS:HE3	2:K:3777:LYS:HB2	1.87	0.40
2:B:1091:GLU:HB3	2:B:1094:TYR:HD2	1.86	0.40
2:B:1785:ASP:OD1	2:B:1788:LYS:NZ	2.50	0.40
2:B:2398:ASP:OD1	2:B:2402:ARG:NH2	2.50	0.40
2:B:4793:PHE:HD1	2:B:4833:GLU:HB2	1.86	0.40
2:E:145:PHE:HD1	2:E:145:PHE:HA	1.76	0.40
2:E:506:HIS:CE1	2:E:564:ARG:HG2	2.56	0.40
2:E:1057:LEU:HB3	2:E:1062:TYR:HB2	2.03	0.40
2:E:1445:TRP:N	2:E:1487:MET:HB2	2.36	0.40
2:E:3871:ILE:O	2:E:3874:SER:OG	2.26	0.40
2:H:228:LEU:HB3	2:H:289:ILE:HB	2.04	0.40
2:H:608:HIS:HB2	2:H:1656:HIS:CD2	2.57	0.40
2:H:1177:LEU:N	2:H:1180:GLU:O	2.55	0.40
2:H:1268:ILE:HD11	2:H:1300:MET:HG3	2.01	0.40
2:H:4582:VAL:O	2:H:4586:PHE:HB2	2.21	0.40
2:H:4793:PHE:HD1	2:H:4833:GLU:HB2	1.86	0.40
2:K:1445:TRP:N	2:K:1487:MET:HB2	2.36	0.40
2:B:1177:LEU:N	2:B:1180:GLU:O	2.55	0.40
2:B:1510:VAL:HG12	2:B:1511:VAL:HG23	2.03	0.40
2:B:4168:GLU:HG3	2:B:4171:ARG:HH11	1.85	0.40
2:E:1162:VAL:O	2:E:1176:THR:OG1	2.33	0.40
2:E:2247:SER:O	2:E:2247:SER:OG	2.37	0.40
2:H:236:LEU:HD12	2:H:236:LEU:HA	1.92	0.40
2:H:1445:TRP:N	2:H:1487:MET:HB2	2.36	0.40
2:H:1644:LEU:HD21	2:H:1651:LEU:HA	2.04	0.40
2:H:4052:ALA:O	2:H:4056:HIS:ND1	2.54	0.40
2:H:4891:ILE:HD11	2:H:4916:LEU:HD13	2.03	0.40
1:J:27:THR:HG23	1:J:100:ASP:HB3	2.03	0.40
2:K:1446:ILE:O	2:K:1540:PHE:N	2.42	0.40
2:K:2168:MET:H	2:K:2168:MET:HG3	1.74	0.40
2:K:2773:ARG:HD3	2:K:2777:LYS:HE3	2.02	0.40
2:B:163:HIS:HA	2:B:164:PRO:HD3	1.93	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:227:TYR:CE1	2:B:355:LYS:HG2	2.57	0.40
2:B:1014:GLN:HA	2:B:1029:ASN:HB2	2.03	0.40
2:B:2103:LEU:HD23	2:B:2103:LEU:HA	1.92	0.40
2:B:4052:ALA:O	2:B:4056:HIS:ND1	2.54	0.40
2:E:643:LEU:H	2:E:643:LEU:HG	1.60	0.40
2:E:1014:GLN:HA	2:E:1029:ASN:HB2	2.03	0.40
2:E:3973:MET:HE3	2:E:4095:ILE:HD13	2.03	0.40
2:E:4780:TYR:OH	2:H:4515:ASN:HB3	2.22	0.40
2:E:4910:THR:HG21	7:E:6003:ATP:C4	2.55	0.40
2:E:4945:TYR:OH	6:E:6002:CFF:H81	2.22	0.40
1:G:11:ASP:OD2	1:G:14:THR:OG1	2.34	0.40
2:H:76:ARG:CZ	2:K:3806:LEU:HD21	2.51	0.40
2:H:123:HIS:CD2	2:H:126:SER:H	2.23	0.40
2:H:227:TYR:CE1	2:H:355:LYS:HG2	2.57	0.40
2:B:228:LEU:HB3	2:B:289:ILE:HB	2.04	0.40
2:B:657:PRO:HB3	2:B:834:VAL:HG22	2.03	0.40
2:B:1809:PRO:O	2:B:1812:GLY:N	2.55	0.40
2:B:1993:ILE:HG23	3:C:112:ASN:HA	2.03	0.40
2:B:4945:TYR:OH	6:B:6002:CFF:H81	2.22	0.40
2:E:228:LEU:HB3	2:E:289:ILE:HB	2.04	0.40
2:E:608:HIS:HB2	2:E:1656:HIS:CD2	2.57	0.40
2:E:2088:LEU:HD23	2:E:2088:LEU:HA	1.89	0.40
2:E:2349:GLU:HA	2:E:2352:ILE:HD11	2.03	0.40
2:E:4668:SER:O	2:E:4672:GLY:N	2.54	0.40
2:H:1446:ILE:HB	2:H:1540:PHE:HB2	2.04	0.40
2:H:1993:ILE:HG23	3:I:112:ASN:HA	2.03	0.40
2:H:3804:LEU:HD13	2:H:3910:ALA:HB2	2.04	0.40
2:H:3831:LEU:HD23	2:H:3906:ASN:HD21	1.86	0.40
2:H:3973:MET:HE3	2:H:4095:ILE:HD13	2.03	0.40
2:H:4923:LEU:HD12	2:H:4923:LEU:HA	1.93	0.40
2:K:32:GLN:O	2:K:53:SER:OG	2.28	0.40
2:K:64:ILE:H	2:K:64:ILE:HG13	1.74	0.40
2:K:439:LYS:HE3	2:K:439:LYS:HB3	1.91	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	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	D	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	G	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
1	J	105/108 (97%)	94 (90%)	11 (10%)	0	100	100
2	B	3386/4968 (68%)	2990 (88%)	383 (11%)	13 (0%)	30	66
2	E	3386/4968 (68%)	2986 (88%)	387 (11%)	13 (0%)	30	66
2	H	3386/4968 (68%)	2989 (88%)	384 (11%)	13 (0%)	30	66
2	K	3386/4968 (68%)	2989 (88%)	384 (11%)	13 (0%)	30	66
3	C	132/149 (89%)	119 (90%)	12 (9%)	1 (1%)	16	52
3	F	132/149 (89%)	119 (90%)	12 (9%)	1 (1%)	16	52
3	I	132/149 (89%)	119 (90%)	12 (9%)	1 (1%)	16	52
3	L	132/149 (89%)	119 (90%)	12 (9%)	1 (1%)	16	52
All	All	14492/20900 (69%)	12806 (88%)	1630 (11%)	56 (0%)	31	66

All (56) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	1477	HIS
2	E	1477	HIS
2	H	1477	HIS
2	K	1477	HIS
2	B	1580	PRO
2	B	4916	LEU
3	C	130	ASP
2	E	1580	PRO
2	E	4916	LEU
3	F	130	ASP
2	H	1580	PRO
2	H	4916	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	I	130	ASP
2	K	1580	PRO
2	K	4916	LEU
3	L	130	ASP
2	B	730	LEU
2	B	1581	GLN
2	B	4071	ALA
2	E	730	LEU
2	E	1581	GLN
2	E	4071	ALA
2	H	730	LEU
2	H	1581	GLN
2	H	4071	ALA
2	K	730	LEU
2	K	1581	GLN
2	K	4071	ALA
2	B	3802	SER
2	E	3802	SER
2	H	3802	SER
2	K	3802	SER
2	B	853	PRO
2	E	853	PRO
2	H	853	PRO
2	K	853	PRO
2	B	3801	CYS
2	B	4164	PRO
2	E	3801	CYS
2	E	4164	PRO
2	H	3801	CYS
2	H	4164	PRO
2	K	3801	CYS
2	K	4164	PRO
2	B	1535	PRO
2	E	1535	PRO
2	H	1535	PRO
2	K	1535	PRO
2	B	828	PRO
2	B	1848	PRO
2	E	828	PRO
2	E	1848	PRO
2	H	828	PRO
2	H	1848	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	K	828	PRO
2	K	1848	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all 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	88/89 (99%)	88 (100%)	0	100	100
1	D	88/89 (99%)	88 (100%)	0	100	100
1	G	88/89 (99%)	88 (100%)	0	100	100
1	J	88/89 (99%)	88 (100%)	0	100	100
2	B	2698/4355 (62%)	2680 (99%)	18 (1%)	76	78
2	E	2698/4355 (62%)	2680 (99%)	18 (1%)	76	78
2	H	2699/4355 (62%)	2680 (99%)	19 (1%)	76	78
2	K	2699/4355 (62%)	2680 (99%)	19 (1%)	76	78
3	C	115/123 (94%)	115 (100%)	0	100	100
3	F	115/123 (94%)	115 (100%)	0	100	100
3	I	115/123 (94%)	115 (100%)	0	100	100
3	L	115/123 (94%)	115 (100%)	0	100	100
All	All	11606/18268 (64%)	11532 (99%)	74 (1%)	76	80

All (74) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	B	113	LEU
2	B	541	ILE
2	B	625	VAL
2	B	643	LEU
2	B	832	LEU
2	B	881	ILE
2	B	925	PRO
2	B	990	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	1042	THR
2	B	1054	VAL
2	B	1089	ARG
2	B	1552	VAL
2	B	2420	ILE
2	B	3726	LEU
2	B	4136	ARG
2	B	4521	TYR
2	B	4652	ARG
2	B	4702	ILE
2	E	113	LEU
2	E	541	ILE
2	E	625	VAL
2	E	643	LEU
2	E	832	LEU
2	E	881	ILE
2	E	925	PRO
2	E	990	PRO
2	E	1042	THR
2	E	1054	VAL
2	E	1089	ARG
2	E	1552	VAL
2	E	2420	ILE
2	E	3726	LEU
2	E	4136	ARG
2	E	4521	TYR
2	E	4652	ARG
2	E	4702	ILE
2	H	113	LEU
2	H	541	ILE
2	H	625	VAL
2	H	643	LEU
2	H	832	LEU
2	H	881	ILE
2	H	925	PRO
2	H	950	VAL
2	H	990	PRO
2	H	1042	THR
2	H	1054	VAL
2	H	1089	ARG
2	H	1552	VAL
2	H	2420	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	3726	LEU
2	H	4136	ARG
2	H	4521	TYR
2	H	4652	ARG
2	H	4702	ILE
2	K	113	LEU
2	K	541	ILE
2	K	625	VAL
2	K	643	LEU
2	K	832	LEU
2	K	881	ILE
2	K	925	PRO
2	K	950	VAL
2	K	990	PRO
2	K	1042	THR
2	K	1054	VAL
2	K	1089	ARG
2	K	1552	VAL
2	K	2420	ILE
2	K	3726	LEU
2	K	4136	ARG
2	K	4521	TYR
2	K	4652	ARG
2	K	4702	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (260) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
2	B	32	GLN
2	B	44	ASN
2	B	57	ASN
2	B	123	HIS
2	B	193	HIS
2	B	261	HIS
2	B	293	GLN
2	B	375	GLN
2	B	394	HIS
2	B	464	HIS
2	B	476	GLN
2	B	487	ASN
2	B	531	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	544	ASN
2	B	593	HIS
2	B	607	ASN
2	B	621	HIS
2	B	776	GLN
2	B	1146	HIS
2	B	1147	GLN
2	B	1242	ASN
2	B	1265	HIS
2	B	1587	HIS
2	B	1602	GLN
2	B	1626	GLN
2	B	1656	HIS
2	B	1669	ASN
2	B	1670	HIS
2	B	1722	ASN
2	B	1746	HIS
2	B	1940	ASN
2	B	1996	GLN
2	B	2060	GLN
2	B	2090	HIS
2	B	2211	ASN
2	B	2212	GLN
2	B	2218	HIS
2	B	2251	ASN
2	B	2252	ASN
2	B	2310	ASN
2	B	2711	ASN
2	B	2820	HIS
2	B	2848	ASN
2	B	3615	HIS
2	B	3666	HIS
2	B	3902	GLN
2	B	3904	GLN
2	B	3916	GLN
2	B	3954	HIS
2	B	3965	GLN
2	B	3976	GLN
2	B	3990	ASN
2	B	3993	ASN
2	B	4089	HIS
2	B	4128	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	4160	GLN
2	B	4172	GLN
2	B	4206	GLN
2	B	4494	ASN
2	B	4499	ASN
2	B	4515	ASN
2	B	4621	GLN
2	B	4918	ASN
3	C	136	GLN
1	D	31	GLN
2	E	32	GLN
2	E	44	ASN
2	E	57	ASN
2	E	123	HIS
2	E	150	GLN
2	E	193	HIS
2	E	261	HIS
2	E	375	GLN
2	E	394	HIS
2	E	476	GLN
2	E	487	ASN
2	E	531	ASN
2	E	544	ASN
2	E	593	HIS
2	E	607	ASN
2	E	621	HIS
2	E	776	GLN
2	E	914	GLN
2	E	1146	HIS
2	E	1147	GLN
2	E	1242	ASN
2	E	1265	HIS
2	E	1587	HIS
2	E	1602	GLN
2	E	1626	GLN
2	E	1656	HIS
2	E	1669	ASN
2	E	1670	HIS
2	E	1722	ASN
2	E	1746	HIS
2	E	1940	ASN
2	E	1996	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	E	2060	GLN
2	E	2090	HIS
2	E	2211	ASN
2	E	2212	GLN
2	E	2218	HIS
2	E	2251	ASN
2	E	2252	ASN
2	E	2711	ASN
2	E	2820	HIS
2	E	2848	ASN
2	E	3615	HIS
2	E	3666	HIS
2	E	3902	GLN
2	E	3904	GLN
2	E	3916	GLN
2	E	3954	HIS
2	E	3965	GLN
2	E	3976	GLN
2	E	3990	ASN
2	E	3993	ASN
2	E	4089	HIS
2	E	4128	ASN
2	E	4172	GLN
2	E	4206	GLN
2	E	4494	ASN
2	E	4499	ASN
2	E	4515	ASN
2	E	4621	GLN
2	E	4788	ASN
2	E	4918	ASN
3	F	54	ASN
3	F	136	GLN
1	G	31	GLN
2	H	32	GLN
2	H	44	ASN
2	H	57	ASN
2	H	123	HIS
2	H	150	GLN
2	H	193	HIS
2	H	261	HIS
2	H	375	GLN
2	H	394	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	395	HIS
2	H	464	HIS
2	H	476	GLN
2	H	487	ASN
2	H	531	ASN
2	H	544	ASN
2	H	593	HIS
2	H	607	ASN
2	H	621	HIS
2	H	1146	HIS
2	H	1147	GLN
2	H	1242	ASN
2	H	1265	HIS
2	H	1587	HIS
2	H	1602	GLN
2	H	1626	GLN
2	H	1656	HIS
2	H	1669	ASN
2	H	1670	HIS
2	H	1722	ASN
2	H	1746	HIS
2	H	1836	ASN
2	H	1996	GLN
2	H	2060	GLN
2	H	2090	HIS
2	H	2211	ASN
2	H	2212	GLN
2	H	2218	HIS
2	H	2251	ASN
2	H	2252	ASN
2	H	2310	ASN
2	H	2711	ASN
2	H	2820	HIS
2	H	2848	ASN
2	H	3615	HIS
2	H	3666	HIS
2	H	3851	HIS
2	H	3902	GLN
2	H	3904	GLN
2	H	3916	GLN
2	H	3954	HIS
2	H	3965	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	H	3976	GLN
2	H	3990	ASN
2	H	3993	ASN
2	H	4089	HIS
2	H	4128	ASN
2	H	4172	GLN
2	H	4206	GLN
2	H	4494	ASN
2	H	4499	ASN
2	H	4515	ASN
2	H	4621	GLN
2	H	4918	ASN
3	I	136	GLN
1	J	31	GLN
2	K	32	GLN
2	K	44	ASN
2	K	57	ASN
2	K	123	HIS
2	K	150	GLN
2	K	193	HIS
2	K	261	HIS
2	K	293	GLN
2	K	375	GLN
2	K	394	HIS
2	K	476	GLN
2	K	487	ASN
2	K	531	ASN
2	K	544	ASN
2	K	593	HIS
2	K	607	ASN
2	K	621	HIS
2	K	776	GLN
2	K	915	HIS
2	K	1146	HIS
2	K	1147	GLN
2	K	1242	ASN
2	K	1265	HIS
2	K	1587	HIS
2	K	1602	GLN
2	K	1626	GLN
2	K	1656	HIS
2	K	1669	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	K	1670	HIS
2	K	1722	ASN
2	K	1746	HIS
2	K	1836	ASN
2	K	1996	GLN
2	K	2060	GLN
2	K	2090	HIS
2	K	2211	ASN
2	K	2212	GLN
2	K	2218	HIS
2	K	2251	ASN
2	K	2252	ASN
2	K	2711	ASN
2	K	2820	HIS
2	K	2848	ASN
2	K	3615	HIS
2	K	3666	HIS
2	K	3902	GLN
2	K	3904	GLN
2	K	3916	GLN
2	K	3954	HIS
2	K	3965	GLN
2	K	3976	GLN
2	K	3990	ASN
2	K	3993	ASN
2	K	4089	HIS
2	K	4128	ASN
2	K	4160	GLN
2	K	4172	GLN
2	K	4206	GLN
2	K	4494	ASN
2	K	4499	ASN
2	K	4515	ASN
2	K	4621	GLN
2	K	4918	ASN
3	L	136	GLN

5.3.3 RNA ⓘ

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 16 ligands modelled in this entry, 8 are monoatomic - leaving 8 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$
6	CFF	H	6002	-	15,15,15	2.11	8 (53%)	23,23,23	2.79	9 (39%)
6	CFF	B	6002	-	15,15,15	2.11	8 (53%)	23,23,23	2.78	9 (39%)
7	ATP	K	6003	-	32,33,33	1.34	6 (18%)	48,52,52	1.77	9 (18%)
6	CFF	K	6002	-	15,15,15	2.11	8 (53%)	23,23,23	2.78	9 (39%)
7	ATP	E	6003	-	32,33,33	1.34	6 (18%)	48,52,52	1.77	9 (18%)
7	ATP	B	6003	-	32,33,33	1.34	6 (18%)	48,52,52	1.77	9 (18%)
6	CFF	E	6002	-	15,15,15	2.11	8 (53%)	23,23,23	2.78	9 (39%)
7	ATP	H	6003	-	32,33,33	1.33	6 (18%)	48,52,52	1.77	9 (18%)

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
6	CFF	H	6002	-	-	-	0/2/2/2
6	CFF	B	6002	-	-	-	0/2/2/2
7	ATP	K	6003	-	-	8/22/38/38	0/3/3/3
6	CFF	K	6002	-	-	-	0/2/2/2
7	ATP	E	6003	-	-	8/22/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
7	ATP	B	6003	-	-	8/22/38/38	0/3/3/3
6	CFF	E	6002	-	-	-	0/2/2/2
7	ATP	H	6003	-	-	8/22/38/38	0/3/3/3

All (56) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	E	6002	CFF	C6-N1	-4.38	1.31	1.40
6	B	6002	CFF	C6-N1	-4.37	1.31	1.40
6	H	6002	CFF	C6-N1	-4.37	1.31	1.40
6	K	6002	CFF	C6-N1	-4.37	1.31	1.40
7	B	6003	ATP	C5-C4	4.03	1.46	1.39
7	E	6003	ATP	C5-C4	4.03	1.46	1.39
7	H	6003	ATP	C5-C4	4.03	1.46	1.39
7	K	6003	ATP	C5-C4	4.03	1.46	1.39
6	B	6002	CFF	C4-N3	-2.90	1.33	1.38
6	E	6002	CFF	C4-N3	-2.90	1.33	1.38
6	H	6002	CFF	C4-N3	-2.90	1.33	1.38
6	K	6002	CFF	C4-N3	-2.90	1.33	1.38
7	B	6003	ATP	C5-N7	-2.80	1.34	1.39
7	E	6003	ATP	C5-N7	-2.76	1.34	1.39
7	K	6003	ATP	C5-N7	-2.74	1.34	1.39
7	H	6003	ATP	C5-N7	-2.73	1.34	1.39
6	B	6002	CFF	C5-N7	-2.70	1.33	1.38
6	E	6002	CFF	C5-N7	-2.70	1.33	1.38
6	H	6002	CFF	C5-N7	-2.70	1.33	1.38
6	K	6002	CFF	C5-N7	-2.70	1.33	1.38
7	E	6003	ATP	C4-N9	-2.36	1.32	1.37
7	K	6003	ATP	C4-N9	-2.36	1.32	1.37
7	B	6003	ATP	C4-N9	-2.35	1.32	1.37
7	H	6003	ATP	C4-N9	-2.35	1.32	1.37
6	K	6002	CFF	O11-C2	-2.31	1.18	1.22
6	B	6002	CFF	O11-C2	-2.30	1.18	1.22
6	E	6002	CFF	O11-C2	-2.30	1.18	1.22
6	H	6002	CFF	O11-C2	-2.30	1.18	1.22
6	E	6002	CFF	C2-N3	-2.29	1.34	1.39
6	E	6002	CFF	C2-N1	-2.27	1.34	1.39
6	B	6002	CFF	C2-N1	-2.26	1.34	1.39
6	H	6002	CFF	C2-N1	-2.26	1.34	1.39
6	H	6002	CFF	C2-N3	-2.25	1.34	1.39
6	K	6002	CFF	C2-N3	-2.25	1.34	1.39
6	K	6002	CFF	C2-N1	-2.24	1.34	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	6002	CFF	C2-N3	-2.22	1.34	1.39
7	B	6003	ATP	C8-N7	2.15	1.35	1.31
7	H	6003	ATP	C8-N7	2.15	1.35	1.31
6	K	6002	CFF	C5-C6	-2.14	1.37	1.43
7	E	6003	ATP	C8-N7	2.12	1.35	1.31
7	K	6003	ATP	C8-N7	2.12	1.35	1.31
6	B	6002	CFF	O13-C6	-2.12	1.18	1.23
6	E	6002	CFF	O13-C6	-2.12	1.18	1.23
6	H	6002	CFF	O13-C6	-2.12	1.18	1.23
6	K	6002	CFF	O13-C6	-2.12	1.18	1.23
6	B	6002	CFF	C5-C6	-2.12	1.37	1.43
6	H	6002	CFF	C5-C6	-2.12	1.37	1.43
6	E	6002	CFF	C5-C6	-2.10	1.37	1.43
7	K	6003	ATP	PB-O3B	2.05	1.61	1.59
7	B	6003	ATP	C5-C6	2.04	1.46	1.41
7	E	6003	ATP	C5-C6	2.04	1.46	1.41
7	H	6003	ATP	C5-C6	2.04	1.46	1.41
7	K	6003	ATP	C5-C6	2.04	1.46	1.41
7	B	6003	ATP	PB-O3B	2.03	1.61	1.59
7	E	6003	ATP	PB-O3B	2.03	1.61	1.59
7	H	6003	ATP	PB-O3B	2.03	1.61	1.59

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	6002	CFF	C14-N7-C8	-7.63	112.01	126.28
6	H	6002	CFF	C14-N7-C8	-7.63	112.01	126.28
6	E	6002	CFF	C14-N7-C8	-7.61	112.04	126.28
6	K	6002	CFF	C14-N7-C8	-7.61	112.04	126.28
7	B	6003	ATP	C5-C4-N3	-5.49	119.16	126.72
7	E	6003	ATP	C5-C4-N3	-5.49	119.16	126.72
7	H	6003	ATP	C5-C4-N3	-5.49	119.16	126.72
7	K	6003	ATP	C5-C4-N3	-5.48	119.17	126.72
6	B	6002	CFF	C14-N7-C5	4.96	139.57	127.77
6	E	6002	CFF	C14-N7-C5	4.96	139.57	127.77
6	H	6002	CFF	C14-N7-C5	4.96	139.57	127.77
6	K	6002	CFF	C14-N7-C5	4.96	139.57	127.77
7	H	6003	ATP	N3-C4-N9	4.72	135.20	127.17
7	E	6003	ATP	N3-C4-N9	4.72	135.19	127.17
7	K	6003	ATP	N3-C4-N9	4.71	135.18	127.17
7	B	6003	ATP	N3-C4-N9	4.70	135.17	127.17
6	B	6002	CFF	C5-C6-N1	4.31	119.96	112.06

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	6002	CFF	C5-C6-N1	4.31	119.96	112.06
6	E	6002	CFF	C5-C6-N1	4.31	119.95	112.06
6	K	6002	CFF	C5-C6-N1	4.30	119.93	112.06
7	B	6003	ATP	C2-N3-C4	3.68	120.81	111.83
7	E	6003	ATP	C2-N3-C4	3.68	120.81	111.83
7	H	6003	ATP	C2-N3-C4	3.67	120.80	111.83
7	K	6003	ATP	C2-N3-C4	3.66	120.77	111.83
6	B	6002	CFF	C6-N1-C2	-3.64	119.74	125.66
6	H	6002	CFF	C6-N1-C2	-3.64	119.74	125.66
6	E	6002	CFF	C6-N1-C2	-3.64	119.74	125.66
6	K	6002	CFF	C6-N1-C2	-3.62	119.78	125.66
7	B	6003	ATP	N3-C2-N1	-3.44	123.38	128.58
7	H	6003	ATP	N3-C2-N1	-3.43	123.39	128.58
7	E	6003	ATP	N3-C2-N1	-3.43	123.39	128.58
7	K	6003	ATP	N3-C2-N1	-3.42	123.40	128.58
6	H	6002	CFF	N3-C4-N9	3.36	131.54	126.27
6	B	6002	CFF	N3-C4-N9	3.34	131.53	126.27
6	E	6002	CFF	N3-C4-N9	3.34	131.53	126.27
6	K	6002	CFF	N3-C4-N9	3.34	131.53	126.27
7	H	6003	ATP	C4-N9-C8	3.15	109.04	105.74
7	E	6003	ATP	C4-N9-C8	3.14	109.04	105.74
7	K	6003	ATP	C4-N9-C8	3.14	109.04	105.74
6	B	6002	CFF	N7-C8-N9	-3.10	107.87	113.48
6	H	6002	CFF	N7-C8-N9	-3.10	107.87	113.48
6	E	6002	CFF	N7-C8-N9	-3.08	107.90	113.48
6	K	6002	CFF	N7-C8-N9	-3.08	107.90	113.48
7	B	6003	ATP	C4-N9-C8	3.08	108.97	105.74
6	E	6002	CFF	N3-C2-N1	2.66	120.46	117.14
6	H	6002	CFF	N3-C2-N1	2.64	120.43	117.14
6	B	6002	CFF	N3-C2-N1	2.62	120.41	117.14
6	K	6002	CFF	N3-C2-N1	2.61	120.40	117.14
7	K	6003	ATP	C4-C5-N7	-2.60	107.61	110.58
6	E	6002	CFF	O13-C6-C5	-2.60	121.06	126.38
7	E	6003	ATP	C4-C5-N7	-2.59	107.62	110.58
6	B	6002	CFF	O13-C6-C5	-2.59	121.08	126.38
6	H	6002	CFF	O13-C6-C5	-2.59	121.08	126.38
6	K	6002	CFF	O13-C6-C5	-2.57	121.11	126.38
7	B	6003	ATP	C4-C5-N7	-2.57	107.65	110.58
7	H	6003	ATP	C4-C5-N7	-2.57	107.65	110.58
6	E	6002	CFF	C6-C5-C4	-2.36	119.94	122.92
6	H	6002	CFF	C6-C5-C4	-2.34	119.97	122.92
7	B	6003	ATP	C3'-C2'-C1'	2.32	105.85	101.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	K	6003	ATP	C3'-C2'-C1'	2.32	105.85	101.46
6	K	6002	CFF	C6-C5-C4	-2.32	120.00	122.92
6	B	6002	CFF	C6-C5-C4	-2.32	120.00	122.92
7	H	6003	ATP	C3'-C2'-C1'	2.32	105.84	101.46
7	E	6003	ATP	C3'-C2'-C1'	2.30	105.82	101.46
7	E	6003	ATP	N9-C8-N7	-2.12	110.92	113.94
7	K	6003	ATP	N9-C8-N7	-2.12	110.92	113.94
7	H	6003	ATP	N9-C8-N7	-2.11	110.94	113.94
7	K	6003	ATP	C5-N7-C8	2.11	106.76	103.45
7	E	6003	ATP	C5-N7-C8	2.11	106.76	103.45
7	B	6003	ATP	N9-C8-N7	-2.08	110.98	113.94
7	B	6003	ATP	C5-N7-C8	2.08	106.72	103.45
7	H	6003	ATP	C5-N7-C8	2.08	106.72	103.45

There are no chirality outliers.

All (32) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	6003	ATP	PB-O3B-PG-O2G
7	B	6003	ATP	PB-O3B-PG-O3G
7	B	6003	ATP	C5'-O5'-PA-O1A
7	B	6003	ATP	C5'-O5'-PA-O2A
7	B	6003	ATP	C5'-O5'-PA-O3A
7	E	6003	ATP	PB-O3B-PG-O2G
7	E	6003	ATP	PB-O3B-PG-O3G
7	E	6003	ATP	C5'-O5'-PA-O1A
7	E	6003	ATP	C5'-O5'-PA-O2A
7	E	6003	ATP	C5'-O5'-PA-O3A
7	H	6003	ATP	PB-O3B-PG-O2G
7	H	6003	ATP	PB-O3B-PG-O3G
7	H	6003	ATP	C5'-O5'-PA-O1A
7	H	6003	ATP	C5'-O5'-PA-O2A
7	H	6003	ATP	C5'-O5'-PA-O3A
7	K	6003	ATP	PB-O3B-PG-O2G
7	K	6003	ATP	PB-O3B-PG-O3G
7	K	6003	ATP	C5'-O5'-PA-O1A
7	K	6003	ATP	C5'-O5'-PA-O2A
7	K	6003	ATP	C5'-O5'-PA-O3A
7	B	6003	ATP	PB-O3A-PA-O1A
7	E	6003	ATP	PB-O3A-PA-O1A
7	H	6003	ATP	PB-O3A-PA-O1A
7	K	6003	ATP	PB-O3A-PA-O1A

Continued on next page...

Continued from previous page...

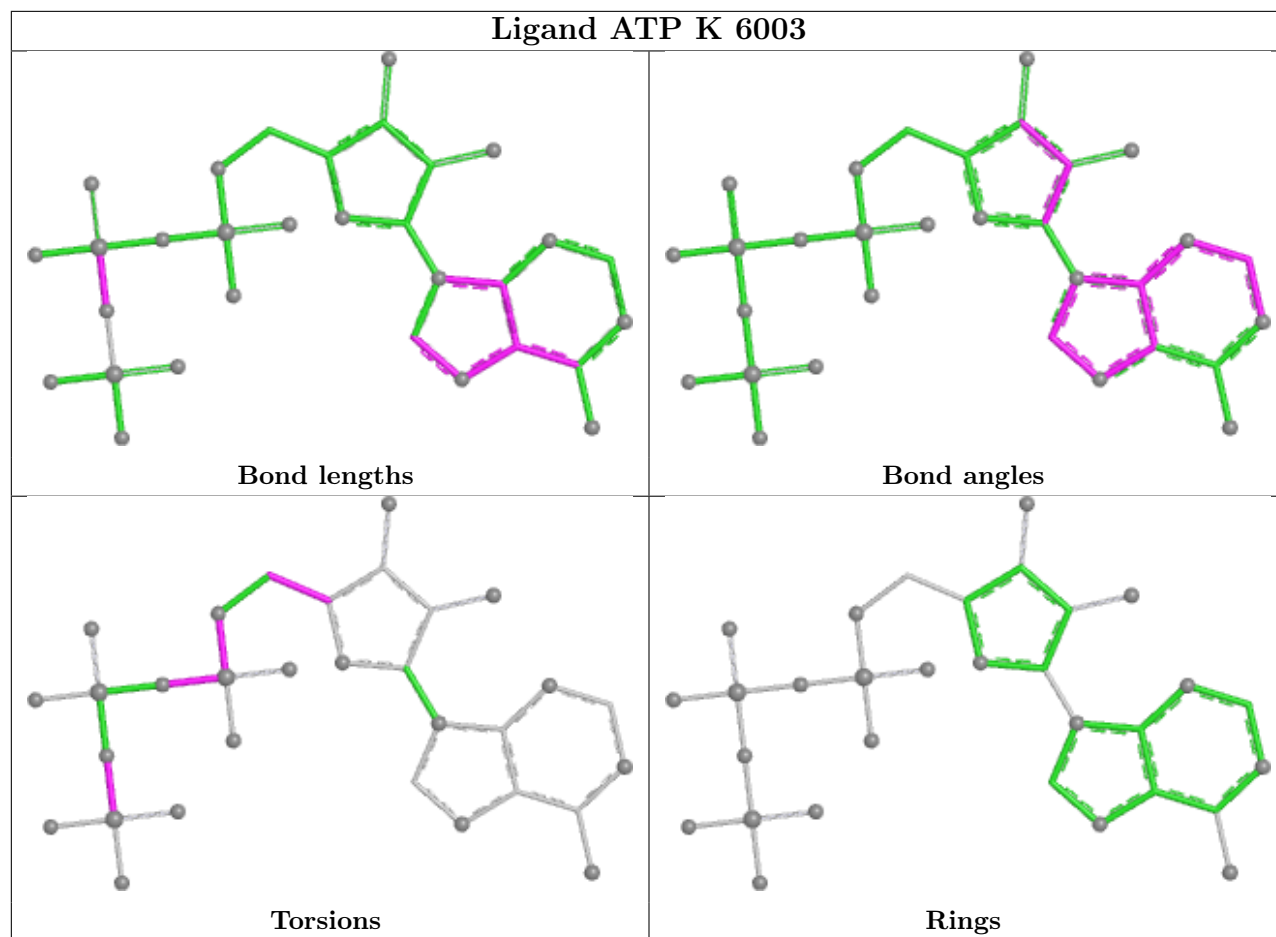
Mol	Chain	Res	Type	Atoms
7	B	6003	ATP	O4'-C4'-C5'-O5'
7	E	6003	ATP	O4'-C4'-C5'-O5'
7	H	6003	ATP	O4'-C4'-C5'-O5'
7	K	6003	ATP	O4'-C4'-C5'-O5'
7	B	6003	ATP	PB-O3A-PA-O2A
7	E	6003	ATP	PB-O3A-PA-O2A
7	H	6003	ATP	PB-O3A-PA-O2A
7	K	6003	ATP	PB-O3A-PA-O2A

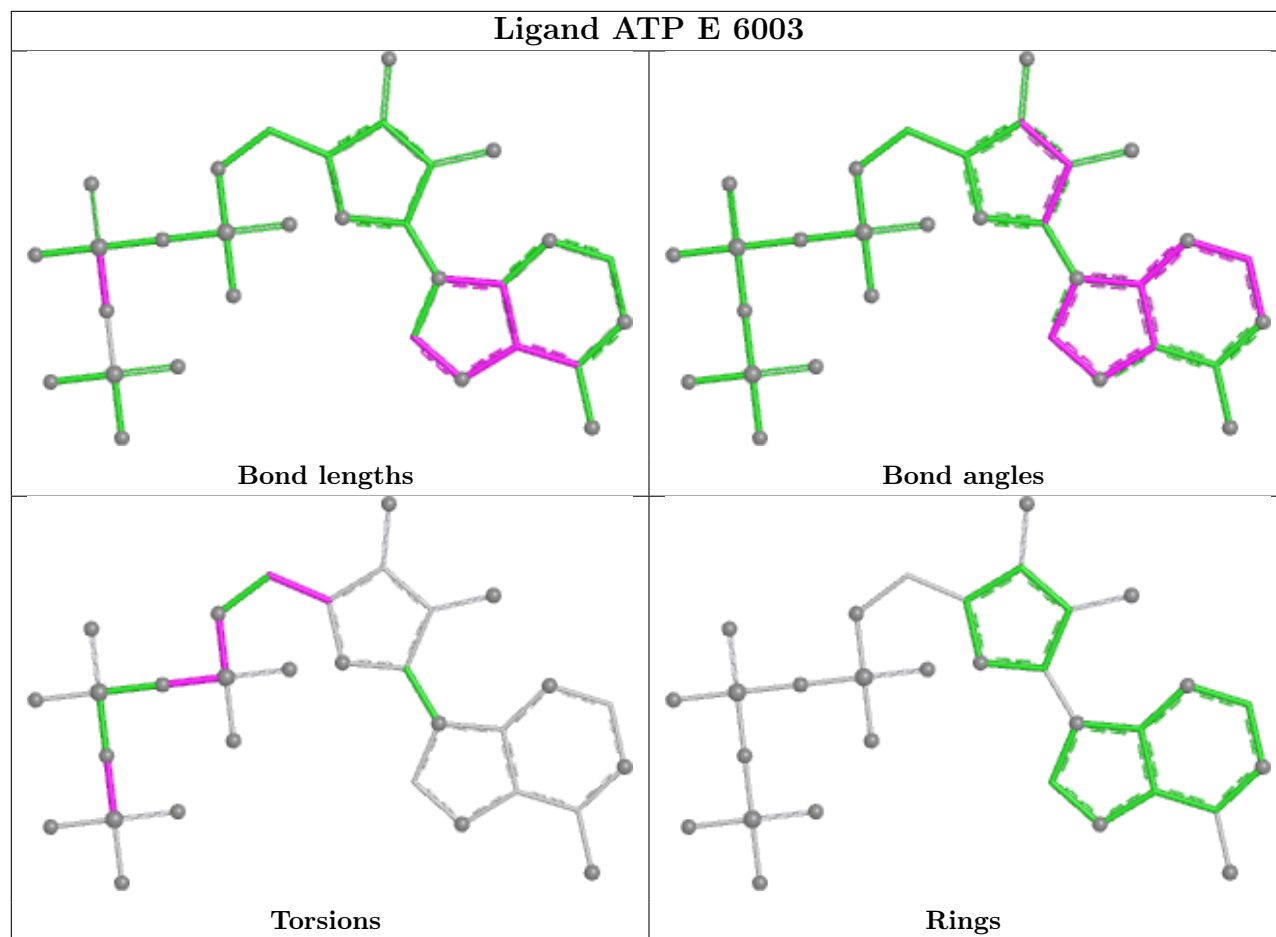
There are no ring outliers.

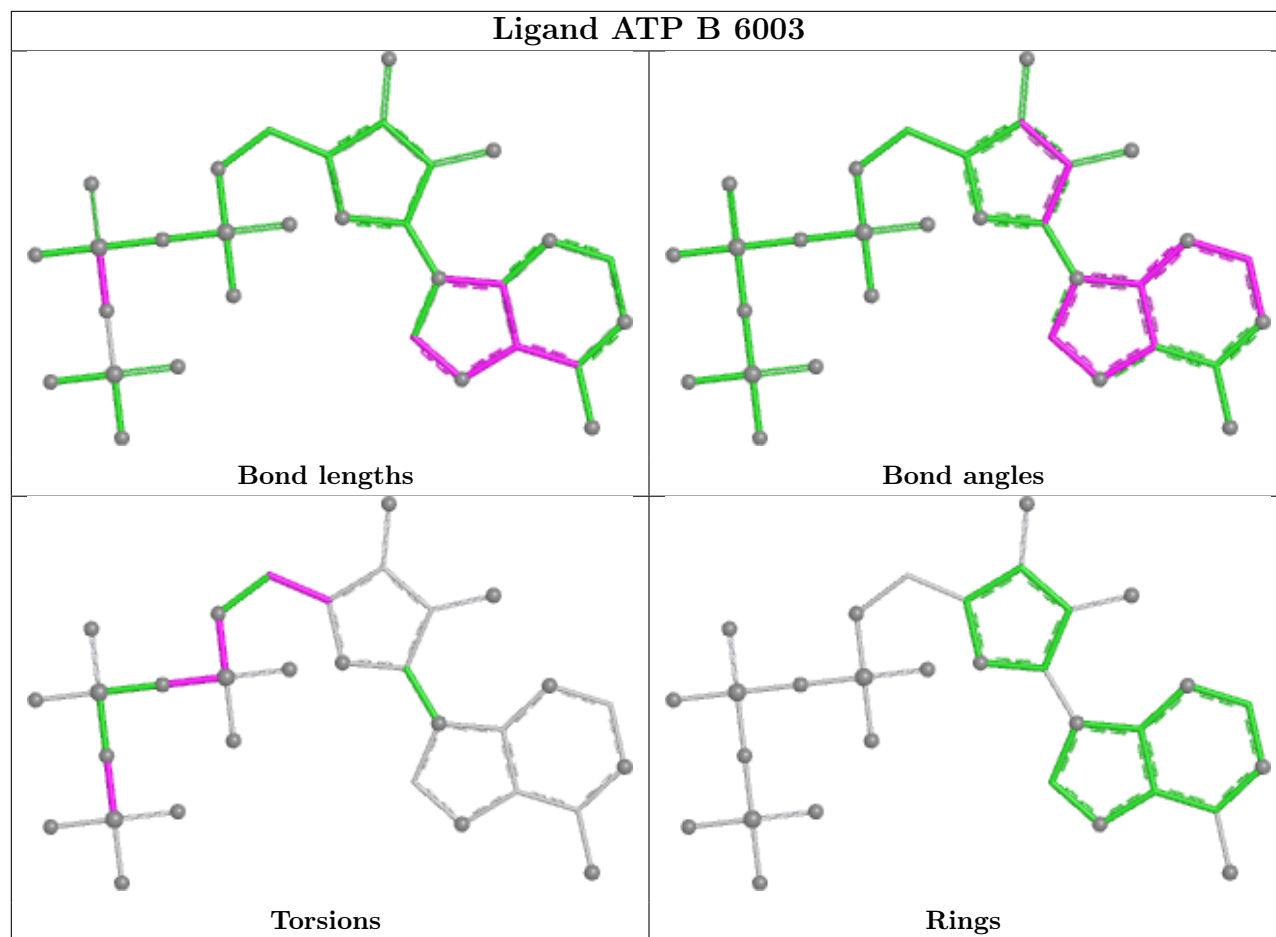
6 monomers are involved in 19 short contacts:

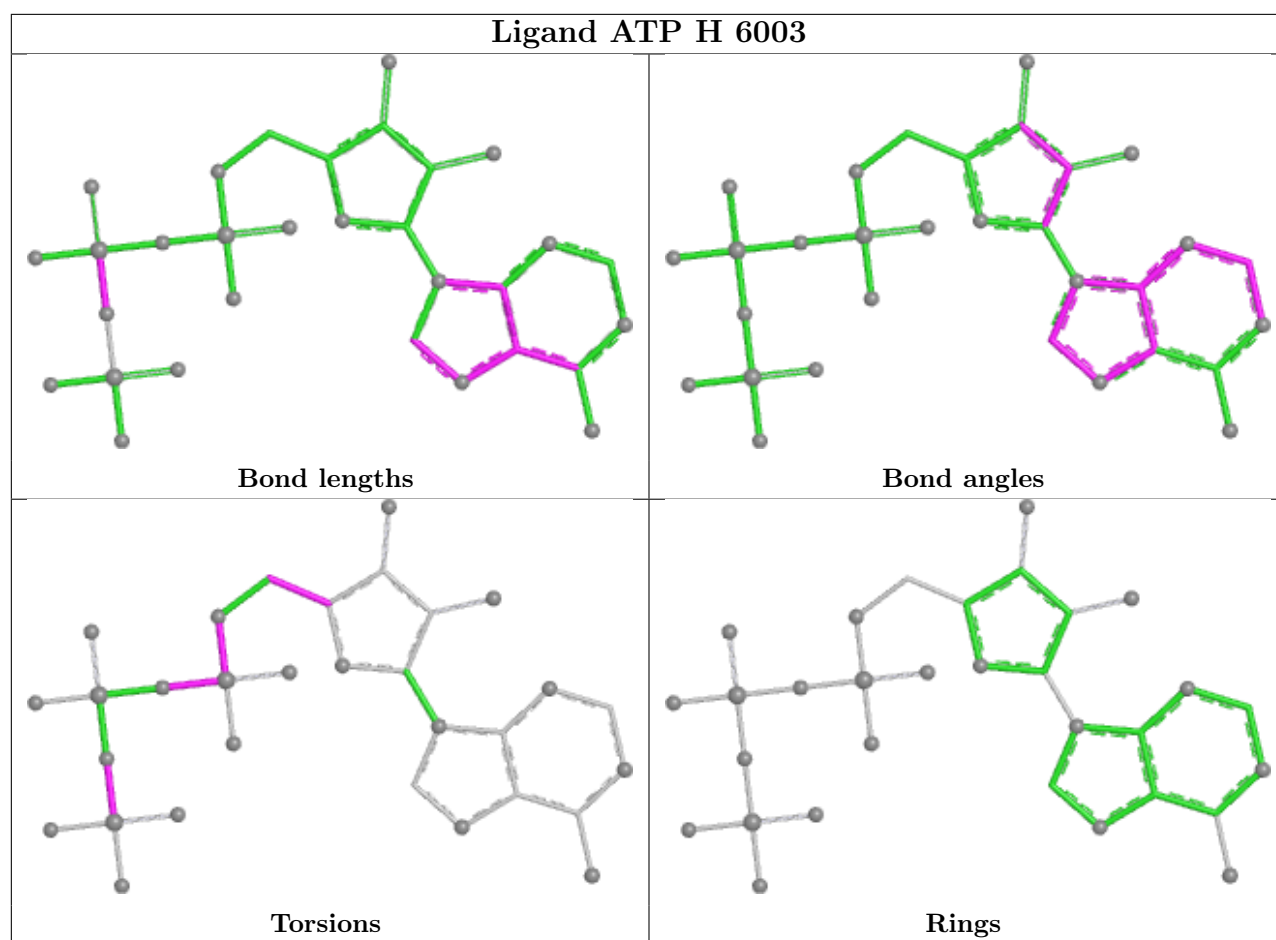
Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	B	6002	CFE	1	0
7	K	6003	ATP	4	0
7	E	6003	ATP	4	0
7	B	6003	ATP	4	0
6	E	6002	CFE	1	0
7	H	6003	ATP	5	0

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.

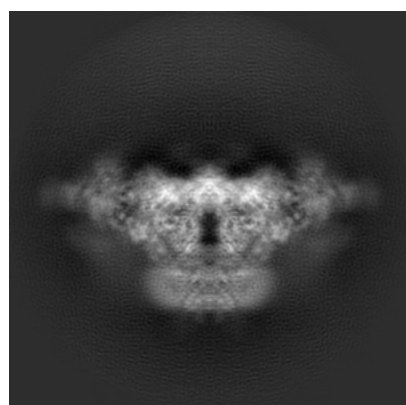
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9834. These allow visual inspection of the internal detail of the map and identification of artifacts.

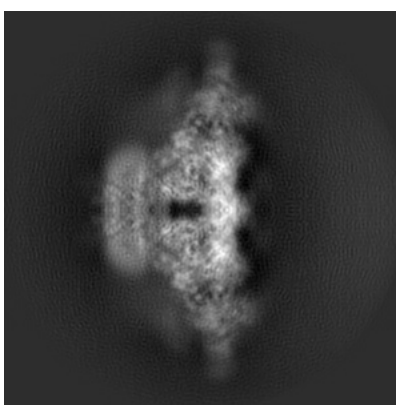
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

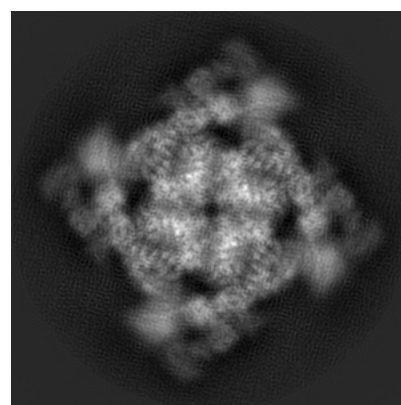
6.1.1 Primary map



X



Y

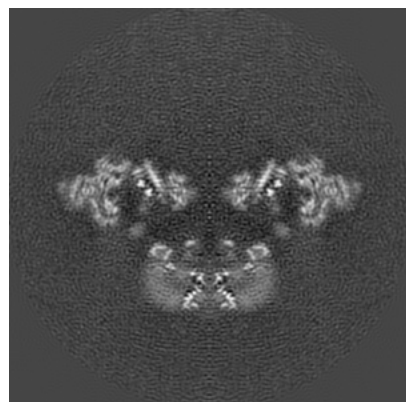


Z

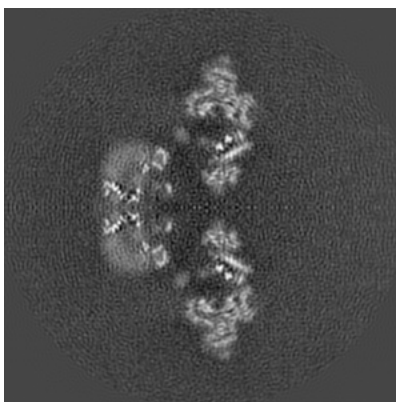
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

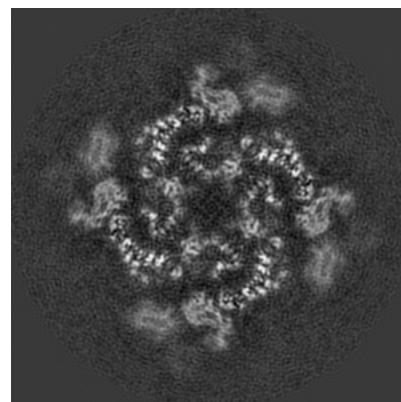
6.2.1 Primary map



X Index: 200



Y Index: 200

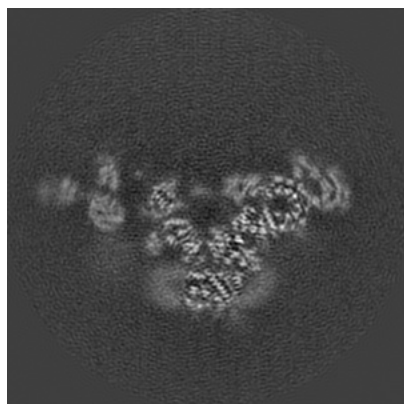


Z Index: 200

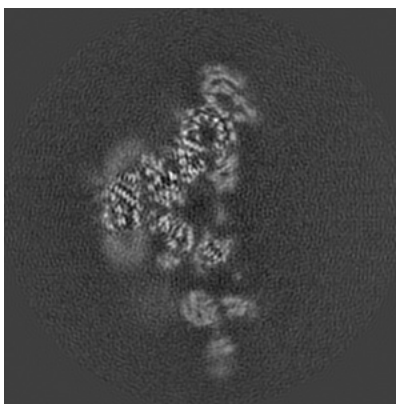
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

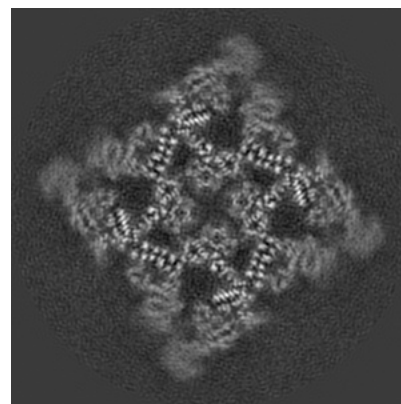
6.3.1 Primary map



X Index: 185



Y Index: 215

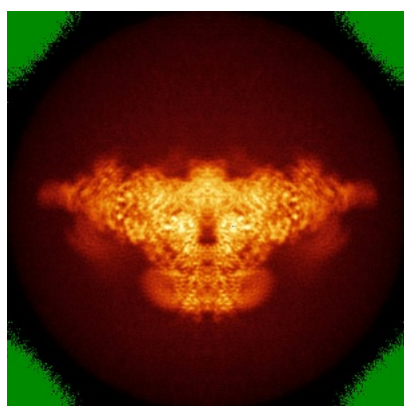


Z Index: 212

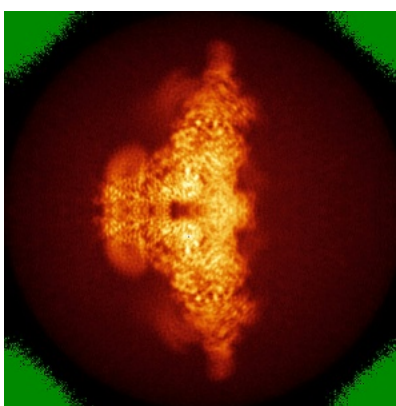
The images above show the largest variance slices of the map in three orthogonal directions.

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

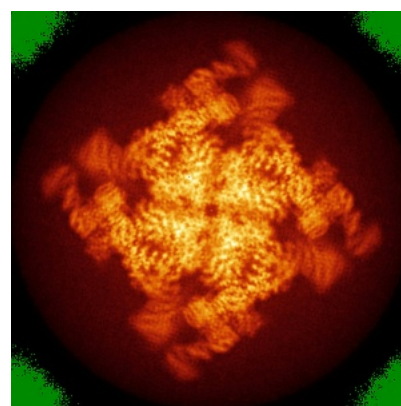
6.4.1 Primary map



X



Y

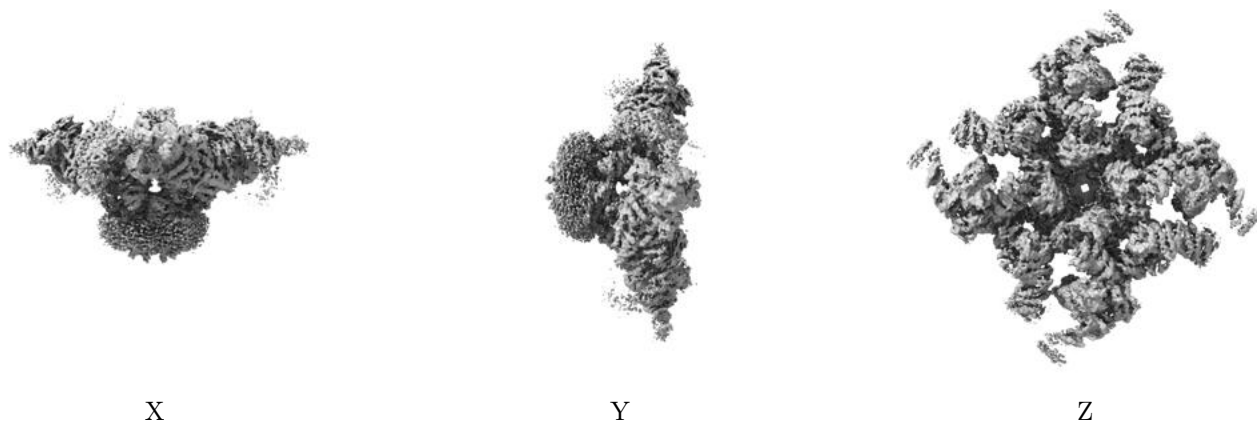


Z

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 0.022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

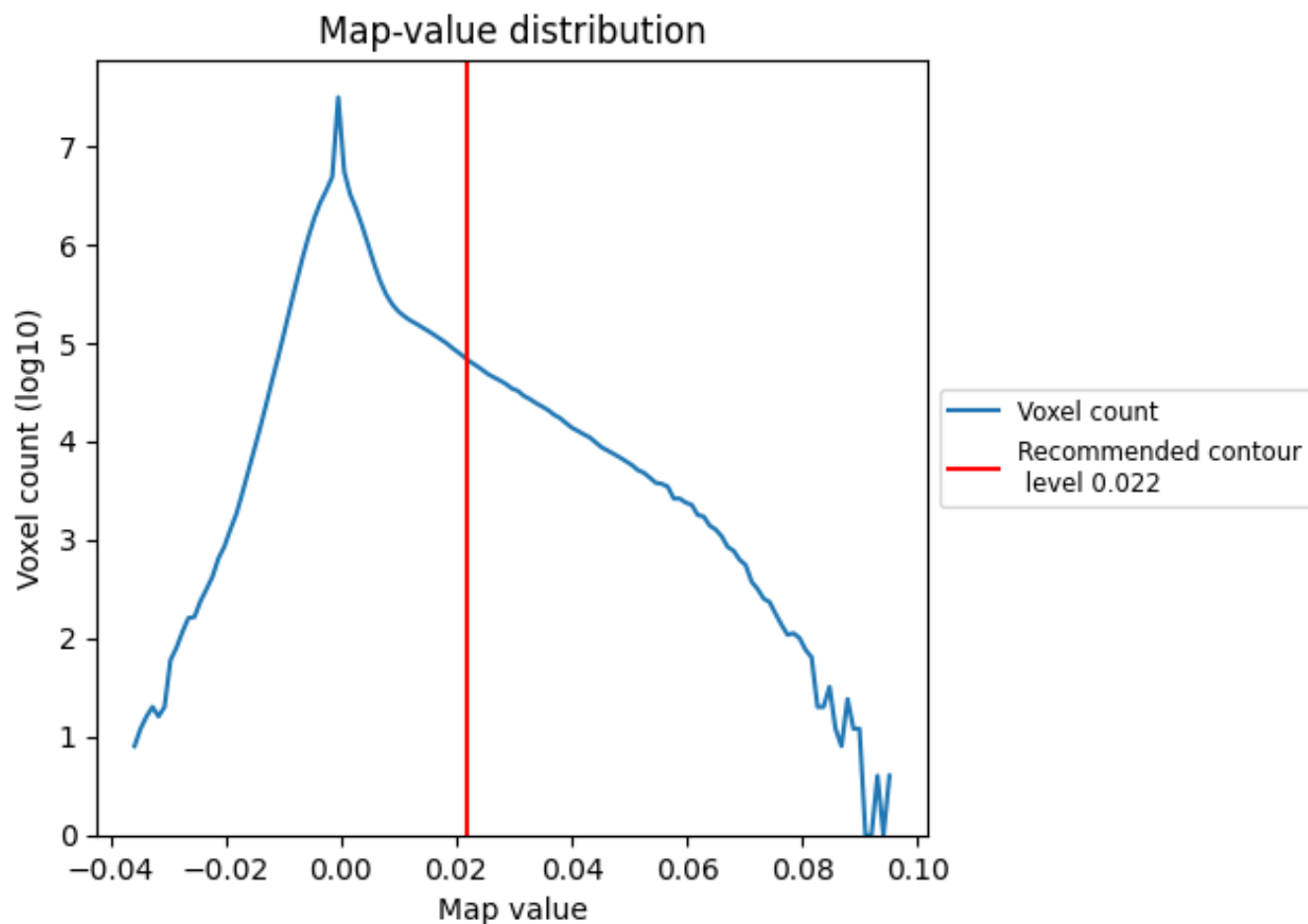
6.6 Mask visualisation [i](#)

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

7 Map analysis [i](#)

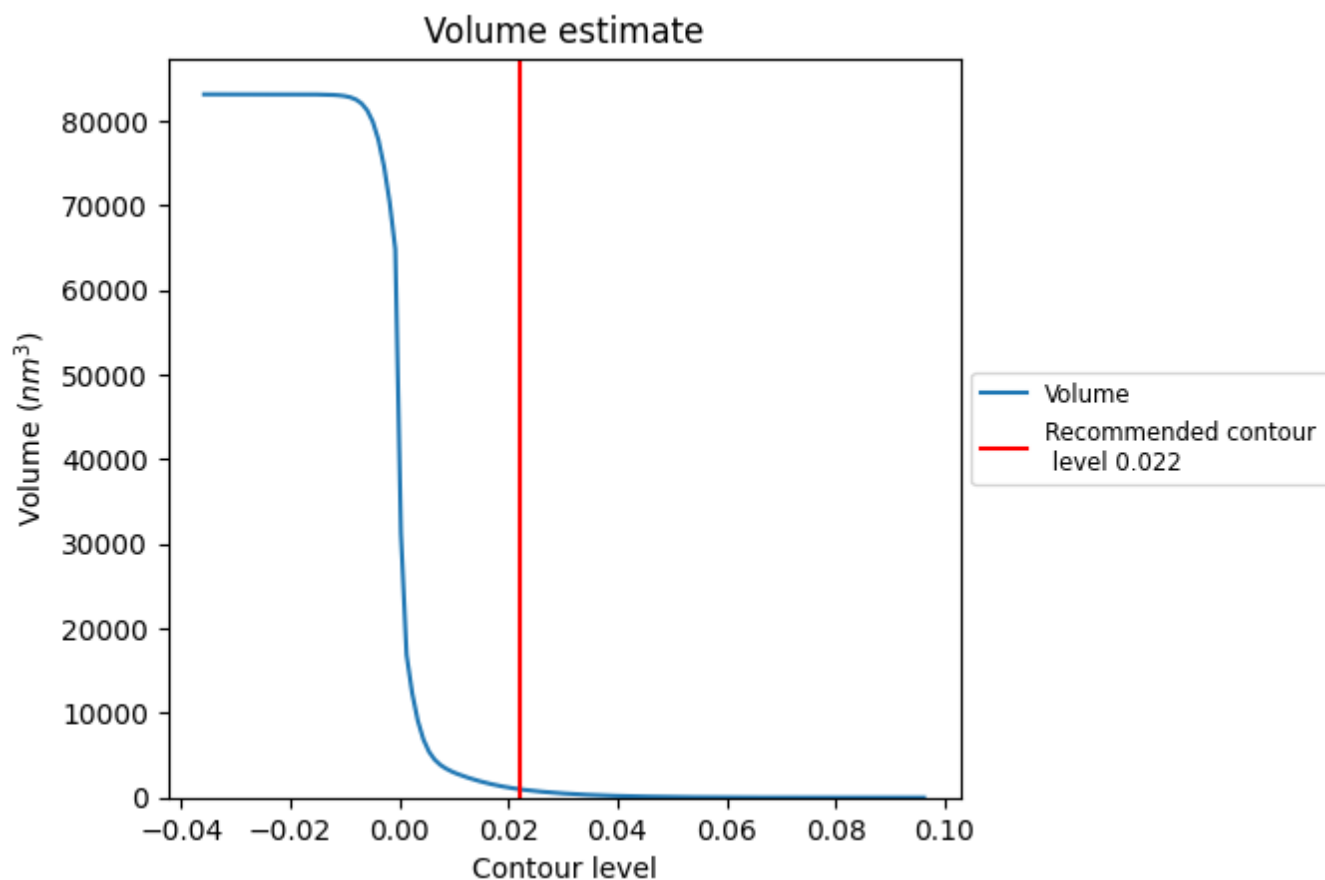
This section contains the results of statistical analysis of the map.

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.

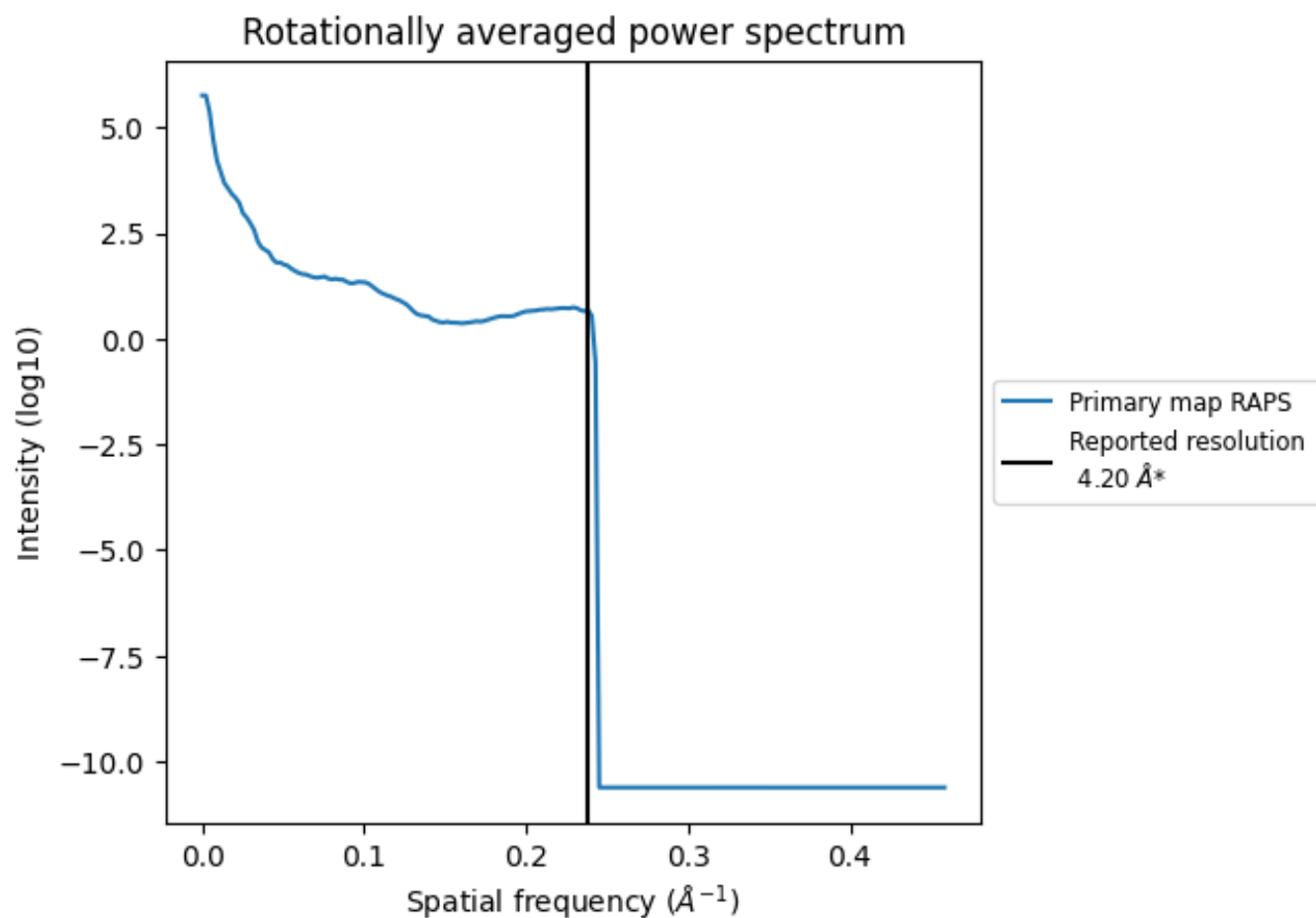
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 992 nm³; this corresponds to an approximate mass of 896 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 ⓘ

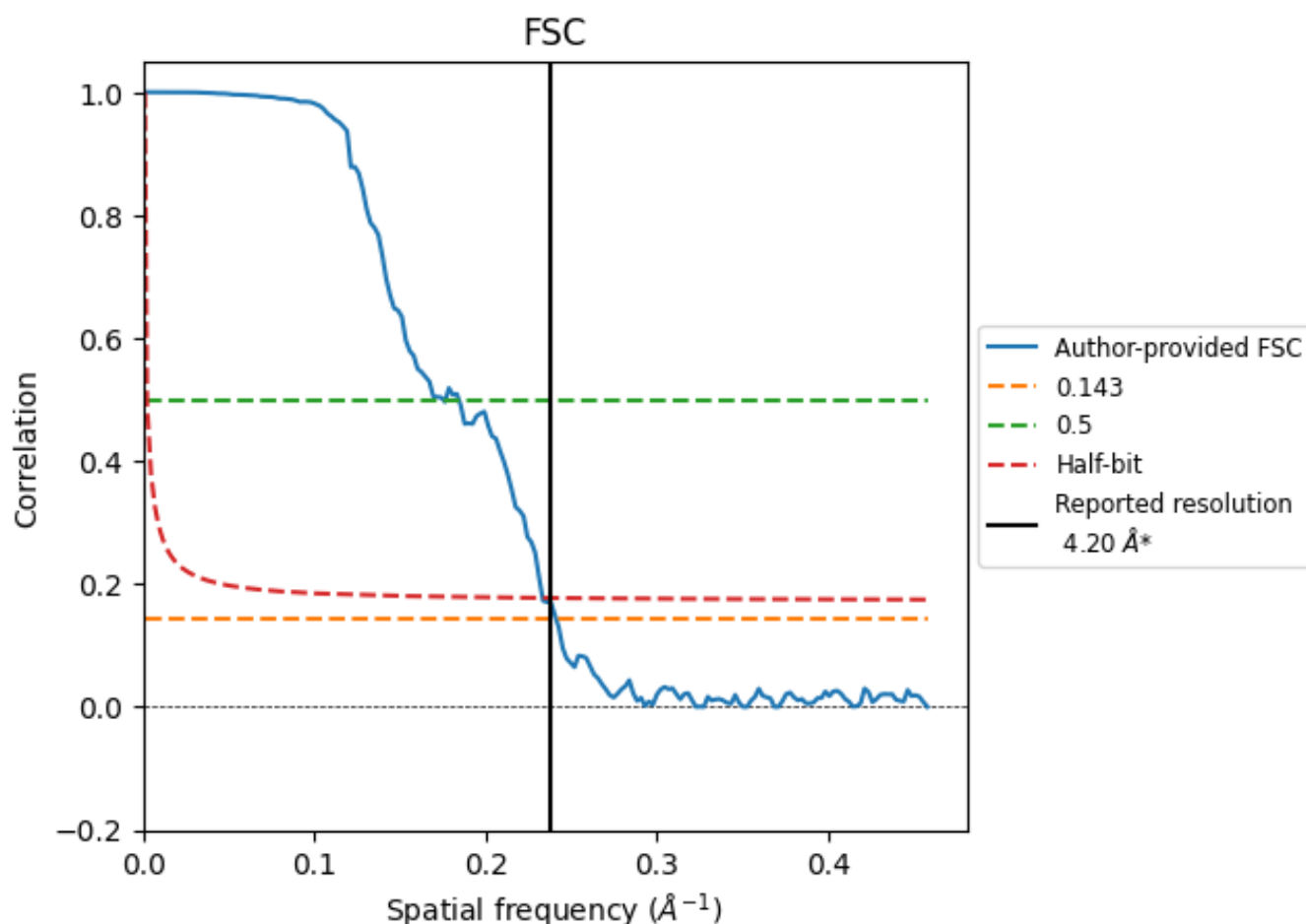


*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.238 Å⁻¹

8.2 Resolution estimates [i](#)

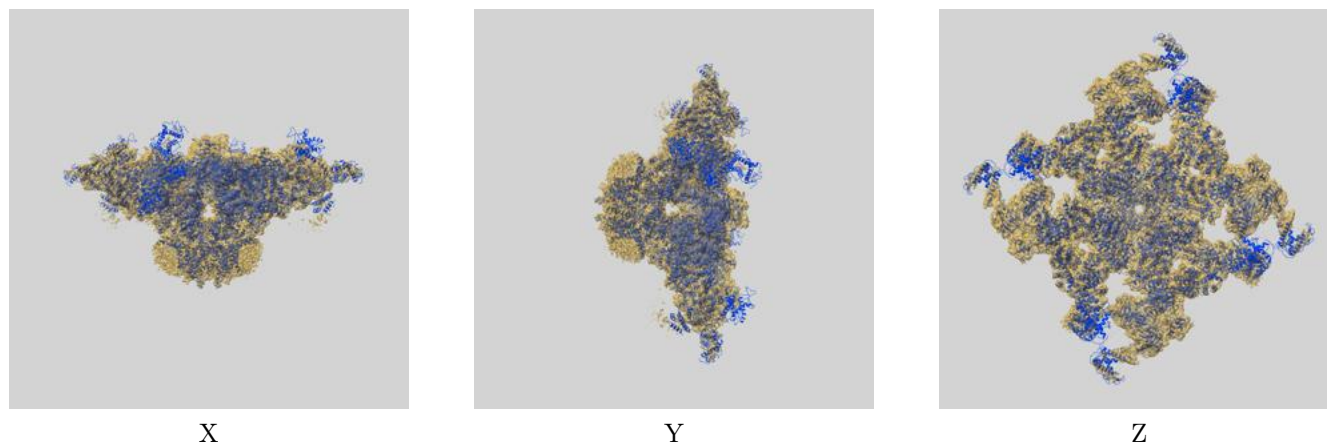
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.20	-	-
Author-provided FSC curve	4.14	5.71	4.28
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

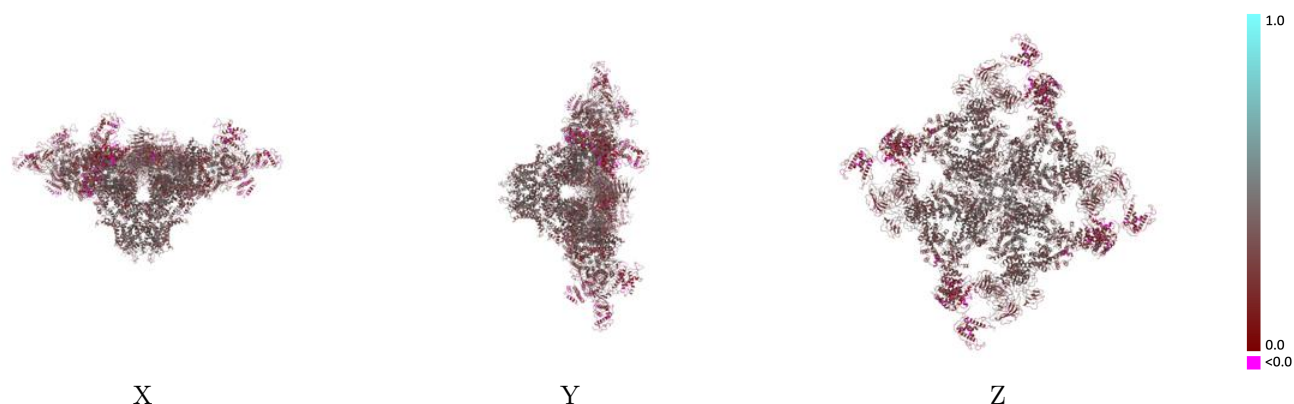
This section contains information regarding the fit between EMDB map EMD-9834 and PDB model 6JII. Per-residue inclusion information can be found in [section 3](#) on [page 8](#).

9.1 Map-model overlay [i](#)



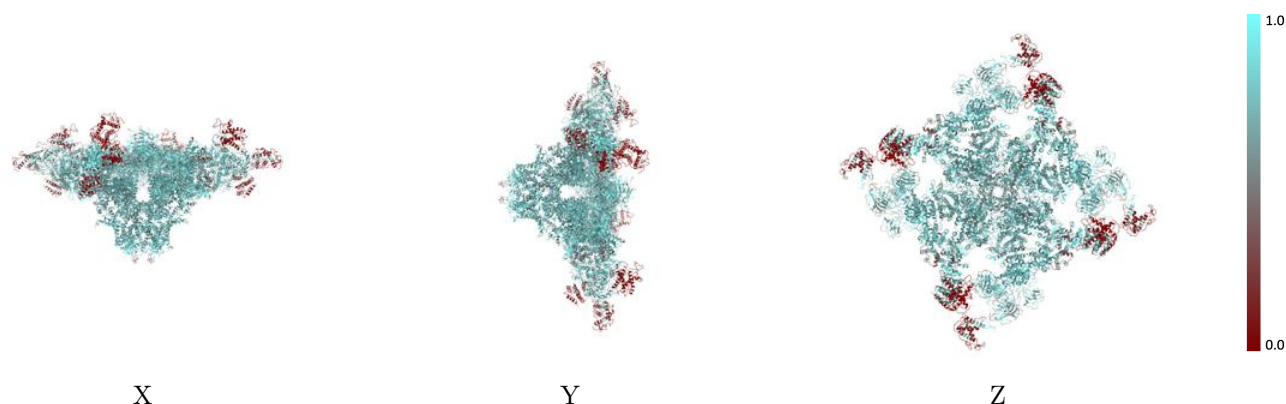
The images above show the 3D surface view of the map at the recommended contour level 0.022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



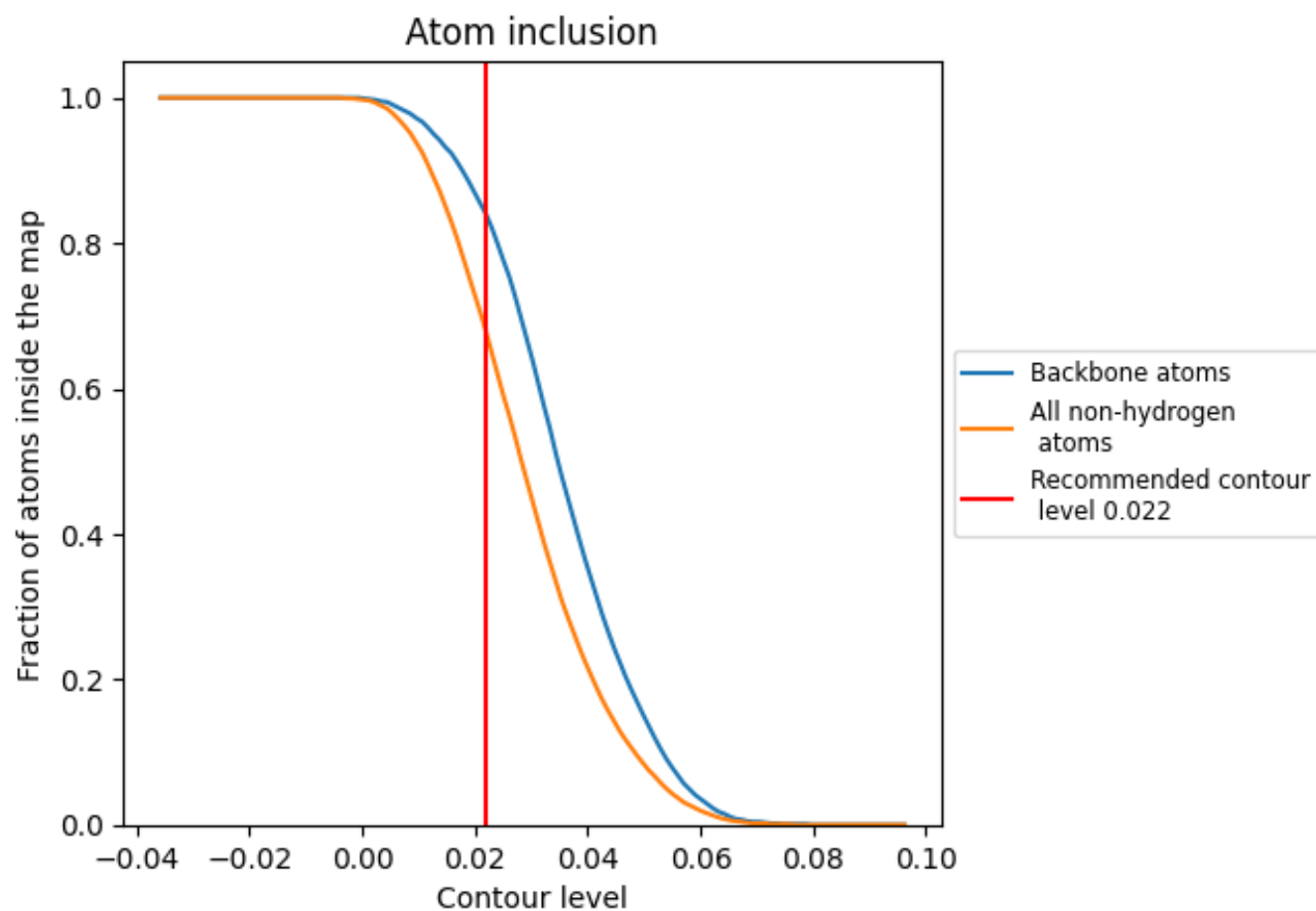
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.022).

9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 68% 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 (0.022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6770	0.3190
A	0.7090	0.3340
B	0.6840	0.3210
C	0.4910	0.2490
D	0.7100	0.3380
E	0.6840	0.3220
F	0.4910	0.2470
G	0.7110	0.3370
H	0.6840	0.3220
I	0.4910	0.2480
J	0.7100	0.3360
K	0.6840	0.3210
L	0.4910	0.2490

