



## Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 11:21 AM UTC

PDB ID : 9E14 / pdb\_00009e14  
EMDB ID : EMD-47383  
Title : Full-length human dynein-1 in phi-like conformation bound to a Lis1 dimer under Nde1-Lis1 condition  
Authors : Yang, J.; Zhang, K.  
Deposited on : 2024-10-21  
Resolution : 5.00 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](mailto: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>.

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

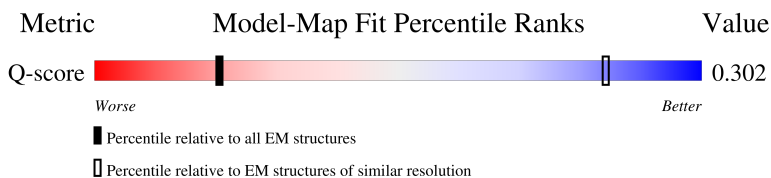
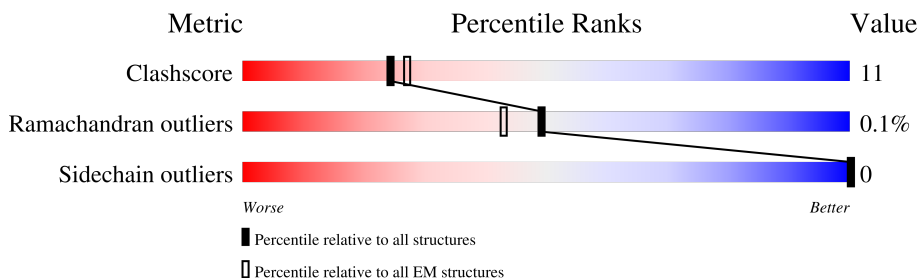
EMDB validation analysis : 0.0.1.dev132  
Mogul : 2022.3.0, CSD as543be (2022)  
MolProbity : 4-5-2 with Phenix2.0  
Buster-report : wwPDB partial adaption of 1.1.7 (2018)  
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)  
EM percentile statistics : 202505.v01 (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 5.00 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.




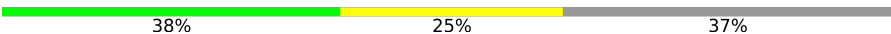








Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	1057 ( 4.50 - 5.50 )

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  $\geq 3$ , 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	4646	<div> <div>10%</div> <div>79%</div> <div>18%</div> <div>.</div> </div>
1	B	4646	<div> <div>6%</div> <div>75%</div> <div>22%</div> <div>.</div> </div>
2	C	638	<div> <div>56%</div> <div>6%</div> <div>38%</div> </div>
2	D	638	<div> <div>36%</div> <div>26%</div> <div>38%</div> </div>

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Mol	Chain	Length	Quality of chain
3	E	492	 61% 37%
3	F	492	 38% 25% 37%
4	G	96	 14% 54% 43%
4	H	96	 70% 27%
5	I	89	 15% 49% 51%
5	J	89	 34% 57% 43%
6	K	113	 60% 75% 25%
6	L	113	 65% 73% 27%
7	O	410	 58% 21% 21%
7	P	410	 53% 25% 22%

## 2 Entry composition [i](#)

There are 10 unique types of molecules in this entry. The entry contains 94479 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 Cytoplasmic dynein 1 heavy chain 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	4542	Total	C	N	O	S	0	0
			36692	23323	6381	6822	166		
1	B	4521	Total	C	N	O	S	0	0
			36527	23221	6349	6791	166		

- Molecule 2 is a protein called Cytoplasmic dynein 1 intermediate chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	C	394	Total	C	N	O	S	0	0
			3112	1962	541	594	15		
2	D	394	Total	C	N	O	S	0	0
			3112	1962	541	594	15		

- Molecule 3 is a protein called Cytoplasmic dynein 1 light intermediate chain 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	E	311	Total	C	N	O	S	0	0
			2518	1614	425	468	11		
3	F	311	Total	C	N	O	S	0	0
			2518	1614	425	468	11		

- Molecule 4 is a protein called Dynein light chain roadblock-type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	G	93	Total	C	N	O	S	0	0
			742	468	128	143	3		
4	H	93	Total	C	N	O	S	0	0
			742	468	128	143	3		

- Molecule 5 is a protein called Dynein light chain 1, cytoplasmic.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	I	89	Total	C	N	O	S	0	0
			728	465	122	135	6		
5	J	89	Total	C	N	O	S	0	0
			728	465	122	135	6		

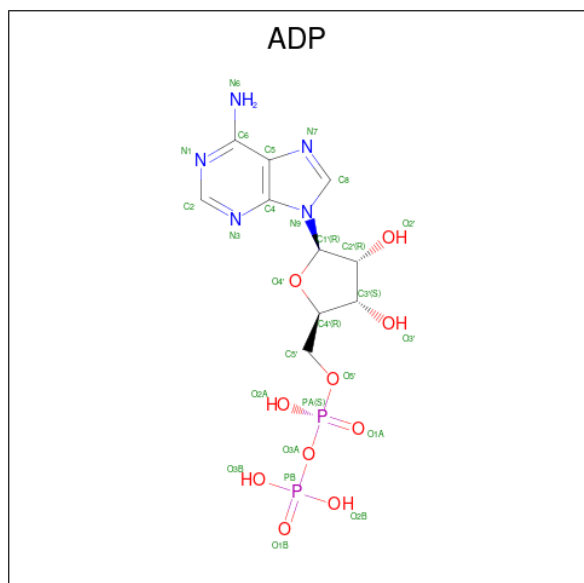
- Molecule 6 is a protein called Dynein light chain Tctex-type 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	K	113	Total	C	N	O	S	0	0
			872	548	142	175	7		
6	L	113	Total	C	N	O	S	0	0
			872	548	142	175	7		

- Molecule 7 is a protein called Platelet-activating factor acetylhydrolase IB subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	O	322	Total	C	N	O	S	0	0
			2557	1608	452	477	20		
7	P	319	Total	C	N	O	S	0	0
			2531	1593	446	472	20		

- Molecule 8 is ADENOSINE-5'-DIPHOSPHATE (CCD ID: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ) (labeled as "Ligand of Interest" by depositor).



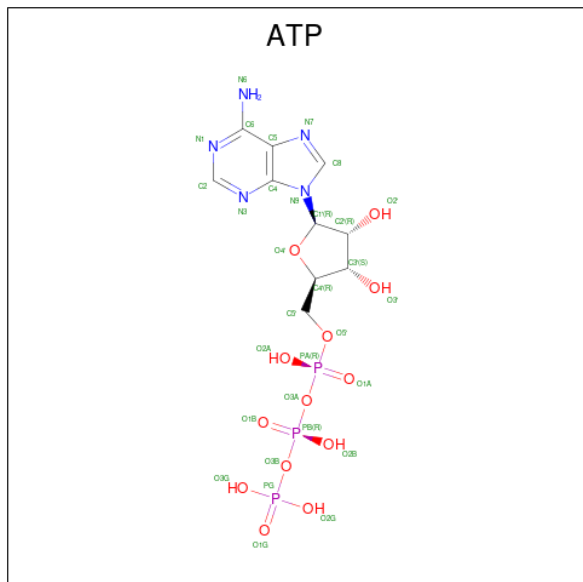
Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	P	0
			27	10	5	10	2	

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Mol	Chain	Residues	Atoms					AltConf
8	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
8	A	1	Total	C	N	O	P	0
			27	10	5	10	2	
8	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
8	B	1	Total	C	N	O	P	0
			27	10	5	10	2	
8	B	1	Total	C	N	O	P	0
			27	10	5	10	2	

- Molecule 9 is ADENOSINE-5'-TRIPHOSPHATE (CCD ID: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
9	A	1	Total	C	N	O	P	0
			31	10	5	13	3	
9	B	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 10 is MAGNESIUM ION (CCD ID: MG) (formula: Mg) (labeled as "Ligand of Interest" by depositor).

Mol	Chain	Residues	Atoms		AltConf
10	A	2	Total	Mg	0
			2	2	

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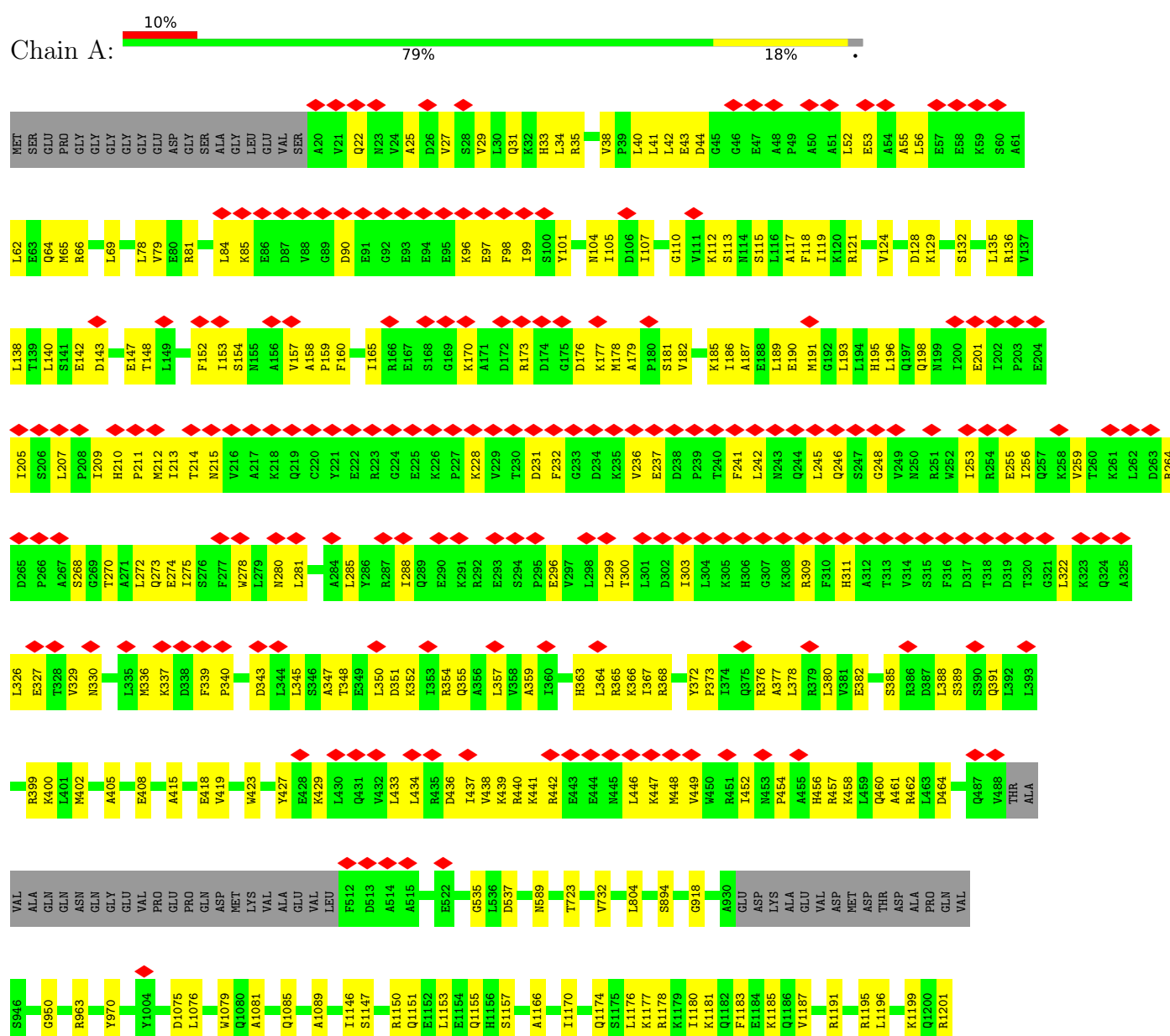
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Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
10	B	2	2	2	0

### 3 Residue-property plots

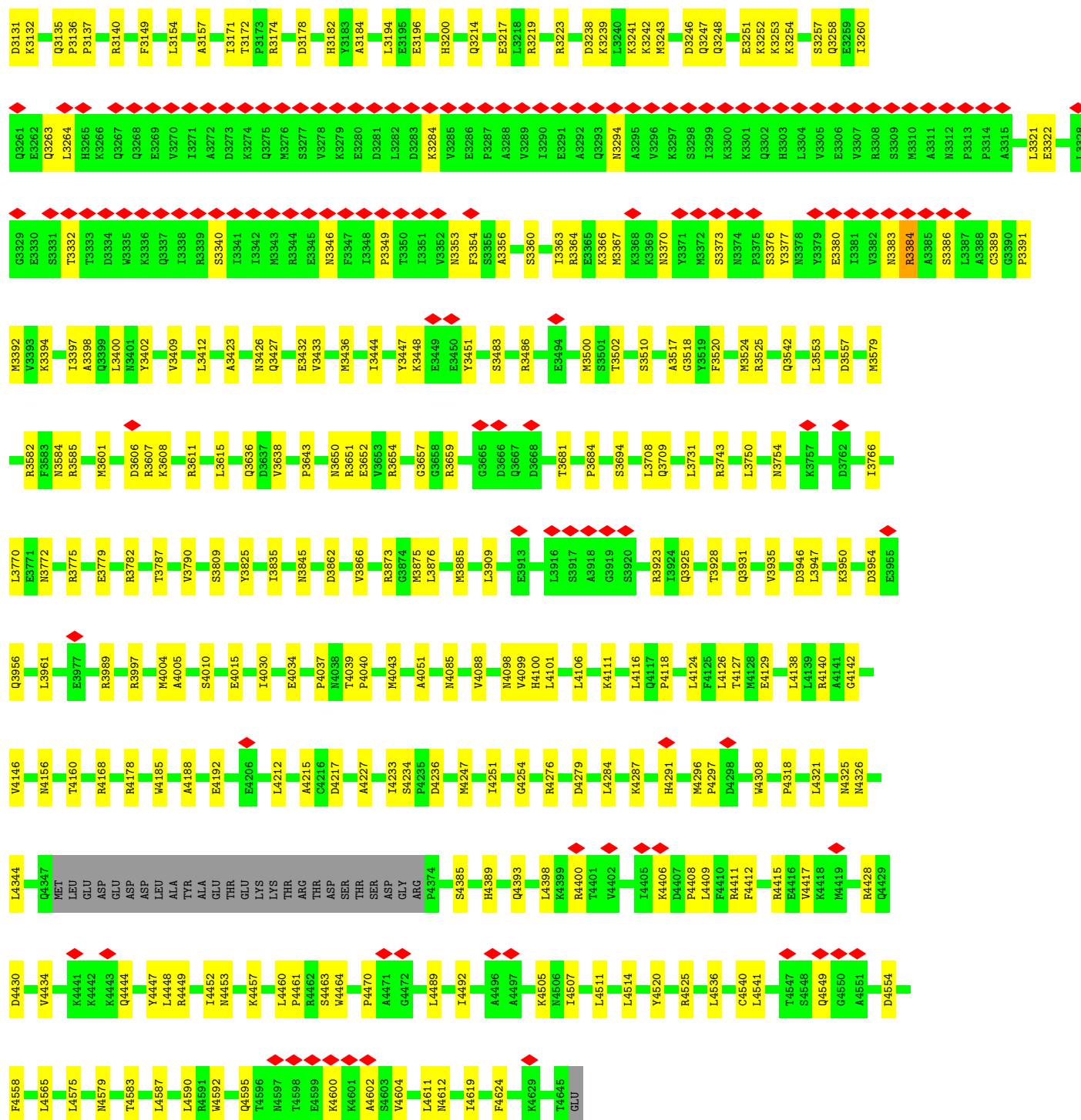
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: Cytoplasmic dynein 1 heavy chain 1

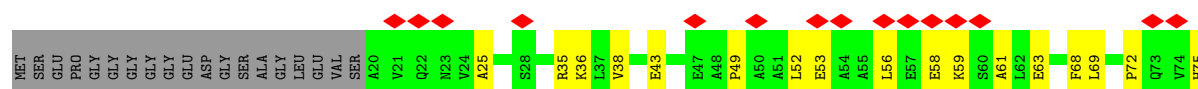
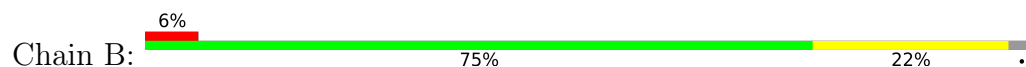




D2975	R2763	G2598	L2449	N2314	E2188	L2039	M1867	I1676	A1577	R1485	K1409	F1302
R2981	F2784	K2601	L2452	D2320	E2189	L2047	Y1868	R1679	K1581	L1486	D1410	Q1203
L2989	I2793	L2605	R2453	D2321	Y2190	Q2051	E1871	I1692	K1584	I1487	R1411	L1209
A2991	Y2794	F2606	C2454	L2324	L2191	L2065	L1879	T1693	S1585	L1415	Q1415	E1215
E2996	S2795	S2607	S2457	E2331	D2195	L2069	C1888	H1695	M1589	M1417	G1219	G1219
S2997	E2814	R2610	S2460	R2332	G2200	I2069	Y1889	I1698	D1590	K1418	N1222	N1222
N2998	R2836	D2614	L2462	M2342	W2203	V2070	M1892	V1699	V1591	K1419	M1225	M1225
V2999	R2836	H2615	H2463	F2343	V2204	P2071	E1700	E1700	L1592	L1420	H1421	H1421
L3000	E2841	E2616	R2467	Q2346	K2206	L2080	K1912	W1701	M1593	H1421	K1228	K1228
F3004	E2841	G2619	D2475	S2357	M2221	D2087	E1914	K1707	I1594	W1424	D1229	D1229
L3005	R2844	S2623	D2475	S2357	M2222	D2087	R1925	V1721	Q1595	W1425	I1232	I1232
E3006	N2860	W2644	M2481	W2361	W2223	R2091	F1926	V1724	G1596	V1426	Q1233	Q1233
R3007	T2877	T2626	Q2485	W2362	G2224	K2094	Y1946	Y1729	Q1598	S1427	Q1327	Q1327
A3013	S2878	E2640	R2492	W2363	S2228	R2105	Q1950	K1729	R1599	E1428	K1350	K1350
N3014	K2879	R2643	R2492	F2364	W2236	R2105	V1951	Y1745	S1600	L1429	A1348	A1348
E3025	V2884	P2645	L2499	W2373	E2242	R2113	G1952	Y1750	L1601	T1430	E1341	E1341
G3036	A2895	N2646	W2500	L2382	R2243	E2117	A1953	V1763	E1602	L1439	D1344	D1344
K3039	K2898	Q2654	L2514	L2387	L2244	E2117	W1954	L1766	R1603	K1441	Q1345	Q1345
E3040	E2902	Q2657	R2519	D2388	E2248	E2120	D1958	L1766	D1606	N1442	E1348	E1348
G3041	E2903	K2657	L2526	D2388	E2248	A2121	E1959	L1766	L1607	N1443	Q1349	Q1349
K3043	E2904	V2660	L2534	D2388	E2248	V2122	G1962	M1769	L1608	A1444	E1349	E1349
L3044	L2905	L2661	E2538	D2388	E2248	D2123	R1966	Q1770	I1611	I1445	P1350	P1350
D3045	D2906	P2669	E2538	D2388	E2248	N2130	Q1973	G1770	I1611	K1446	P1350	P1350
S3046	E2912	V2669	E2538	D2388	E2248	Q2134	C1977	G1771	K1612	K1447	Q1361	Q1361
H3047	E2913	L2669	E2538	D2388	E2248	L2137	I1978	G1771	K1612	D1448	N1362	N1362
E3048	E2914	Q2685	E2538	D2388	E2248	D2137	I1978	G1771	K1612	V1449	L1363	L1363
E3049	H2918	Q2685	E2538	D2388	E2248	D2137	I1978	G1771	K1612	L1450	D1364	D1364
K3052	E2922	L2703	E2538	D2388	E2248	D2137	I1978	G1771	K1612	L1451	D1364	D1364
Q3057	L2934	Q2707	E2554	D2388	E2248	D2137	I1978	G1771	K1612	L1452	A1365	A1365
R3060	L2935	F2708	T2555	D2388	E2248	D2137	I1978	G1771	K1612	Q1453	S1372	S1372
N3061	K2943	V2709	E2555	D2388	E2248	D2137	I1978	G1771	K1612	F1373	F1373	F1373
V3064	E2943	P2714	E2556	D2388	E2248	D2137	I1978	G1771	K1612	P1374	P1374	P1374
T3067	L2956	R2726	D2573	D2388	E2248	D2137	I1978	G1771	K1612	V1386	V1386	V1386
N3068	E2961	R2726	R2576	D2388	E2248	D2137	I1978	G1771	K1612	L1390	L1390	L1390
R3078	K2962	H2730	L2580	D2388	E2248	D2137	I1978	G1771	K1612	Y1393	Y1393	Y1393
K3088	V2963	V2731	W2584	D2388	E2248	D2137	I1978	G1771	K1612	M1394	M1394	M1394
R3088	H2964	P2732	W2584	D2388	E2248	D2137	I1978	G1771	K1612	K1395	K1395	K1395
K3113	R2965	Y2738	P2590	D2388	E2248	D2137	I1978	G1771	K1612	L1463	L1463	L1463
D3114	K2966	Y2738	L2591	D2388	E2248	D2137	I1978	G1771	K1612	Q1465	Q1465	Q1465
V3129	Y2967	R2753	V2592	D2388	E2248	D2137	I1978	G1771	K1612	I1466	I1466	I1466
Y3130	D2973	R2757	P2596	D2388	E2248	D2137	I1978	G1771	K1612	R1467	R1467	R1467
	E2974			D2388	E2248	D2137	I1978	G1771	K1612	N1471	N1471	N1471
				D2388	E2248	D2137	I1978	G1771	K1612	L1475	L1475	L1475
				D2388	E2248	D2137	I1978	G1771	K1612	D1476	D1476	D1476
				D2388	E2248	D2137	I1978	G1771	K1612	L1477	L1477	L1477
				D2388	E2248	D2137	I1978	G1771	K1612	V1478	V1478	V1478
				D2388	E2248	D2137	I1978	G1771	K1612	Q1481	Q1481	Q1481
				D2388	E2248	D2137	I1978	G1771	K1612	N1482	N1482	N1482
				D2388	E2248	D2137	I1978	G1771	K1612	A1407	A1407	A1407
				D2388	E2248	D2137	I1978	G1771	K1612	S1405	S1405	S1405
				D2388	E2248	D2137	I1978	G1771	K1612	E1406	E1406	E1406
				D2388	E2248	D2137	I1978	G1771	K1612	A1407	A1407	A1407
				D2388	E2248	D2137	I1978	G1771	K1612	L1408	L1408	L1408

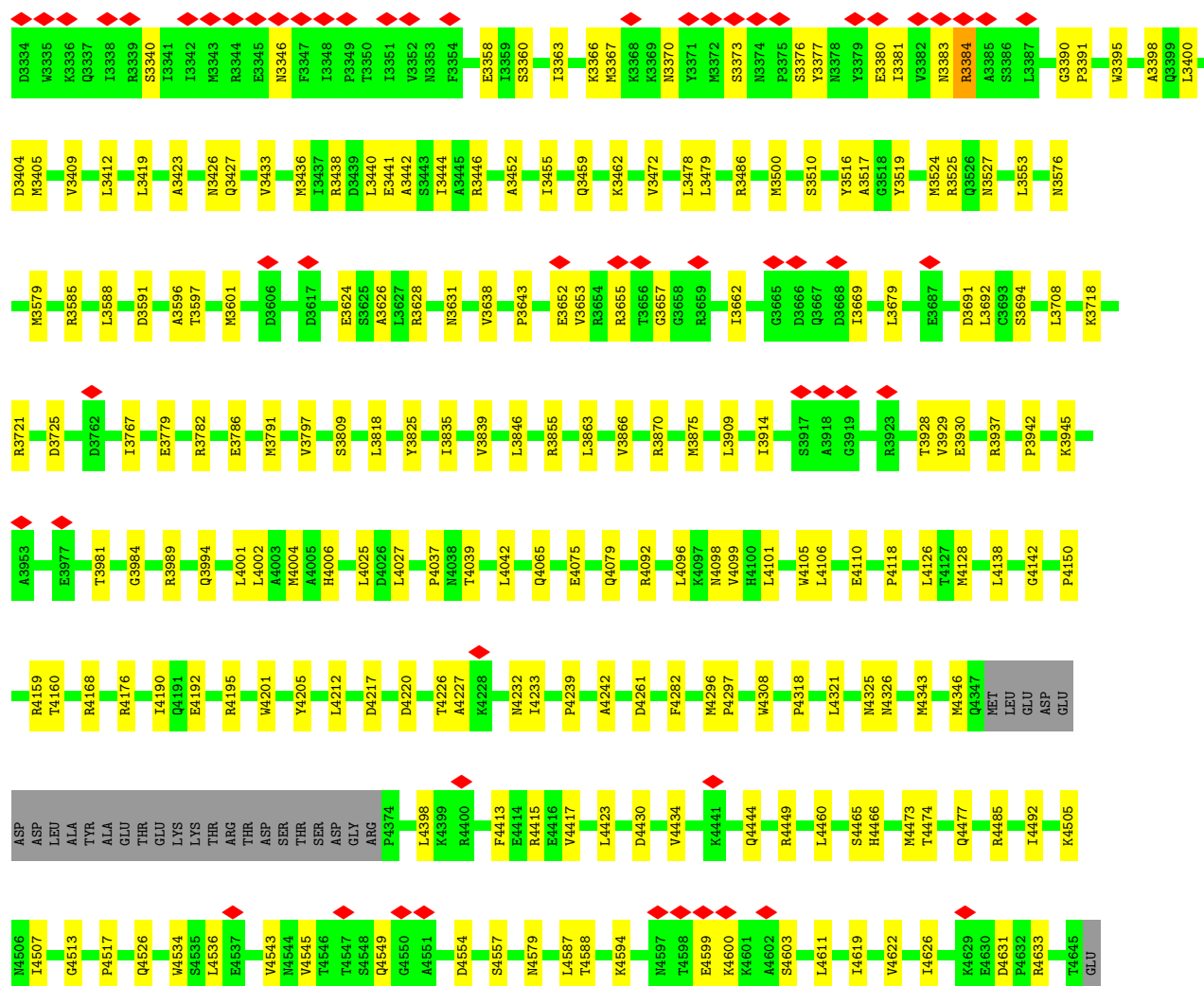


• Molecule 1: Cytoplasmic dynein 1 heavy chain 1



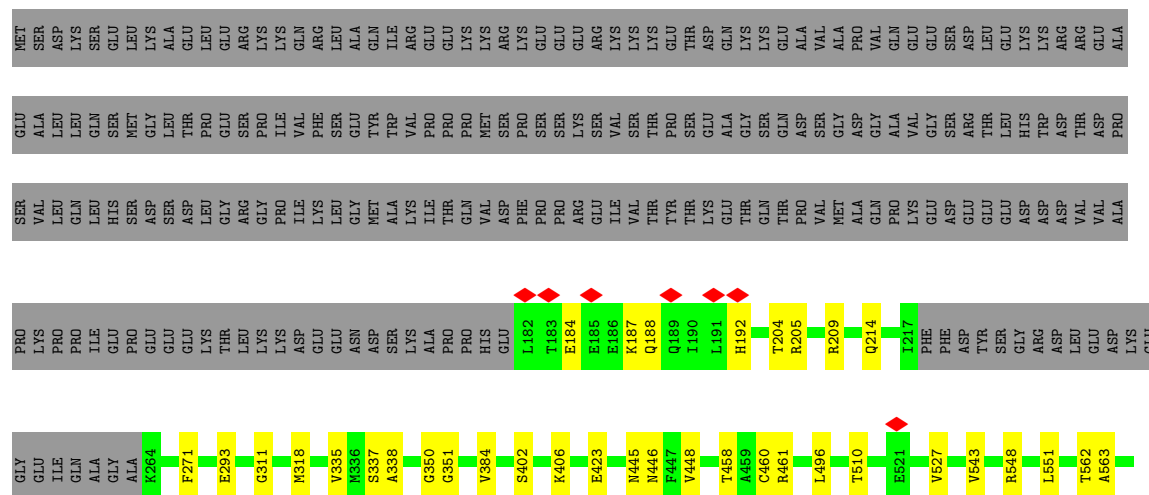






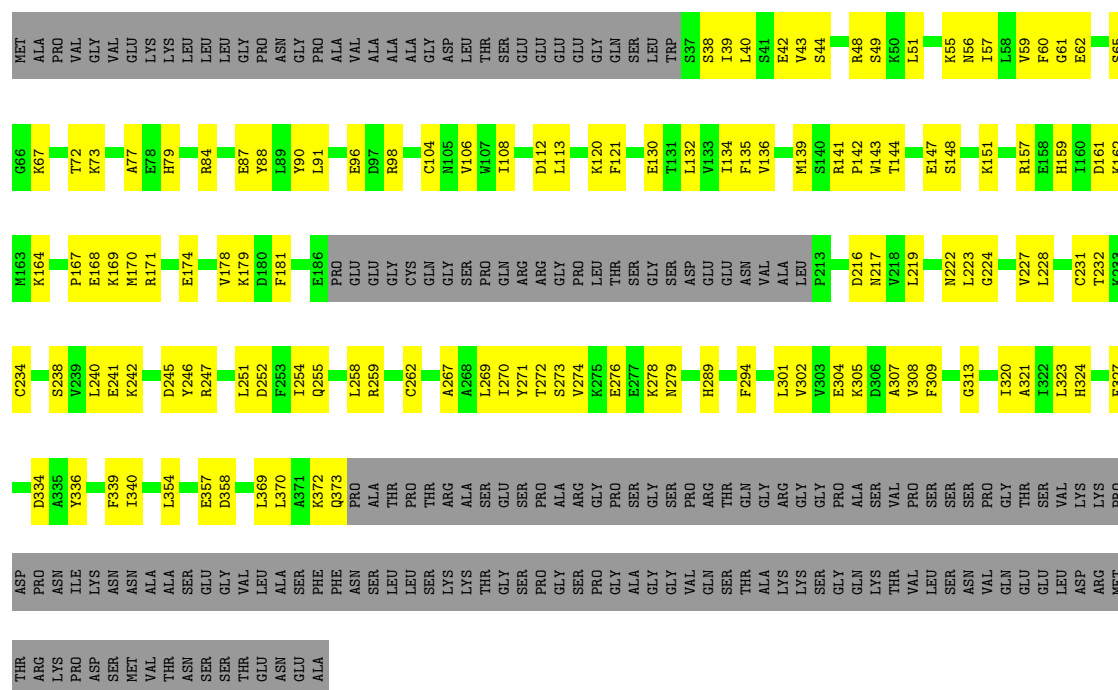
● Molecule 2: Cytoplasmic dynein 1 intermediate chain 2

Chain C:



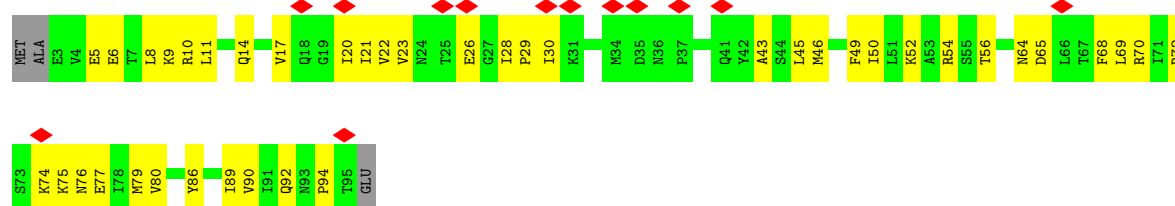


Chain F:  38% 25% 37%



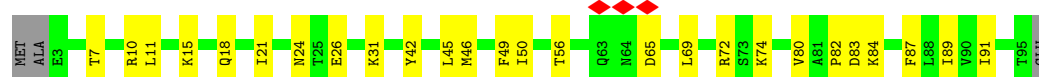
• Molecule 4: Dynein light chain roadblock-type 1

Chain G:  14% 54% 43% .



• Molecule 4: Dynein light chain roadblock-type 1

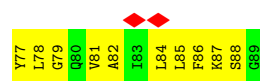
Chain H:  70% 27% .



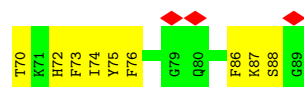
• Molecule 5: Dynein light chain 1, cytoplasmic

Chain I:  15% 49% 51%

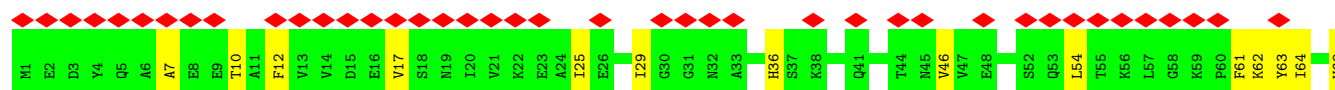
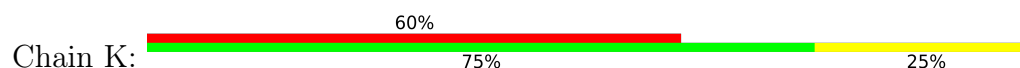




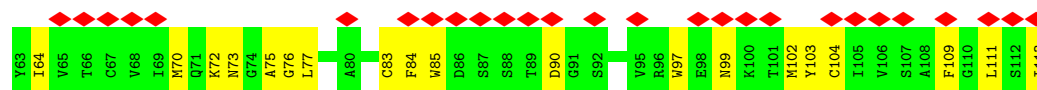
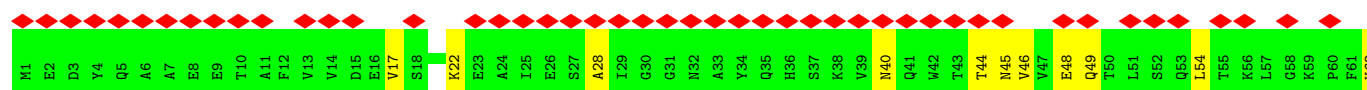
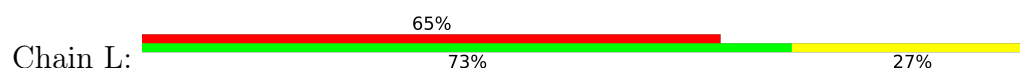
• Molecule 5: Dynein light chain 1, cytoplasmic



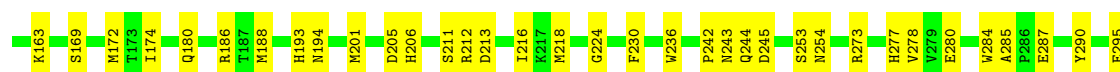
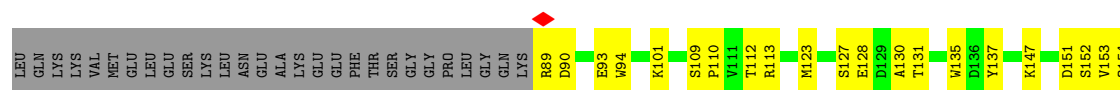
• Molecule 6: Dynein light chain Tctex-type 1



• Molecule 6: Dynein light chain Tctex-type 1



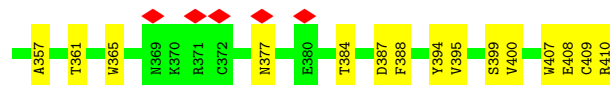
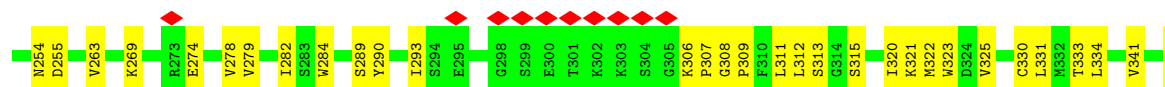
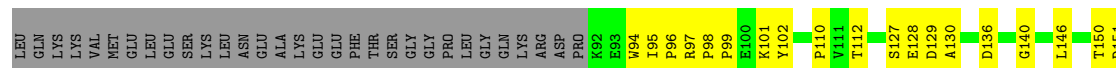
• Molecule 7: Platelet-activating factor acetylhydrolase IB subunit beta







- Molecule 7: Platelet-activating factor acetylhydrolase IB subunit beta



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	61684	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS GLACIOS	Depositor
Voltage (kV)	200	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	40	Depositor
Minimum defocus (nm)	1200	Depositor
Maximum defocus (nm)	2600	Depositor
Magnification	45000	Depositor
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	1.773	Depositor
Minimum map value	0.000	Depositor
Average map value	0.002	Depositor
Map value standard deviation	0.016	Depositor
Recommended contour level	0.15	Depositor
Map size (Å)	729.12, 729.12, 729.12	wwPDB
Map dimensions	420, 420, 420	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.736, 1.736, 1.736	Depositor

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, MG, ADP

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	0.10	0/37419	0.28	0/50625
1	B	0.11	0/37248	0.29	0/50392
2	C	0.11	0/3195	0.32	0/4351
2	D	0.10	0/3195	0.30	0/4351
3	E	0.13	0/2573	0.34	0/3473
3	F	0.11	0/2573	0.32	0/3473
4	G	0.15	0/752	0.41	0/1017
4	H	0.12	0/752	0.31	0/1017
5	I	0.18	0/744	0.43	0/997
5	J	0.13	0/744	0.35	0/997
6	K	0.10	0/888	0.28	0/1203
6	L	0.10	0/888	0.30	0/1203
7	O	0.12	0/2624	0.29	0/3555
7	P	0.13	0/2597	0.33	0/3518
All	All	0.11	0/96192	0.29	0/130172

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
1	B	0	1
2	D	0	1
All	All	0	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	471	ARG	Sidechain
2	D	526	TYR	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	36692	0	36961	580	0
1	B	36527	0	36808	753	0
2	C	3112	0	2964	25	0
2	D	3112	0	2964	116	0
3	E	2518	0	2525	6	0
3	F	2518	0	2525	101	0
4	G	742	0	768	40	0
4	H	742	0	768	22	0
5	I	728	0	714	54	0
5	J	728	0	714	45	0
6	K	872	0	846	27	0
6	L	872	0	846	24	0
7	O	2557	0	2487	61	0
7	P	2531	0	2463	73	0
8	A	81	0	36	5	0
8	B	81	0	36	3	0
9	A	31	0	12	1	0
9	B	31	0	12	1	0
10	A	2	0	0	0	0
10	B	2	0	0	0	0
All	All	94479	0	94449	1824	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 11.

All (1824) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1937:ASP:HA	1:B:1967:MET:HE1	1.44	0.98
1:B:471:ARG:NH1	1:B:472:GLN:HG3	1.81	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:471:ARG:HH12	1:B:472:GLN:HG3	1.29	0.92
1:B:4296:MET:HE3	1:B:4297:PRO:HD2	1.53	0.90
7:P:306:LYS:HD3	7:P:308:GLY:H	1.37	0.87
1:B:3257:SER:HA	1:B:3260:ILE:HD12	1.58	0.85
7:P:199:ALA:HB2	7:P:241:ARG:HH21	1.41	0.85
1:B:462:ARG:NH1	1:B:466:MET:SD	2.51	0.84
1:B:1170:ILE:HG22	1:B:1174:GLN:HE22	1.45	0.80
1:B:853:ILE:HG21	1:B:888:LEU:HD21	1.64	0.80
1:B:2905:LEU:HD11	1:B:3652:GLU:HB2	1.63	0.79
5:I:4:ARG:NH2	5:I:78:LEU:O	2.16	0.79
1:A:182:VAL:HA	1:A:185:LYS:HG2	1.65	0.77
1:B:246:GLN:NE2	1:B:309:ARG:HD3	2.00	0.77
7:P:239:MET:SD	7:P:241:ARG:NH1	2.57	0.77
1:A:1170:ILE:HD11	1:A:1232:ILE:HG12	1.66	0.77
1:A:357:LEU:HD21	1:A:388:LEU:HD21	1.66	0.77
5:I:4:ARG:HE	5:I:78:LEU:HG	1.48	0.77
1:A:115:SER:H	1:A:140:LEU:HB3	1.49	0.77
1:B:162:LYS:HG2	1:B:166:ARG:HE	1.50	0.77
1:A:2956:LEU:HD23	1:A:2989:LYS:HB3	1.68	0.76
1:B:333:ASN:HA	1:B:336:MET:HE2	1.67	0.76
1:B:798:ARG:HH12	1:B:855:GLU:HB3	1.50	0.76
1:B:468:LYS:O	1:B:471:ARG:NH1	2.18	0.75
3:F:91:LEU:HB3	3:F:104:CYS:HB3	1.68	0.75
1:A:3242:LYS:HZ3	1:A:3447:TYR:HD2	1.32	0.75
1:B:399:ARG:HH22	1:B:404:VAL:HG11	1.49	0.75
1:A:3243:MET:HE2	1:A:3448:LYS:HG3	1.69	0.75
1:B:246:GLN:HA	1:B:249:VAL:HG12	1.69	0.75
1:A:246:GLN:HB2	1:A:309:ARG:HD3	1.69	0.75
1:B:3981:THR:HG23	1:B:3984:GLY:H	1.52	0.74
1:B:718:PHE:HA	1:B:738:ASN:H	1.52	0.74
1:B:3818:LEU:HD23	1:B:4346:MET:HE1	1.69	0.74
2:D:509:TRP:HB3	2:D:516:PRO:HA	1.69	0.73
5:J:8:ILE:HG23	5:J:76:PHE:HB3	1.70	0.73
1:B:343:ASP:OD1	1:B:352:LYS:NZ	2.22	0.72
1:A:2644:THR:HG22	1:A:2646:ASN:H	1.55	0.72
1:A:350:LEU:HB3	1:A:419:VAL:HG21	1.72	0.72
1:A:2189:MET:HG3	1:A:2191:LEU:HD23	1.71	0.72
6:K:62:LYS:HE2	6:K:113:ILE:HD13	1.69	0.72
1:B:874:PHE:HB3	1:B:996:LEU:HD21	1.72	0.72
1:A:1229:ASP:O	1:A:1233:GLN:NE2	2.23	0.71
1:B:609:ILE:HG21	1:B:678:GLU:HB3	1.72	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:754:LYS:HZ1	1:B:760:VAL:H	1.37	0.71
1:B:483:VAL:O	1:B:567:ARG:NH1	2.23	0.71
1:A:4043:MET:HE2	1:A:4051:ALA:HB1	1.73	0.71
1:B:264:ARG:HD3	1:B:274:GLU:HG2	1.73	0.71
3:F:62:GLU:HG3	3:F:65:SER:HB2	1.73	0.71
2:D:211:LEU:HG	4:H:15:LYS:HE3	1.73	0.70
1:B:150:HIS:HB2	1:B:193:LEU:HB3	1.72	0.70
1:B:223:ARG:NH1	1:B:225:GLU:OE2	2.23	0.70
4:G:54:ARG:HH12	4:G:65:ASP:HA	1.56	0.70
5:I:29:LEU:HD13	5:I:38:ILE:HD13	1.72	0.70
1:B:266:PRO:HB2	1:B:379:ARG:HB2	1.73	0.70
1:B:482:ARG:O	1:B:487:GLN:NE2	2.24	0.70
1:A:2457:SER:HB2	1:A:2732:PRO:HB3	1.74	0.70
1:B:2457:SER:HB3	1:B:2732:PRO:HB3	1.72	0.70
1:A:402:MET:HA	1:A:535:GLY:HA3	1.73	0.70
1:B:813:GLN:NE2	3:F:357:GLU:OE1	2.25	0.70
1:A:159:PRO:HD2	1:B:107:ILE:HD11	1.74	0.70
1:A:1966:ARG:HA	1:A:4101:LEU:HD13	1.74	0.70
1:B:653:GLN:NE2	2:D:503:ASP:OD2	2.25	0.70
2:D:445:ASN:HD21	2:D:463:GLY:H	1.37	0.69
5:I:57:ILE:HB	5:I:84:LEU:HB3	1.74	0.69
1:A:40:LEU:O	1:B:132:SER:OG	2.10	0.69
1:A:327:GLU:O	1:A:330:ASN:ND2	2.26	0.69
1:B:266:PRO:HB3	1:B:376:ARG:HG3	1.73	0.69
1:B:2684:ARG:NH1	1:B:2688:GLU:OE1	2.25	0.69
2:D:506:VAL:H	2:D:520:PHE:HB3	1.57	0.69
1:B:864:LEU:HD23	1:B:907:ILE:HD11	1.74	0.69
1:B:981:LYS:NZ	3:F:90:TYR:OH	2.25	0.69
1:A:189:LEU:HG	1:B:189:LEU:HD11	1.74	0.69
1:B:130:PRO:HB2	1:B:133:SER:HB2	1.74	0.69
1:A:3517:ALA:HB1	1:A:3525:ARG:HG2	1.73	0.69
1:B:4326:ASN:ND2	1:B:4579:ASN:O	2.26	0.68
7:P:243:ASN:ND2	7:P:245:ASP:OD1	2.26	0.68
1:B:379:ARG:NH2	1:B:451:ARG:O	2.26	0.68
1:B:581:MET:HG2	1:B:611:ARG:HH21	1.57	0.68
1:A:343:ASP:OD1	1:A:352:LYS:NZ	2.22	0.68
1:B:722:SER:HB3	1:B:731:ASN:HD21	1.57	0.68
1:A:3253:LYS:HD3	1:A:3436:MET:HG3	1.74	0.68
1:B:977:GLU:HB3	1:B:981:LYS:HZ3	1.58	0.68
1:B:1170:ILE:O	1:B:1174:GLN:NE2	2.26	0.68
4:G:80:VAL:HG12	4:G:89:ILE:HG22	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1461:GLU:HG3	1:B:1464:LYS:HZ2	1.59	0.68
1:B:330:ASN:HA	1:B:333:ASN:HB2	1.76	0.67
5:I:64:SER:OG	5:J:36:LYS:NZ	2.26	0.67
1:B:462:ARG:HD2	1:B:465:GLN:NE2	2.10	0.67
1:A:337:LYS:HZ1	1:A:367:ILE:HB	1.58	0.67
3:F:167:PRO:HA	3:F:170:MET:HE3	1.76	0.67
5:I:57:ILE:HD12	5:I:84:LEU:HD23	1.74	0.67
5:I:67:THR:HG23	5:J:43:LYS:HE3	1.76	0.67
1:B:441:LYS:O	1:B:445:ASN:N	2.28	0.67
1:B:462:ARG:HH21	1:B:537:ASP:HB2	1.59	0.67
1:A:3611:ARG:NH1	1:A:3636:GLN:OE1	2.28	0.67
1:A:3657:GLY:O	1:A:3659:ARG:NH1	2.28	0.67
1:A:4505:LYS:NZ	1:A:4554:ASP:O	2.28	0.67
4:G:8:LEU:HD23	4:G:20:ILE:HG22	1.77	0.67
1:B:386:ARG:NH2	1:B:453:ASN:O	2.28	0.66
7:P:322:MET:HE1	7:P:331:LEU:HD12	1.76	0.66
1:B:1082:LEU:HD21	3:F:39:ILE:HG21	1.76	0.66
6:K:73:ASN:HD21	6:L:75:ALA:HB2	1.60	0.66
1:A:3247:GLN:HG3	1:A:3444:ILE:HD13	1.77	0.66
1:B:669:LEU:HD22	1:B:673:TRP:HB3	1.78	0.66
2:D:187:LYS:HE3	4:H:24:ASN:H	1.59	0.66
5:I:9:LYS:HG2	5:I:76:PHE:HA	1.77	0.66
1:A:3257:SER:HA	1:A:3260:ILE:HD12	1.76	0.66
1:B:399:ARG:NH2	1:B:408:GLU:OE1	2.28	0.66
2:C:548:ARG:HA	2:C:566:SER:HA	1.76	0.66
1:A:2271:ASN:OD1	1:A:2272:THR:N	2.29	0.66
1:B:2590:PRO:HG3	1:B:2687:VAL:HG21	1.78	0.66
2:D:313:ALA:HB3	2:D:329:PHE:HB3	1.78	0.66
1:B:1148:LYS:NZ	1:B:1152:GLU:OE2	2.29	0.66
1:A:78:LEU:HB3	1:A:104:ASN:HB2	1.77	0.66
2:D:356:GLN:NE2	2:D:373:THR:O	2.28	0.66
1:A:132:SER:O	1:A:136:ARG:NH2	2.28	0.66
1:B:3178:ASP:OD2	1:B:3585:ARG:NE	2.29	0.66
4:G:74:LYS:NZ	4:H:65:ASP:OD1	2.29	0.66
2:D:358:VAL:HG13	2:D:369:PRO:HB3	1.78	0.65
1:A:359:ALA:O	1:A:363:HIS:ND1	2.29	0.65
1:B:365:ARG:NH2	1:B:429:LYS:O	2.29	0.65
1:B:442:ARG:O	1:B:445:ASN:ND2	2.29	0.65
3:F:273:SER:HB3	3:F:276:GLU:HG2	1.78	0.65
2:C:445:ASN:O	2:C:461:ARG:N	2.30	0.65
6:K:85:TRP:CD1	6:K:90:ASP:HB2	2.32	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:P:183:GLU:OE1	7:P:183:GLU:N	2.29	0.65
1:A:3363:ILE:HG22	1:A:3367:MET:HE1	1.77	0.65
1:B:516:ASP:HA	1:B:563:ARG:HH12	1.62	0.65
1:A:447:LYS:HD3	1:A:449:VAL:HG22	1.79	0.65
1:A:4600:LYS:HG3	1:A:4602:ALA:H	1.62	0.65
1:B:3045:ASP:OD1	1:B:3046:SER:N	2.30	0.65
1:A:201:GLU:HA	1:A:280:ASN:HD21	1.61	0.65
1:A:2449:LEU:HA	1:A:2453:ARG:HH21	1.61	0.64
1:B:257:GLN:NE2	1:B:319:ASP:O	2.30	0.64
1:B:1958:ASP:HA	1:B:2017:THR:HB	1.78	0.64
1:A:1594:ILE:HB	1:A:1597:VAL:HB	1.79	0.64
1:A:1565:THR:HG22	1:A:1569:GLN:HE22	1.63	0.64
1:A:3584:ASN:O	1:A:3651:ARG:NH1	2.30	0.64
1:B:1196:LEU:HD23	1:B:1199:LYS:HE2	1.80	0.64
1:B:1461:GLU:HA	1:B:1464:LYS:HG2	1.78	0.64
1:B:3229:LEU:O	1:B:3233:ASN:ND2	2.31	0.64
4:H:26:GLU:HA	4:H:87:PHE:HE2	1.62	0.64
1:A:195:HIS:O	1:A:198:GLN:HG2	1.98	0.64
1:A:4470:PRO:HG3	1:A:4612:ASN:HD22	1.60	0.64
5:I:20:ASP:OD2	5:I:50:TYR:OH	2.15	0.64
2:D:272:PHE:HB2	2:D:593:GLN:HG3	1.79	0.64
1:A:2162:SER:OG	1:A:4406:LYS:NZ	2.29	0.64
1:A:4326:ASN:ND2	1:A:4579:ASN:O	2.31	0.64
2:D:392:THR:HG23	2:D:394:ASN:H	1.62	0.64
1:B:2220:LEU:HD23	1:B:2342:MET:HE3	1.80	0.64
1:A:38:VAL:HG21	1:A:52:LEU:HD22	1.79	0.64
1:B:530:VAL:N	1:B:553:TYR:OH	2.28	0.64
3:F:142:PRO:O	3:F:336:TYR:OH	2.16	0.64
3:F:302:VAL:HA	3:F:308:VAL:HG13	1.79	0.64
1:A:270:THR:HG23	1:A:273:GLN:H	1.63	0.64
1:A:1222:ASN:HA	1:A:1225:MET:HG2	1.79	0.63
1:B:3479:LEU:O	1:B:3486:ARG:NH2	2.31	0.63
2:D:337:SER:O	2:D:351:GLY:N	2.31	0.63
1:A:3044:LEU:HD12	1:A:3049:GLU:HG3	1.79	0.63
1:A:160:PHE:HB2	1:B:107:ILE:HD12	1.79	0.63
1:A:2903:GLU:O	1:A:3654:ARG:NH2	2.30	0.63
1:B:260:THR:HG23	1:B:261:LYS:HD3	1.81	0.63
1:A:2000:GLU:OE1	1:A:2005:GLN:NE2	2.32	0.63
1:B:4505:LYS:NZ	1:B:4554:ASP:O	2.26	0.63
1:A:64:GLN:HE21	1:A:105:ILE:HB	1.64	0.63
1:A:121:ARG:HD2	1:A:136:ARG:HG2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:4192:GLU:HG3	1:A:4321:LEU:HD11	1.79	0.63
1:A:4489:LEU:HD13	1:A:4492:ILE:HD11	1.79	0.63
1:B:396:LEU:HD11	1:B:536:LEU:HD22	1.81	0.63
1:B:666:GLU:OE1	1:B:673:TRP:NE1	2.32	0.63
2:C:337:SER:O	2:C:351:GLY:N	2.28	0.63
2:D:445:ASN:OD1	2:D:446:ASN:N	2.29	0.63
7:O:320:ILE:HB	7:O:334:LEU:HB2	1.79	0.63
1:B:530:VAL:HG13	1:B:553:TYR:CZ	2.34	0.63
1:B:649:ILE:O	1:B:653:GLN:HG2	1.99	0.63
1:A:2047:GLN:HA	1:A:2070:VAL:HG21	1.82	0.62
2:D:505:THR:OG1	2:D:521:GLU:OE2	2.16	0.62
1:A:3423:ALA:O	1:A:3427:GLN:N	2.28	0.62
1:A:3708:LEU:HD23	1:A:3809:SER:HA	1.80	0.62
1:B:3721:ARG:HH11	1:B:3797:VAL:HG13	1.65	0.62
1:B:4398:LEU:HG	1:B:4417:VAL:HG11	1.81	0.62
3:F:289:HIS:ND1	3:F:294:PHE:O	2.25	0.62
1:A:42:LEU:HB3	1:A:81:ARG:HH21	1.64	0.62
1:A:4318:PRO:HG2	1:A:4325:ASN:HA	1.81	0.62
2:D:400:SER:HB3	2:D:410:TRP:HZ3	1.65	0.62
1:A:1612:GLN:NE2	1:A:1635:GLU:OE1	2.32	0.62
2:D:457:TYR:HB3	2:D:468:ILE:HD12	1.82	0.62
6:K:78:HIS:NE2	6:L:40:ASN:OD1	2.32	0.62
1:A:2242:GLU:HG2	1:A:2248:GLU:HA	1.81	0.62
1:B:68:PHE:HZ	1:B:135:LEU:HD11	1.63	0.62
3:F:278:LYS:HE2	3:F:307:ALA:HB2	1.81	0.62
4:G:75:LYS:HD2	4:G:76:ASN:HB2	1.79	0.62
1:A:354:ARG:HD2	1:A:419:VAL:HG22	1.80	0.62
1:A:1888:CYS:O	1:A:1892:MET:HG2	2.00	0.62
1:B:25:ALA:HB3	1:B:69:LEU:HD21	1.81	0.62
1:B:255:GLU:HA	1:B:258:LYS:HE3	1.81	0.62
1:B:659:THR:OG1	1:B:690:ARG:NH2	2.33	0.62
1:B:2573:ASP:OD1	1:B:2576:ARG:NH2	2.33	0.62
1:A:348:THR:O	1:A:399:ARG:NH2	2.31	0.62
1:B:1174:GLN:OE1	1:B:1233:GLN:NE2	2.33	0.62
1:B:3194:LEU:HD23	1:B:3500:MET:HG2	1.82	0.62
3:F:136:VAL:HG13	3:F:232:THR:HG21	1.81	0.62
7:P:243:ASN:ND2	7:P:247:THR:OG1	2.32	0.62
1:A:3946:ASP:OD2	1:A:3950:LYS:NZ	2.32	0.61
1:B:701:ASP:OD1	1:B:704:ARG:NH2	2.32	0.61
1:B:1477:LEU:HB3	1:B:1485:ARG:HG3	1.80	0.61
1:A:118:PHE:HB3	1:A:135:LEU:HD21	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:423:TRP:HE1	1:A:457:ARG:HH12	1.46	0.61
7:P:309:PRO:HB2	7:P:325:VAL:HB	1.81	0.61
1:A:2981:ARG:HH22	1:A:3025:GLU:HG3	1.66	0.61
1:B:1170:ILE:HG23	1:B:1233:GLN:HE21	1.65	0.61
2:C:575:ARG:O	2:C:588:GLY:N	2.29	0.61
2:D:215:ILE:HG13	2:D:217:ILE:H	1.64	0.61
5:J:46:PHE:HB3	5:J:54:TRP:CD1	2.35	0.61
1:A:4453:ASN:O	1:A:4457:LYS:NZ	2.33	0.61
1:B:3718:LYS:NZ	1:B:3725:ASP:OD2	2.33	0.61
1:B:3825:TYR:CZ	1:B:3875:MET:HG3	2.35	0.61
1:B:4075:GLU:O	1:B:4079:GLN:NE2	2.33	0.61
1:A:1201:ARG:HH21	1:B:1061:TRP:HD1	1.48	0.61
1:A:1533:LEU:HD11	1:A:1597:VAL:HG22	1.81	0.61
1:A:3845:ASN:ND2	1:A:3862:ASP:OD2	2.32	0.61
1:B:2629:GLU:OE1	1:B:2629:GLU:N	2.33	0.61
1:B:3130:TYR:CZ	1:B:3132:LYS:HB2	2.36	0.61
1:B:3404:ASP:C	1:B:3405:MET:HE2	2.26	0.61
1:A:4398:LEU:HG	1:A:4417:VAL:HG21	1.83	0.61
1:B:761:PRO:HD2	1:B:764:ILE:HD12	1.82	0.61
1:B:2841:GLU:OE1	1:B:2844:ARG:NH2	2.33	0.61
2:D:315:VAL:HB	2:D:327:TYR:HB2	1.83	0.61
1:A:170:LYS:NZ	1:A:176:ASP:O	2.31	0.61
1:B:1933:ASP:HB2	1:B:1962:ARG:HH21	1.65	0.61
1:A:1461:GLU:HA	1:A:1464:LYS:HG2	1.82	0.61
1:A:3238:ASP:HA	1:A:3241:LYS:HD2	1.83	0.61
1:B:462:ARG:HD2	1:B:465:GLN:HE21	1.66	0.61
1:B:2449:LEU:HA	1:B:2453:ARG:HH21	1.66	0.61
1:B:2481:MET:HE3	1:B:2485:GLN:HG2	1.83	0.61
2:D:291:TYR:HE1	2:D:345:PRO:HB2	1.66	0.61
1:A:4040:PRO:HB3	1:A:4124:LEU:HD23	1.82	0.61
2:C:406:LYS:HA	2:C:423:GLU:HA	1.83	0.61
2:D:531:MET:HG2	2:D:578:TRP:H	1.66	0.61
2:D:539:LEU:HD21	2:D:551:LEU:HD11	1.83	0.61
4:H:80:VAL:HG22	4:H:82:PRO:HD3	1.82	0.61
1:A:439:LYS:HG2	1:A:442:ARG:HE	1.65	0.60
1:B:3782:ARG:NH1	1:B:3786:GLU:OE2	2.34	0.60
1:A:1181:LYS:HG2	1:A:1185:LYS:HZ1	1.66	0.60
1:B:484:LEU:HD13	1:B:564:ILE:HG12	1.83	0.60
1:B:468:LYS:O	1:B:471:ARG:HD3	2.01	0.60
1:B:3708:LEU:HD23	1:B:3809:SER:HA	1.83	0.60
1:A:205:ILE:HD13	1:A:255:GLU:HG2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2060:ARG:NH1	1:B:2128:ALA:O	2.34	0.60
1:B:3253:LYS:HA	1:B:3256:MET:HG2	1.83	0.60
3:F:87:GLU:HB2	3:F:108:ILE:HG23	1.83	0.60
2:D:607:ARG:NH1	2:D:610:GLU:OE2	2.34	0.60
1:B:465:GLN:HE22	1:B:546:TRP:HE1	1.50	0.60
1:B:613:LYS:HG3	1:B:682:LEU:HD12	1.83	0.60
1:B:1982:LEU:HD11	1:B:2012:MET:HB3	1.83	0.60
1:A:4168:ARG:NH2	1:A:4217:ASP:OD1	2.35	0.60
3:F:259:ARG:HD3	3:F:320:ILE:HG22	1.84	0.60
4:H:21:ILE:HG12	4:H:89:ILE:HD11	1.84	0.60
7:O:295:GLU:OE2	7:O:368:LYS:NZ	2.34	0.60
1:A:1491:ASP:O	1:A:1495:ASN:ND2	2.34	0.60
1:B:2257:LYS:NZ	1:B:2308:ASP:OD2	2.29	0.60
1:B:3073:GLU:OE2	1:B:3073:GLU:N	2.32	0.60
2:D:338:ALA:HA	2:D:350:GLY:HA2	1.84	0.60
2:D:551:LEU:HB3	2:D:563:ALA:HB3	1.82	0.60
7:P:95:ILE:HD11	7:P:352:PHE:HD2	1.66	0.60
6:K:36:HIS:CD2	6:L:76:GLY:HA3	2.36	0.60
1:B:195:HIS:O	1:B:198:GLN:NE2	2.35	0.59
1:B:485:ARG:O	1:B:487:GLN:NE2	2.35	0.59
1:B:3294:ASN:HB3	1:B:3391:PRO:HB3	1.84	0.59
1:B:3591:ASP:OD2	1:B:3596:ALA:N	2.35	0.59
3:F:178:VAL:HG22	3:F:219:LEU:HD13	1.83	0.59
1:A:44:ASP:HB2	1:B:130:PRO:HB3	1.84	0.59
1:A:119:ILE:HD12	1:B:155:ASN:HB2	1.84	0.59
1:A:2382:LEU:O	1:A:2416:GLN:NE2	2.34	0.59
1:A:3961:LEU:O	1:A:3997:ARG:NH1	2.34	0.59
2:D:485:HIS:NE2	2:D:487:ALA:O	2.35	0.59
1:A:147:GLU:HA	1:A:196:LEU:HD13	1.84	0.59
1:B:648:ILE:HD11	1:B:698:ILE:HB	1.82	0.59
1:B:2181:GLU:HG3	1:B:2244:LEU:HB2	1.83	0.59
1:B:2839:GLU:OE2	1:B:2839:GLU:N	2.29	0.59
3:F:231:CYS:HB2	3:F:271:TYR:HD1	1.68	0.59
1:A:2260:SER:OG	1:A:2262:ASP:OD1	2.17	0.59
1:A:3557:ASP:OD1	1:A:3743:ARG:NH1	2.34	0.59
1:A:4039:THR:HG23	1:A:4142:GLY:HA2	1.84	0.59
1:B:88:VAL:HG22	1:B:90:ASP:H	1.66	0.59
1:B:4039:THR:HG23	1:B:4142:GLY:HA2	1.83	0.59
1:B:4150:PRO:O	1:B:4195:ARG:NH2	2.35	0.59
6:L:45:ASN:HB3	6:L:49:GLN:HE22	1.67	0.59
1:A:1201:ARG:NH2	1:B:967:GLN:O	2.36	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:277:HIS:ND1	7:O:316:ARG:HB2	2.18	0.59
1:A:2841:GLU:OE1	1:A:2844:ARG:NH2	2.35	0.59
1:B:456:HIS:HA	1:B:459:LEU:HB2	1.85	0.59
1:B:1085:GLN:HE22	3:F:39:ILE:HD12	1.66	0.59
2:D:480:THR:OG1	2:D:528:TYR:O	2.17	0.59
5:J:54:TRP:CZ3	5:J:87:LYS:HB2	2.38	0.59
7:O:188:MET:HE2	7:O:224:GLY:HA2	1.85	0.59
7:O:211:SER:OG	7:O:213:ASP:OD1	2.18	0.59
1:A:81:ARG:HD3	1:A:99:ILE:HG13	1.85	0.59
1:B:177:LYS:O	1:B:177:LYS:HD3	2.03	0.59
1:B:1267:VAL:O	1:B:1382:SER:N	2.36	0.59
1:A:4444:GLN:HE21	1:A:4449:ARG:HA	1.67	0.59
1:A:4611:LEU:HB2	1:A:4619:ILE:HD11	1.85	0.59
1:B:581:MET:HE1	1:B:608:LEU:HD12	1.85	0.59
4:G:46:MET:SD	4:G:89:ILE:HG21	2.43	0.59
7:O:90:ASP:HB3	7:O:93:GLU:HB3	1.85	0.59
7:O:123:MET:HE3	7:O:137:TYR:HB3	1.84	0.59
1:A:4100:HIS:NE2	1:A:4129:GLU:OE2	2.36	0.59
1:B:721:GLU:OE2	1:B:736:LYS:NZ	2.36	0.59
1:B:864:LEU:HB2	1:B:877:ILE:HG21	1.85	0.58
1:B:869:TYR:HB2	1:B:914:ARG:HH21	1.68	0.58
2:D:559:GLU:HG2	2:D:560:VAL:HG13	1.85	0.58
4:G:69:LEU:H	4:G:79:MET:HE1	1.69	0.58
6:K:70:MET:HE1	6:L:77:LEU:HD13	1.83	0.58
1:A:1174:GLN:HA	1:A:1177:LYS:HG2	1.85	0.58
1:B:153:ILE:O	1:B:157:VAL:HG12	2.04	0.58
2:D:607:ARG:HG2	2:D:610:GLU:HG2	1.84	0.58
1:A:207:LEU:HG	1:A:209:ILE:HG12	1.84	0.58
1:A:296:GLU:OE2	1:A:300:THR:OG1	2.22	0.58
1:B:365:ARG:HD3	1:B:433:LEU:HD22	1.86	0.58
1:B:1131:PHE:O	1:B:1135:LEU:HG	2.03	0.58
1:A:274:GLU:OE1	1:A:376:ARG:NH2	2.36	0.58
4:G:46:MET:HA	4:G:49:PHE:CE2	2.38	0.58
1:B:552:ARG:O	1:B:555:GLU:HG2	2.03	0.58
1:B:2078:GLU:O	1:B:4415:ARG:NH1	2.36	0.58
3:F:62:GLU:O	3:F:67:LYS:NZ	2.37	0.58
5:I:8:ILE:HD13	5:I:18:GLN:NE2	2.18	0.58
6:K:54:LEU:HB3	6:K:63:TYR:CE2	2.38	0.58
1:A:2793:ILE:O	1:A:2836:ARG:NH1	2.37	0.58
1:A:3638:VAL:HG12	1:A:3681:THR:HB	1.86	0.58
1:B:3380:GLU:HA	1:B:3383:ASN:HD22	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:83:ASP:OD1	4:H:84:LYS:N	2.34	0.58
1:A:2626:THR:HB	1:A:2669:PRO:HG3	1.85	0.58
5:I:68:HIS:CG	5:I:73:PHE:HB2	2.38	0.58
1:A:185:LYS:HE3	1:B:189:LEU:HD23	1.86	0.58
1:A:405:ALA:HB3	1:A:408:GLU:HG2	1.86	0.58
1:B:584:ILE:HG23	1:B:587:ARG:HH21	1.69	0.58
1:A:3178:ASP:OD2	1:A:3585:ARG:NE	2.37	0.58
1:B:2102:ASN:OD1	1:B:2105:ARG:NH2	2.37	0.58
1:B:3367:MET:HE1	1:B:3400:LEU:HB3	1.85	0.58
7:O:309:PRO:HG2	7:O:325:VAL:HB	1.86	0.58
1:A:3172:THR:HG21	1:A:3694:SER:HB3	1.86	0.57
1:A:1695:HIS:HB3	1:A:1700:GLU:HG3	1.85	0.57
1:B:1453:ALA:O	1:B:1457:MET:HG2	2.04	0.57
1:B:4492:ILE:HG13	1:B:4507:ILE:HD13	1.86	0.57
3:F:72:THR:HG21	3:F:79:HIS:HA	1.85	0.57
7:O:147:LYS:NZ	7:P:136:ASP:OD2	2.34	0.57
7:P:94:TRP:HB3	7:P:409:CYS:HB3	1.85	0.57
1:A:1464:LYS:HA	1:A:1467:ARG:HB2	1.85	0.57
1:A:2172:ARG:HH22	1:A:2205:GLU:HG3	1.69	0.57
1:A:2877:LEU:HD11	1:A:2884:VAL:HG23	1.87	0.57
1:B:89:GLY:HA2	1:B:244:GLN:HG2	1.86	0.57
1:B:4096:LEU:HD13	1:B:4105:TRP:HH2	1.69	0.57
1:A:117:ALA:N	1:A:138:LEU:O	2.33	0.57
1:A:2091:ARG:HD2	1:A:2357:SER:HB2	1.87	0.57
1:A:4178:ARG:HH21	1:A:4296:MET:HG3	1.69	0.57
1:B:3172:THR:HG21	1:B:3694:SER:HB3	1.86	0.57
1:A:236:VAL:HG23	1:A:303:ILE:HB	1.85	0.57
1:B:264:ARG:NH2	1:B:268:SER:O	2.36	0.57
2:D:446:ASN:HA	2:D:460:CYS:HA	1.84	0.57
4:G:43:ALA:HA	4:G:46:MET:HG2	1.86	0.57
1:A:1195:ARG:NH2	3:F:96:GLU:O	2.37	0.57
1:A:2573:ASP:OD1	1:A:2576:ARG:NH2	2.38	0.57
1:A:2753:ARG:O	1:A:2763:ARG:NH1	2.28	0.57
1:B:4318:PRO:HG2	1:B:4325:ASN:HA	1.86	0.57
3:F:241:GLU:HA	3:F:246:TYR:HB2	1.86	0.57
6:L:62:LYS:HE3	6:L:113:ILE:HG12	1.86	0.57
1:B:2414:GLN:NE2	1:B:2418:ASP:OD2	2.29	0.57
1:B:4444:GLN:HE21	1:B:4449:ARG:HA	1.69	0.57
6:K:83:CYS:HB3	6:L:64:ILE:HA	1.86	0.57
7:P:174:ILE:HD11	7:P:195:VAL:HG11	1.85	0.57
1:B:264:ARG:NH1	1:B:274:GLU:OE2	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:361:PHE:CG	1:B:426:GLU:HG3	2.40	0.57
1:A:1623:ARG:NH2	1:A:1634:ASP:OD1	2.38	0.57
1:B:2063:GLU:O	1:B:2067:ASN:ND2	2.38	0.57
2:D:538:ALA:HB1	2:D:554:LEU:HB2	1.86	0.57
5:I:62:PHE:HE2	5:I:64:SER:HB3	1.69	0.57
5:J:43:LYS:NZ	5:J:47:ASP:OD2	2.37	0.57
1:A:4227:ALA:HB2	1:A:4233:ILE:HD12	1.85	0.56
1:B:2562:VAL:HG11	1:B:2755:MET:HB2	1.85	0.56
2:D:447:PHE:HE2	2:D:461:ARG:HD3	1.70	0.56
7:P:243:ASN:HB3	7:P:284:TRP:CZ3	2.40	0.56
1:A:2499:LEU:HD12	1:A:2514:LEU:HD23	1.87	0.56
1:B:1484:CYS:SG	1:B:1485:ARG:N	2.78	0.56
2:D:511:THR:HG23	2:D:512:LYS:HD3	1.86	0.56
1:A:3174:ARG:NH1	1:A:3650:ASN:OD1	2.38	0.56
1:B:264:ARG:O	1:B:376:ARG:NH1	2.37	0.56
1:B:1193:GLY:HA2	1:B:1196:LEU:HD12	1.86	0.56
1:B:3030:MET:HA	1:B:3030:MET:HE3	1.87	0.56
1:B:4168:ARG:NH2	1:B:4217:ASP:OD1	2.37	0.56
2:D:299:TYR:HB3	2:D:312:VAL:HB	1.88	0.56
2:D:359:LEU:HD22	2:D:415:LEU:HD13	1.87	0.56
1:A:1085:GLN:O	1:A:1089:ALA:N	2.35	0.56
1:B:2867:MET:HA	1:B:2867:MET:HE3	1.87	0.56
2:D:352:THR:HG23	2:D:354:SER:H	1.71	0.56
1:A:1491:ASP:OD1	1:A:1492:ASP:N	2.38	0.56
1:A:2961:ILE:HD11	1:A:2998:ASN:HB3	1.87	0.56
1:A:4492:ILE:HG22	1:A:4507:ILE:HD13	1.88	0.56
2:D:284:CYS:HB2	2:D:337:SER:HA	1.88	0.56
5:I:13:MET:SD	5:I:74:ILE:HB	2.45	0.56
1:A:3825:TYR:CZ	1:A:3875:MET:HG3	2.41	0.56
1:B:1210:TYR:HB2	1:B:1213:ASN:OD1	2.05	0.56
1:B:1213:ASN:HD21	5:J:8:ILE:HG22	1.71	0.56
1:B:1984:GLU:O	1:B:1987:ASN:ND2	2.38	0.56
2:C:496:LEU:HA	2:C:510:THR:HA	1.88	0.56
2:D:287:TRP:CD1	2:D:579:THR:HA	2.41	0.56
6:K:83:CYS:HB2	6:K:85:TRP:CZ3	2.40	0.56
7:O:244:GLN:NE2	7:O:285:ALA:O	2.39	0.56
1:A:55:ALA:HB3	1:A:101:TYR:HD2	1.70	0.56
1:B:116:LEU:HD23	1:B:139:THR:HB	1.86	0.56
1:A:3260:ILE:O	1:A:3264:LEU:N	2.34	0.56
1:A:3349:PRO:O	1:A:3353:ASN:ND2	2.39	0.56
1:B:4517:PRO:HG3	1:B:4611:LEU:HD13	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:384:VAL:HA	2:C:402:SER:HA	1.87	0.56
4:G:65:ASP:HB3	4:H:74:LYS:HD3	1.88	0.56
7:O:216:ILE:HB	7:O:230:PHE:HB2	1.87	0.56
1:A:1879:LEU:HD11	1:A:1914:GLU:HB3	1.86	0.56
1:A:2091:ARG:NH1	1:A:2320:ASP:OD1	2.38	0.56
1:B:38:VAL:HB	1:B:52:LEU:HD21	1.88	0.56
1:B:485:ARG:NH1	1:B:486:PRO:O	2.39	0.56
1:B:3124:ASP:OD1	1:B:3125:TYR:N	2.39	0.56
2:D:551:LEU:N	2:D:563:ALA:O	2.38	0.56
1:B:283:ARG:HG3	1:B:287:ARG:HH12	1.71	0.56
7:P:236:TRP:HB3	7:P:254:ASN:ND2	2.21	0.56
1:A:2757:ARG:HA	1:A:2763:ARG:HD3	1.88	0.55
1:B:231:ASP:OD1	1:B:232:PHE:N	2.39	0.55
1:B:956:LYS:N	1:B:985:GLU:OE2	2.39	0.55
1:B:3510:SER:HB3	1:B:3553:LEU:HD21	1.87	0.55
1:B:3779:GLU:OE2	1:B:3782:ARG:NH2	2.37	0.55
1:B:4611:LEU:HB2	1:B:4619:ILE:HD11	1.89	0.55
1:B:3276:MET:HE1	1:B:3412:LEU:HD13	1.88	0.55
1:A:1673:VAL:HG23	1:A:1692:ILE:HD11	1.87	0.55
1:A:3247:GLN:O	1:A:3251:GLU:N	2.34	0.55
1:A:4010:SER:HB2	1:A:4015:GLU:HA	1.88	0.55
1:B:2047:GLN:NE2	1:B:2067:ASN:OD1	2.40	0.55
2:D:359:LEU:HB2	2:D:415:LEU:HD22	1.88	0.55
1:B:3626:ALA:HA	1:B:3631:ASN:HB2	1.88	0.55
6:L:64:ILE:HB	6:L:109:PHE:HB2	1.88	0.55
7:O:110:PRO:HB3	7:O:400:VAL:HA	1.89	0.55
1:A:2686:MET:HE3	1:A:2703:LEU:HD11	1.89	0.55
1:B:2430:ASN:O	1:B:2435:LYS:NZ	2.39	0.55
1:B:3263:GLN:CD	1:B:3426:ASN:HB3	2.31	0.55
1:B:4543:VAL:HG11	1:B:4622:VAL:HB	1.89	0.55
2:C:551:LEU:O	2:C:562:THR:N	2.39	0.55
2:D:475:HIS:HD2	2:D:507:LYS:HE3	1.72	0.55
1:A:1763:GLU:OE2	1:A:1838:TRP:NE1	2.32	0.55
1:A:3659:ARG:NH2	1:B:3631:ASN:OD1	2.39	0.55
1:B:529:ASN:HB3	1:B:553:TYR:HE1	1.72	0.55
1:B:3270:VAL:HG22	1:B:3419:LEU:HB3	1.88	0.55
3:F:38:SER:O	3:F:40:LEU:N	2.39	0.55
4:G:11:LEU:HG	4:G:20:ILE:HD12	1.87	0.55
5:I:15:GLU:O	5:I:18:GLN:HB2	2.06	0.55
1:A:1219:GLY:HA2	1:A:1222:ASN:HD21	1.70	0.55
1:A:1554:SER:O	1:A:1558:LYS:NZ	2.35	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:186:ILE:O	1:B:190:GLU:HG2	2.07	0.55
1:B:1174:GLN:O	1:B:1178:ARG:NH1	2.40	0.55
1:B:2091:ARG:NH2	8:B:4701:ADP:O3A	2.40	0.55
5:I:77:TYR:CE2	5:I:82:ALA:HB2	2.42	0.55
1:B:399:ARG:O	1:B:399:ARG:NH1	2.35	0.55
1:B:1623:ARG:NH1	1:B:1629:PHE:O	2.39	0.55
5:I:43:LYS:HE3	5:J:67:THR:H	1.72	0.55
7:O:353:ILE:HB	7:O:365:TRP:HB2	1.89	0.55
1:A:256:ILE:HA	1:A:259:VAL:HG12	1.89	0.55
1:A:2228:SER:N	9:A:4702:ATP:O1B	2.40	0.55
7:O:186:ARG:HD3	7:O:224:GLY:HA3	1.88	0.55
1:B:1672:VAL:HA	1:B:1691:SER:HA	1.89	0.55
5:J:9:LYS:N	5:J:75:TYR:O	2.35	0.55
1:A:2174:GLU:OE1	1:A:2176:THR:OG1	2.22	0.54
1:A:3008:MET:HE1	1:A:3064:VAL:HG11	1.89	0.54
1:B:3046:SER:OG	1:B:3048:GLU:OE1	2.26	0.54
1:B:3114:ASP:O	1:B:3140:ARG:NH2	2.40	0.54
3:F:241:GLU:HA	3:F:246:TYR:H	1.72	0.54
1:A:236:VAL:HG13	1:A:237:GLU:HG2	1.88	0.54
1:A:382:GLU:HG3	1:A:452:ILE:HG13	1.88	0.54
1:B:561:GLU:OE1	1:B:594:ARG:NH1	2.40	0.54
1:B:1075:ASP:HB3	1:B:1078:LYS:HB3	1.88	0.54
1:A:85:LYS:HE2	1:A:112:LYS:HE3	1.89	0.54
1:A:2619:GLY:O	1:A:3014:ASN:ND2	2.36	0.54
1:A:4215:ALA:HB1	1:A:4247:MET:HE2	1.89	0.54
1:B:2644:THR:OG1	1:B:2647:GLY:O	2.23	0.54
1:B:3219:ARG:NH2	1:B:3472:VAL:HG13	2.23	0.54
2:D:555:ASN:ND2	2:D:610:GLU:OE1	2.26	0.54
1:A:25:ALA:O	1:A:66:ARG:NH1	2.34	0.54
1:A:1464:LYS:HB3	1:A:1467:ARG:HH21	1.70	0.54
1:A:3380:GLU:HA	1:A:3383:ASN:HD22	1.71	0.54
1:B:1969:SER:OG	1:B:4098:ASN:ND2	2.36	0.54
1:B:4485:ARG:HG2	1:B:4513:GLY:HA2	1.90	0.54
1:A:113:SER:H	1:A:142:GLU:HG3	1.72	0.54
1:B:186:ILE:HA	1:B:189:LEU:HD12	1.89	0.54
1:B:2956:LEU:HD13	1:B:2989:LYS:HB3	1.90	0.54
2:D:440:PRO:HG2	2:D:443:ASP:HB3	1.88	0.54
1:A:963:ARG:N	1:A:970:TYR:O	2.40	0.54
1:A:1699:ASN:OD1	1:A:1700:GLU:N	2.41	0.54
1:A:1958:ASP:HA	1:A:2017:THR:HB	1.89	0.54
1:B:257:GLN:NE2	1:B:319:ASP:OD1	2.34	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:530:VAL:HG12	1:B:549:ALA:HB1	1.90	0.54
5:I:53:THR:H	5:I:87:LYS:HE2	1.73	0.54
1:A:3243:MET:HE1	1:B:3243:MET:HE1	1.90	0.54
1:A:4549:GLN:HG3	1:A:4587:LEU:HB2	1.89	0.54
1:B:88:VAL:HB	1:B:95:GLU:HA	1.89	0.54
1:B:391:GLN:O	1:B:394:LYS:HG2	2.08	0.54
1:B:3366:LYS:O	1:B:3370:ASN:N	2.39	0.54
1:B:755:TRP:CG	2:D:453:GLU:HG3	2.43	0.54
1:B:2452:LEU:HD13	1:B:2729:ARG:HH21	1.73	0.54
1:B:2808:GLU:OE1	1:B:2811:ARG:NH2	2.36	0.54
1:B:3914:ILE:O	1:B:3937:ARG:NH1	2.41	0.54
1:B:3942:PRO:O	1:B:3945:LYS:NZ	2.35	0.54
5:I:65:TYR:CD2	5:J:40:ALA:HA	2.43	0.54
1:A:446:LEU:HD23	1:A:446:LEU:H	1.73	0.54
1:B:636:SER:HB2	1:B:641:LEU:HB3	1.89	0.54
1:B:991:MET:HE1	1:B:1020:ARG:HH21	1.72	0.54
1:B:1139:MET:O	1:B:1143:HIS:ND1	2.41	0.54
1:B:4042:LEU:HD23	1:B:4142:GLY:HA3	1.89	0.54
1:A:3364:ARG:HA	1:A:3367:MET:HE2	1.90	0.54
1:A:4088:VAL:HG11	1:A:4116:LEU:HD21	1.90	0.54
1:B:904:ASP:HA	1:B:907:ILE:HG22	1.90	0.54
1:B:2671:MET:HE3	1:B:2721:LYS:HB3	1.89	0.54
5:I:55:HIS:NE2	5:I:88:SER:O	2.39	0.54
5:J:18:GLN:HG2	5:J:74:ILE:HD12	1.90	0.54
6:K:70:MET:HB2	6:K:103:TYR:HB2	1.89	0.54
7:P:110:PRO:HB3	7:P:400:VAL:HA	1.90	0.54
1:A:152:PHE:CZ	1:B:121:ARG:HA	2.43	0.53
1:A:1565:THR:O	1:A:1569:GLN:NE2	2.41	0.53
1:B:251:ARG:NH1	1:B:251:ARG:O	2.40	0.53
1:B:1879:LEU:HD13	1:B:1918:ALA:HB2	1.88	0.53
4:G:54:ARG:NH2	4:G:64:ASN:O	2.39	0.53
7:P:101:LYS:HE3	7:P:394:TYR:HE2	1.73	0.53
1:A:210:HIS:CD2	1:A:212:MET:HG2	2.43	0.53
1:A:228:LYS:N	1:A:231:ASP:OD2	2.41	0.53
1:B:1213:ASN:HA	5:J:10:ASN:HA	1.90	0.53
1:A:53:GLU:HA	1:A:56:LEU:HB3	1.90	0.53
1:A:78:LEU:HD13	1:A:107:ILE:HG22	1.89	0.53
1:A:242:LEU:HB3	1:A:309:ARG:HE	1.73	0.53
1:A:3114:ASP:O	1:A:3140:ARG:NH2	2.41	0.53
1:B:83:THR:O	1:B:112:LYS:NZ	2.40	0.53
6:K:25:ILE:HA	6:K:46:VAL:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1467:ARG:HG2	1:A:1523:TRP:HZ2	1.72	0.53
1:B:1210:TYR:CE2	5:J:7:VAL:HA	2.44	0.53
1:B:1213:ASN:HB3	5:J:11:ALA:HB3	1.91	0.53
1:B:1964:GLU:HB2	1:B:1967:MET:HB2	1.91	0.53
3:F:272:THR:HA	3:F:279:ASN:HD22	1.74	0.53
4:H:69:LEU:HB3	4:H:80:VAL:HG13	1.90	0.53
5:I:77:TYR:CZ	5:I:82:ALA:HB2	2.43	0.53
1:A:1201:ARG:NH1	1:B:1058:GLN:OE1	2.39	0.53
1:A:2973:ASP:OD2	1:A:3007:ARG:NH2	2.40	0.53
1:A:3042:LEU:HB3	1:A:3044:LEU:HD23	1.89	0.53
1:B:653:GLN:NE2	2:D:476:GLN:OE1	2.34	0.53
1:B:906:GLU:OE2	1:B:909:ARG:NH2	2.42	0.53
1:B:2943:LYS:N	8:B:4704:ADP:O1B	2.39	0.53
3:F:132:LEU:HD11	3:F:228:LEU:HD23	1.90	0.53
5:J:68:HIS:ND1	5:J:69:GLU:O	2.30	0.53
1:A:96:LYS:NZ	1:A:97:GLU:O	2.40	0.53
1:A:2269:ASP:OD2	1:A:2272:THR:OG1	2.24	0.53
1:A:2607:SER:HA	1:A:2610:ARG:HE	1.73	0.53
1:B:631:GLN:HA	1:B:634:LYS:HE2	1.91	0.53
1:B:1183:PHE:O	1:B:1187:VAL:HG23	2.09	0.53
1:B:1188:GLU:O	1:B:1191:ARG:HG2	2.09	0.53
1:A:1507:MET:HE2	1:A:1507:MET:N	2.24	0.53
1:A:2262:ASP:HB2	1:A:2267:THR:HG22	1.90	0.53
1:B:1892:MET:HA	1:B:1892:MET:HE3	1.90	0.53
7:P:334:LEU:HD23	7:P:365:TRP:HE3	1.73	0.53
1:A:2018:MET:HE1	1:A:2028:LEU:HD13	1.91	0.53
1:A:2592:VAL:HG23	1:A:2731:VAL:HG21	1.90	0.53
1:A:2943:LYS:N	8:A:4704:ADP:O1B	2.41	0.53
1:B:694:ASN:ND2	1:B:697:GLU:OE1	2.42	0.53
1:B:1161:ALA:C	1:B:1163:THR:H	2.17	0.53
4:G:79:MET:HB3	4:G:90:VAL:HB	1.90	0.53
1:B:78:LEU:HB3	1:B:104:ASN:HB2	1.91	0.53
3:F:245:ASP:OD1	3:F:247:ARG:NH1	2.41	0.53
4:G:26:GLU:HG3	4:G:28:ILE:HG12	1.90	0.53
7:P:216:ILE:HB	7:P:230:PHE:HB2	1.91	0.53
1:A:2684:ARG:CZ	1:A:2726:ARG:HD3	2.39	0.53
1:B:213:ILE:HD13	1:B:300:THR:HG22	1.91	0.53
2:D:584:GLU:HA	2:D:598:ASP:HA	1.91	0.53
3:F:73:LYS:HD2	3:F:274:VAL:HG23	1.91	0.53
7:P:101:LYS:HG2	7:P:102:TYR:CD2	2.44	0.53
1:A:1219:GLY:HA2	1:A:1222:ASN:ND2	2.25	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:91:GLU:HA	1:B:243:ASN:HB3	1.91	0.52
5:I:36:LYS:NZ	5:I:37:ASP:OD1	2.39	0.52
1:A:400:LYS:HD2	1:A:400:LYS:O	2.09	0.52
1:A:2457:SER:O	1:A:2460:SER:OG	2.27	0.52
1:B:1213:ASN:HD22	5:J:10:ASN:C	2.16	0.52
1:B:3478:LEU:HD13	1:B:3767:ILE:HG23	1.91	0.52
7:O:322:MET:HE3	7:O:331:LEU:HD12	1.91	0.52
1:A:186:ILE:O	1:A:190:GLU:HG2	2.09	0.52
1:A:2935:LEU:HB2	1:A:3067:THR:HG22	1.92	0.52
2:D:475:HIS:HB2	2:D:507:LYS:HD2	1.91	0.52
2:D:527:VAL:HA	2:D:544:ASP:HA	1.92	0.52
6:L:62:LYS:HG3	6:L:113:ILE:HG12	1.91	0.52
1:A:2262:ASP:OD1	1:A:2263:HIS:N	2.42	0.52
1:A:3772:ASN:OD1	1:A:3775:ARG:NH1	2.42	0.52
1:B:4239:PRO:HB2	1:B:4242:ALA:HB3	1.91	0.52
1:A:2538:GLU:HB3	1:A:2548:TRP:CE2	2.44	0.52
2:D:427:LYS:O	2:D:430:LYS:HG3	2.09	0.52
1:A:1174:GLN:O	1:A:1178:ARG:NH1	2.38	0.52
1:A:2446:ILE:HD11	1:A:2714:PRO:HB3	1.91	0.52
1:B:961:GLU:OE2	1:B:963:ARG:NH2	2.42	0.52
1:B:1043:ILE:HA	1:B:1102:PHE:HE2	1.75	0.52
1:B:1213:ASN:ND2	5:J:8:ILE:HG22	2.25	0.52
1:B:1937:ASP:CG	1:B:2273:ARG:HH22	2.17	0.52
7:P:212:ARG:HD3	7:P:236:TRP:CG	2.45	0.52
1:B:717:ILE:HA	1:B:824:TRP:HE3	1.73	0.52
1:B:819:GLY:HA3	1:B:832:TYR:CZ	2.45	0.52
1:B:1026:MET:HE3	1:B:1028:ASP:HB2	1.91	0.52
1:B:2481:MET:HE2	1:B:2486:LEU:HA	1.90	0.52
2:D:346:ASN:OD1	2:D:363:ARG:N	2.38	0.52
5:I:64:SER:H	5:J:36:LYS:HD3	1.75	0.52
1:A:152:PHE:HZ	1:B:121:ARG:HA	1.74	0.52
1:A:153:ILE:O	1:A:157:VAL:HG22	2.10	0.52
1:A:1147:SER:O	1:A:1151:GLN:HG2	2.10	0.52
1:A:1745:TYR:O	1:A:1807:LYS:NZ	2.36	0.52
1:A:2614:ASP:HA	1:A:2657:LYS:NZ	2.25	0.52
1:A:3284:LYS:O	1:A:3402:TYR:OH	2.20	0.52
1:B:997:PRO:HA	1:B:1018:PHE:HA	1.90	0.52
3:E:135:PHE:H	3:E:229:VAL:HA	1.73	0.52
1:A:84:LEU:HB3	1:A:98:PHE:HB3	1.91	0.52
1:B:852:ILE:O	1:B:855:GLU:HG3	2.10	0.52
1:B:1627:PRO:HB3	1:B:1950:GLN:HB3	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1959:GLU:OE1	1:B:2025:ARG:NH1	2.42	0.52
1:B:2290:SER:HB2	1:B:2295:LEU:HG	1.92	0.52
1:B:3199:MET:HG3	7:P:150:THR:O	2.10	0.52
1:A:1912:LYS:N	8:A:4701:ADP:O1B	2.38	0.52
1:B:285:LEU:HB2	1:B:322:LEU:HD11	1.91	0.52
2:D:413:ASP:OD1	2:D:414:MET:N	2.43	0.52
7:O:201:MET:HE2	7:O:201:MET:HA	1.93	0.52
1:A:1962:ARG:NH2	1:A:2314:ASN:OD1	2.44	0.51
1:A:2302:VAL:HA	1:A:2342:MET:HB3	1.91	0.51
1:A:3254:LYS:O	1:A:3258:GLN:N	2.42	0.51
1:A:3483:SER:HA	1:A:3486:ARG:HE	1.75	0.51
2:D:613:ARG:HA	2:D:616:ARG:HG2	1.92	0.51
3:F:139:MET:HA	3:F:142:PRO:HB3	1.92	0.51
3:F:252:ASP:HB3	3:F:327:PHE:HE1	1.75	0.51
5:I:74:ILE:HG12	5:I:76:PHE:HD1	1.74	0.51
5:J:34:ILE:O	5:J:38:ILE:HG12	2.09	0.51
7:O:366:ASP:HB2	7:O:373:MET:SD	2.49	0.51
1:A:3135:GLN:O	1:A:3137:PRO:HD3	2.10	0.51
1:A:4106:LEU:HD13	1:A:4138:LEU:HD22	1.93	0.51
1:B:480:ILE:HG23	1:B:484:LEU:HB2	1.92	0.51
1:B:1508:LYS:HG2	1:B:1513:TYR:CZ	2.46	0.51
4:G:56:THR:HG23	4:H:45:LEU:HG	1.92	0.51
1:A:29:VAL:O	1:A:33:HIS:ND1	2.43	0.51
1:A:3502:THR:HG22	1:A:3542:GLN:HB3	1.91	0.51
1:B:243:ASN:HA	1:B:246:GLN:OE1	2.09	0.51
1:B:1937:ASP:HA	1:B:1967:MET:CE	2.28	0.51
1:B:3340:SER:O	1:B:3346:ASN:ND2	2.43	0.51
2:D:332:GLN:OE1	2:D:372:ARG:NH1	2.43	0.51
4:G:23:VAL:HA	4:G:29:PRO:HA	1.92	0.51
1:A:3251:GLU:HA	1:A:3254:LYS:HB2	1.92	0.51
1:A:3366:LYS:O	1:A:3370:ASN:N	2.40	0.51
1:B:420:PHE:CE2	1:B:460:GLN:HG2	2.46	0.51
1:B:448:MET:HA	1:B:448:MET:HE3	1.91	0.51
1:B:960:HIS:ND1	1:B:978:CYS:SG	2.83	0.51
1:B:1166:ALA:O	1:B:1170:ILE:HG12	2.10	0.51
4:G:45:LEU:HD21	4:H:56:THR:HA	1.92	0.51
1:A:3322:GLU:OE2	1:A:3377:TYR:OH	2.27	0.51
1:A:3909:LEU:HB3	1:A:4344:LEU:HD13	1.93	0.51
1:B:465:GLN:HE22	1:B:546:TRP:NE1	2.09	0.51
1:B:613:LYS:HE2	1:B:682:LEU:HB2	1.92	0.51
1:B:3292:ALA:HA	1:B:3395:TRP:HZ2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:8:ILE:HA	5:I:76:PHE:CB	2.40	0.51
5:I:29:LEU:HD22	5:I:38:ILE:HG21	1.91	0.51
1:A:1455:GLY:HA3	1:A:1512:TYR:HE2	1.76	0.51
1:B:689:PHE:HA	1:B:692:LYS:HE3	1.92	0.51
1:B:4190:ILE:HD12	1:B:4201:TRP:HZ2	1.75	0.51
5:I:74:ILE:HG22	5:I:85:LEU:O	2.10	0.51
1:A:2956:LEU:HD13	1:A:2991:ALA:HB2	1.91	0.51
1:B:479:VAL:HG11	1:B:590:ALA:HB2	1.92	0.51
1:B:1085:GLN:HA	1:B:1088:LYS:HE3	1.93	0.51
1:B:1191:ARG:HA	1:B:1194:GLN:HG3	1.93	0.51
1:B:1623:ARG:NH2	1:B:1634:ASP:OD1	2.44	0.51
5:J:13:MET:HG2	5:J:73:PHE:O	2.11	0.51
7:O:151:ASP:CG	7:O:152:SER:H	2.18	0.51
7:P:290:TYR:HD2	7:P:307:PRO:HG2	1.76	0.51
1:A:253:ILE:HD12	1:A:256:ILE:HD11	1.91	0.51
1:A:1835:SER:OG	1:A:1837:GLU:OE1	2.29	0.51
1:A:2094:LYS:HZ2	8:A:4701:ADP:HO2'	1.56	0.51
7:O:243:ASN:ND2	7:O:245:ASP:OD1	2.44	0.51
7:P:96:PRO:HA	7:P:408:GLU:O	2.11	0.51
1:A:4409:LEU:HD11	1:A:4558:PHE:HE2	1.76	0.51
1:B:3517:ALA:HB1	1:B:3525:ARG:HG2	1.93	0.51
1:A:1462:PHE:O	1:A:1466:ILE:HD12	2.11	0.51
1:A:2285:ARG:NH1	1:A:2331:GLU:OE2	2.35	0.51
1:B:242:LEU:HD23	1:B:309:ARG:HE	1.76	0.51
1:B:3129:VAL:HG21	1:B:3149:PHE:HB2	1.92	0.51
3:F:120:LYS:HD3	3:F:162:LYS:HE2	1.93	0.51
3:F:227:VAL:HG13	3:F:267:ALA:HB2	1.93	0.51
4:H:18:GLN:HB2	4:H:91:ILE:HG23	1.93	0.51
4:H:82:PRO:HB3	4:H:87:PHE:HD1	1.76	0.51
6:K:54:LEU:HB3	6:K:63:TYR:CD2	2.46	0.51
6:L:22:LYS:HE2	6:L:97:TRP:HD1	1.76	0.51
1:A:189:LEU:O	1:A:193:LEU:HD23	2.11	0.50
1:A:447:LYS:O	1:A:448:MET:HE2	2.11	0.50
1:A:2290:SER:HB2	1:A:2295:LEU:HG	1.92	0.50
1:A:2989:LYS:HD2	1:A:3061:ASN:HD22	1.75	0.50
1:A:3263:GLN:CD	1:A:3426:ASN:HB3	2.37	0.50
1:B:35:ARG:HD2	1:B:56:LEU:HD11	1.93	0.50
1:B:241:PHE:O	1:B:245:LEU:HG	2.11	0.50
1:B:905:MET:O	1:B:908:GLU:HG2	2.11	0.50
1:B:1514:LYS:HA	1:B:1517:GLU:OE2	2.11	0.50
7:P:186:ARG:NH2	7:P:222:GLN:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3161:LEU:HD11	1:B:3524:MET:HE1	1.93	0.50
1:B:3253:LYS:HD3	1:B:3436:MET:HG3	1.93	0.50
6:K:61:PHE:HD1	6:K:112:SER:HA	1.77	0.50
6:L:17:VAL:HG13	6:L:54:LEU:HD21	1.93	0.50
7:O:201:MET:HG3	7:O:206:HIS:HB2	1.92	0.50
1:A:179:ALA:HA	1:A:182:VAL:HG22	1.93	0.50
1:A:2181:GLU:HG3	1:A:2244:LEU:HB2	1.93	0.50
1:B:158:ALA:HB3	1:B:159:PRO:HD3	1.94	0.50
1:B:180:PRO:O	1:B:184:LYS:NZ	2.45	0.50
1:B:440:ARG:NH1	1:B:444:GLU:HB2	2.26	0.50
1:B:569:ARG:NH1	1:B:603:GLU:OE1	2.45	0.50
1:B:1032:ALA:HA	1:B:1035:GLU:HG2	1.94	0.50
1:B:2592:VAL:HG23	1:B:2731:VAL:HG11	1.93	0.50
1:B:4099:VAL:HB	1:B:4106:LEU:HD21	1.92	0.50
5:I:57:ILE:HD13	5:J:57:ILE:HD12	1.92	0.50
5:J:8:ILE:HA	5:J:76:PHE:HA	1.93	0.50
1:A:1350:PRO:HA	1:A:1430:THR:HA	1.93	0.50
1:B:210:HIS:CD2	1:B:244:GLN:HB3	2.47	0.50
1:B:1978:ILE:HD11	1:B:2001:LEU:HD11	1.92	0.50
1:B:2085:HIS:HB2	1:B:2361:MET:HE2	1.93	0.50
1:B:4545:VAL:HG12	1:B:4588:THR:HG22	1.93	0.50
1:A:185:LYS:HE3	1:B:189:LEU:HA	1.93	0.50
1:A:456:HIS:NE2	1:A:460:GLN:OE1	2.43	0.50
1:A:1229:ASP:CG	1:A:1233:GLN:HE22	2.19	0.50
1:A:2039:LEU:HD12	1:A:4254:GLY:HA2	1.94	0.50
1:A:2556:GLU:OE2	1:A:2753:ARG:NH1	2.44	0.50
1:A:3394:LYS:HA	1:A:3397:ILE:HD12	1.93	0.50
1:A:4030:ILE:HA	1:A:4034:GLU:HG3	1.94	0.50
1:B:2910:VAL:HG11	1:B:3105:VAL:HA	1.93	0.50
2:D:275:ARG:O	2:D:280:ARG:NH1	2.43	0.50
2:D:481:GLY:HA3	2:D:529:ASP:HA	1.94	0.50
4:G:14:GLN:NE2	4:G:92:GLN:OE1	2.43	0.50
7:O:350:GLY:O	7:O:367:TYR:OH	2.30	0.50
1:A:1533:LEU:HD13	1:A:1598:GLN:OE1	2.12	0.50
1:A:2221:MET:HG3	1:A:2343:PHE:HB2	1.93	0.50
1:A:3360:SER:HA	1:A:3363:ILE:HD12	1.93	0.50
5:J:12:ASP:N	5:J:73:PHE:O	2.44	0.50
5:J:13:MET:HE1	5:J:54:TRP:CH2	2.47	0.50
1:A:2134:GLN:HE21	1:A:2165:PHE:HD2	1.60	0.50
1:B:1126:GLU:OE1	1:B:1130:LYS:NZ	2.37	0.50
1:B:1194:GLN:HG2	1:B:1211:ILE:HG21	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3597:THR:O	1:B:3601:MET:HG2	2.12	0.50
2:C:551:LEU:N	2:C:563:ALA:O	2.36	0.50
1:A:339:PHE:HB2	1:A:340:PRO:HD3	1.94	0.50
1:B:349:GLU:OE1	1:B:349:GLU:N	2.45	0.50
1:B:354:ARG:HH22	1:B:418:GLU:HG2	1.76	0.50
1:B:921:ALA:O	1:B:924:GLN:HG3	2.10	0.50
1:B:1539:ASP:OD2	1:B:2292:ARG:NH2	2.45	0.50
1:B:1612:GLN:NE2	1:B:1635:GLU:OE1	2.44	0.50
1:B:3230:GLU:HA	1:B:3233:ASN:HD21	1.77	0.50
1:B:3791:MET:HE2	1:B:3791:MET:N	2.27	0.50
3:F:216:ASP:OD1	3:F:217:ASN:N	2.44	0.50
5:J:86:PHE:HE2	5:J:88:SER:HB3	1.76	0.50
1:A:1153:LEU:HD11	1:A:1228:LYS:HG3	1.94	0.50
1:A:1769:MET:SD	1:A:1777:PRO:HD2	2.52	0.50
1:A:2080:LEU:O	1:A:4415:ARG:NH1	2.45	0.50
1:A:2481:MET:SD	1:A:2485:GLN:HB3	2.52	0.50
1:A:3246:ASP:HB3	1:A:3444:ILE:HD11	1.93	0.50
1:B:1519:ASP:OD1	1:B:1520:ALA:N	2.44	0.50
6:L:99:ASN:ND2	6:L:102:MET:SD	2.84	0.50
1:A:1978:ILE:HD11	1:A:2001:LEU:HD11	1.93	0.49
1:A:2162:SER:HG	1:A:4406:LYS:NZ	2.09	0.49
1:A:3129:VAL:HG21	1:A:3149:PHE:HB2	1.94	0.49
1:A:3157:ALA:HB1	1:A:3524:MET:HE2	1.94	0.49
1:B:913:VAL:O	1:B:916:GLN:HG2	2.12	0.49
1:B:2488:ARG:O	1:B:2492:ARG:HG2	2.11	0.49
1:B:3657:GLY:HA2	7:O:172:MET:SD	2.52	0.49
3:F:39:ILE:HA	3:F:42:GLU:HG2	1.92	0.49
7:P:254:ASN:HA	7:P:278:VAL:HG13	1.94	0.49
1:A:1146:ILE:HG22	1:A:1150:ARG:HE	1.75	0.49
1:A:1467:ARG:O	1:A:1471:ASN:ND2	2.45	0.49
1:A:3750:LEU:O	1:A:3754:ASN:ND2	2.44	0.49
1:B:414:VAL:HA	1:B:417:PHE:HD2	1.77	0.49
1:B:960:HIS:CE1	1:B:1107:ILE:HG22	2.47	0.49
6:K:61:PHE:HB2	6:K:63:TYR:CE1	2.47	0.49
1:A:213:ILE:HB	1:A:241:PHE:HZ	1.77	0.49
1:A:272:LEU:HD13	1:A:275:ILE:HD11	1.94	0.49
1:A:3935:VAL:HG13	1:A:3947:LEU:HD23	1.94	0.49
1:B:80:GLU:O	1:B:102:ASN:N	2.42	0.49
1:B:1457:MET:O	1:B:1460:GLU:HG3	2.12	0.49
1:B:1897:GLU:O	1:B:1899:ARG:NH1	2.45	0.49
1:B:2347:ASP:OD1	1:B:2348:LEU:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2684:ARG:HD2	1:B:2726:ARG:HG2	1.94	0.49
1:B:3930:GLU:OE1	1:B:3930:GLU:N	2.42	0.49
4:G:46:MET:O	4:G:50:ILE:HG12	2.12	0.49
5:I:4:ARG:CZ	5:I:79:GLY:HA3	2.43	0.49
1:A:415:ALA:O	1:A:418:GLU:HG3	2.12	0.49
1:A:3377:TYR:HB3	1:A:3397:ILE:HD11	1.93	0.49
1:B:146:TYR:CG	1:B:196:LEU:HB3	2.48	0.49
1:B:1198:GLU:O	1:B:1201:ARG:NH1	2.45	0.49
1:B:1457:MET:O	1:B:1460:GLU:N	2.45	0.49
1:B:2388:ASP:OD1	1:B:2389:GLU:N	2.46	0.49
1:B:3158:ASN:ND2	1:B:3169:MET:O	2.42	0.49
1:B:4037:PRO:HB2	1:B:4118:PRO:HG2	1.94	0.49
3:F:56:ASN:OD1	3:F:57:ILE:N	2.45	0.49
5:J:60:ARG:NH1	5:J:61:ASN:HB3	2.27	0.49
5:J:68:HIS:CG	5:J:73:PHE:HB2	2.47	0.49
1:A:1393:TYR:O	1:A:1395:LYS:N	2.45	0.49
1:A:2175:MET:SD	1:A:2175:MET:N	2.85	0.49
1:A:3294:ASN:HB3	1:A:3391:PRO:HB3	1.94	0.49
1:B:170:LYS:NZ	1:B:176:ASP:O	2.45	0.49
1:B:292:ARG:NH2	1:B:316:PHE:O	2.44	0.49
2:D:422:MET:HE1	2:D:424:LEU:HA	1.94	0.49
1:A:165:ILE:HG23	1:A:170:LYS:HB3	1.93	0.49
1:A:193:LEU:HD13	1:B:182:VAL:HG11	1.93	0.49
1:A:423:TRP:NE1	1:A:457:ARG:HH12	2.10	0.49
1:A:1973:GLN:NE2	1:A:1977:CYS:SG	2.86	0.49
1:B:406:TYR:CD2	1:B:474:GLU:HG2	2.48	0.49
2:D:282:VAL:HG12	2:D:575:ARG:HH12	1.76	0.49
2:D:382:HIS:CG	2:D:404:ASP:HB2	2.47	0.49
5:I:8:ILE:HG23	5:I:76:PHE:HB3	1.95	0.49
1:B:1457:MET:HA	1:B:1460:GLU:HG3	1.94	0.49
1:B:1667:ASN:ND2	1:B:1672:VAL:HG12	2.27	0.49
3:E:229:VAL:O	3:E:269:LEU:HA	2.12	0.49
1:A:434:LEU:O	1:A:438:VAL:HG23	2.13	0.49
1:A:3885:MET:HE1	1:A:4005:ALA:HB1	1.93	0.49
1:A:4385:SER:O	1:A:4389:HIS:ND1	2.40	0.49
1:B:854:GLU:HA	1:B:857:ILE:HG22	1.95	0.49
1:B:922:TRP:CH2	1:B:986:MET:HB3	2.48	0.49
1:B:1013:THR:OG1	1:B:1014:GLU:N	2.38	0.49
1:B:1533:LEU:HD11	1:B:1597:VAL:HG22	1.94	0.49
1:B:2138:ILE:HD12	1:B:2161:LEU:HD22	1.94	0.49
2:D:504:TRP:CD1	2:D:523:ASN:H	2.31	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:68:HIS:CD2	5:I:73:PHE:HB2	2.47	0.49
1:A:1952:GLY:HA2	1:A:2012:MET:HB2	1.94	0.49
1:A:3659:ARG:HH12	1:B:3631:ASN:HD21	1.61	0.49
1:B:80:GLU:HB3	1:B:102:ASN:HB2	1.95	0.49
1:B:264:ARG:NH1	1:B:265:ASP:O	2.46	0.49
1:B:537:ASP:O	1:B:543:THR:OG1	2.19	0.49
1:B:650:TRP:CE2	1:B:654:ILE:HD11	2.48	0.49
1:B:842:ASN:O	1:B:845:GLU:HG3	2.13	0.49
1:B:3653:VAL:HG12	1:B:3662:ILE:HB	1.94	0.49
2:D:297:ALA:HB3	2:D:314:LEU:HB3	1.95	0.49
2:D:390:VAL:HG11	2:D:447:PHE:HZ	1.77	0.49
3:F:234:CYS:SG	3:F:271:TYR:HB3	2.53	0.49
7:P:321:LYS:HG2	7:P:333:THR:HG22	1.94	0.49
1:A:2934:LEU:HD11	1:A:3068:MET:HE2	1.95	0.49
1:B:121:ARG:NH1	1:B:133:SER:O	2.42	0.49
1:B:2065:LEU:HD21	1:B:2134:GLN:HG2	1.95	0.49
1:B:2999:VAL:HG11	1:B:3005:LEU:HG	1.95	0.49
1:A:1478:VAL:HG23	1:A:1488:ARG:NH1	2.28	0.48
1:B:3928:THR:HG22	1:B:3929:VAL:H	1.78	0.48
4:G:76:ASN:HA	4:G:94:PRO:HD3	1.93	0.48
7:P:312:LEU:HD21	7:P:320:ILE:HG23	1.94	0.48
1:A:34:LEU:O	1:A:38:VAL:HG13	2.13	0.48
1:A:3606:ASP:OD1	1:A:3607:ARG:N	2.46	0.48
1:B:129:LYS:HD2	1:B:130:PRO:HD2	1.95	0.48
1:B:254:ARG:NH2	1:B:257:GLN:OE1	2.35	0.48
1:B:1204:PHE:H	5:J:5:LYS:HE3	1.78	0.48
1:B:3024:ASP:OD1	1:B:3025:GLU:N	2.46	0.48
1:B:3030:MET:HG3	1:B:3047:HIS:CE1	2.47	0.48
1:B:4227:ALA:HB2	1:B:4233:ILE:HD12	1.95	0.48
6:L:72:LYS:HG2	6:L:103:TYR:CE2	2.49	0.48
1:A:189:LEU:HD13	1:B:185:LYS:HE2	1.96	0.48
1:B:246:GLN:CD	1:B:309:ARG:HD3	2.38	0.48
1:B:988:ALA:O	1:B:992:VAL:HG23	2.12	0.48
1:B:1495:ASN:HA	1:B:1498:LYS:HZ2	1.79	0.48
3:F:238:SER:O	3:F:241:GLU:HG2	2.12	0.48
4:G:22:VAL:HG11	4:G:86:TYR:HB3	1.93	0.48
4:G:49:PHE:O	4:G:52:LYS:HG2	2.14	0.48
4:G:69:LEU:HD11	4:H:69:LEU:HD11	1.96	0.48
7:P:228:LYS:NZ	7:P:263:VAL:O	2.46	0.48
1:A:128:ASP:OD1	1:A:129:LYS:N	2.45	0.48
1:A:1476:ASP:HB3	1:A:1488:ARG:CZ	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:TYR:O	1:B:290:GLU:HG2	2.13	0.48
1:B:585:PHE:CD2	1:B:668:VAL:HG23	2.49	0.48
1:B:1126:GLU:O	1:B:1129:SER:OG	2.29	0.48
1:B:1839:LEU:O	1:B:1843:ARG:NH1	2.46	0.48
1:B:2917:ASP:OD2	1:B:2921:ARG:NH2	2.45	0.48
1:B:3135:GLN:O	1:B:3137:PRO:HD3	2.13	0.48
1:B:3381:ILE:HD12	1:B:3390:GLY:HA2	1.95	0.48
1:B:4160:THR:HG23	1:B:4212:LEU:HD21	1.94	0.48
2:C:187:LYS:HZ2	4:G:30:ILE:HA	1.77	0.48
2:C:204:THR:HA	4:G:10:ARG:HH12	1.79	0.48
1:A:3510:SER:HB3	1:A:3553:LEU:HD21	1.95	0.48
1:B:246:GLN:NE2	1:B:309:ARG:CD	2.75	0.48
2:D:296:VAL:HG13	2:D:340:PHE:CZ	2.48	0.48
1:B:804:LEU:HD11	1:B:899:TRP:CD1	2.49	0.48
1:B:1060:LEU:HD22	1:B:1119:LYS:HE2	1.96	0.48
1:B:2855:LEU:HD21	1:B:2863:ARG:HG2	1.95	0.48
1:B:3360:SER:HA	1:B:3363:ILE:HD12	1.96	0.48
2:D:334:ALA:O	2:D:353:TYR:N	2.39	0.48
4:G:21:ILE:HG23	4:G:89:ILE:HG13	1.95	0.48
7:P:196:SER:OG	7:P:236:TRP:NE1	2.36	0.48
1:A:354:ARG:NH1	1:A:355:GLN:HG2	2.28	0.48
1:A:4549:GLN:HA	1:A:4587:LEU:HD22	1.96	0.48
1:B:779:ILE:HA	1:B:782:ILE:HG22	1.95	0.48
1:B:790:ARG:O	1:B:794:LYS:HG2	2.14	0.48
1:B:1071:ARG:NH1	3:F:43:VAL:HA	2.28	0.48
1:B:2969:GLY:HA2	1:B:3004:PHE:HE1	1.77	0.48
1:B:3440:LEU:O	1:B:3444:ILE:N	2.35	0.48
2:C:188:GLN:O	2:C:192:HIS:ND1	2.43	0.48
2:D:504:TRP:CD1	2:D:522:ASP:H	2.30	0.48
7:P:218:MET:HE3	7:P:228:LYS:HE2	1.96	0.48
1:A:209:ILE:HA	1:A:248:GLY:HA3	1.96	0.48
1:A:285:LEU:HA	1:A:288:ILE:HG12	1.96	0.48
1:B:582:PHE:CE1	1:B:668:VAL:HG11	2.48	0.48
1:B:770:GLN:HG2	1:B:773:GLN:HE21	1.79	0.48
1:B:1546:TYR:OH	1:B:1612:GLN:OE1	2.25	0.48
1:B:1560:LEU:HD23	1:B:1561:LEU:HG	1.95	0.48
1:B:2488:ARG:HG2	1:B:2492:ARG:HH12	1.78	0.48
1:B:4025:LEU:HG	1:B:4027:LEU:HD22	1.95	0.48
1:A:437:ILE:HG22	1:A:441:LYS:HD2	1.96	0.48
1:A:458:LYS:O	1:A:462:ARG:HG3	2.13	0.48
1:B:1137:SER:O	1:B:1140:THR:OG1	2.28	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1150:ARG:HG3	5:J:70:THR:HG21	1.96	0.48
1:B:2629:GLU:O	1:B:2633:LYS:HG2	2.13	0.48
1:B:3459:GLN:HA	1:B:3462:LYS:HD2	1.96	0.48
1:B:3638:VAL:HG21	1:B:3679:LEU:HB3	1.94	0.48
1:B:4099:VAL:HG22	1:B:4128:MET:HB3	1.96	0.48
1:B:4474:THR:H	1:B:4477:GLN:HE21	1.60	0.48
2:D:504:TRP:HA	2:D:527:VAL:HG12	1.95	0.48
7:O:366:ASP:OD1	7:O:369:ASN:N	2.42	0.48
1:A:213:ILE:HB	1:A:241:PHE:CZ	2.49	0.48
1:A:1628:ARG:NH2	1:A:1871:GLU:OE1	2.46	0.48
1:A:4098:ASN:N	1:A:4127:THR:O	2.46	0.48
1:A:4463:SER:HG	1:A:4464:TRP:CD1	2.32	0.48
1:B:438:VAL:HG13	1:B:448:MET:HE2	1.96	0.48
1:B:1561:LEU:HD11	1:B:1618:TYR:HB2	1.96	0.48
2:D:479:ILE:HD12	2:D:499:THR:HB	1.96	0.48
3:F:159:HIS:HA	3:F:162:LYS:HG2	1.96	0.48
3:F:181:PHE:CE1	3:F:313:GLY:HA2	2.48	0.48
1:A:1166:ALA:O	1:A:1170:ILE:HG12	2.14	0.47
1:A:3447:TYR:HB3	1:A:3451:TYR:OH	2.14	0.47
2:D:504:TRP:HE1	2:D:522:ASP:HB2	1.79	0.47
3:F:271:TYR:CE2	3:F:308:VAL:HB	2.49	0.47
3:F:370:LEU:HA	3:F:373:GLN:HG2	1.96	0.47
6:K:90:ASP:OD1	6:K:112:SER:N	2.46	0.47
1:A:272:LEU:HD21	1:A:345:LEU:HD21	1.96	0.47
1:A:1513:TYR:HE1	1:A:1520:ALA:HB3	1.79	0.47
1:A:1530:ILE:HD11	1:A:1589:MET:HE1	1.96	0.47
1:A:4460:LEU:HD12	1:A:4461:PRO:HD2	1.96	0.47
1:B:79:VAL:HG23	1:B:116:LEU:HB2	1.95	0.47
1:B:185:LYS:O	1:B:188:GLU:HG3	2.13	0.47
1:B:1038:SER:O	1:B:1041:MET:HG3	2.13	0.47
1:B:1136:GLY:HA2	1:B:1139:MET:HE2	1.95	0.47
1:A:1836:PHE:HA	1:A:1839:LEU:HB2	1.96	0.47
1:A:2452:LEU:HD13	1:A:2729:ARG:HH21	1.79	0.47
1:A:3923:ARG:HH12	1:A:3925:GLN:HA	1.78	0.47
1:A:368:ARG:HH11	1:A:437:ILE:HD13	1.79	0.47
1:A:1079:TRP:C	1:A:1081:ALA:H	2.22	0.47
1:A:4037:PRO:HB2	1:A:4118:PRO:HG2	1.96	0.47
1:B:204:GLU:HA	1:B:288:ILE:HD11	1.97	0.47
1:B:1164:SER:O	1:B:1168:THR:OG1	2.27	0.47
1:B:2091:ARG:HD2	1:B:2357:SER:HB2	1.96	0.47
1:B:2423:MET:HE1	1:B:2462:LEU:HD13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3989:ARG:HG3	1:B:4004:MET:HE2	1.96	0.47
2:D:508:LEU:O	2:D:517:LEU:N	2.42	0.47
3:F:164:LYS:O	3:F:164:LYS:HD3	2.15	0.47
5:I:55:HIS:N	5:I:86:PHE:O	2.39	0.47
1:A:182:VAL:HG21	1:B:196:LEU:HD11	1.97	0.47
1:A:1750:VAL:HG12	1:A:1811:LEU:HD21	1.96	0.47
3:F:57:ILE:HD13	3:F:106:VAL:HG22	1.96	0.47
6:L:85:TRP:CD1	6:L:90:ASP:HB2	2.49	0.47
1:B:2060:ARG:HG3	1:B:2061:THR:HG23	1.96	0.47
1:B:3438:ARG:HA	1:B:3441:GLU:HB2	1.94	0.47
3:F:51:LEU:HB3	3:F:98:ARG:HE	1.79	0.47
3:F:174:GLU:HA	3:F:224:GLY:HA2	1.96	0.47
5:I:61:ASN:HB3	5:J:60:ARG:CZ	2.44	0.47
1:A:336:MET:HB3	1:A:363:HIS:CD2	2.50	0.47
1:A:368:ARG:NH1	1:A:437:ILE:HD13	2.29	0.47
1:A:1222:ASN:HA	1:A:1225:MET:HE3	1.97	0.47
1:A:1839:LEU:O	1:A:1843:ARG:NH1	2.48	0.47
1:A:2461:MET:HE2	1:A:2461:MET:HB3	1.83	0.47
1:A:4099:VAL:HG11	1:A:4126:LEU:HD22	1.96	0.47
1:A:4156:ASN:ND2	1:A:4188:ALA:HA	2.30	0.47
1:B:213:ILE:HG13	1:B:232:PHE:CE1	2.50	0.47
1:B:468:LYS:HA	1:B:471:ARG:CD	2.44	0.47
1:B:709:ARG:HD2	1:B:711:LEU:HG	1.94	0.47
1:B:717:ILE:HG22	1:B:718:PHE:HD2	1.78	0.47
1:B:724:ARG:HH11	1:B:726:ARG:HH21	1.63	0.47
1:B:1093:PHE:HE2	1:B:1117:ASN:HB2	1.79	0.47
1:B:1170:ILE:O	1:B:1173:VAL:HG12	2.15	0.47
1:B:2297:LYS:O	1:B:2338:ASN:ND2	2.36	0.47
2:D:535:THR:O	2:D:606:PRO:HG3	2.14	0.47
7:P:306:LYS:HD3	7:P:308:GLY:N	2.19	0.47
1:A:195:HIS:ND1	1:A:268:SER:O	2.46	0.47
1:A:804:LEU:HA	1:A:894:SER:O	2.14	0.47
1:A:2449:LEU:HD11	1:A:2454:CYS:SG	2.55	0.47
1:A:3518:GLY:CA	1:A:3579:MET:HE1	2.44	0.47
1:B:1220:ALA:O	1:B:1224:ILE:HG12	2.15	0.47
1:B:2228:SER:N	9:B:4702:ATP:O1B	2.46	0.47
1:B:3251:GLU:HA	1:B:3254:LYS:HB2	1.97	0.47
2:D:537:PRO:HB3	2:D:611:TRP:CZ3	2.50	0.47
3:F:168:GLU:HB2	3:F:171:ARG:HH21	1.80	0.47
7:P:289:SER:O	7:P:293:ILE:HG12	2.15	0.47
7:P:361:THR:HG22	7:P:377:ASN:HA	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:363:HIS:HA	1:A:366:LYS:HZ3	1.78	0.47
1:A:3383:ASN:O	1:A:3384:ARG:HB3	2.15	0.47
1:B:2123:ASP:HB3	1:B:2126:GLU:HG2	1.96	0.47
1:B:2221:MET:HG2	1:B:2343:PHE:HB2	1.97	0.47
1:B:4460:LEU:HD21	1:B:4465:SER:HB3	1.97	0.47
5:I:78:LEU:O	5:I:81:VAL:N	2.48	0.47
6:K:83:CYS:HB2	6:K:85:TRP:HZ3	1.79	0.47
7:O:212:ARG:HG3	7:O:236:TRP:CG	2.50	0.47
7:P:399:SER:OG	7:P:400:VAL:N	2.48	0.47
1:A:62:LEU:O	1:A:66:ARG:HG2	2.15	0.47
1:A:2388:ASP:OD1	1:A:2389:GLU:N	2.48	0.47
1:A:4434:VAL:HG13	1:A:4452:ILE:HD11	1.97	0.47
4:H:7:THR:O	4:H:11:LEU:HD23	2.15	0.47
5:I:28:ALA:HB1	5:I:38:ILE:HG23	1.97	0.47
1:A:241:PHE:O	1:A:245:LEU:HG	2.15	0.46
1:A:427:TYR:OH	1:A:452:ILE:HG12	2.15	0.46
1:B:78:LEU:HD11	1:B:115:SER:HB2	1.97	0.46
1:B:180:PRO:O	1:B:184:LYS:HG2	2.14	0.46
1:B:991:MET:HE1	1:B:994:LEU:HD23	1.96	0.46
1:B:1041:MET:HA	1:B:1044:VAL:HG12	1.97	0.46
1:B:3373:SER:HB3	1:B:3376:SER:OG	2.15	0.46
1:B:3383:ASN:O	1:B:3384:ARG:HB3	2.14	0.46
3:F:113:LEU:HD21	3:F:151:LYS:HD2	1.97	0.46
1:A:364:LEU:O	1:A:367:ILE:HG22	2.16	0.46
1:A:2895:ALA:HA	1:A:2898:LYS:HD2	1.97	0.46
1:A:2903:GLU:HG3	1:A:2904:GLU:OE1	2.14	0.46
1:A:4525:ARG:NH1	1:A:4536:LEU:HG	2.30	0.46
1:B:210:HIS:HB3	1:B:213:ILE:HG22	1.96	0.46
1:B:431:GLN:O	1:B:435:ARG:HG2	2.15	0.46
1:B:1497:VAL:HG21	1:B:1531:MET:HE3	1.97	0.46
1:B:1721:VAL:HA	1:B:1724:VAL:HG12	1.97	0.46
1:B:4176:ARG:NH1	1:B:4220:ASP:OD1	2.48	0.46
1:B:4473:MET:HG2	1:B:4477:GLN:HE21	1.81	0.46
1:B:4549:GLN:HG3	1:B:4587:LEU:HB2	1.97	0.46
2:D:301:ASN:OD1	2:D:302:ASN:N	2.48	0.46
1:A:2203:TRP:HH2	1:A:2236:VAL:HG21	1.81	0.46
1:A:2605:LEU:HD11	1:A:2709:VAL:HG11	1.98	0.46
1:A:4430:ASP:OD2	1:A:4447:TYR:OH	2.34	0.46
1:B:486:PRO:HA	1:B:567:ARG:NH2	2.29	0.46
1:B:635:MET:O	1:B:639:ARG:HG2	2.15	0.46
1:B:1041:MET:HG2	3:F:121:PHE:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:I:7:VAL:O	5:I:76:PHE:HB2	2.15	0.46
7:P:211:SER:OG	7:P:212:ARG:N	2.49	0.46
7:P:311:LEU:HB3	7:P:323:TRP:HB2	1.98	0.46
1:A:3989:ARG:HB3	1:A:4004:MET:CE	2.44	0.46
1:B:146:TYR:CZ	1:B:196:LEU:HD22	2.50	0.46
1:B:304:LEU:HD13	1:B:312:ALA:HB3	1.96	0.46
1:B:825:GLU:HA	1:B:829:LEU:HD11	1.98	0.46
1:B:1541:GLN:O	1:B:1545:VAL:HG23	2.16	0.46
1:B:3321:LEU:HD22	1:B:3332:THR:HA	1.97	0.46
5:I:43:LYS:HE3	5:J:67:THR:N	2.30	0.46
7:O:163:LYS:HG2	7:O:180:GLN:HE22	1.79	0.46
7:P:127:SER:OG	7:P:128:GLU:N	2.48	0.46
7:P:195:VAL:HA	7:P:211:SER:HB2	1.96	0.46
1:A:65:MET:O	1:A:69:LEU:HG	2.15	0.46
1:A:1698:ILE:HD12	1:A:1701:TRP:HE1	1.81	0.46
1:A:1861:MET:HE1	1:A:1889:TYR:HB3	1.98	0.46
1:A:2654:GLN:HG3	1:A:2657:LYS:HB2	1.96	0.46
1:A:2964:HIS:HA	1:A:3643:PRO:HD2	1.97	0.46
1:A:3013:ALA:HA	1:A:3088:ARG:HG3	1.98	0.46
1:A:3366:LYS:HD2	1:A:3400:LEU:HD21	1.98	0.46
1:A:3876:LEU:HD23	1:A:4146:VAL:HG11	1.97	0.46
1:B:864:LEU:HA	1:B:867:CYS:HB2	1.97	0.46
1:B:3423:ALA:O	1:B:3427:GLN:N	2.33	0.46
2:C:311:GLY:HA3	2:C:335:VAL:H	1.80	0.46
5:I:74:ILE:O	5:I:84:LEU:HD12	2.16	0.46
7:P:191:HIS:HB2	7:P:217:LYS:HD2	1.97	0.46
1:A:1176:LEU:O	1:A:1180:ILE:HG13	2.16	0.46
1:A:3248:GLN:O	1:A:3252:LYS:N	2.38	0.46
1:A:3354:PHE:CE2	1:A:3356:ALA:HB3	2.50	0.46
1:A:3928:THR:H	1:A:3931:GLN:HE21	1.62	0.46
1:B:977:GLU:O	1:B:981:LYS:HG2	2.16	0.46
2:D:374:PRO:HD3	2:D:416:SER:HA	1.97	0.46
7:P:206:HIS:CE1	7:P:220:GLU:HG2	2.51	0.46
7:P:243:ASN:HD21	7:P:247:THR:H	1.64	0.46
1:B:464:ASP:O	1:B:467:ARG:HG2	2.15	0.46
1:B:895:ASN:HB2	3:F:354:LEU:HD23	1.98	0.46
1:B:1099:LYS:HD3	1:B:1107:ILE:O	2.16	0.46
1:B:1966:ARG:HA	1:B:4101:LEU:HD13	1.98	0.46
1:B:3835:ILE:HG23	1:B:3866:VAL:HG12	1.97	0.46
5:I:54:TRP:HA	5:I:87:LYS:HA	1.98	0.46
5:I:62:PHE:CE2	5:I:64:SER:HB3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:723:THR:O	1:A:732:VAL:N	2.48	0.46
1:A:1495:ASN:HA	1:A:1498:LYS:HE3	1.97	0.46
1:B:148:THR:HG23	1:B:152:PHE:CE2	2.51	0.46
1:B:734:LYS:NZ	1:B:789:GLU:OE2	2.41	0.46
1:B:801:ILE:HD11	1:B:850:LEU:HB3	1.97	0.46
1:B:872:LYS:O	1:B:875:SER:N	2.49	0.46
1:B:3133:LEU:HD11	1:B:3141:GLU:HB3	1.98	0.46
3:F:61:GLY:HA3	3:F:67:LYS:HD3	1.97	0.46
1:A:1627:PRO:HB3	1:A:1950:GLN:HB3	1.97	0.46
1:B:1063:MET:SD	3:F:44:SER:HA	2.55	0.46
1:B:1399:LEU:O	1:B:1403:LEU:N	2.48	0.46
1:B:2964:HIS:HA	1:B:3643:PRO:HD2	1.98	0.46
2:D:607:ARG:HG3	2:D:609:ASP:HB3	1.97	0.46
3:F:301:LEU:HB3	3:F:309:PHE:HB3	1.98	0.46
3:F:321:ALA:HA	3:F:324:HIS:NE2	2.31	0.46
7:P:95:ILE:HD11	7:P:352:PHE:CD2	2.47	0.46
1:A:373:PRO:HB2	1:A:376:ARG:HB3	1.98	0.46
1:A:1155:GLN:NE2	1:A:1157:SER:H	2.14	0.46
1:A:1618:TYR:HD2	1:A:1619:LEU:HD22	1.81	0.46
1:A:4276:ARG:NH1	1:A:4279:ASP:OD2	2.48	0.46
1:B:1142:PHE:CE2	1:B:1214:ILE:HD12	2.51	0.46
1:B:1214:ILE:HA	1:B:1217:GLU:HG2	1.98	0.46
1:B:1666:LEU:HD23	1:B:1673:VAL:HA	1.97	0.46
1:B:3039:LYS:HB3	7:O:273:ARG:HH21	1.80	0.46
1:B:3256:MET:HE3	1:B:3256:MET:HB2	1.83	0.46
1:B:4517:PRO:HG2	1:B:4619:ILE:HD12	1.98	0.46
2:D:620:GLU:HG3	2:D:621:ILE:HG12	1.98	0.46
3:F:258:LEU:HB3	3:F:269:LEU:HD11	1.97	0.46
3:F:321:ALA:HA	3:F:324:HIS:CD2	2.51	0.46
1:A:2596:PRO:HB2	1:A:2738:TYR:CZ	2.51	0.45
1:B:464:ASP:OD1	1:B:465:GLN:N	2.50	0.45
1:B:479:VAL:HG11	1:B:590:ALA:CB	2.46	0.45
1:B:513:ASP:HB3	1:B:516:ASP:HB2	1.98	0.45
1:B:1188:GLU:HA	1:B:1191:ARG:HE	1.80	0.45
1:B:2047:GLN:HA	1:B:2070:VAL:HG21	1.98	0.45
1:B:2906:ASP:OD2	1:B:3655:ARG:HG2	2.15	0.45
1:B:3442:ALA:O	1:B:3446:ARG:HG2	2.16	0.45
2:D:336:MET:HE3	2:D:353:TYR:HB2	1.97	0.45
2:D:429:SER:O	2:D:429:SER:OG	2.33	0.45
5:I:9:LYS:HE3	5:I:77:TYR:CD1	2.51	0.45
6:K:64:ILE:HD11	6:L:111:LEU:HD21	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:PHE:HZ	1:A:299:LEU:HD13	1.81	0.45
1:A:1647:VAL:HA	1:A:1650:LEU:HD12	1.98	0.45
1:A:3321:LEU:HD22	1:A:3332:THR:HA	1.98	0.45
1:A:3601:MET:CE	1:A:3611:ARG:HB2	2.46	0.45
1:B:58:GLU:HG3	1:B:61:ALA:H	1.80	0.45
1:B:81:ARG:N	1:B:114:ASN:O	2.49	0.45
1:B:263:ASP:HA	1:B:277:PHE:HE2	1.81	0.45
1:B:557:ILE:HA	1:B:560:VAL:HG22	1.97	0.45
2:D:475:HIS:CE1	2:D:477:GLY:H	2.34	0.45
3:F:48:ARG:HD2	3:F:49:SER:HB2	1.97	0.45
3:F:278:LYS:HG3	3:F:279:ASN:ND2	2.32	0.45
3:F:369:LEU:HA	3:F:372:LYS:HG2	1.98	0.45
7:P:282:ILE:HG22	7:P:313:SER:HA	1.97	0.45
7:P:341:VAL:HA	7:P:357:ALA:HA	1.97	0.45
1:A:110:GLY:H	1:A:140:LEU:HD21	1.81	0.45
1:A:2623:SER:H	1:A:2626:THR:HG1	1.58	0.45
1:A:3182:HIS:NE2	1:A:3582:ARG:O	2.49	0.45
1:A:3219:ARG:O	1:A:3223:ARG:NE	2.38	0.45
1:A:3238:ASP:OD1	1:A:3239:LYS:N	2.49	0.45
1:A:3779:GLU:HB2	1:A:3782:ARG:HH22	1.80	0.45
1:A:4234:SER:OG	1:A:4236:ASP:OD1	2.29	0.45
1:A:4525:ARG:HD2	1:A:4592:TRP:CH2	2.51	0.45
1:B:635:MET:SD	1:B:636:SER:N	2.90	0.45
1:B:869:TYR:OH	1:B:989:TRP:O	2.33	0.45
1:B:1589:MET:N	1:B:1589:MET:SD	2.89	0.45
1:B:3160:ARG:HG2	1:B:3164:ARG:HH22	1.82	0.45
1:B:3292:ALA:HA	1:B:3395:TRP:CZ2	2.51	0.45
1:B:4150:PRO:HB3	1:B:4159:ARG:HE	1.81	0.45
2:D:199:PHE:HA	2:D:202:HIS:CD2	2.51	0.45
5:J:60:ARG:H	5:J:60:ARG:HD3	1.82	0.45
7:P:274:GLU:HG3	7:P:323:TRP:CH2	2.50	0.45
1:A:388:LEU:O	1:A:391:GLN:HG3	2.16	0.45
1:A:2179:ARG:NH2	1:A:2195:ASP:OD1	2.50	0.45
1:A:2277:ASP:OD2	1:A:2285:ARG:NE	2.45	0.45
1:A:4287:LYS:NZ	1:A:4291:HIS:O	2.38	0.45
2:D:483:HIS:ND1	2:D:532:TRP:HD1	2.14	0.45
2:D:495:HIS:HB2	2:D:511:THR:HG22	1.99	0.45
3:F:305:LYS:HD3	3:F:305:LYS:HA	1.74	0.45
1:A:1450:LEU:O	1:A:1453:ALA:N	2.50	0.45
1:A:1609:GLY:O	1:A:1613:LYS:HG2	2.16	0.45
1:B:253:ILE:HA	1:B:256:ILE:HG12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1051:VAL:O	1:B:1055:LEU:N	2.36	0.45
1:B:2596:PRO:HB2	1:B:2738:TYR:CZ	2.52	0.45
1:B:2631:LEU:HD13	1:B:2686:MET:HE1	1.99	0.45
1:B:3216:GLU:OE2	1:B:3220:ARG:NH1	2.48	0.45
1:B:4065:GLN:HB3	1:B:4092:ARG:HH21	1.80	0.45
1:A:35:ARG:HD3	1:A:53:GLU:HG2	1.97	0.45
1:A:462:ARG:NH1	1:A:537:ASP:O	2.50	0.45
1:A:1203:GLN:HB2	1:B:1062:ASP:O	2.16	0.45
1:A:4412:PHE:CZ	1:A:4520:TYR:HB2	2.52	0.45
1:B:232:PHE:HB3	1:B:235:LYS:HB2	1.98	0.45
1:B:635:MET:O	1:B:639:ARG:N	2.49	0.45
1:B:1479:ASN:HD21	1:B:1482:ASN:H	1.65	0.45
1:B:3588:LEU:HD11	1:B:3638:VAL:HG11	1.98	0.45
3:F:262:CYS:HB2	3:F:267:ALA:HB3	1.98	0.45
7:O:201:MET:HE1	7:O:242:PRO:HB3	1.99	0.45
1:A:41:LEU:HD13	1:B:132:SER:HB2	1.99	0.45
1:A:253:ILE:HA	1:A:256:ILE:HG12	1.98	0.45
1:A:1476:ASP:HB3	1:A:1488:ARG:NH1	2.32	0.45
1:A:1661:VAL:HG22	1:A:1676:ILE:HD12	1.99	0.45
1:B:718:PHE:CD1	1:B:735:LEU:HD11	2.52	0.45
4:G:68:PHE:HD2	4:H:72:ARG:HB3	1.81	0.45
5:I:9:LYS:N	5:I:75:TYR:O	2.42	0.45
6:K:75:ALA:HB2	6:L:73:ASN:HD21	1.80	0.45
7:O:254:ASN:HD22	7:O:278:VAL:HG21	1.81	0.45
1:A:187:ALA:O	1:A:191:MET:HG3	2.15	0.45
1:A:2176:THR:O	1:A:2180:GLU:HG2	2.16	0.45
1:A:2185:VAL:HG13	1:A:2189:MET:HE3	1.99	0.45
1:B:130:PRO:O	1:B:134:GLN:N	2.50	0.45
1:B:150:HIS:CE1	1:B:194:LEU:HB3	2.51	0.45
1:B:1135:LEU:HD22	1:B:1190:TYR:CD1	2.52	0.45
1:B:1674:LEU:HB3	1:B:1685:MET:HE1	1.99	0.45
1:B:2175:MET:HE2	1:B:2208:LEU:HD22	1.99	0.45
1:B:3251:GLU:O	1:B:3255:VAL:HG23	2.17	0.45
1:B:3366:LYS:HD2	1:B:3400:LEU:HD21	1.99	0.45
1:B:3409:VAL:HA	1:B:3412:LEU:HD12	1.97	0.45
3:F:251:LEU:O	3:F:254:ILE:HG22	2.17	0.45
5:I:13:MET:HE3	5:I:17:MET:CE	2.47	0.45
6:K:7:ALA:HA	6:K:10:THR:HG22	1.98	0.45
7:O:280:GLU:OE2	7:O:316:ARG:NE	2.50	0.45
1:A:79:VAL:C	1:A:115:SER:HG	2.25	0.45
1:A:2222:MET:HG2	1:A:2364:PHE:CE1	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3036:GLY:HA2	1:A:3039:LYS:NZ	2.32	0.45
1:A:3046:SER:HB3	1:A:3049:GLU:CD	2.42	0.45
1:A:3263:GLN:NE2	1:A:3426:ASN:HB3	2.32	0.45
1:B:798:ARG:O	1:B:801:ILE:HG22	2.17	0.45
1:B:1156:HIS:NE2	1:B:1166:ALA:HA	2.32	0.45
1:B:1188:GLU:HA	1:B:1191:ARG:NE	2.32	0.45
1:B:2639:CYS:HA	1:B:2652:PRO:HA	1.98	0.45
3:E:174:GLU:HA	3:E:224:GLY:HA3	1.99	0.45
7:O:112:THR:HG21	7:O:154:GLN:HA	1.98	0.45
7:O:337:HIS:NE2	7:O:355:SER:OG	2.38	0.45
7:P:212:ARG:HD3	7:P:236:TRP:HB2	1.98	0.45
1:A:368:ARG:HH12	1:A:436:ASP:C	2.25	0.45
1:A:2519:ARG:HG3	1:A:2526:LEU:HD12	1.98	0.45
1:A:2584:TRP:HE3	1:A:2591:LEU:HD22	1.82	0.45
1:A:2623:SER:OG	1:A:3006:GLU:OE1	2.34	0.45
1:A:2661:LEU:HD22	1:A:2708:PHE:CE1	2.52	0.45
1:B:578:ALA:HB2	1:B:611:ARG:HG2	1.99	0.45
1:B:1836:PHE:HA	1:B:1839:LEU:HB2	1.98	0.45
6:K:63:TYR:HB2	6:L:84:PHE:CE1	2.52	0.45
1:A:2538:GLU:OE2	1:A:2551:LYS:NZ	2.35	0.44
1:B:283:ARG:HH11	1:B:287:ARG:HH22	1.63	0.44
2:D:538:ALA:HB2	2:D:614:PHE:CG	2.52	0.44
3:F:255:GLN:OE1	3:F:323:LEU:HD21	2.17	0.44
3:F:304:GLU:HG2	3:F:307:ALA:HB3	1.99	0.44
4:G:70:ARG:NH2	4:G:72:ARG:HH21	2.16	0.44
1:A:178:MET:HE1	1:B:196:LEU:HG	1.99	0.44
1:A:3380:GLU:OE1	1:A:3380:GLU:N	2.50	0.44
1:B:375:GLN:HB2	1:B:447:LYS:HZ3	1.83	0.44
1:B:786:ARG:NH1	1:B:790:ARG:HH12	2.16	0.44
1:B:1213:ASN:HD21	5:J:8:ILE:C	2.25	0.44
1:B:2106:GLU:O	1:B:2110:LYS:N	2.39	0.44
2:D:330:HIS:HB3	2:D:367:ARG:HG3	2.00	0.44
3:F:120:LYS:HA	3:F:159:HIS:CE1	2.52	0.44
5:J:13:MET:HB2	5:J:18:GLN:HG3	1.99	0.44
5:J:55:HIS:HB2	5:J:86:PHE:CE1	2.51	0.44
7:P:97:ARG:HE	7:P:410:ARG:HB2	1.82	0.44
7:P:130:ALA:HA	7:P:153:VAL:HG23	1.98	0.44
1:A:42:LEU:HD23	1:A:81:ARG:HE	1.83	0.44
1:A:177:LYS:HD3	1:A:177:LYS:HA	1.75	0.44
1:A:178:MET:HE2	1:B:195:HIS:CD2	2.53	0.44
1:A:1571:ILE:HD11	1:A:1607:LEU:HD12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1721:VAL:HA	1:A:1724:VAL:HG12	1.99	0.44
1:A:2257:LYS:NZ	1:A:2308:ASP:OD2	2.43	0.44
1:A:3135:GLN:HB3	1:A:3136:PRO:HD3	1.99	0.44
1:A:4540:CYS:SG	1:A:4595:GLN:NE2	2.91	0.44
1:B:153:ILE:HG13	1:B:154:SER:N	2.33	0.44
1:B:257:GLN:HA	1:B:260:THR:HG22	2.00	0.44
1:B:547:GLU:HA	1:B:550:MET:HE3	2.00	0.44
1:B:642:PRO:HB2	1:B:749:GLU:OE2	2.17	0.44
2:D:504:TRP:CD2	2:D:523:ASN:HB3	2.52	0.44
3:F:120:LYS:HA	3:F:159:HIS:HE1	1.82	0.44
3:F:142:PRO:HB2	3:F:254:ILE:HD11	2.00	0.44
3:F:238:SER:C	3:F:242:LYS:HZ2	2.26	0.44
4:H:42:TYR:O	4:H:46:MET:HG2	2.18	0.44
7:P:235:GLU:HB2	7:P:255:ASP:HB3	2.00	0.44
1:A:242:LEU:HB3	1:A:309:ARG:NE	2.31	0.44
1:A:4215:ALA:HA	1:A:4251:ILE:HD13	1.98	0.44
1:B:270:THR:HG23	1:B:273:GLN:H	1.83	0.44
1:B:718:PHE:HD1	1:B:735:LEU:HD11	1.83	0.44
1:B:754:LYS:NZ	1:B:760:VAL:HG22	2.33	0.44
1:B:908:GLU:HB2	1:B:1019:TYR:CZ	2.52	0.44
1:B:1146:ILE:O	1:B:1150:ARG:HG2	2.17	0.44
1:B:4473:MET:HG2	1:B:4477:GLN:NE2	2.32	0.44
2:D:287:TRP:HZ3	2:D:318:MET:HE1	1.83	0.44
1:A:351:ASP:OD1	1:A:352:LYS:N	2.49	0.44
1:A:1460:GLU:OE1	1:A:1460:GLU:N	2.48	0.44
1:A:3253:LYS:HB3	1:A:3433:VAL:HG13	1.98	0.44
1:B:212:MET:HA	1:B:215:ASN:HD21	1.82	0.44
1:B:893:TYR:HB2	1:B:896:LEU:HD21	1.99	0.44
1:B:2905:LEU:CD1	1:B:3652:GLU:HB2	2.40	0.44
2:C:338:ALA:HA	2:C:350:GLY:HA2	2.00	0.44
2:D:523:ASN:CG	2:D:524:ALA:H	2.25	0.44
2:D:578:TRP:HA	2:D:585:ILE:HD12	2.00	0.44
7:O:89:ARG:NH2	7:O:409:CYS:O	2.51	0.44
7:O:131:THR:HG22	7:O:147:LYS:HG2	1.98	0.44
1:A:326:LEU:HA	1:A:329:VAL:HG12	1.98	0.44
1:A:1515:VAL:HG23	1:A:1516:PHE:CD2	2.53	0.44
1:A:2387:LEU:HD21	1:A:2463:HIS:HB3	1.99	0.44
1:A:3057:GLN:OE1	1:A:3060:ARG:NH1	2.51	0.44
1:B:311:HIS:HA	1:B:314:VAL:HG22	2.00	0.44
1:B:516:ASP:HA	1:B:563:ARG:NH1	2.30	0.44
1:B:718:PHE:CE1	1:B:820:ILE:HD13	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:724:ARG:HH21	1:B:729:THR:HA	1.81	0.44
1:B:1090:ARG:HH21	1:B:1121:ASP:HA	1.83	0.44
1:B:1135:LEU:HD22	1:B:1190:TYR:HD1	1.83	0.44
1:B:2107:ARG:HD3	1:B:2136:ILE:HG12	2.00	0.44
1:B:3452:ALA:O	1:B:3455:ILE:HG22	2.17	0.44
2:D:339:THR:HG22	2:D:387:VAL:HG23	1.99	0.44
1:A:1568:PHE:O	1:A:1572:SER:N	2.43	0.44
1:A:2591:LEU:HA	1:A:2731:VAL:HG23	2.00	0.44
1:B:35:ARG:NH2	1:B:53:GLU:OE2	2.51	0.44
1:B:2885:ASP:HB3	1:B:2888:GLU:OE1	2.18	0.44
2:D:287:TRP:HZ2	2:D:586:ALA:HB2	1.83	0.44
2:D:359:LEU:O	2:D:370:VAL:N	2.47	0.44
7:O:123:MET:N	7:O:135:TRP:O	2.38	0.44
1:A:158:ALA:HB3	1:A:159:PRO:HD3	2.00	0.44
1:A:365:ARG:NH2	1:A:429:LYS:O	2.50	0.44
1:A:1539:ASP:O	1:A:1543:ARG:HG2	2.18	0.44
1:A:1619:LEU:HD21	1:A:1638:LEU:HD21	2.00	0.44
1:A:1698:ILE:HD12	1:A:1701:TRP:NE1	2.33	0.44
1:A:2607:SER:HA	1:A:2610:ARG:NE	2.32	0.44
1:A:2660:VAL:HG22	1:A:2707:GLN:HB3	2.00	0.44
1:A:2999:VAL:HG13	1:A:3004:PHE:HB2	2.00	0.44
1:A:3196:GLU:O	1:A:3200:HIS:ND1	2.32	0.44
1:A:3398:ALA:C	1:A:3400:LEU:H	2.26	0.44
1:A:3607:ARG:O	1:A:3608:LYS:HG2	2.18	0.44
1:A:3954:ASP:OD2	1:A:3956:GLN:NE2	2.50	0.44
1:B:332:TYR:CE1	1:B:335:LEU:HD22	2.53	0.44
1:B:567:ARG:O	1:B:571:GLN:HG3	2.18	0.44
1:B:1090:ARG:HH22	1:B:1124:HIS:CB	2.31	0.44
1:B:4534:TRP:CD2	1:B:4594:LYS:HD3	2.52	0.44
2:C:187:LYS:HB3	4:G:30:ILE:HG13	2.00	0.44
3:F:59:VAL:HG12	3:F:108:ILE:HA	2.00	0.44
3:F:231:CYS:HB2	3:F:271:TYR:CD1	2.52	0.44
3:F:259:ARG:HH11	3:F:323:LEU:HD22	1.83	0.44
7:O:218:MET:HG3	7:O:230:PHE:HE1	1.82	0.44
7:O:287:GLU:HA	7:O:290:TYR:CE1	2.53	0.44
7:P:269:LYS:NZ	7:P:325:VAL:O	2.50	0.44
1:A:143:ASP:N	1:A:143:ASP:OD1	2.50	0.44
1:A:1959:GLU:N	1:A:2017:THR:O	2.51	0.44
1:B:1204:PHE:H	5:J:5:LYS:CE	2.31	0.44
1:B:1478:VAL:HG11	1:B:1488:ARG:HH21	1.83	0.44
1:B:1661:VAL:HG22	1:B:1676:ILE:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1965:GLU:HB3	1:B:4101:LEU:HD22	2.00	0.44
1:B:3433:VAL:HA	1:B:3436:MET:HE2	1.99	0.44
1:B:4554:ASP:OD2	1:B:4557:SER:OG	2.28	0.44
5:J:52:PRO:HA	5:J:53:THR:HA	1.66	0.44
1:A:52:LEU:HD12	1:A:101:TYR:CD1	2.53	0.43
1:A:2661:LEU:HD22	1:A:2708:PHE:HE1	1.83	0.43
1:A:3386:SER:OG	1:A:3389:CYS:SG	2.76	0.43
1:B:344:LEU:HD23	1:B:356:ALA:HB1	2.00	0.43
1:B:845:GLU:HA	1:B:848:ASP:OD2	2.17	0.43
1:B:1654:PHE:HA	1:B:1657:MET:HE2	2.00	0.43
1:B:1709:MET:HE3	1:B:1871:GLU:HA	1.99	0.43
1:B:2446:ILE:HD11	1:B:2714:PRO:HB3	1.99	0.43
1:B:3096:ASP:OD1	1:B:3097:TRP:N	2.51	0.43
2:D:426:HIS:ND1	2:D:427:LYS:HG2	2.33	0.43
3:F:219:LEU:HD22	3:F:222:ASN:CG	2.43	0.43
6:L:45:ASN:O	6:L:46:VAL:C	2.61	0.43
1:A:22:GLN:NE2	1:A:124:VAL:O	2.51	0.43
1:A:136:ARG:HG3	1:B:152:PHE:CZ	2.52	0.43
1:A:170:LYS:HG2	1:A:179:ALA:HB3	2.00	0.43
1:A:385:SER:HB2	1:A:454:PRO:HB3	1.99	0.43
1:A:3731:LEU:HD21	1:A:3790:VAL:HB	2.00	0.43
1:B:463:LEU:HA	1:B:466:MET:HE3	2.01	0.43
1:B:810:LYS:HD3	1:B:810:LYS:HA	1.68	0.43
1:B:1194:GLN:CD	1:B:1211:ILE:HD13	2.43	0.43
1:B:1667:ASN:ND2	1:B:1669:ASP:OD1	2.52	0.43
1:B:2363:TRP:HE1	1:B:2365:SER:HB2	1.83	0.43
2:C:446:ASN:HA	2:C:460:CYS:HA	2.00	0.43
3:F:334:ASP:OD2	3:F:339:PHE:HB2	2.18	0.43
1:A:27:VAL:O	1:A:31:GLN:HB2	2.17	0.43
1:A:154:SER:O	1:A:158:ALA:HB3	2.19	0.43
1:A:461:ALA:HA	1:A:464:ASP:OD2	2.18	0.43
1:A:1209:LEU:HD23	1:A:1209:LEU:H	1.83	0.43
1:A:1805:ARG:NE	1:A:2105:ARG:HH21	2.16	0.43
1:A:2640:GLU:N	1:A:2640:GLU:OE1	2.51	0.43
1:A:3520:PHE:HB3	1:A:3524:MET:HB3	1.99	0.43
1:B:1550:ILE:O	1:B:1554:SER:OG	2.29	0.43
1:B:2536:ASP:OD1	1:B:2576:ARG:NH1	2.51	0.43
1:B:2691:GLY:HA2	1:B:2703:LEU:HG	2.00	0.43
1:B:3624:GLU:O	1:B:3628:ARG:HG2	2.19	0.43
1:B:4099:VAL:HG11	1:B:4126:LEU:HD22	2.00	0.43
1:B:4413:PHE:CD2	1:B:4492:ILE:HG21	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4631:ASP:OD2	1:B:4633:ARG:NH2	2.51	0.43
7:O:94:TRP:HB2	7:O:409:CYS:HB3	2.00	0.43
1:A:215:ASN:C	1:A:215:ASN:HD22	2.27	0.43
1:A:385:SER:O	1:A:388:LEU:HB2	2.18	0.43
1:A:1183:PHE:O	1:A:1187:VAL:HG23	2.19	0.43
1:A:2492:ARG:HG2	1:A:2545:TRP:NE1	2.33	0.43
1:A:3253:LYS:O	1:A:3257:SER:N	2.49	0.43
1:B:2641:TYR:CE1	1:B:2650:LEU:HD13	2.53	0.43
2:D:425:VAL:HG11	2:D:429:SER:HA	2.00	0.43
2:D:427:LYS:HG3	2:D:428:GLN:OE1	2.19	0.43
5:J:10:ASN:O	5:J:75:TYR:N	2.51	0.43
7:O:354:LEU:HD12	7:O:362:LEU:HD11	2.00	0.43
7:P:212:ARG:HA	7:P:236:TRP:CD1	2.54	0.43
1:A:1867:ASN:O	1:A:1925:ARG:NH1	2.38	0.43
1:B:388:LEU:O	1:B:391:GLN:HG3	2.19	0.43
1:B:657:GLN:HE21	2:D:503:ASP:HB3	1.84	0.43
1:B:793:GLU:HA	1:B:796:GLU:HG3	2.00	0.43
1:B:1182:GLN:CD	1:B:1185:LYS:HZ3	2.26	0.43
3:F:144:THR:HA	3:F:147:GLU:OE2	2.18	0.43
5:I:13:MET:HA	5:I:71:LYS:HA	1.99	0.43
6:K:76:GLY:O	6:L:70:MET:HE2	2.18	0.43
7:P:101:LYS:HE3	7:P:394:TYR:CE2	2.52	0.43
7:P:243:ASN:CG	7:P:248:LEU:H	2.26	0.43
7:P:323:TRP:CZ3	7:P:330:CYS:HB2	2.53	0.43
1:A:2590:PRO:O	1:A:2732:PRO:HD2	2.18	0.43
1:A:3601:MET:HE1	1:A:3611:ARG:HB2	2.00	0.43
1:A:4575:LEU:HG	1:A:4624:PHE:HB3	2.01	0.43
1:B:68:PHE:O	1:B:120:LYS:NZ	2.30	0.43
1:B:72:PRO:O	1:B:75:HIS:NE2	2.51	0.43
1:B:378:LEU:HG	1:B:379:ARG:HH21	1.83	0.43
1:B:382:GLU:O	1:B:386:ARG:HG2	2.18	0.43
1:B:386:ARG:HH11	1:B:455:ALA:HB2	1.84	0.43
1:B:612:VAL:O	1:B:616:ILE:HG12	2.18	0.43
1:B:660:ALA:HA	1:B:663:LYS:HG2	2.00	0.43
1:B:1664:ILE:HG22	1:B:1676:ILE:HG22	2.01	0.43
1:B:1769:MET:HB3	1:B:1831:ASP:HB2	2.01	0.43
1:B:2190:TYR:CE2	1:B:2385:ILE:HD11	2.54	0.43
1:B:2437:LEU:HD21	1:B:2451:ARG:HG3	2.01	0.43
1:B:2855:LEU:HD11	1:B:2863:ARG:HD2	2.00	0.43
1:B:3032:GLN:HA	1:B:3035:GLU:HB3	2.00	0.43
1:B:3191:ARG:O	1:B:3195:GLU:HG2	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:4192:GLU:HB2	1:B:4321:LEU:HD21	1.99	0.43
2:D:495:HIS:CD2	2:D:495:HIS:H	2.36	0.43
3:E:56:ASN:O	3:E:131:THR:HA	2.19	0.43
3:F:38:SER:OG	3:F:39:ILE:N	2.51	0.43
4:G:72:ARG:HA	4:G:77:GLU:HA	2.00	0.43
7:O:312:LEU:HD21	7:O:353:ILE:HD13	2.00	0.43
1:A:1464:LYS:HA	1:A:1467:ARG:HE	1.84	0.43
1:A:3363:ILE:HG23	1:A:3400:LEU:HD22	2.00	0.43
1:B:568:LEU:O	1:B:572:LEU:N	2.46	0.43
1:B:1018:PHE:CZ	1:B:1020:ARG:HD2	2.53	0.43
1:B:1211:ILE:HG13	1:B:1212:ASP:N	2.34	0.43
1:B:1594:ILE:HB	1:B:1597:VAL:HB	2.01	0.43
1:B:3039:LYS:HB3	7:O:273:ARG:NH2	2.33	0.43
3:F:358:ASP:OD1	3:F:358:ASP:N	2.51	0.43
4:G:5:GLU:HA	4:G:8:LEU:HD12	2.00	0.43
5:I:8:ILE:HA	5:I:76:PHE:HB3	2.00	0.43
5:J:70:THR:O	5:J:72:HIS:ND1	2.48	0.43
7:O:123:MET:HE1	7:O:406:VAL:HG22	2.01	0.43
7:O:174:ILE:HB	7:O:188:MET:HB2	2.00	0.43
1:A:185:LYS:NZ	1:B:192:GLY:HA3	2.33	0.43
1:B:462:ARG:HH21	1:B:537:ASP:CB	2.27	0.43
1:B:641:LEU:HA	1:B:748:LYS:HZ1	1.84	0.43
1:B:1037:TYR:HB3	3:F:121:PHE:CZ	2.54	0.43
1:B:3044:LEU:HD23	1:B:3049:GLU:HB2	2.01	0.43
1:B:3835:ILE:HG12	1:B:3870:ARG:HD2	2.01	0.43
2:D:579:THR:HG21	2:D:584:GLU:CD	2.44	0.43
3:F:141:ARG:HB2	3:F:143:TRP:HE1	1.84	0.43
3:F:168:GLU:HG2	3:F:169:LYS:HD3	2.01	0.43
7:O:127:SER:OG	7:O:128:GLU:N	2.51	0.43
7:P:136:ASP:O	7:P:140:GLY:N	2.47	0.43
1:A:148:THR:O	1:A:152:PHE:HD1	2.01	0.43
1:A:173:ARG:HD2	1:B:283:ARG:NH2	2.34	0.43
1:A:211:PRO:O	1:A:214:THR:OG1	2.33	0.43
1:A:1529:ARG:HE	1:A:1592:LEU:HD11	1.84	0.43
1:A:2065:LEU:HD22	1:A:2137:LEU:HD22	2.00	0.43
1:A:2446:ILE:HD12	1:A:2446:ILE:HA	1.88	0.43
1:B:178:MET:O	1:B:182:VAL:HG13	2.19	0.43
1:B:1213:ASN:HA	5:J:11:ALA:H	1.83	0.43
1:B:2914:GLU:OE1	1:B:2914:GLU:N	2.49	0.43
1:B:3039:LYS:HE2	7:O:273:ARG:NH2	2.34	0.43
7:P:129:ASP:OD1	7:P:129:ASP:N	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:2091:ARG:NH2	8:A:4701:ADP:O2A	2.52	0.43
1:A:2784:PHE:HB2	1:A:2794:TYR:HE2	1.84	0.43
1:A:3389:CYS:HA	1:A:3392:MET:HE2	2.01	0.43
1:B:52:LEU:O	1:B:56:LEU:HG	2.18	0.43
1:B:1882:THR:HA	1:B:2048:LEU:HD23	2.01	0.43
1:B:2900:PHE:CE2	1:B:2905:LEU:HB3	2.53	0.43
1:B:4110:GLU:HG3	1:B:4138:LEU:HA	2.00	0.43
2:D:576:VAL:HG12	2:D:587:VAL:HG22	2.00	0.43
3:F:60:PHE:HE2	3:F:148:SER:HB2	1.83	0.43
5:I:2:CYS:C	5:I:4:ARG:H	2.26	0.43
7:O:194:ASN:O	7:O:212:ARG:N	2.50	0.43
7:O:212:ARG:HA	7:O:236:TRP:CD1	2.54	0.43
7:P:387:ASP:OD1	7:P:388:PHE:N	2.52	0.43
1:A:1446:VAL:O	1:A:1450:LEU:N	2.43	0.42
1:A:1671:SER:HB2	1:A:1693:THR:HG23	2.01	0.42
1:A:1926:PHE:O	1:A:1954:TRP:N	2.49	0.42
1:A:2047:GLN:NE2	1:A:2051:GLN:OE1	2.49	0.42
1:A:2324:LEU:HD22	1:A:2332:ARG:HB3	2.01	0.42
1:A:2616:GLU:OE1	1:A:2654:GLN:NE2	2.52	0.42
1:A:2905:LEU:HD12	1:A:2905:LEU:HA	1.90	0.42
1:A:3615:LEU:HD11	1:A:4111:LYS:HD3	2.00	0.42
1:B:871:HIS:HB2	1:B:992:VAL:HG13	2.01	0.42
1:B:981:LYS:NZ	3:F:90:TYR:HH	2.15	0.42
1:B:2654:GLN:NE2	1:B:2657:LYS:O	2.48	0.42
1:B:2837:LEU:HD13	1:B:2842:GLU:HB3	2.01	0.42
1:B:3839:VAL:HG21	1:B:3863:LEU:HA	2.00	0.42
1:B:4423:LEU:HD11	1:B:4466:HIS:ND1	2.34	0.42
2:D:327:TYR:HB3	2:D:360:TRP:HH2	1.84	0.42
5:I:74:ILE:HG12	5:I:76:PHE:CD1	2.54	0.42
7:O:152:SER:C	7:O:169:SER:HG	2.26	0.42
7:O:371:ARG:NH1	7:O:373:MET:HG3	2.34	0.42
1:A:388:LEU:O	1:A:389:SER:C	2.63	0.42
1:A:1766:LEU:HD13	1:A:1833:ALA:HA	2.01	0.42
1:B:38:VAL:HG11	1:B:52:LEU:HD11	2.00	0.42
1:B:1061:TRP:C	1:B:1063:MET:H	2.26	0.42
1:B:1079:TRP:O	1:B:1083:LEU:HD23	2.20	0.42
1:B:4002:LEU:O	1:B:4006:HIS:ND1	2.45	0.42
2:D:267:LEU:HA	2:D:597:TYR:HB3	2.01	0.42
2:D:288:SER:HB2	2:D:340:PHE:CE2	2.54	0.42
2:D:347:LEU:HD23	2:D:359:LEU:HD11	2.01	0.42
2:D:401:ILE:HD12	2:D:406:LYS:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:96:LYS:HE3	1:A:96:LYS:HB3	1.90	0.42
1:A:2150:VAL:HA	1:A:2363:TRP:CD1	2.54	0.42
1:B:1039:ALA:O	1:B:1043:ILE:HG12	2.18	0.42
1:B:2419:ALA:O	1:B:2423:MET:HG2	2.18	0.42
1:B:3322:GLU:OE2	1:B:3377:TYR:OH	2.33	0.42
1:B:3909:LEU:HD21	1:B:4343:MET:HE3	2.02	0.42
2:C:184:GLU:HA	2:C:187:LYS:HE2	2.01	0.42
5:J:13:MET:HE2	5:J:73:PHE:C	2.43	0.42
6:K:70:MET:HE3	6:L:70:MET:HE1	2.00	0.42
7:P:151:ASP:OD1	7:P:152:SER:N	2.47	0.42
1:A:31:GLN:HE21	1:A:56:LEU:HG	1.84	0.42
1:A:372:TYR:HD2	1:A:377:ALA:HB2	1.84	0.42
1:A:1558:LYS:HG3	1:A:1565:THR:HG21	2.01	0.42
1:A:3154:LEU:HB3	1:A:3171:ILE:HG13	2.01	0.42
1:B:1535:ASP:OD1	1:B:2292:ARG:NH2	2.46	0.42
1:B:4226:THR:HG21	1:B:4239:PRO:HD3	2.02	0.42
1:B:4282:PHE:HB3	1:B:4296:MET:HB2	2.01	0.42
2:C:271:PHE:O	2:C:594:ILE:N	2.51	0.42
3:F:59:VAL:HG23	3:F:134:ILE:O	2.19	0.42
6:K:97:TRP:HE3	6:K:104:CYS:HB3	1.85	0.42
1:A:264:ARG:NH1	1:A:274:GLU:OE1	2.53	0.42
1:A:1196:LEU:HA	1:A:1199:LYS:HG2	2.02	0.42
1:A:1526:LYS:HB2	1:A:1526:LYS:HE3	1.80	0.42
1:A:2149:LEU:HD11	1:A:2157:LEU:HD13	2.01	0.42
1:A:2964:HIS:H	1:A:2967:TYR:HB2	1.84	0.42
1:A:3835:ILE:HG23	1:A:3866:VAL:HG12	2.02	0.42
1:A:4160:THR:HG23	1:A:4212:LEU:HD21	2.02	0.42
1:A:4185:TRP:CD1	1:A:4284:LEU:HD22	2.55	0.42
1:B:642:PRO:HG2	1:B:749:GLU:HG2	2.01	0.42
1:B:1698:ILE:HD12	1:B:1701:TRP:HE1	1.85	0.42
1:B:2901:TYR:HA	1:B:2905:LEU:O	2.20	0.42
1:B:3662:ILE:HG23	1:B:3669:ILE:HB	2.01	0.42
4:G:14:GLN:HB3	4:G:17:VAL:HG21	2.01	0.42
7:O:109:SER:HB3	7:O:128:GLU:HB2	2.01	0.42
1:A:441:LYS:HE3	1:A:448:MET:HE1	2.01	0.42
1:A:1537:TRP:HE3	1:A:1601:LEU:HD11	1.83	0.42
1:A:2069:ILE:HB	1:A:2137:LEU:HD21	2.02	0.42
1:B:309:ARG:HG3	1:B:311:HIS:CE1	2.55	0.42
1:B:578:ALA:HB1	1:B:582:PHE:CE2	2.55	0.42
1:B:634:LYS:O	1:B:638:VAL:HG23	2.20	0.42
1:B:916:GLN:HB2	1:B:1026:MET:HE1	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3008:MET:HA	1:B:3008:MET:HE3	2.02	0.42
1:B:3381:ILE:HG23	1:B:3390:GLY:HA2	2.00	0.42
3:F:139:MET:SD	3:F:139:MET:N	2.74	0.42
5:I:13:MET:HE3	5:I:17:MET:SD	2.60	0.42
5:J:11:ALA:HA	5:J:74:ILE:HA	2.02	0.42
7:O:113:ARG:HA	7:O:385:SER:OG	2.20	0.42
1:B:750:VAL:O	1:B:754:LYS:HG2	2.19	0.42
1:B:1020:ARG:HH22	3:F:84:ARG:N	2.17	0.42
1:B:1090:ARG:HH22	1:B:1124:HIS:HB2	1.85	0.42
1:B:2094:LYS:HE3	8:B:4701:ADP:O2'	2.20	0.42
1:B:2773:MET:HG2	1:B:2825:TRP:HE1	1.85	0.42
1:B:4232:ASN:OD1	1:B:4233:ILE:N	2.53	0.42
2:D:273:ASP:O	2:D:277:SER:OG	2.23	0.42
2:D:536:HIS:HB3	2:D:539:LEU:HB3	2.00	0.42
4:H:46:MET:O	4:H:50:ILE:HG12	2.20	0.42
5:I:63:GLY:HA2	5:J:36:LYS:HG2	2.01	0.42
7:O:128:GLU:HA	7:O:152:SER:HB2	2.00	0.42
1:A:376:ARG:O	1:A:380:LEU:HG	2.20	0.42
1:A:1181:LYS:HG2	1:A:1185:LYS:NZ	2.34	0.42
1:A:1591:VAL:HA	1:A:1594:ILE:HG13	2.00	0.42
1:A:4565:LEU:O	1:A:4583:THR:N	2.50	0.42
1:B:49:PRO:HG3	1:B:81:ARG:NH2	2.35	0.42
1:B:292:ARG:HH12	1:B:320:THR:HG22	1.85	0.42
1:B:336:MET:HA	1:B:339:PHE:HE2	1.84	0.42
1:B:484:LEU:HD11	1:B:563:ARG:NH1	2.35	0.42
1:B:1859:ILE:N	1:B:1866:PHE:O	2.47	0.42
1:B:2206:LYS:HA	1:B:2206:LYS:HD3	1.84	0.42
1:B:3380:GLU:OE1	1:B:3380:GLU:N	2.52	0.42
1:B:4603:SER:O	1:B:4626:ILE:HG12	2.20	0.42
2:D:485:HIS:HA	2:D:532:TRP:CD1	2.54	0.42
3:F:55:LYS:HZ3	3:F:130:GLU:HA	1.83	0.42
3:F:141:ARG:HB2	3:F:143:TRP:NE1	2.35	0.42
1:A:40:LEU:C	1:B:132:SER:HG	2.22	0.42
1:A:214:THR:HA	1:A:296:GLU:OE1	2.20	0.42
1:A:3131:ASP:OD1	1:A:3132:LYS:N	2.53	0.42
1:A:3214:GLN:O	1:A:3217:GLU:HG3	2.20	0.42
1:A:4106:LEU:HD23	1:A:4106:LEU:HA	1.87	0.42
1:B:85:LYS:HE3	1:B:95:GLU:HB2	2.02	0.42
1:B:977:GLU:OE1	1:B:977:GLU:N	2.37	0.42
1:B:1965:GLU:OE2	1:B:2026:SER:HB3	2.19	0.42
1:B:2172:ARG:NH1	1:B:2173:GLY:O	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3524:MET:HA	1:B:3527:ASN:HB2	2.02	0.42
1:B:3846:LEU:HD22	1:B:3855:ARG:HD2	2.00	0.42
2:C:214:GLN:HB2	2:D:209:ARG:NH1	2.34	0.42
3:F:39:ILE:O	3:F:43:VAL:HG13	2.20	0.42
5:I:10:ASN:HB2	5:I:75:TYR:HB3	2.02	0.42
7:P:217:LYS:HG2	7:P:229:THR:HG23	2.02	0.42
1:A:1458:ALA:HA	1:A:1461:GLU:CD	2.44	0.42
1:A:2156:LEU:HD21	1:A:4400:ARG:HH12	1.85	0.42
1:A:2224:GLY:O	1:A:2346:GLN:HA	2.20	0.42
1:A:3432:GLU:O	1:A:3436:MET:HG2	2.20	0.42
1:A:3709:GLN:HG3	1:A:3809:SER:HB3	2.02	0.42
1:B:143:ASP:OD1	1:B:143:ASP:N	2.53	0.42
1:B:413:MET:HA	1:B:416:CYS:SG	2.60	0.42
1:B:526:ALA:O	1:B:553:TYR:CZ	2.73	0.42
1:B:655:ASP:OD1	1:B:690:ARG:NE	2.53	0.42
1:B:716:ARG:H	1:B:738:ASN:HD22	1.68	0.42
1:B:1054:TRP:HE1	1:B:1112:VAL:HG21	1.85	0.42
1:B:1138:ASN:OD1	1:B:1139:MET:N	2.53	0.42
1:B:1933:ASP:HA	1:B:1962:ARG:HE	1.84	0.42
1:B:2713:ASN:OD1	1:B:2720:ARG:NH2	2.47	0.42
1:B:3175:HIS:HB3	1:B:3516:TYR:CE1	2.55	0.42
1:B:4526:GLN:OE1	1:B:4536:LEU:HD11	2.20	0.42
2:D:485:HIS:HE1	2:D:537:PRO:HA	1.85	0.42
4:G:6:GLU:O	4:G:9:LYS:HG3	2.20	0.42
4:G:52:LYS:HZ2	4:H:49:PHE:HA	1.85	0.42
7:O:253:SER:OG	7:O:254:ASN:N	2.53	0.42
7:P:330:CYS:SG	7:P:331:LEU:N	2.93	0.42
1:A:285:LEU:HB2	1:A:322:LEU:HD21	2.01	0.41
1:A:1191:ARG:NH2	1:A:1215:GLU:OE2	2.53	0.41
1:A:2363:TRP:HE1	1:A:2365:SER:HB3	1.85	0.41
1:A:3196:GLU:HG3	1:A:3200:HIS:HE1	1.85	0.41
1:A:3885:MET:HE2	1:A:3885:MET:HB2	1.78	0.41
1:A:4178:ARG:NH2	1:A:4297:PRO:O	2.53	0.41
1:B:782:ILE:HA	1:B:785:VAL:HG12	2.02	0.41
1:B:2444:GLU:H	1:B:2510:MET:HE2	1.85	0.41
1:B:3260:ILE:HA	1:B:3263:GLN:CD	2.45	0.41
2:D:266:SER:O	2:D:597:TYR:HB2	2.20	0.41
3:E:95:ASP:O	3:E:99:ASP:N	2.48	0.41
3:F:254:ILE:O	3:F:258:LEU:HG	2.20	0.41
4:H:21:ILE:HD12	4:H:31:LYS:HB2	2.02	0.41
7:O:193:HIS:HD1	7:O:194:ASN:H	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:193:HIS:HB3	7:O:212:ARG:HB3	2.02	0.41
7:P:112:THR:HA	7:P:384:THR:HG21	2.02	0.41
7:P:165:LEU:HB3	7:P:177:TRP:HB2	2.02	0.41
7:P:243:ASN:ND2	7:P:248:LEU:H	2.17	0.41
7:P:248:LEU:HB3	7:P:284:TRP:HH2	1.85	0.41
1:A:2148:LYS:HB2	1:A:2361:MET:HB2	2.02	0.41
1:A:4408:PRO:HB3	1:A:4411:ARG:HH21	1.86	0.41
1:B:43:GLU:OE2	1:B:81:ARG:NH2	2.40	0.41
1:B:543:THR:O	1:B:547:GLU:OE1	2.37	0.41
1:B:1141:GLU:O	1:B:1145:GLN:HG2	2.20	0.41
1:B:2374:ILE:H	1:B:2374:ILE:HG13	1.71	0.41
1:B:3005:LEU:HD23	1:B:3005:LEU:HA	1.94	0.41
4:G:43:ALA:HA	4:G:46:MET:CG	2.48	0.41
6:L:44:THR:O	6:L:48:GLU:HG2	2.20	0.41
1:A:25:ALA:HB3	1:A:69:LEU:HD13	2.01	0.41
1:A:1598:GLN:O	1:A:1602:GLU:HG2	2.20	0.41
1:A:2427:PHE:CE1	1:A:2433:VAL:HG21	2.56	0.41
1:A:2996:GLU:OE1	1:A:2996:GLU:N	2.51	0.41
1:A:3684:PRO:HD2	1:A:4140:ARG:NH2	2.35	0.41
1:B:401:LEU:HD12	1:B:409:PHE:HE1	1.85	0.41
1:B:2427:PHE:CD1	1:B:2433:VAL:HG21	2.55	0.41
1:B:4599:GLU:C	1:B:4600:LYS:HD2	2.45	0.41
4:G:45:LEU:HD12	4:G:45:LEU:HA	1.87	0.41
4:G:70:ARG:HH21	4:G:72:ARG:HH21	1.69	0.41
5:I:8:ILE:HD13	5:I:18:GLN:HE22	1.84	0.41
1:A:1525:ASP:OD2	1:A:1529:ARG:NH1	2.50	0.41
1:A:1707:LYS:O	1:A:1707:LYS:HD3	2.21	0.41
1:A:1888:CYS:HA	1:A:2039:LEU:HD22	2.03	0.41
1:A:2967:TYR:OH	1:A:2975:ASP:OD2	2.31	0.41
1:A:4099:VAL:HB	1:A:4106:LEU:HD21	2.02	0.41
1:B:794:LYS:HA	1:B:794:LYS:HD3	1.80	0.41
1:B:1071:ARG:CZ	3:F:43:VAL:HG12	2.51	0.41
1:B:1224:ILE:HD12	1:B:1228:LYS:NZ	2.36	0.41
1:B:1495:ASN:HA	1:B:1498:LYS:NZ	2.36	0.41
1:B:2879:LYS:HE2	7:O:336:GLY:HA2	2.01	0.41
1:B:2943:LYS:HG2	1:B:3094:PHE:HD2	1.85	0.41
1:B:3040:GLU:OE2	1:B:3042:LEU:HB2	2.19	0.41
3:E:273:SER:O	3:E:277:GLU:N	2.53	0.41
3:F:179:LYS:HE3	3:F:179:LYS:HB3	1.83	0.41
3:F:222:ASN:OD1	3:F:223:LEU:N	2.53	0.41
6:K:29:ILE:HD11	6:K:69:ILE:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:K:68:VAL:CG1	6:K:70:MET:HE2	2.51	0.41
1:A:90:ASP:N	1:A:90:ASP:OD1	2.52	0.41
1:A:309:ARG:HG3	1:A:311:HIS:CE1	2.56	0.41
1:A:3409:VAL:HA	1:A:3412:LEU:HD12	2.02	0.41
1:A:3585:ARG:NH1	1:A:3694:SER:O	2.39	0.41
1:A:3873:ARG:HD3	1:A:3873:ARG:HA	1.81	0.41
1:A:4297:PRO:HG3	1:A:4308:TRP:CG	2.55	0.41
1:A:4511:LEU:HD23	1:A:4511:LEU:HA	1.91	0.41
1:A:4600:LYS:HZ1	1:A:4604:VAL:H	1.68	0.41
1:B:969:ILE:HD13	1:B:969:ILE:HA	1.94	0.41
1:B:971:LEU:HB3	1:B:974:PRO:HA	2.02	0.41
1:B:976:GLU:HB2	3:F:88:TYR:OH	2.20	0.41
1:B:2385:ILE:O	1:B:2416:GLN:NE2	2.46	0.41
1:B:2859:PRO:O	1:B:2861:ILE:HG23	2.20	0.41
1:B:2876:TRP:CE2	1:B:2953:MET:HE1	2.55	0.41
1:B:3691:ASP:OD1	1:B:3692:LEU:N	2.53	0.41
2:C:214:GLN:C	2:D:209:ARG:HH12	2.29	0.41
2:D:456:VAL:O	2:D:472:PHE:HB2	2.21	0.41
2:D:472:PHE:HA	2:D:514:ASN:OD1	2.20	0.41
3:F:55:LYS:HE2	3:F:130:GLU:HB3	2.02	0.41
3:F:72:THR:OG1	3:F:77:ALA:HB3	2.20	0.41
4:H:10:ARG:HG3	4:H:11:LEU:HD22	2.01	0.41
6:L:97:TRP:HE3	6:L:104:CYS:HB3	1.86	0.41
7:O:340:TRP:HB2	7:O:358:ASP:OD2	2.19	0.41
7:P:146:LEU:HB3	7:P:177:TRP:CZ3	2.55	0.41
1:A:178:MET:O	1:A:181:SER:OG	2.26	0.41
1:A:918:GLY:HA2	1:A:950:GLY:HA2	2.02	0.41
1:A:2071:PRO:HB3	1:A:4536:LEU:HD23	2.02	0.41
1:B:368:ARG:HD2	1:B:368:ARG:HA	1.81	0.41
1:B:1196:LEU:O	1:B:1200:GLN:HG2	2.20	0.41
1:B:1581:LYS:HA	1:B:1584:LYS:NZ	2.36	0.41
1:B:2896:ARG:HA	1:B:2896:ARG:HD3	1.85	0.41
1:B:3112:LYS:HD3	1:B:3112:LYS:HA	1.82	0.41
1:B:3928:THR:HG22	1:B:3929:VAL:N	2.36	0.41
1:B:4297:PRO:HG3	1:B:4308:TRP:CD2	2.55	0.41
7:P:395:VAL:HG23	7:P:407:TRP:HD1	1.86	0.41
1:A:81:ARG:HA	1:A:101:TYR:HA	2.02	0.41
1:A:2534:ILE:H	1:A:2534:ILE:HD12	1.86	0.41
1:A:3196:GLU:HG3	1:A:3200:HIS:CE1	2.55	0.41
1:A:4541:LEU:HD21	1:A:4590:LEU:HD12	2.03	0.41
1:B:180:PRO:HA	1:B:183:GLU:CD	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:242:LEU:O	1:B:246:GLN:OE1	2.39	0.41
1:B:722:SER:HB3	1:B:731:ASN:ND2	2.30	0.41
1:B:865:GLU:HG2	1:B:910:ILE:HD13	2.02	0.41
1:B:1135:LEU:HD13	1:B:1190:TYR:HE1	1.85	0.41
1:B:1698:ILE:O	1:B:1702:LEU:HD23	2.20	0.41
1:B:2308:ASP:O	1:B:2312:VAL:HG12	2.21	0.41
1:B:2654:GLN:NE2	1:B:2657:LYS:HB2	2.35	0.41
2:C:448:VAL:HA	2:C:458:THR:HA	2.02	0.41
2:D:445:ASN:OD1	2:D:461:ARG:N	2.50	0.41
3:F:62:GLU:CD	3:F:141:ARG:HH12	2.28	0.41
4:G:23:VAL:HG11	4:G:43:ALA:HB1	2.02	0.41
5:I:36:LYS:HE3	5:I:36:LYS:HB3	1.87	0.41
7:O:130:ALA:HA	7:O:153:VAL:HG23	2.02	0.41
7:P:194:ASN:C	7:P:211:SER:HG	2.27	0.41
1:A:2601:LYS:N	8:A:4703:ADP:O1B	2.54	0.41
1:B:633:CYS:SG	1:B:634:LYS:HD3	2.61	0.41
1:B:1817:HIS:CD2	1:B:1881:GLN:HG2	2.56	0.41
1:B:3263:GLN:HA	1:B:3266:LYS:HD2	2.02	0.41
3:F:142:PRO:HB2	3:F:254:ILE:CD1	2.51	0.41
3:F:240:LEU:HB3	3:F:246:TYR:CD2	2.56	0.41
6:L:28:ALA:HB2	6:L:49:GLN:NE2	2.36	0.41
1:A:27:VAL:HA	1:A:65:MET:HE1	2.03	0.41
1:A:43:GLU:HG3	1:A:81:ARG:HH22	1.86	0.41
1:A:347:ALA:HA	1:A:352:LYS:HD3	2.03	0.41
1:A:1476:ASP:O	1:A:1487:ILE:HA	2.21	0.41
1:A:2270:PRO:HA	1:A:2273:ARG:NH1	2.36	0.41
1:A:3005:LEU:HD11	1:A:3078:ARG:HE	1.85	0.41
1:A:3194:LEU:HD23	1:A:3500:MET:HE2	2.03	0.41
1:A:3731:LEU:HG	1:A:3787:THR:HG23	2.03	0.41
1:A:4085:ASN:HB3	7:O:205:ASP:OD2	2.21	0.41
1:B:232:PHE:CE2	1:B:303:ILE:HG21	2.56	0.41
1:B:718:PHE:HB2	1:B:736:LYS:O	2.20	0.41
1:B:783:GLU:HG2	2:D:375:LEU:HD22	2.03	0.41
1:B:974:PRO:HD2	1:B:977:GLU:CD	2.46	0.41
1:B:980:TYR:HD2	3:F:90:TYR:HH	1.64	0.41
1:B:1125:LYS:HA	1:B:1128:LEU:HD12	2.03	0.41
1:B:1150:ARG:O	1:B:1153:LEU:HG	2.21	0.41
1:B:1494:PHE:O	1:B:1498:LYS:HG3	2.21	0.41
1:B:2211:TYR:O	1:B:2214:THR:OG1	2.36	0.41
1:B:2894:LYS:HB2	1:B:2894:LYS:HE3	1.85	0.41
1:B:2976:LEU:HD23	1:B:2976:LEU:HA	1.88	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:3248:GLN:O	1:B:3252:LYS:N	2.42	0.41
1:B:3358:GLU:OE1	1:B:3366:LYS:NZ	2.48	0.41
1:B:3638:VAL:CG2	1:B:3679:LEU:HB3	2.51	0.41
2:D:205:ARG:HH21	2:D:327:TYR:HE1	1.69	0.41
4:H:26:GLU:HA	4:H:87:PHE:CE2	2.49	0.41
5:I:46:PHE:HD2	5:I:54:TRP:CD2	2.38	0.41
7:O:273:ARG:O	7:O:273:ARG:HG2	2.21	0.41
7:P:163:LYS:HE3	7:P:163:LYS:HB2	1.80	0.41
7:P:243:ASN:ND2	7:P:247:THR:H	2.19	0.41
7:P:279:VAL:HA	7:P:315:SER:HA	2.02	0.41
1:A:1075:ASP:O	1:A:1076:LEU:C	2.64	0.41
1:A:1859:ILE:HD11	1:A:1868:TYR:HD1	1.86	0.41
1:A:2596:PRO:HB2	1:A:2738:TYR:CE1	2.56	0.41
1:A:2905:LEU:HD11	1:A:3652:GLU:HB3	2.03	0.41
1:A:4511:LEU:HD23	1:A:4514:LEU:HD12	2.02	0.41
1:B:205:ILE:HD12	1:B:255:GLU:CD	2.47	0.41
1:B:539:SER:O	1:B:541:GLU:N	2.54	0.41
1:B:801:ILE:HD11	1:B:850:LEU:CB	2.51	0.41
1:B:1195:ARG:O	1:B:1199:LYS:HG2	2.20	0.41
1:B:3253:LYS:HB3	1:B:3433:VAL:HG13	2.03	0.41
3:F:270:ILE:HG22	3:F:271:TYR:N	2.36	0.41
1:A:40:LEU:HD11	1:B:36:LYS:HD2	2.02	0.40
1:A:210:HIS:NE2	1:A:212:MET:HG2	2.36	0.40
1:A:278:TRP:O	1:A:281:LEU:HG	2.21	0.40
1:A:368:ARG:NH2	1:A:440:ARG:HG3	2.35	0.40
1:A:1477:LEU:HB3	1:A:1485:ARG:HB3	2.03	0.40
1:A:1643:ASN:CG	1:A:1649:LYS:HD2	2.46	0.40
1:A:2598:GLY:HA3	1:A:2795:SER:HB2	2.03	0.40
1:A:2912:PHE:CE2	1:A:2914:GLU:HB2	2.56	0.40
1:A:4296:MET:HE2	1:A:4296:MET:HA	2.03	0.40
1:B:59:LYS:HZ1	1:B:63:GLU:HB2	1.85	0.40
1:B:1464:LYS:O	1:B:1467:ARG:N	2.50	0.40
1:B:4430:ASP:O	1:B:4434:VAL:HG23	2.20	0.40
3:F:134:ILE:HG13	3:F:135:PHE:N	2.37	0.40
5:I:4:ARG:HH22	5:I:81:VAL:HG23	1.86	0.40
1:A:365:ARG:HD3	1:A:433:LEU:HD22	2.03	0.40
1:A:2206:LYS:HD3	1:A:2206:LYS:HA	1.86	0.40
1:A:2500:TRP:HB3	1:A:2580:LEU:HD11	2.03	0.40
1:A:4430:ASP:O	1:A:4434:VAL:HG23	2.21	0.40
1:A:4448:LEU:HD23	1:A:4448:LEU:HA	1.94	0.40
1:B:716:ARG:HD2	1:B:820:ILE:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:780:SER:O	1:B:783:GLU:HG3	2.22	0.40
1:B:1561:LEU:HD22	1:B:1564:GLU:OE2	2.21	0.40
1:B:1728:GLY:O	1:B:1729:LYS:HG2	2.21	0.40
1:B:1930:PHE:HA	1:B:2326:THR:HG21	2.03	0.40
1:B:3190:LYS:HD3	1:B:3190:LYS:HA	1.85	0.40
1:B:3576:ASN:HA	1:B:3579:MET:HE3	2.03	0.40
2:D:426:HIS:CD2	2:D:468:ILE:HG21	2.57	0.40
5:J:17:MET:HE2	5:J:50:TYR:CD1	2.56	0.40
5:J:32:TYR:HB2	5:J:38:ILE:HD13	2.03	0.40
7:O:101:LYS:NZ	7:O:408:GLU:OE2	2.44	0.40
1:A:378:LEU:O	1:A:382:GLU:OE1	2.39	0.40
1:A:1146:ILE:HD11	1:A:1183:PHE:CE2	2.56	0.40
1:A:1946:VAL:HG22	1:A:2006:VAL:HG21	2.03	0.40
1:A:2918:HIS:O	1:A:2922:ILE:HG12	2.21	0.40
1:A:3048:GLU:O	1:A:3052:LYS:HG2	2.21	0.40
1:A:3373:SER:HB3	1:A:3376:SER:OG	2.21	0.40
1:A:3989:ARG:HB3	1:A:4004:MET:HE3	2.03	0.40
1:B:479:VAL:HG13	1:B:480:ILE:HG12	2.02	0.40
1:B:659:THR:HA	1:B:662:MET:HG2	2.03	0.40
1:B:961:GLU:HG2	1:B:972:ASN:O	2.22	0.40
1:B:1698:ILE:HD12	1:B:1701:TRP:NE1	2.36	0.40
1:B:1792:LEU:HD12	1:B:1815:LEU:HD22	2.03	0.40
1:B:2668:LEU:N	1:B:2669:PRO:HD2	2.37	0.40
2:C:205:ARG:NH2	2:C:209:ARG:HH21	2.20	0.40
2:C:293:GLU:O	2:C:318:MET:N	2.53	0.40
2:D:412:LEU:HD12	2:D:412:LEU:HA	1.96	0.40
3:F:157:ARG:NH1	3:F:161:ASP:OD1	2.37	0.40
5:I:46:PHE:HD2	5:I:54:TRP:CE2	2.40	0.40
7:P:155:ASP:OD1	7:P:156:ILE:N	2.54	0.40
1:A:1458:ALA:HA	1:A:1461:GLU:OE2	2.21	0.40
1:A:1661:VAL:HG13	1:A:1676:ILE:HB	2.02	0.40
1:A:2200:GLY:HA2	1:A:2373:MET:HE1	2.03	0.40
1:A:3113:MET:SD	1:A:3184:ALA:HA	2.60	0.40
1:A:3340:SER:O	1:A:3346:ASN:ND2	2.55	0.40
1:A:3766:ILE:O	1:A:3770:LEU:HG	2.20	0.40
1:B:857:ILE:HD11	1:B:881:VAL:HG22	2.04	0.40
1:B:964:ILE:HG13	1:B:968:VAL:C	2.47	0.40
1:B:3169:MET:HG2	1:B:3519:TYR:CE2	2.56	0.40
1:B:3398:ALA:C	1:B:3400:LEU:H	2.28	0.40
1:B:3994:GLN:HB2	1:B:4001:LEU:HD21	2.03	0.40
1:B:4205:TYR:OH	1:B:4261:ASP:OD2	2.31	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:287:TRP:CZ3	2:D:318:MET:HE1	2.56	0.40
3:F:336:TYR:CZ	3:F:340:ILE:HD11	2.56	0.40
6:K:12:PHE:CZ	6:K:17:VAL:HG21	2.55	0.40
6:K:64:ILE:HG23	6:L:83:CYS:SG	2.61	0.40
1:A:193:LEU:HA	1:B:178:MET:HE3	2.04	0.40
1:A:1959:GLU:HB3	1:A:1962:ARG:HD3	2.04	0.40
1:A:4393:GLN:HG3	1:A:4428:ARG:CZ	2.52	0.40
1:B:483:VAL:HG21	1:B:588:PHE:HB2	2.03	0.40
1:B:870:ASP:HB3	1:B:873:THR:HG22	2.04	0.40
1:B:1478:VAL:HG11	1:B:1488:ARG:HE	1.86	0.40
1:B:1972:SER:OG	1:B:2031:ASN:ND2	2.54	0.40
2:C:204:THR:HA	4:G:10:ARG:NH1	2.36	0.40
2:C:527:VAL:HA	2:C:543:VAL:O	2.22	0.40
2:D:475:HIS:CE1	2:D:503:ASP:HB2	2.56	0.40
4:G:43:ALA:HA	4:G:46:MET:HE3	2.03	0.40
7:O:284:TRP:HZ3	7:O:309:PRO:HB2	1.86	0.40
7:P:98:PRO:N	7:P:99:PRO:HD2	2.37	0.40
7:P:169:SER:OG	7:P:170:ALA:N	2.55	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	4530/4646 (98%)	4400 (97%)	128 (3%)	2 (0%)	100	100
1	B	4507/4646 (97%)	4375 (97%)	129 (3%)	3 (0%)	48	83
2	C	390/638 (61%)	369 (95%)	21 (5%)	0	100	100
2	D	390/638 (61%)	369 (95%)	21 (5%)	0	100	100
3	E	307/492 (62%)	298 (97%)	9 (3%)	0	100	100
3	F	307/492 (62%)	294 (96%)	12 (4%)	1 (0%)	36	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	G	91/96 (95%)	86 (94%)	5 (6%)	0	100	100
4	H	91/96 (95%)	83 (91%)	8 (9%)	0	100	100
5	I	87/89 (98%)	80 (92%)	7 (8%)	0	100	100
5	J	87/89 (98%)	83 (95%)	4 (5%)	0	100	100
6	K	111/113 (98%)	110 (99%)	1 (1%)	0	100	100
6	L	111/113 (98%)	107 (96%)	4 (4%)	0	100	100
7	O	320/410 (78%)	306 (96%)	14 (4%)	0	100	100
7	P	317/410 (77%)	303 (96%)	14 (4%)	0	100	100
All	All	11646/12968 (90%)	11263 (97%)	377 (3%)	6 (0%)	49	83

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	3384	ARG
1	B	540	LYS
1	B	3384	ARG
1	A	589	ASN
1	B	1161	ALA
3	F	112	ASP

### 5.3.2 Protein sidechains [i](#)

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	4044/4125 (98%)	4044 (100%)	0	100	100
1	B	4028/4125 (98%)	4028 (100%)	0	100	100
2	C	344/557 (62%)	344 (100%)	0	100	100
2	D	344/557 (62%)	344 (100%)	0	100	100
3	E	279/422 (66%)	279 (100%)	0	100	100
3	F	279/422 (66%)	279 (100%)	0	100	100
4	G	87/89 (98%)	87 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
4	H	87/89 (98%)	87 (100%)	0	100	100
5	I	78/78 (100%)	78 (100%)	0	100	100
5	J	78/78 (100%)	78 (100%)	0	100	100
6	K	97/97 (100%)	97 (100%)	0	100	100
6	L	97/97 (100%)	97 (100%)	0	100	100
7	O	287/364 (79%)	287 (100%)	0	100	100
7	P	284/364 (78%)	284 (100%)	0	100	100
All	All	10413/11464 (91%)	10413 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (115) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	64	GLN
1	A	114	ASN
1	A	198	GLN
1	A	215	ASN
1	A	219	GLN
1	A	244	GLN
1	A	280	ASN
1	A	355	GLN
1	A	421	GLN
1	A	1186	GLN
1	A	1233	GLN
1	A	1465	GLN
1	A	1569	GLN
1	A	1855	GLN
1	A	1856	GLN
1	A	1950	GLN
1	A	1973	GLN
1	A	1974	GLN
1	A	2171	HIS
1	A	2215	GLN
1	A	2263	HIS
1	A	2464	GLN
1	A	2468	ASN
1	A	2476	HIS
1	A	2485	GLN

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Mol	Chain	Res	Type
1	A	2549	GLN
1	A	2588	HIS
1	A	2698	GLN
1	A	2849	ASN
1	A	3061	ASN
1	A	3152	GLN
1	A	3158	ASN
1	A	3353	ASN
1	A	3383	ASN
1	A	3427	GLN
1	A	3499	GLN
1	A	3526	GLN
1	A	3538	GLN
1	A	3735	GLN
1	A	3754	ASN
1	A	3820	GLN
1	A	3877	HIS
1	A	3952	GLN
1	A	4029	HIS
1	A	4429	GLN
1	A	4444	GLN
1	A	4490	GLN
1	A	4506	ASN
1	A	4530	GLN
1	A	4566	GLN
1	A	4589	GLN
1	B	195	HIS
1	B	280	ASN
1	B	421	GLN
1	B	465	GLN
1	B	487	GLN
1	B	680	GLN
1	B	731	ASN
1	B	871	HIS
1	B	879	ASN
1	B	1174	GLN
1	B	1213	ASN
1	B	1233	GLN
1	B	1495	ASN
1	B	1559	HIS
1	B	1755	GLN
1	B	1841	GLN

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Mol	Chain	Res	Type
1	B	1974	GLN
1	B	1987	ASN
1	B	2031	ASN
1	B	2047	GLN
1	B	2067	ASN
1	B	2212	GLN
1	B	2482	GLN
1	B	2485	GLN
1	B	2827	HIS
1	B	2918	HIS
1	B	3014	ASN
1	B	3233	ASN
1	B	3353	ASN
1	B	3383	ASN
1	B	3427	GLN
1	B	3735	GLN
1	B	3744	GLN
1	B	3792	GLN
1	B	3820	GLN
1	B	3826	GLN
1	B	3877	HIS
1	B	3952	GLN
1	B	4079	GLN
1	B	4098	ASN
1	B	4249	GLN
1	B	4258	ASN
1	B	4325	ASN
1	B	4386	ASN
1	B	4389	HIS
1	B	4393	GLN
1	B	4425	GLN
1	B	4444	GLN
1	B	4477	GLN
1	B	4566	GLN
2	C	188	GLN
2	D	270	GLN
2	D	393	GLN
2	D	419	GLN
2	D	426	HIS
3	F	295	HIS
4	H	64	ASN
5	I	18	GLN

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Mol	Chain	Res	Type
5	I	51	ASN
6	K	41	GLN
6	K	71	GLN
7	O	154	GLN
7	O	254	ASN
7	P	154	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 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
8	ADP	A	4701	10	28,29,29	1.40	4 (14%)	43,45,45	1.84	10 (23%)
8	ADP	B	4704	-	28,29,29	1.40	4 (14%)	43,45,45	1.84	9 (20%)
9	ATP	B	4702	10	32,33,33	0.31	0	48,52,52	0.28	0
8	ADP	B	4701	10	28,29,29	1.39	4 (14%)	43,45,45	1.86	8 (18%)
8	ADP	A	4704	-	28,29,29	1.40	4 (14%)	43,45,45	1.83	9 (20%)
8	ADP	B	4703	-	28,29,29	1.40	4 (14%)	43,45,45	1.88	8 (18%)
9	ATP	A	4702	10	32,33,33	0.30	0	48,52,52	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
8	ADP	A	4703	-	28,29,29	1.40	4 (14%)	43,45,45	1.86	8 (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
8	ADP	A	4701	10	-	1/16/32/32	0/3/3/3
8	ADP	B	4704	-	-	1/16/32/32	0/3/3/3
9	ATP	B	4702	10	-	3/22/38/38	0/3/3/3
8	ADP	B	4701	10	-	2/16/32/32	0/3/3/3
8	ADP	A	4704	-	-	1/16/32/32	0/3/3/3
8	ADP	B	4703	-	-	5/16/32/32	0/3/3/3
9	ATP	A	4702	10	-	5/22/38/38	0/3/3/3
8	ADP	A	4703	-	-	5/16/32/32	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	4703	ADP	C5-C4	4.73	1.47	1.39
8	B	4703	ADP	C5-C4	4.68	1.47	1.39
8	B	4701	ADP	C5-C4	4.66	1.47	1.39
8	B	4704	ADP	C5-C4	4.65	1.47	1.39
8	A	4704	ADP	C5-C4	4.63	1.47	1.39
8	A	4701	ADP	C5-C4	4.60	1.47	1.39
8	A	4704	ADP	C5-C6	2.70	1.48	1.41
8	B	4704	ADP	C5-C6	2.69	1.48	1.41
8	A	4703	ADP	C5-C6	2.68	1.48	1.41
8	B	4703	ADP	C5-C6	2.68	1.48	1.41
8	A	4701	ADP	C5-C6	2.67	1.48	1.41
8	B	4701	ADP	C5-C6	2.64	1.48	1.41
8	B	4701	ADP	C5-N7	-2.39	1.34	1.39
8	B	4703	ADP	C5-N7	-2.35	1.34	1.39
8	A	4703	ADP	C5-N7	-2.34	1.34	1.39
8	A	4704	ADP	C5-N7	-2.34	1.34	1.39
8	A	4701	ADP	C5-N7	-2.33	1.34	1.39
8	B	4704	ADP	C5-N7	-2.33	1.34	1.39
8	A	4701	ADP	C8-N7	2.32	1.36	1.31
8	A	4704	ADP	C8-N7	2.31	1.36	1.31
8	B	4704	ADP	C8-N7	2.27	1.36	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	A	4703	ADP	C8-N7	2.27	1.36	1.31
8	B	4703	ADP	C8-N7	2.26	1.36	1.31
8	B	4701	ADP	C8-N7	2.22	1.36	1.31

All (52) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	B	4703	ADP	C5-C4-N3	-6.16	118.24	126.72
8	A	4703	ADP	C5-C4-N3	-6.01	118.44	126.72
8	B	4701	ADP	C5-C4-N3	-5.90	118.59	126.72
8	B	4704	ADP	C5-C4-N3	-5.81	118.72	126.72
8	A	4701	ADP	C5-C4-N3	-5.80	118.72	126.72
8	A	4704	ADP	C5-C4-N3	-5.78	118.75	126.72
8	B	4703	ADP	N3-C4-N9	4.91	135.51	127.17
8	A	4703	ADP	N3-C4-N9	4.85	135.41	127.17
8	B	4701	ADP	N3-C4-N9	4.71	135.18	127.17
8	B	4704	ADP	N3-C4-N9	4.64	135.06	127.17
8	A	4704	ADP	N3-C4-N9	4.59	134.97	127.17
8	A	4701	ADP	N3-C4-N9	4.55	134.90	127.17
8	B	4703	ADP	C2-N3-C4	3.85	121.23	111.83
8	A	4703	ADP	C2-N3-C4	3.76	121.02	111.83
8	B	4701	ADP	C2-N3-C4	3.73	120.95	111.83
8	A	4704	ADP	C2-N3-C4	3.69	120.84	111.83
8	A	4701	ADP	C2-N3-C4	3.68	120.81	111.83
8	B	4704	ADP	C2-N3-C4	3.66	120.77	111.83
8	A	4701	ADP	C4-C5-N7	-3.53	106.55	110.58
8	B	4704	ADP	C4-C5-N7	-3.45	106.64	110.58
8	A	4704	ADP	C4-C5-N7	-3.42	106.68	110.58
8	B	4703	ADP	C4-C5-N7	-3.38	106.72	110.58
8	B	4701	ADP	C4-C5-N7	-3.37	106.73	110.58
8	A	4703	ADP	C4-C5-N7	-3.35	106.75	110.58
8	B	4703	ADP	N3-C2-N1	-3.29	123.59	128.58
8	A	4703	ADP	N3-C2-N1	-3.26	123.65	128.58
8	B	4701	ADP	N3-C2-N1	-3.24	123.69	128.58
8	A	4704	ADP	N3-C2-N1	-3.23	123.69	128.58
8	A	4701	ADP	N3-C2-N1	-3.21	123.73	128.58
8	B	4704	ADP	N3-C2-N1	-3.16	123.79	128.58
8	B	4704	ADP	C4-N9-C8	2.73	108.61	105.74
8	A	4701	ADP	C4-N9-C8	2.65	108.52	105.74
8	B	4703	ADP	C3'-C2'-C1'	2.63	106.44	101.46
8	A	4704	ADP	C4-N9-C8	2.63	108.50	105.74
8	A	4701	ADP	C5-N7-C8	2.59	107.52	103.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	A	4703	ADP	C4-N9-C8	2.58	108.44	105.74
8	B	4701	ADP	C4-N9-C8	2.55	108.41	105.74
8	A	4703	ADP	C3'-C2'-C1'	2.53	106.26	101.46
8	A	4704	ADP	C3'-C2'-C1'	2.52	106.23	101.46
8	B	4704	ADP	C5-N7-C8	2.52	107.40	103.45
8	A	4704	ADP	C5-N7-C8	2.50	107.38	103.45
8	B	4704	ADP	C3'-C2'-C1'	2.49	106.18	101.46
8	B	4703	ADP	C5-N7-C8	2.49	107.36	103.45
8	A	4703	ADP	C5-N7-C8	2.48	107.35	103.45
8	B	4701	ADP	C5-N7-C8	2.48	107.34	103.45
8	B	4701	ADP	C3'-C2'-C1'	2.43	106.06	101.46
8	B	4703	ADP	C4-N9-C8	2.42	108.28	105.74
8	A	4701	ADP	C3'-C2'-C1'	2.15	105.54	101.46
8	A	4701	ADP	C6-C5-N7	2.11	136.16	132.09
8	A	4704	ADP	C6-C5-N7	2.05	136.05	132.09
8	B	4704	ADP	C6-C5-N7	2.04	136.02	132.09
8	A	4701	ADP	N9-C8-N7	-2.04	111.05	113.94

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
8	A	4701	ADP	C5'-O5'-PA-O2A
8	A	4703	ADP	C5'-O5'-PA-O1A
8	A	4703	ADP	C5'-O5'-PA-O3A
8	B	4701	ADP	C5'-O5'-PA-O2A
8	B	4701	ADP	C5'-O5'-PA-O3A
8	B	4703	ADP	C5'-O5'-PA-O1A
8	B	4703	ADP	C5'-O5'-PA-O3A
9	A	4702	ATP	O4'-C4'-C5'-O5'
8	A	4703	ADP	O4'-C4'-C5'-O5'
9	B	4702	ATP	O4'-C4'-C5'-O5'
8	A	4703	ADP	C3'-C4'-C5'-O5'
8	B	4703	ADP	O4'-C4'-C5'-O5'
8	B	4703	ADP	C3'-C4'-C5'-O5'
9	A	4702	ATP	C3'-C4'-C5'-O5'
9	B	4702	ATP	PB-O3B-PG-O3G
9	B	4702	ATP	C3'-C4'-C5'-O5'
8	A	4703	ADP	C5'-O5'-PA-O2A
8	A	4704	ADP	C5'-O5'-PA-O1A
8	B	4703	ADP	C5'-O5'-PA-O2A
8	B	4704	ADP	C5'-O5'-PA-O1A

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Mol	Chain	Res	Type	Atoms
9	A	4702	ATP	PB-O3B-PG-O1G
9	A	4702	ATP	PB-O3B-PG-O2G
9	A	4702	ATP	PB-O3B-PG-O3G

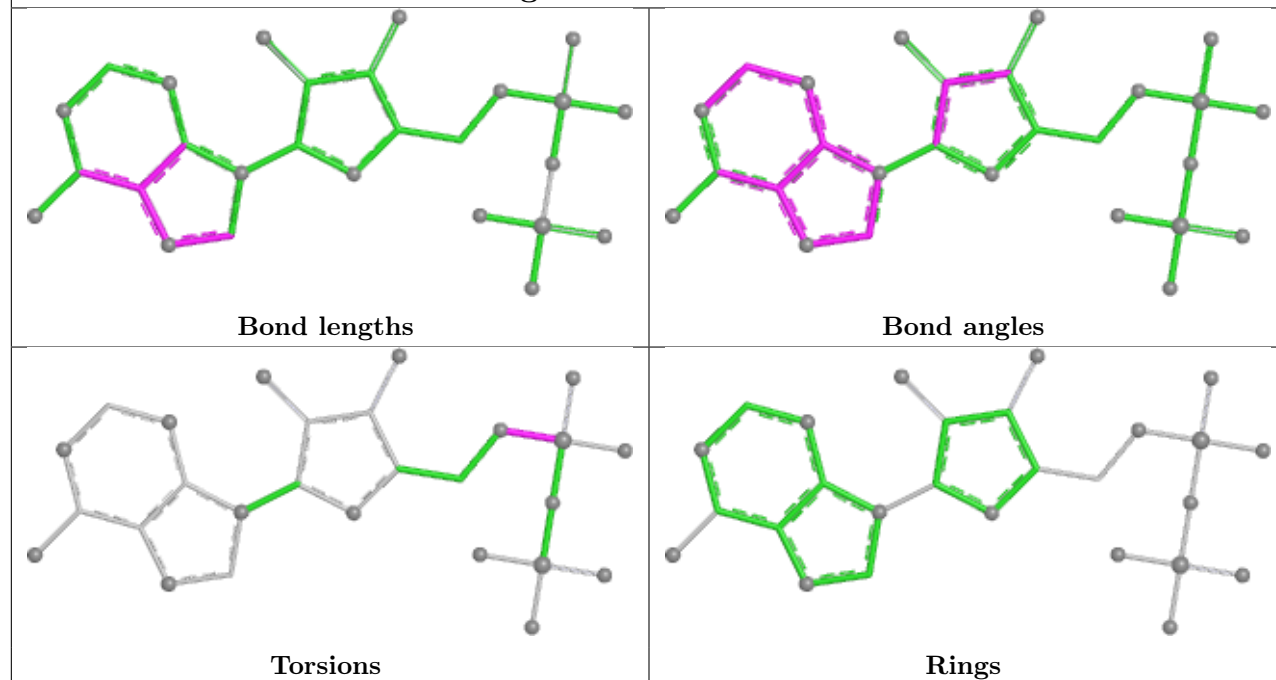
There are no ring outliers.

7 monomers are involved in 10 short contacts:

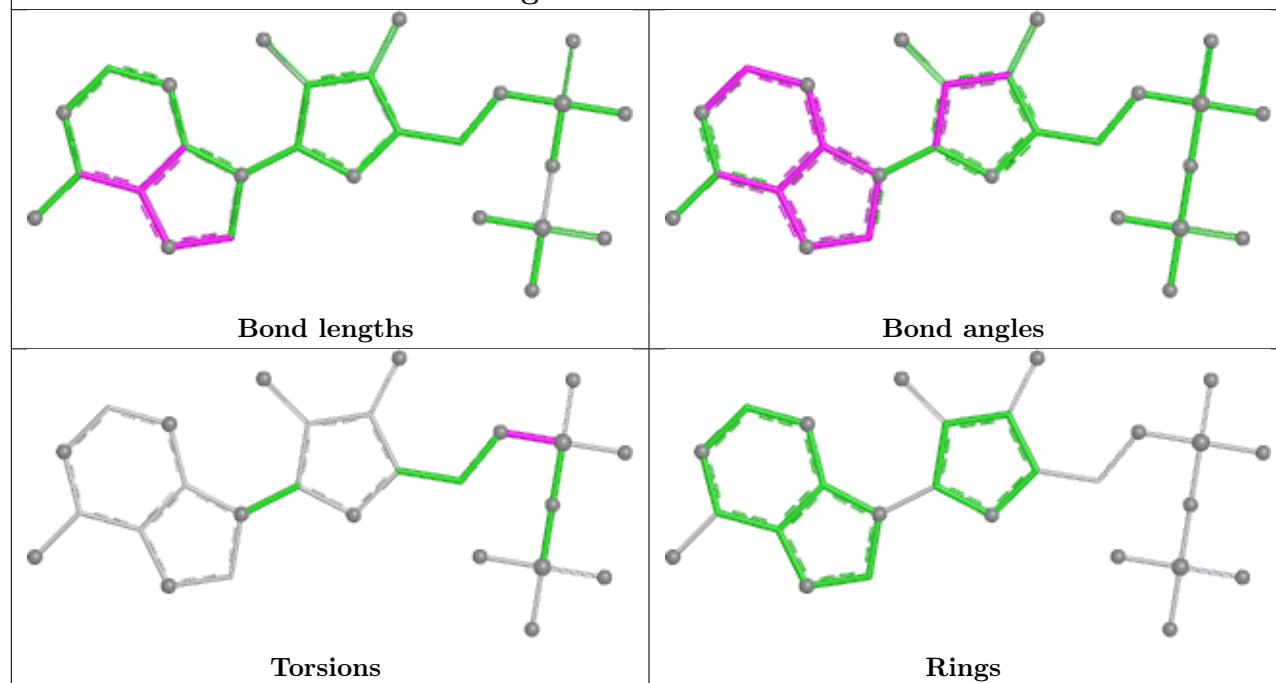
Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	A	4701	ADP	3	0
8	B	4704	ADP	1	0
9	B	4702	ATP	1	0
8	B	4701	ADP	2	0
8	A	4704	ADP	1	0
9	A	4702	ATP	1	0
8	A	4703	ADP	1	0

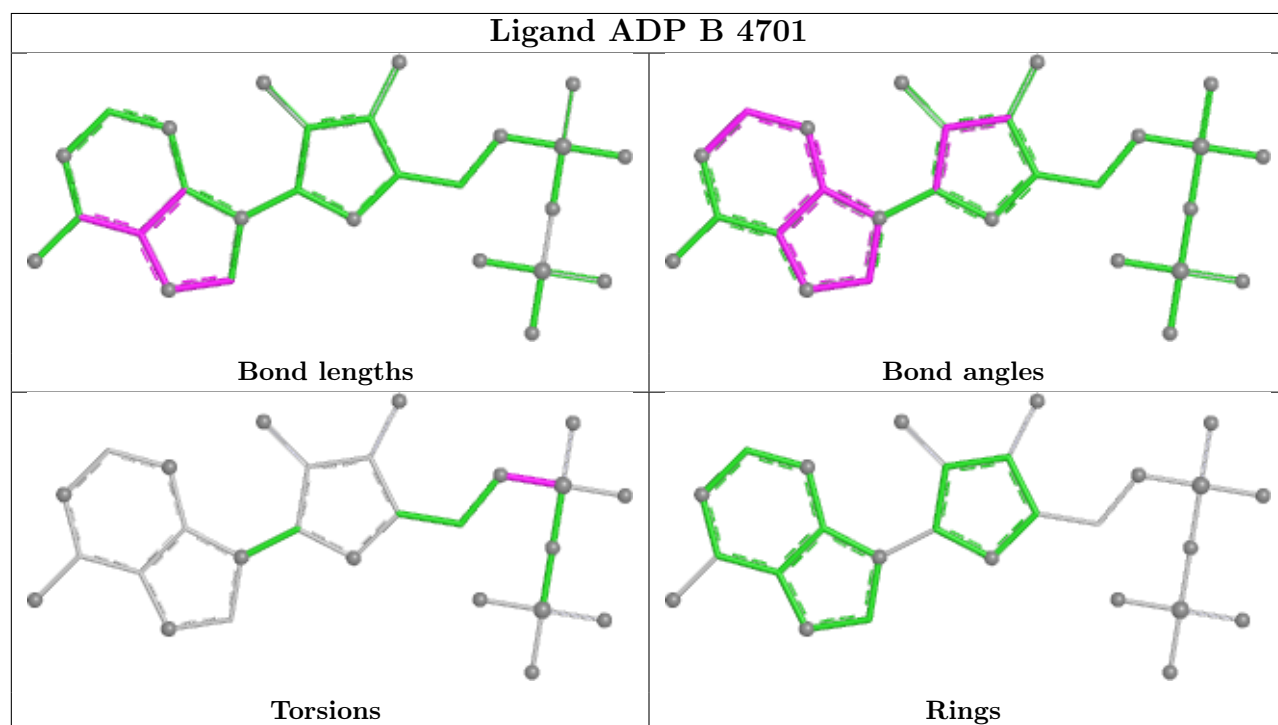
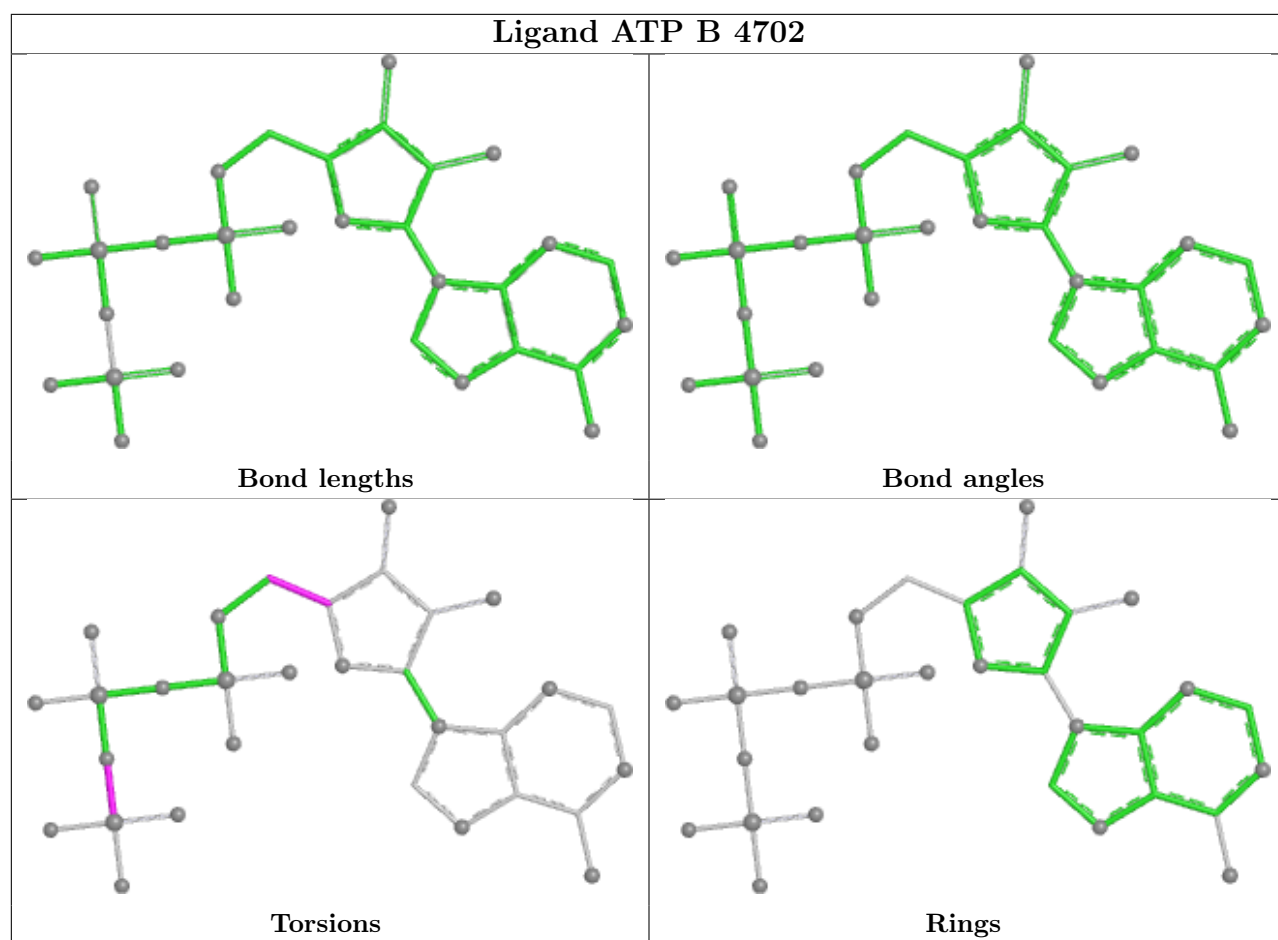
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

## Ligand ADP A 4701

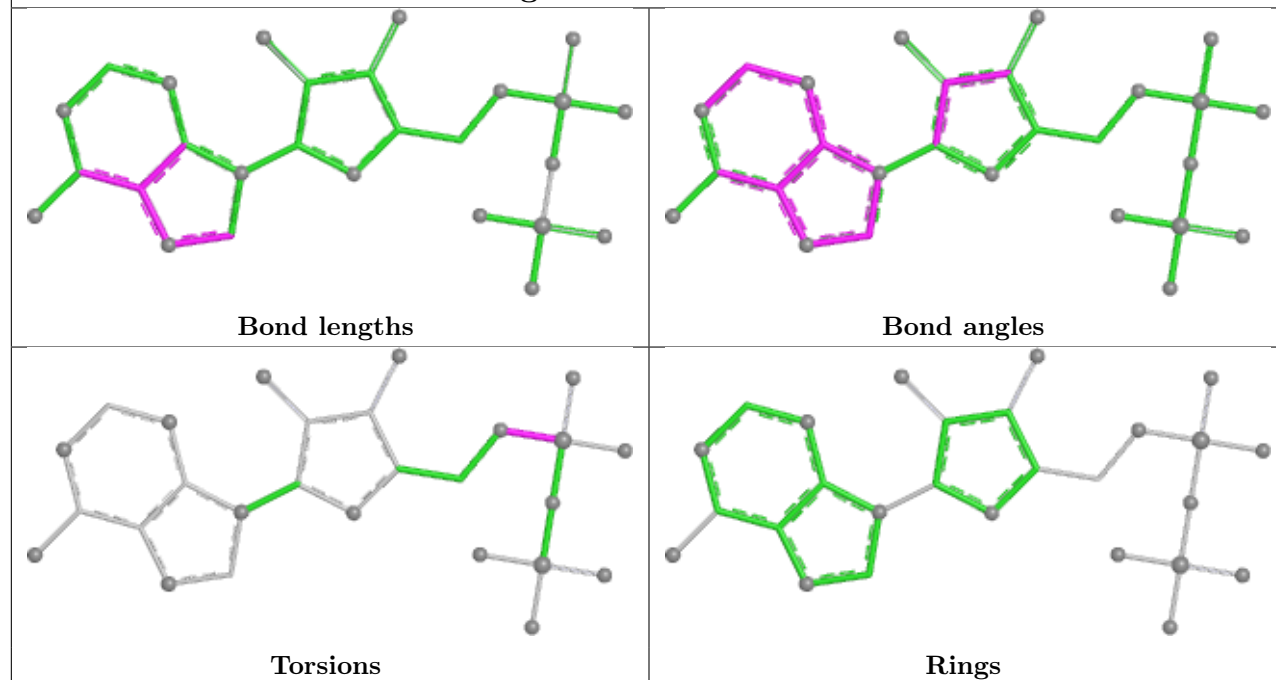


## Ligand ADP B 4704

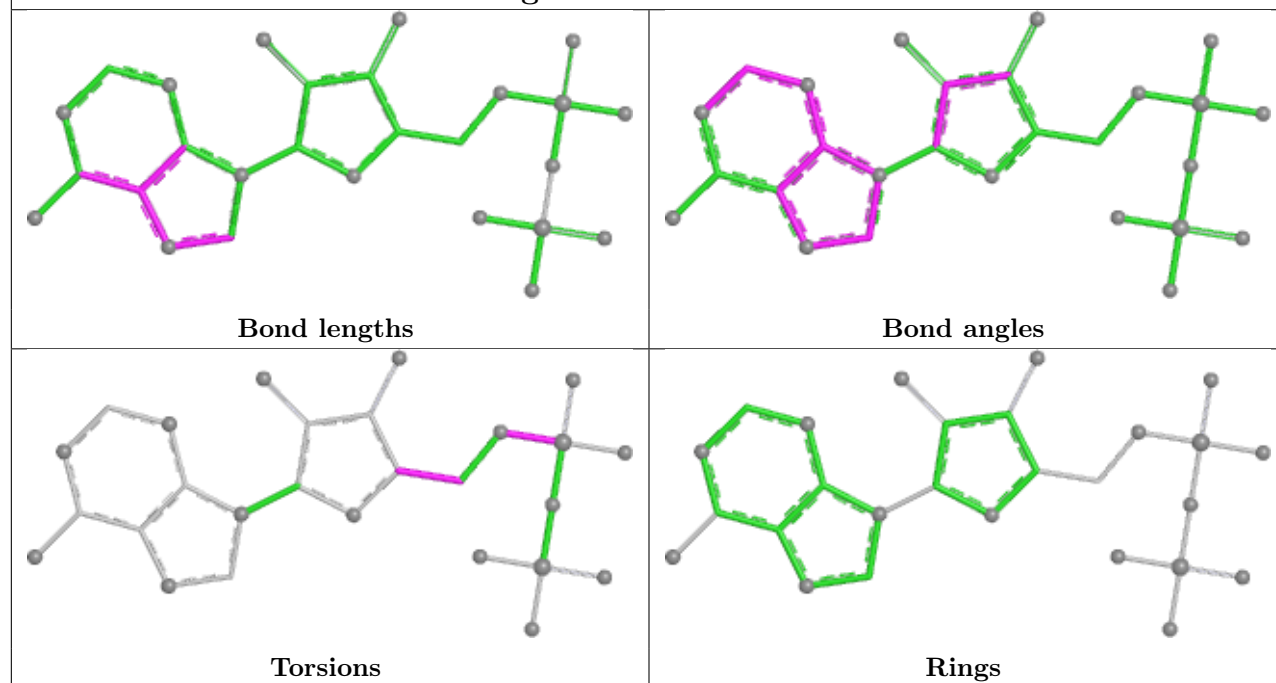




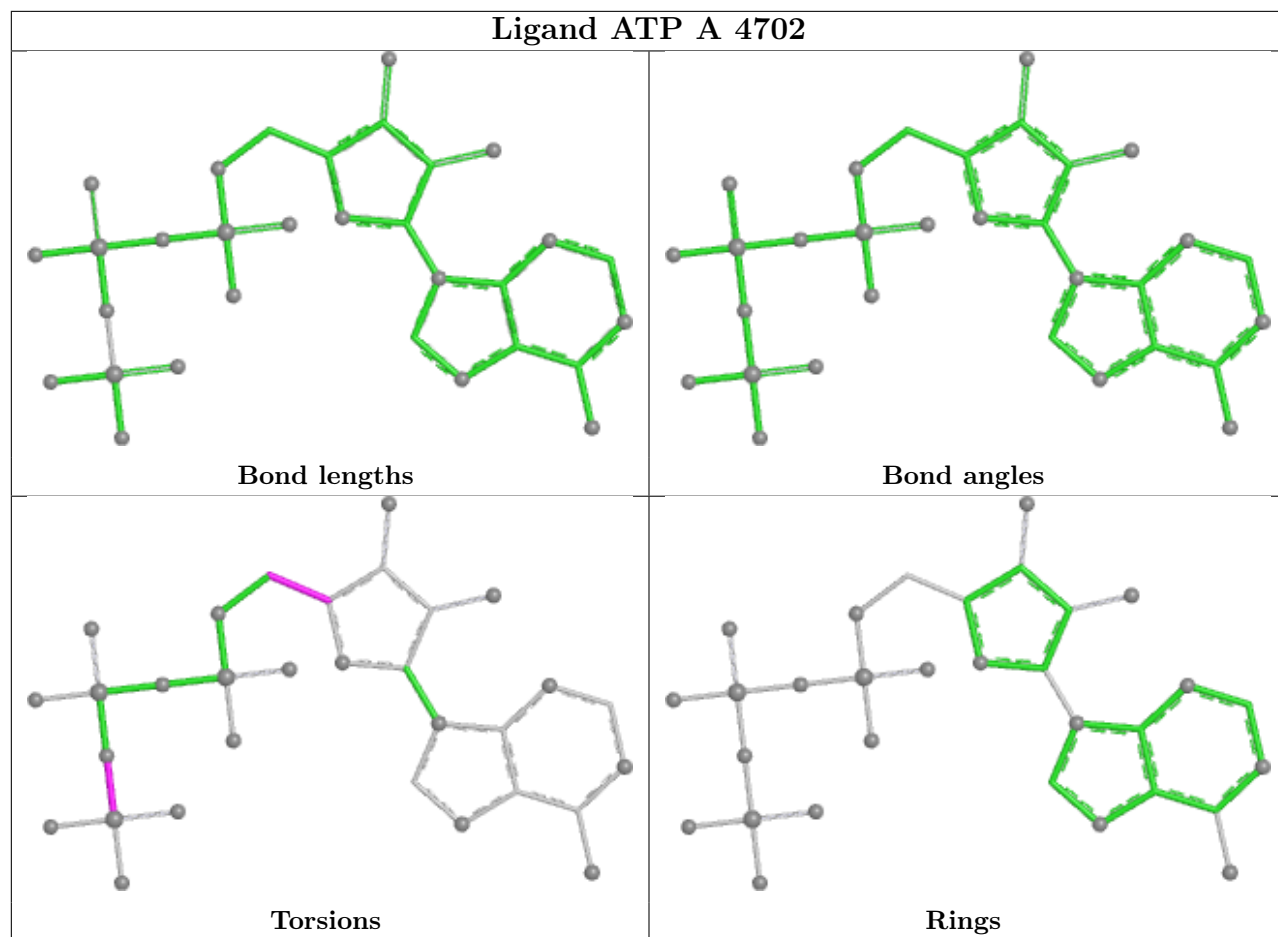
## Ligand ADP A 4704



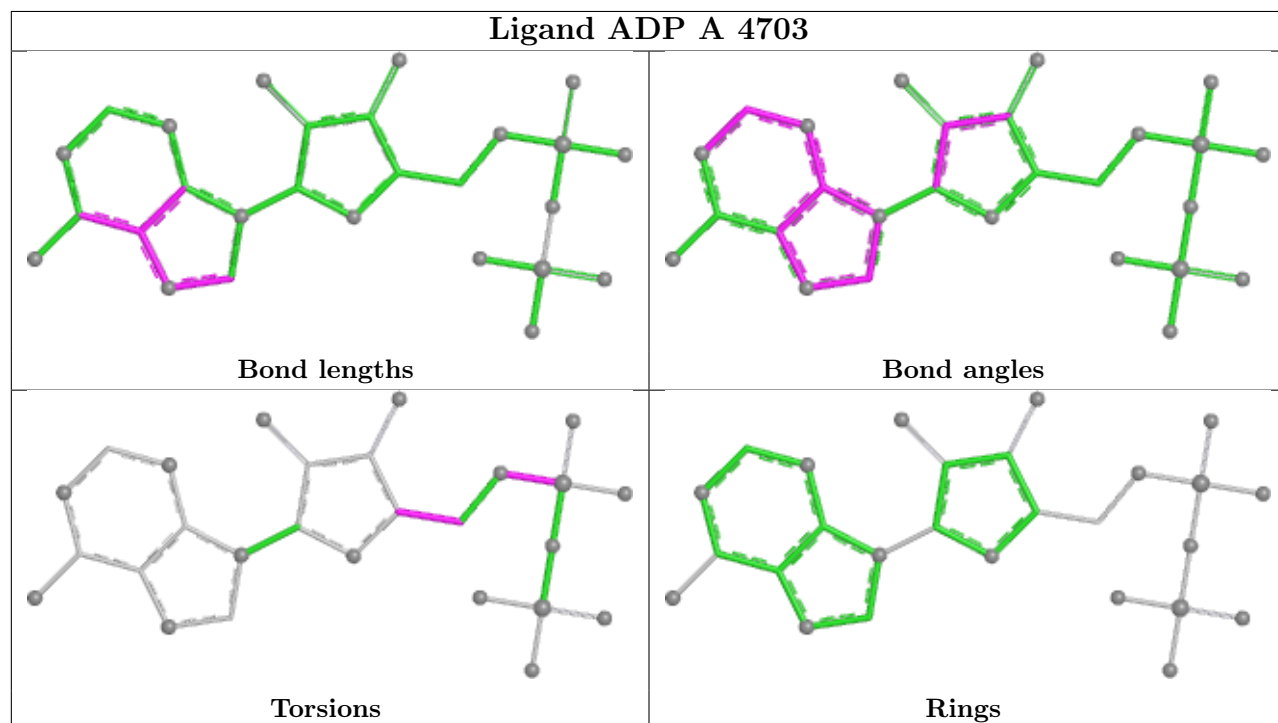
## Ligand ADP B 4703



## Ligand ATP A 4702



## Ligand ADP A 4703



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	B	1
1	A	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	1394:MET	C	1395:LYS	N	8.85
1	A	1394:MET	C	1395:LYS	N	3.62

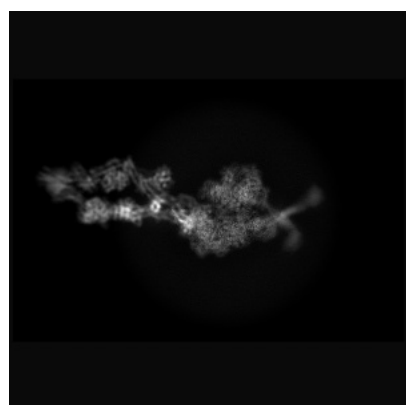
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-47383. These allow visual inspection of the internal detail of the map and identification of artifacts.

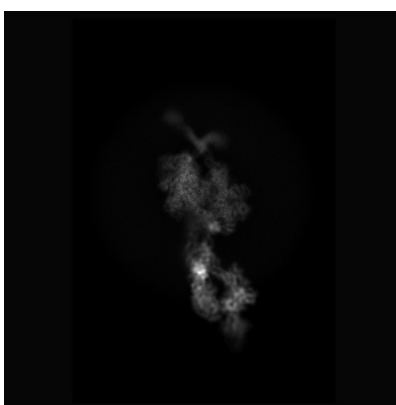
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

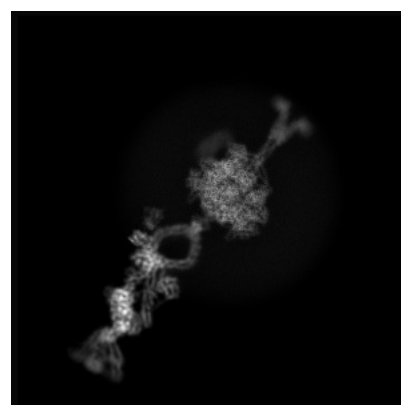
#### 6.1.1 Primary map



X



Y

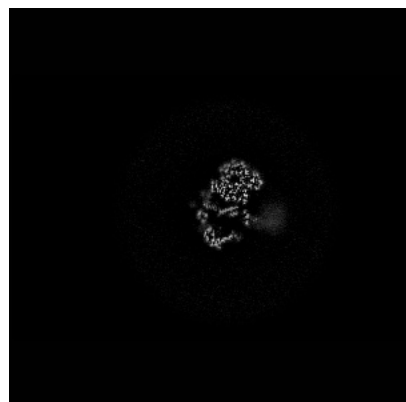


Z

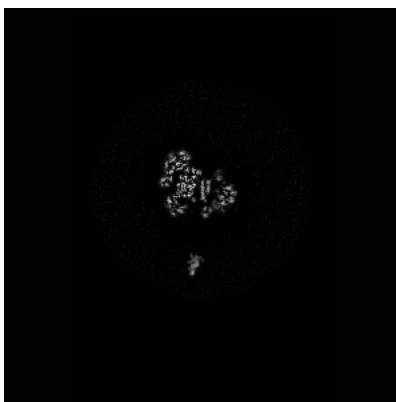
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

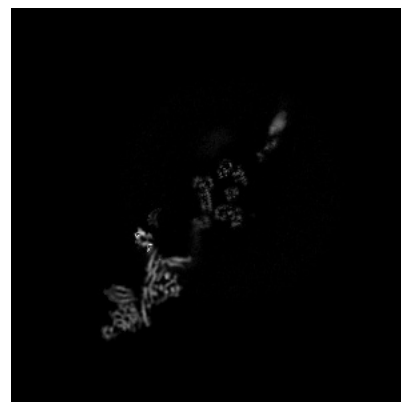
#### 6.2.1 Primary map



X Index: 210



Y Index: 210



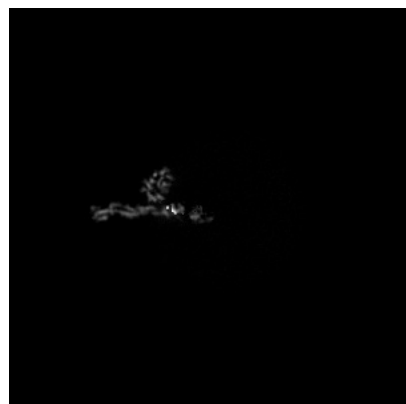
Z Index: 210



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

## 6.3 Largest variance slices [i](#)

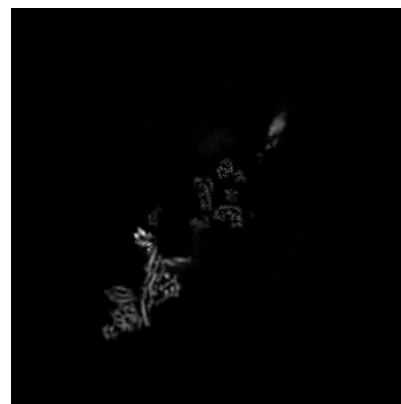
### 6.3.1 Primary map



X Index: 144



Y Index: 156

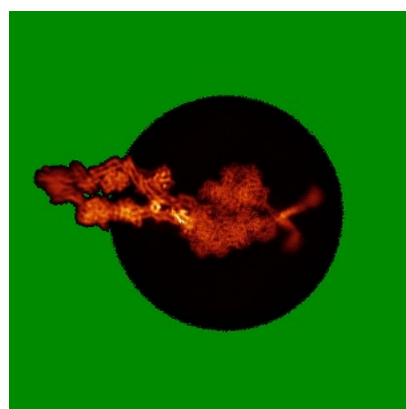


Z Index: 209

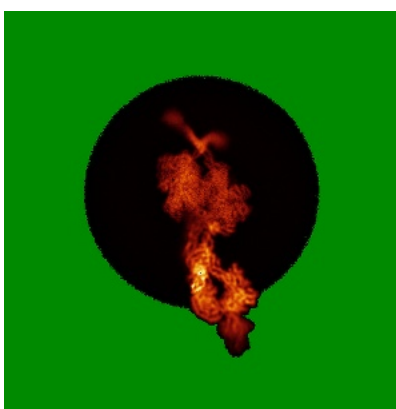
The images above show the largest variance slices of the map in three orthogonal directions.

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

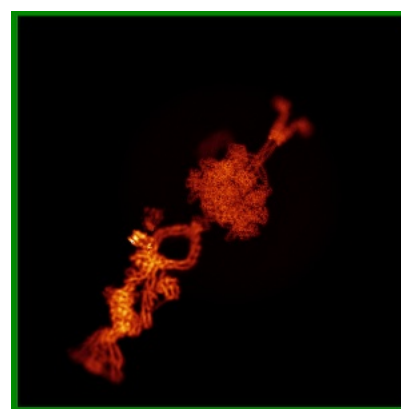
### 6.4.1 Primary map



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

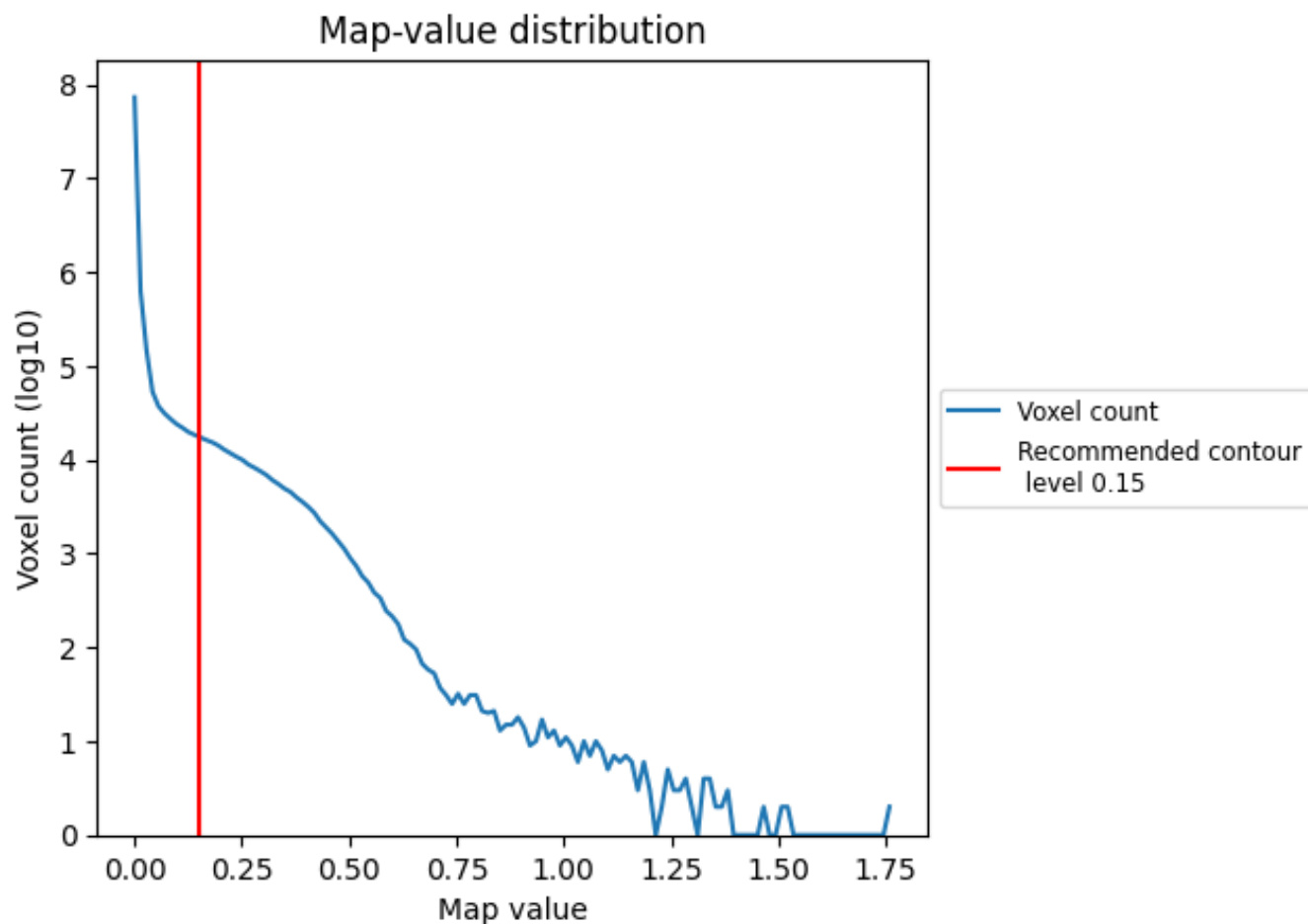
## 6.6 Mask visualisation [i](#)

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

## 7 Map analysis [i](#)

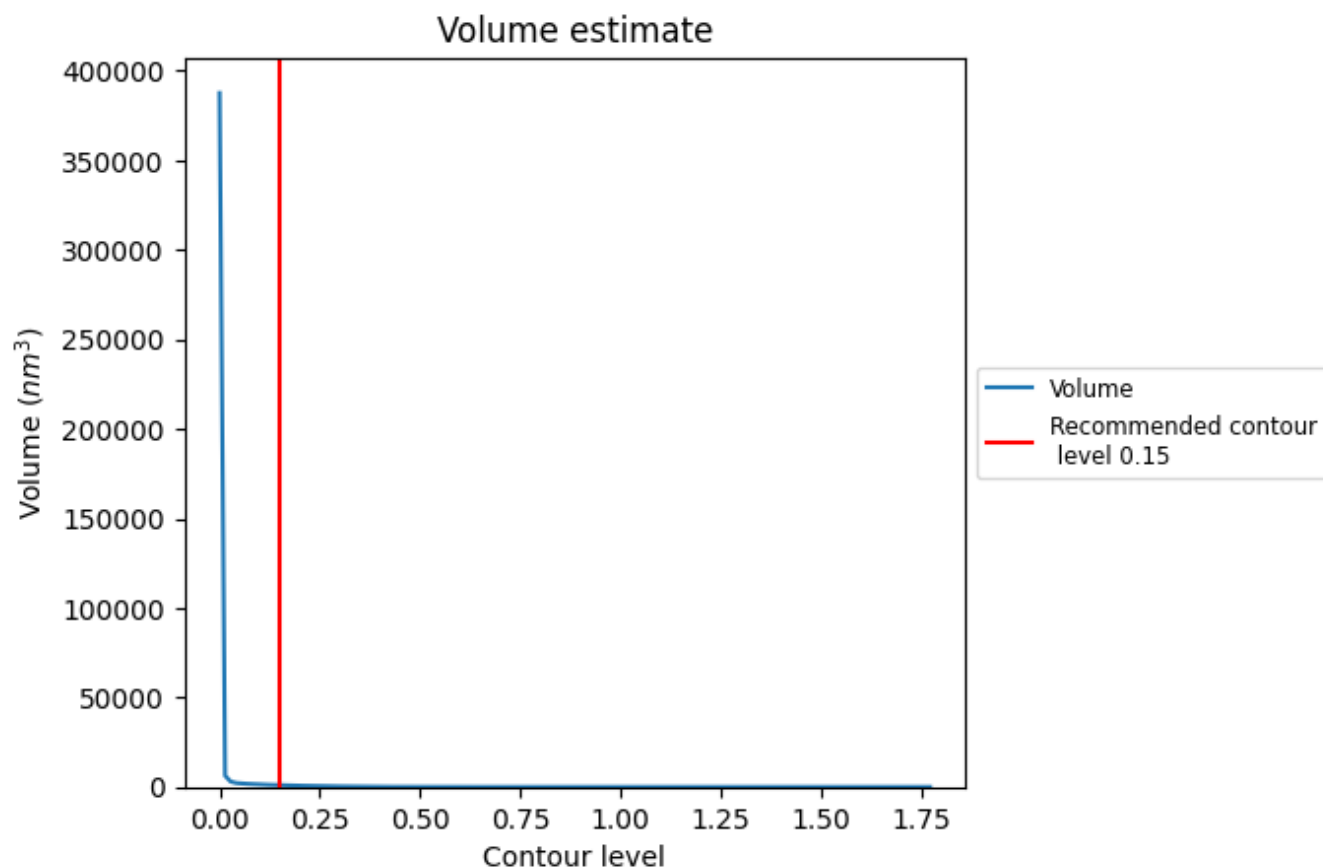
This section contains the results of statistical analysis of the map.

### 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.

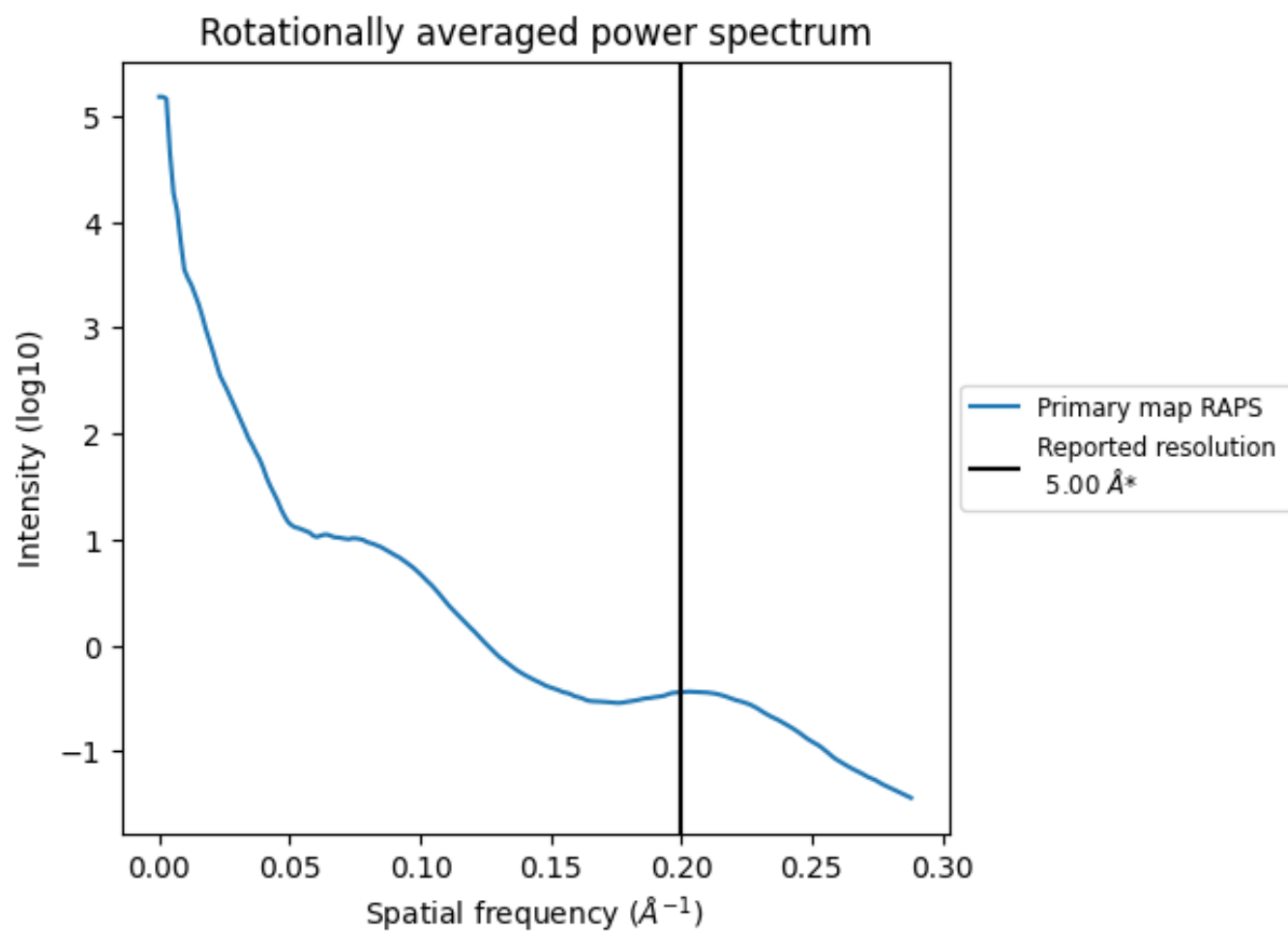
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1005  $\text{nm}^3$ ; this corresponds to an approximate mass of 908 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 0.200 Å<sup>-1</sup>

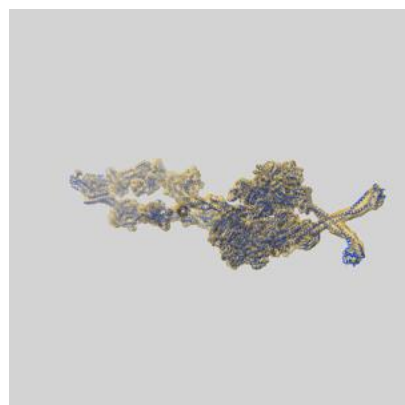
## 8 Fourier-Shell correlation

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

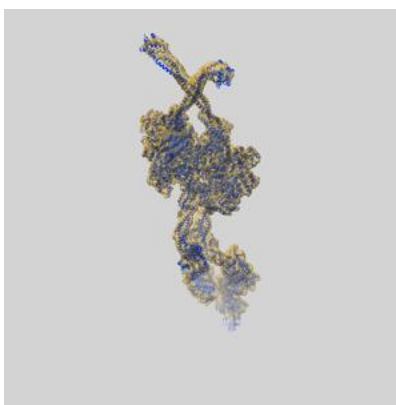
## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-47383 and PDB model 9E14. Per-residue inclusion information can be found in section [3](#) on page [8](#).

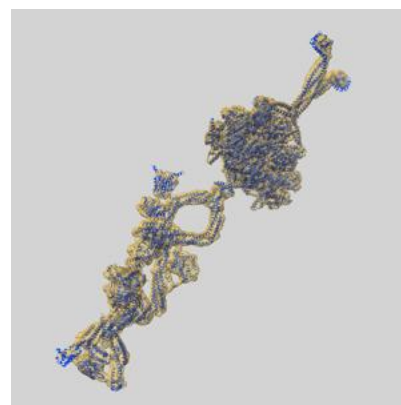
### 9.1 Map-model overlay [i](#)



X



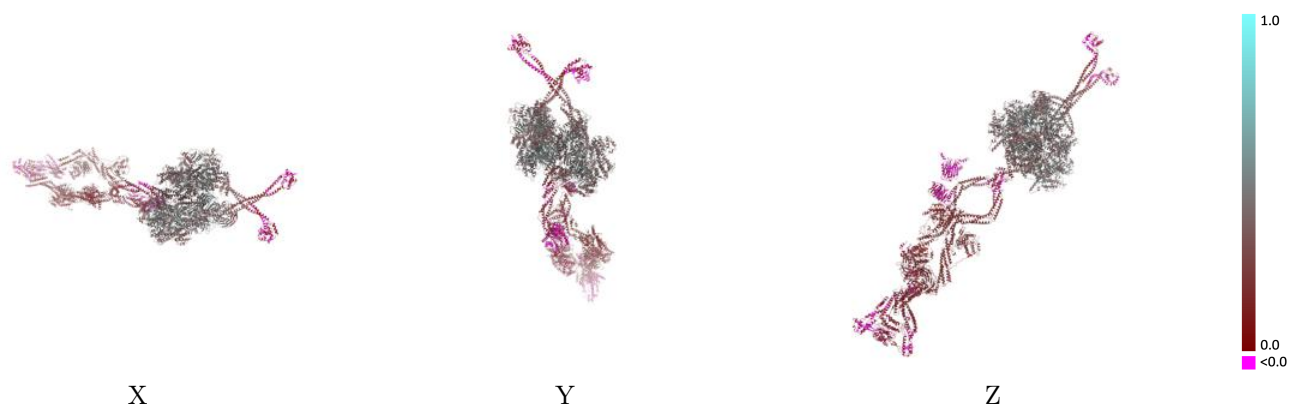
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.15 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 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.

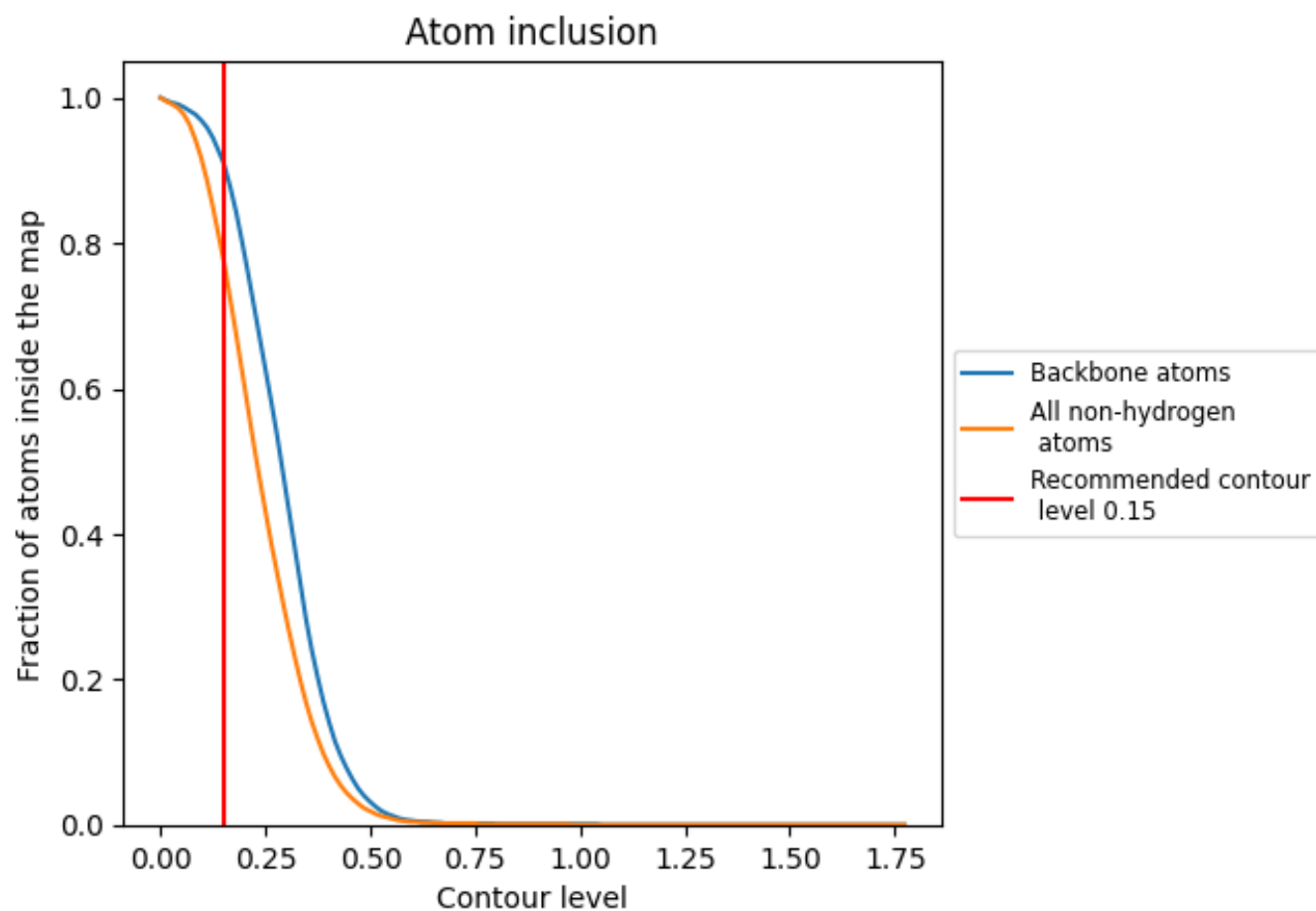
## 9.3 Atom inclusion mapped to coordinate model [i](#)



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 (0.15).



## 9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 78% 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 (0.15) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	<div></div> 0.7770	<div></div> 0.3020
A	<div></div> 0.7410	<div></div> 0.3160
B	<div></div> 0.7900	<div></div> 0.3320
C	<div></div> 0.9210	<div></div> 0.2070
D	<div></div> 0.9250	<div></div> 0.1850
E	<div></div> 0.9320	<div></div> 0.2040
F	<div></div> 0.9220	<div></div> 0.1970
G	<div></div> 0.7570	<div></div> 0.1070
H	<div></div> 0.8730	<div></div> 0.1490
I	<div></div> 0.7660	<div></div> 0.0700
J	<div></div> 0.6230	<div></div> 0.0360
K	<div></div> 0.3560	<div></div> 0.0150
L	<div></div> 0.3330	<div></div> 0.0080
O	<div></div> 0.8120	<div></div> 0.4860
P	<div></div> 0.7490	<div></div> 0.3860

1.0

0.0

<0.0