



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 8, 2018 – 11:38 PM EST

PDB ID : 2WIN
Title : C3 convertase (C3bBb) stabilized by SCIN
Authors : Wu, J.; Janssen, B.J.; Gros, P.
Deposited on : 2009-05-13
Resolution : 3.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20030736
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

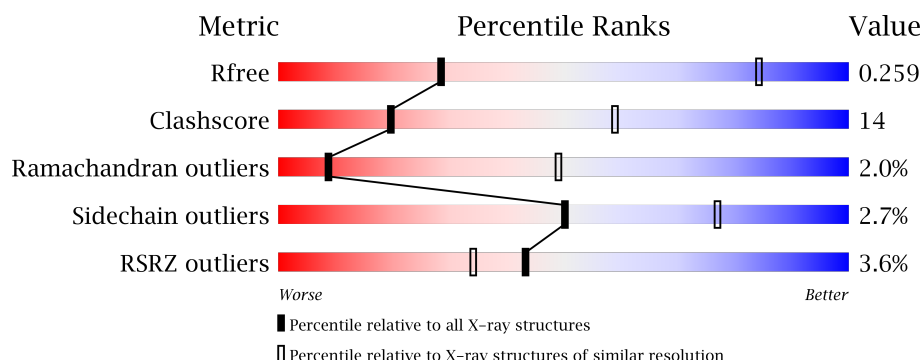
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.90 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	100719	1007 (4.20-3.60)
Clashscore	112137	1103 (4.20-3.60)
Ramachandran outliers	110173	1062 (4.20-3.60)
Sidechain outliers	110143	1053 (4.20-3.60)
RSRZ outliers	101464	1020 (4.20-3.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	645	<div> <div>2%</div> <div>72%</div> <div>25%</div> <div>..</div> </div>
1	C	645	<div> <div>2%</div> <div>72%</div> <div>26%</div> <div>..</div> </div>
1	E	645	<div> <div>2%</div> <div>72%</div> <div>26%</div> <div>..</div> </div>
1	G	645	<div> <div>9%</div> <div>71%</div> <div>27%</div> <div>..</div> </div>
2	B	915	<div> <div>3%</div> <div>69%</div> <div>26%</div> <div>...</div> </div>

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Mol	Chain	Length	Quality of chain
2	D	915	
2	F	915	
2	H	915	
3	I	507	
3	J	507	
3	K	507	
3	L	507	
4	M	92	
4	N	92	
4	P	92	
4	Q	92	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
5	NDG	B	2642	X	-	-	-
5	NDG	C	1646	X	-	-	-
5	NDG	D	2642	X	-	-	-
5	NDG	E	1646	X	-	-	-
5	NDG	G	1646	X	-	-	-
5	NDG	H	2642	X	-	-	-
5	NDG	I	1743	X	-	-	-
5	NDG	I	1746	X	-	-	-
5	NDG	J	1743	X	-	-	-
5	NDG	K	1743	X	-	-	-
5	NDG	L	1743	X	-	-	-
5	NDG	L	1746	X	-	-	-
8	MAN	H	2644	X	-	-	-
8	MAN	H	2645	X	-	-	-
8	MAN	I	1745	X	-	-	-
8	MAN	J	1745	X	-	-	-
8	MAN	K	1745	X	-	-	-
8	MAN	K	1746	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
8	MAN	K	1748	X	-	-	-

2 Entry composition

There are 10 unique types of molecules in this entry. The entry contains 67989 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called COMPLEMENT C3 BETA CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	638	Total	C	N	O	S	0	0	0
			4958	3157	841	945	15			
1	C	638	Total	C	N	O	S	0	0	0
			4958	3157	841	945	15			
1	E	638	Total	C	N	O	S	0	0	0
			4958	3157	841	945	15			
1	G	638	Total	C	N	O	S	0	0	0
			4958	3157	841	945	15			

- Molecule 2 is a protein called COMPLEMENT C3B ALPHA' CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	901	Total	C	N	O	S	0	0	0
			7177	4545	1209	1386	37			
2	D	901	Total	C	N	O	S	0	0	0
			7166	4537	1208	1384	37			
2	F	900	Total	C	N	O	S	0	0	0
			7172	4545	1206	1384	37			
2	H	900	Total	C	N	O	S	2313	0	0
			7175	4547	1209	1382	37			

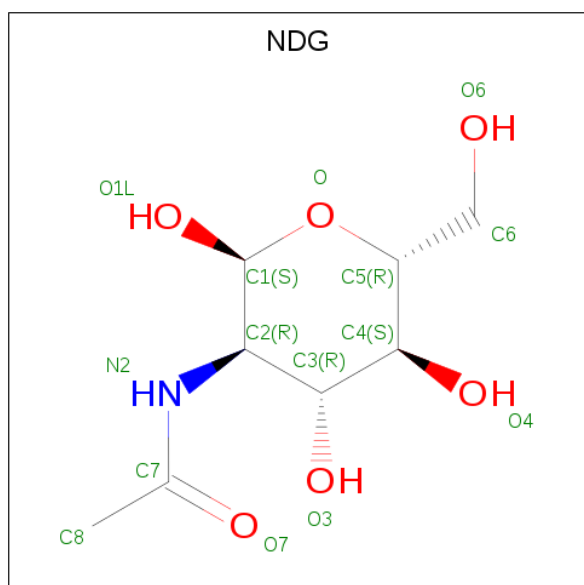
- Molecule 3 is a protein called COMPLEMENT FACTOR B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	I	507	Total	C	N	O	S	0	0	0
			4004	2543	685	756	20			
3	J	507	Total	C	N	O	S	0	0	0
			4004	2543	685	756	20			
3	K	507	Total	C	N	O	S	0	0	0
			4004	2543	685	756	20			
3	L	507	Total	C	N	O	S	0	0	0
			4004	2543	685	756	20			

- Molecule 4 is a protein called STAPHYLOCOCCAL COMPLEMENT INHIBITOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	M	84	Total	C	N	O	S	0	0	0
			682	432	111	137	2			
4	N	84	Total	C	N	O	S	0	0	0
			682	432	111	137	2			
4	P	84	Total	C	N	O	S	0	0	0
			682	432	111	137	2			
4	Q	84	Total	C	N	O	S	0	0	0
			682	432	111	137	2			

- Molecule 5 is 2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE (three-letter code: NDG) (formula: $C_8H_{15}NO_6$).



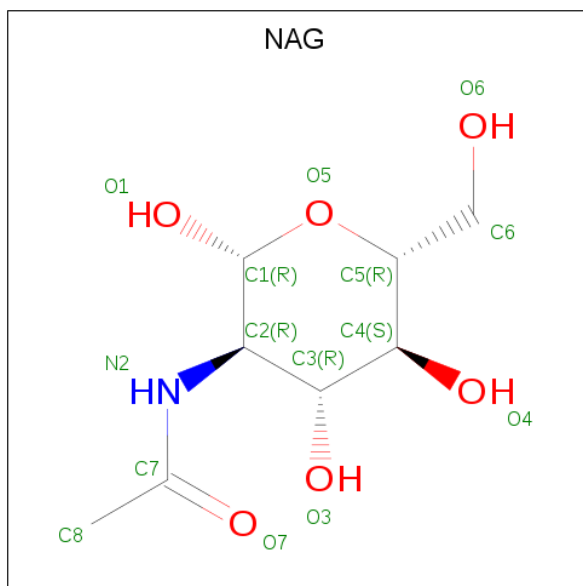
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	N	O	0	0
			14	8	1	5		
5	B	1	Total	C	N	O	0	0
			14	8	1	5		
5	C	1	Total	C	N	O	0	0
			14	8	1	5		
5	D	1	Total	C	N	O	0	0
			14	8	1	5		
5	E	1	Total	C	N	O	0	0
			14	8	1	5		
5	F	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	G	1	Total	C	N	O	0	0
			14	8	1	5		
5	H	1	Total	C	N	O	0	0
			14	8	1	5		
5	I	1	Total	C	N	O	0	0
			14	8	1	5		
5	I	1	Total	C	N	O	0	0
			14	8	1	5		
5	J	1	Total	C	N	O	0	0
			14	8	1	5		
5	K	1	Total	C	N	O	0	0
			14	8	1	5		
5	K	1	Total	C	N	O	0	0
			14	8	1	5		
5	L	1	Total	C	N	O	0	0
			14	8	1	5		
5	L	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 6 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula: $C_8H_{15}NO_6$).



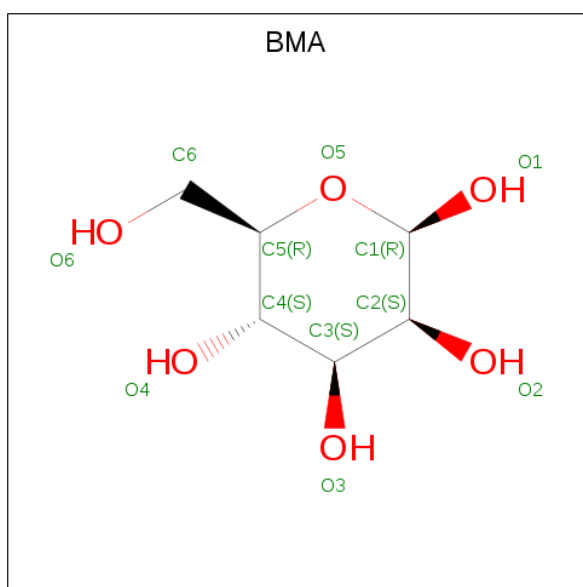
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	0
			14	8	1	5		
6	B	1	Total	C	N	O	0	0
			14	8	1	5		

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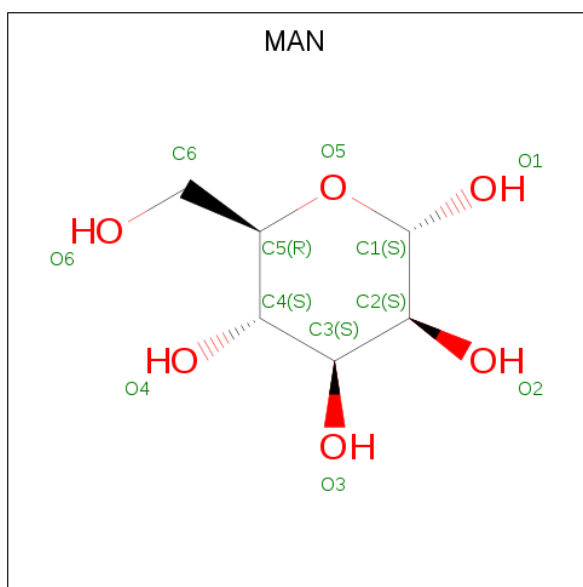
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			14	8	1	5		
6	D	1	Total	C	N	O	0	0
			14	8	1	5		
6	E	1	Total	C	N	O	0	0
			14	8	1	5		
6	F	1	Total	C	N	O	0	0
			14	8	1	5		
6	G	1	Total	C	N	O	0	0
			14	8	1	5		
6	H	1	Total	C	N	O	0	0
			14	8	1	5		
6	I	1	Total	C	N	O	0	0
			14	8	1	5		
6	I	1	Total	C	N	O	0	0
			14	8	1	5		
6	J	1	Total	C	N	O	0	0
			14	8	1	5		
6	K	1	Total	C	N	O	0	0
			14	8	1	5		
6	L	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 7 is BETA-D-MANNOSE (three-letter code: BMA) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			11	6	5		
7	A	1	Total	C	O	0	0
			11	6	5		
7	B	1	Total	C	O	0	0
			11	6	5		
7	B	1	Total	C	O	0	0
			11	6	5		
7	B	1	Total	C	O	0	0
			11	6	5		
7	C	1	Total	C	O	0	0
			11	6	5		
7	C	1	Total	C	O	0	0
			11	6	5		
7	C	1	Total	C	O	0	0
			11	6	5		
7	D	1	Total	C	O	0	0
			11	6	5		
7	D	1	Total	C	O	0	0
			11	6	5		
7	E	1	Total	C	O	0	0
			11	6	5		
7	E	1	Total	C	O	0	0
			11	6	5		
7	F	1	Total	C	O	0	0
			11	6	5		
7	F	1	Total	C	O	0	0
			11	6	5		
7	F	1	Total	C	O	0	0
			11	6	5		
7	F	1	Total	C	O	0	0
			11	6	5		
7	G	1	Total	C	O	0	0
			11	6	5		
7	G	1	Total	C	O	0	0
			11	6	5		
7	G	1	Total	C	O	0	0
			11	6	5		
7	K	1	Total	C	O	0	0
			11	6	5		
7	L	1	Total	C	O	0	0
			11	6	5		

- Molecule 8 is ALPHA-D-MANNOSE (three-letter code: MAN) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	G	1	Total	C	O	0	0
			11	6	5		
8	H	1	Total	C	O	0	0
			11	6	5		
8	H	1	Total	C	O	0	0
			11	6	5		
8	I	1	Total	C	O	0	0
			11	6	5		
8	J	1	Total	C	O	0	0
			11	6	5		
8	K	1	Total	C	O	0	0
			11	6	5		
8	K	1	Total	C	O	0	0
			11	6	5		
8	K	1	Total	C	O	0	0
			11	6	5		

- Molecule 9 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	J	1	Total	Mg	0	0
			1	1		
9	I	1	Total	Mg	0	0
			1	1		
9	L	1	Total	Mg	0	0
			1	1		
9	K	1	Total	Mg	0	0
			1	1		

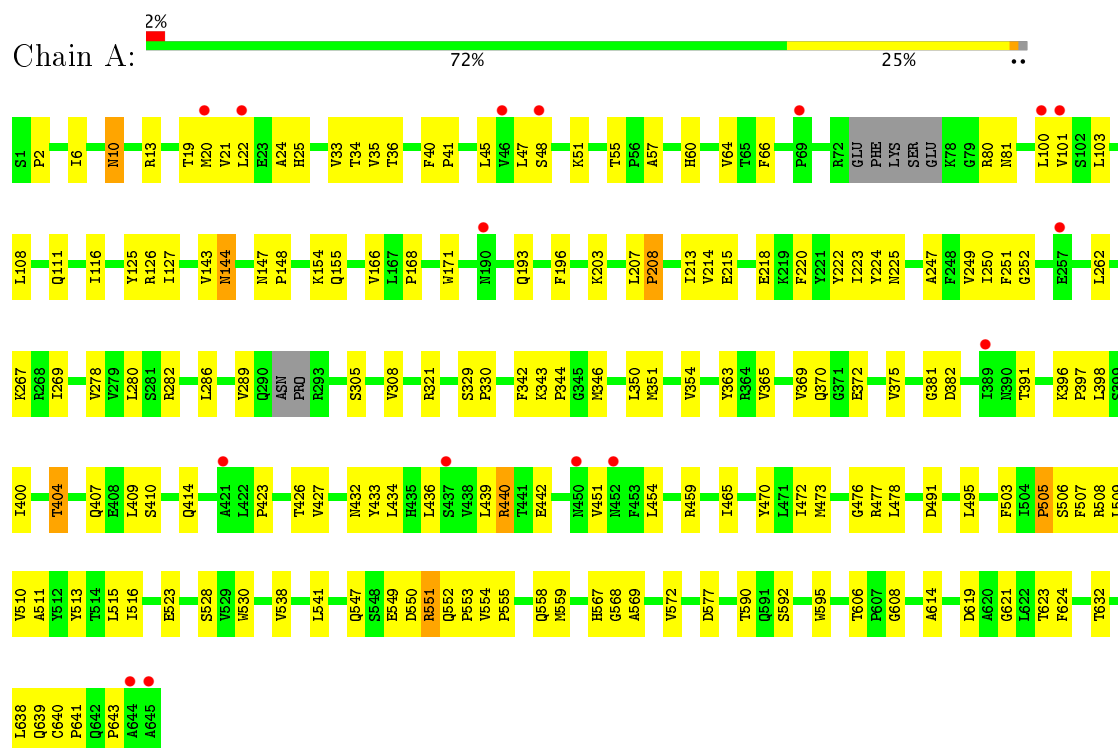
- Molecule 10 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
10	B	1	Total 1	O 1	0	0
10	I	2	Total 2	O 2	0	0
10	J	2	Total 2	O 2	0	0
10	K	2	Total 2	O 2	0	0
10	L	1	Total 1	O 1	0	0

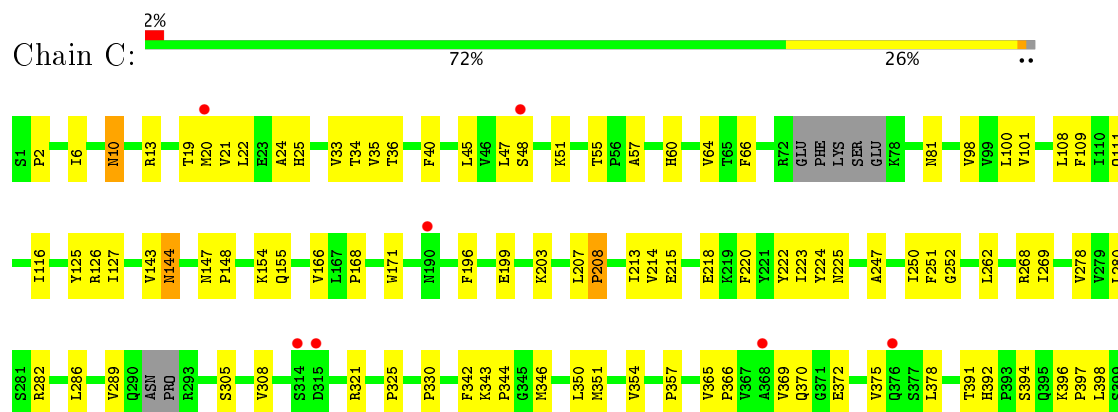
3 Residue-property plots

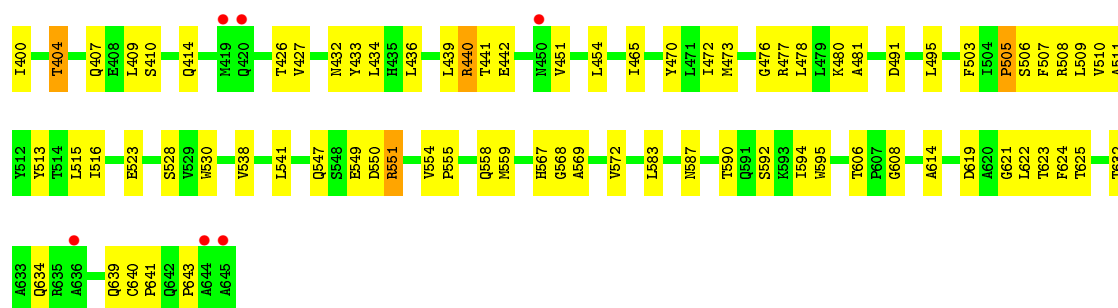
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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 dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). 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: COMPLEMENT C3 BETA CHAIN

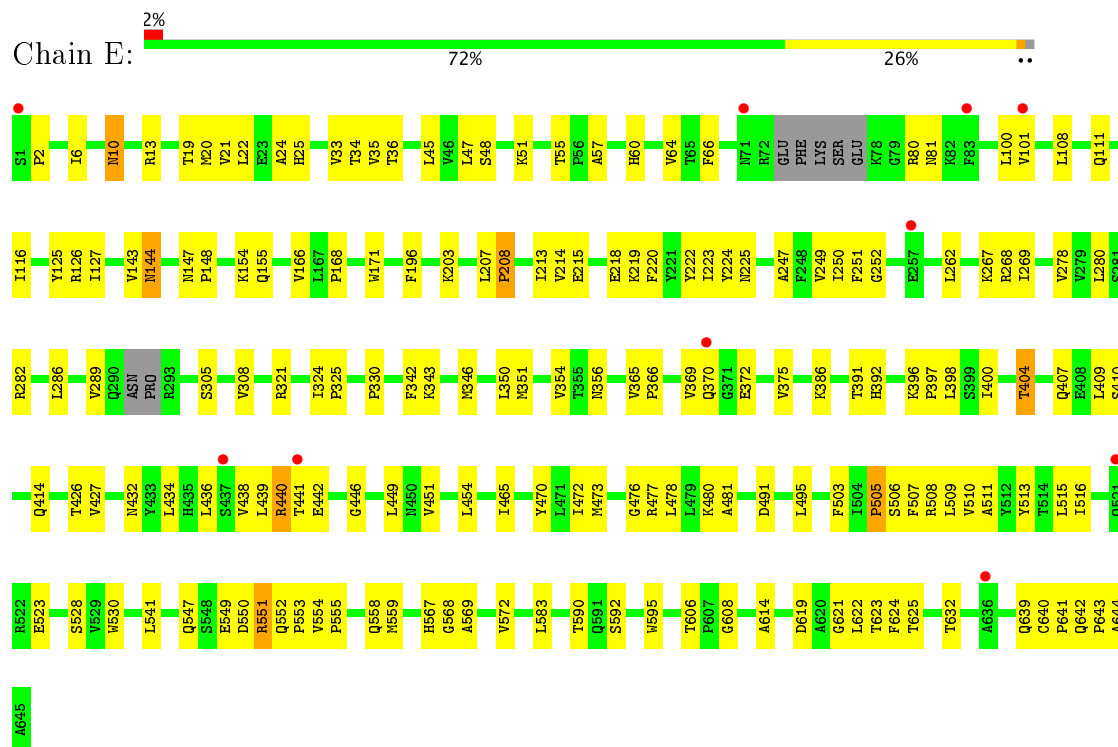


• Molecule 1: COMPLEMENT C3 BETA CHAIN

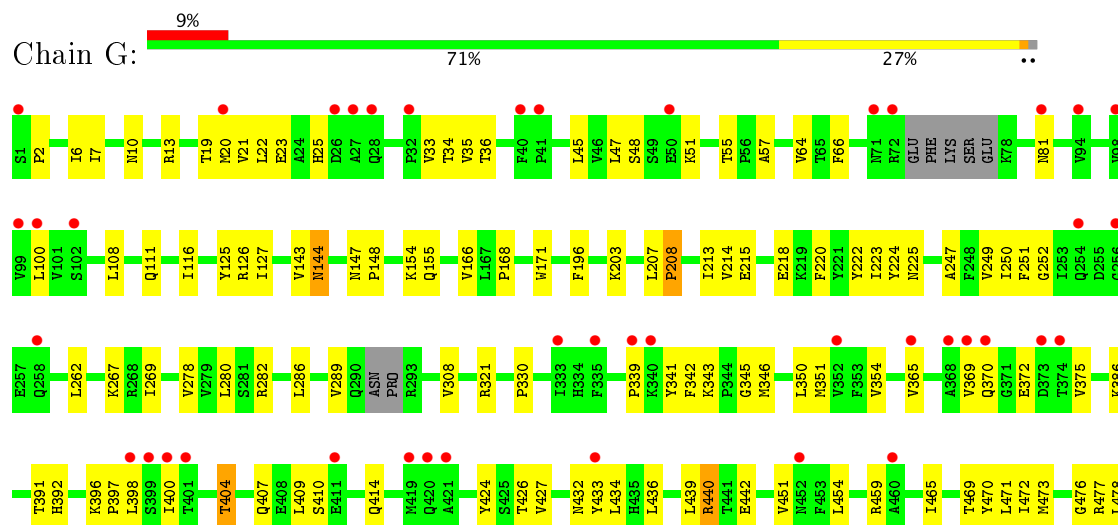


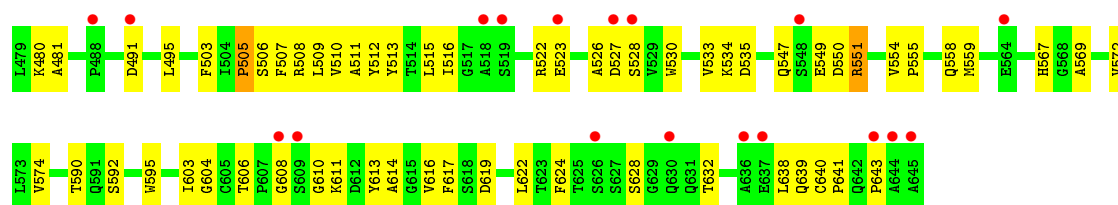


• Molecule 1: COMPLEMENT C3 BETA CHAIN

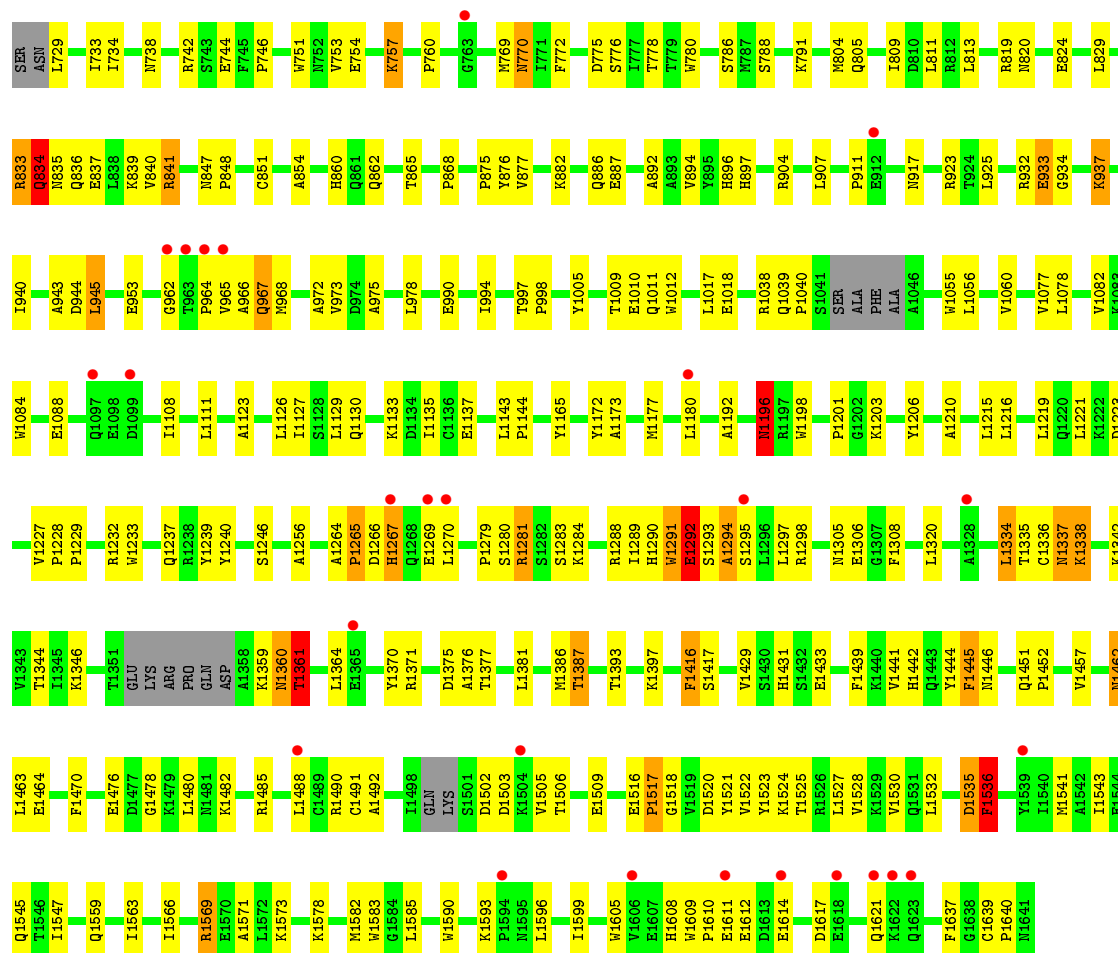


• Molecule 1: COMPLEMENT C3 BETA CHAIN

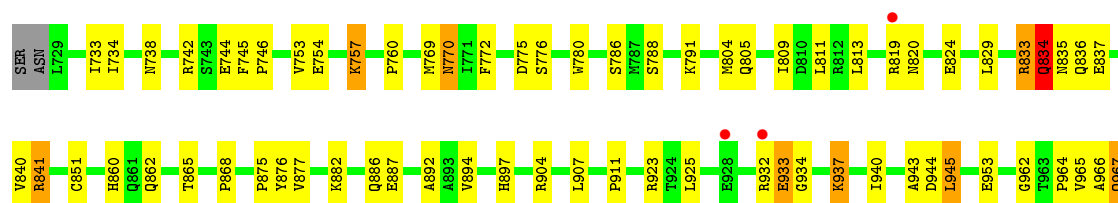




• Molecule 2: COMPLEMENT C3B ALPHA' CHAIN

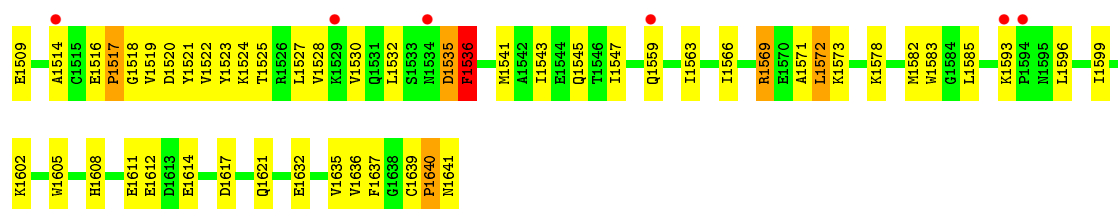


• Molecule 2: COMPLEMENT C3B ALPHA' CHAIN

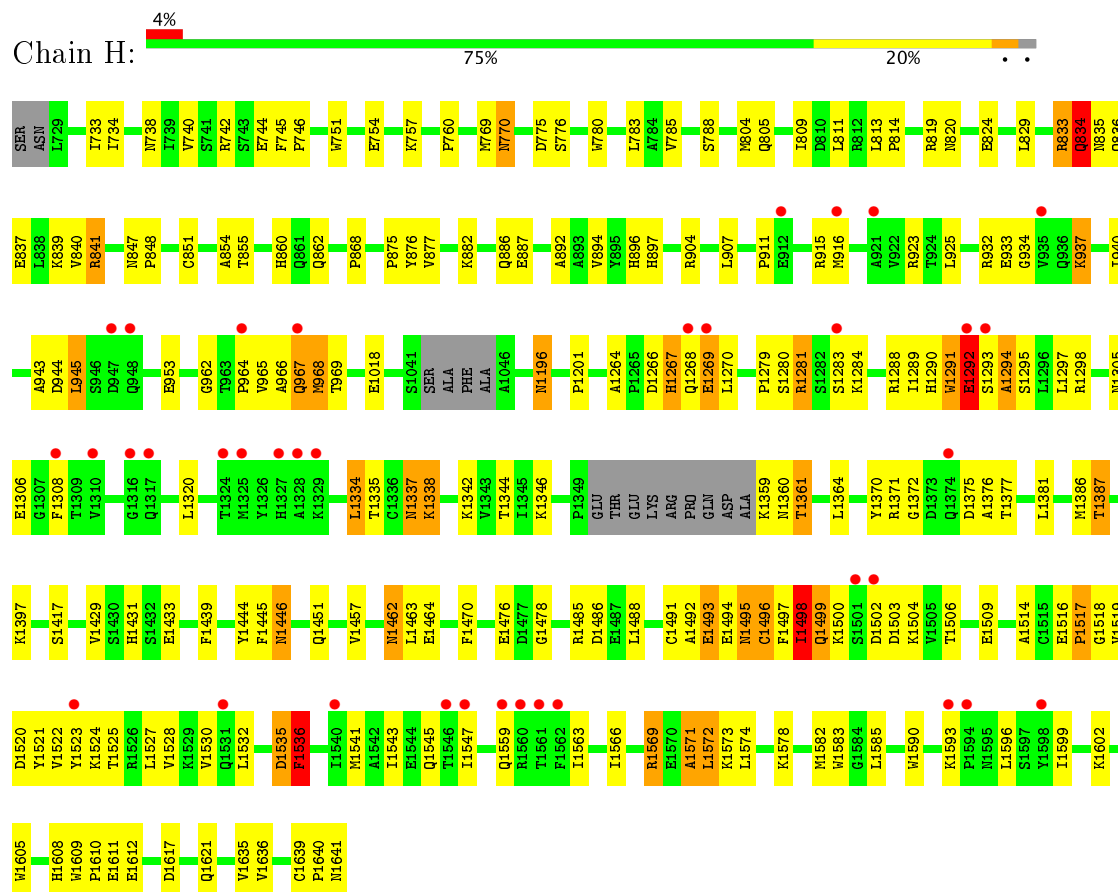




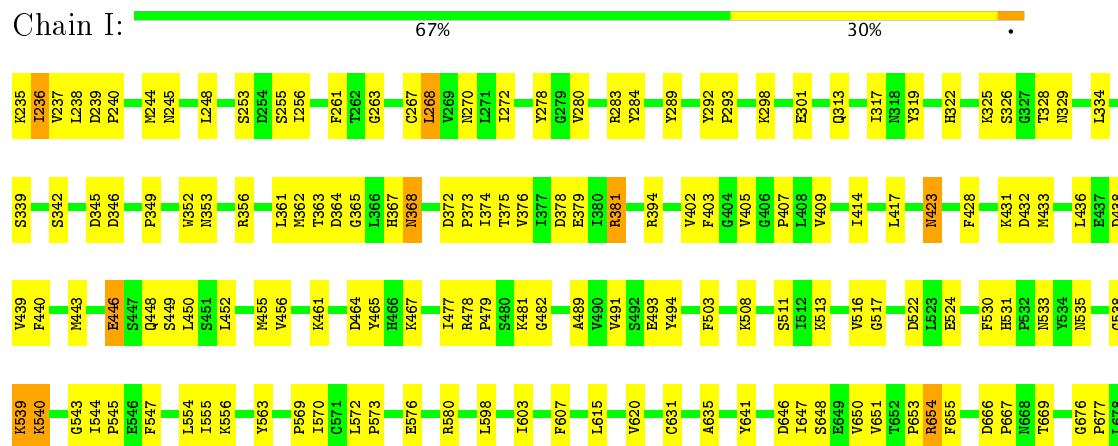
D1373	K1284	L1180	L1056	G962	V840	SER
D1375	R1288	K1181	V1060	T963	R841	ASN
A1376	I1289	P1183		P964		L729
T1377	H1290		I1073	V865	N847	I733
M1378	W1291	A1192	D1074	A868	P846	I734
	E1292	K1193	S1075	Q967		
L1381	S1293	D1194	Q1076	R968	A854	N738
	A1294	K1195	V1077	T955	T855	I739
M1386	S1295	N1196	L1078	E870	V740	V740
T1387	L1296	R1197	C1079	H860	S741	S741
	L1297	W1198		A872	Q861	R742
A1390	R1298	P1201	V1082	V973	Q862	S743
P1391	N1305	G1202	K1083	D874	E744	E744
	E1306	K1203	W1084	A975	F745	F745
K1397	G1307			P868	P746	P746
S1417	F1308	Y1206	E1088	L878	P875	V753
	K1315	A1210	D1093	G987	V876	E754
V1429	L1320	L1215	G1094	E990	K882	K757
H1430		L1216	I1108	I994	Q886	E758
H1431			L1111	T997	E887	P759
S1432	H1327	L1219	E1116	R998	A892	M769
E1433	A1328	K1329	K1117	T999	A893	N770
F1439	A1330	L1220	D1118	V1000	V894	
F1445	K1331	K1222	M1119	Y1005	H895	D775
M1446	L1334	D1223			H896	S776
	T1335	V1227	T1122		R897	
Q1451	C1336	P1228	A1123	T1009	R904	M780
V1457	N1337	P1229	L1126	Q1010	Q1011	
	K1338		S1128	I1127	W1012	S786
K1342		R1232	W1233	L1017	P911	S787
V1343		W1237	L1129	E1018	E912	S788
I1345		K1238	Q1130	Q1038	N904	Q805
K1346		Y1239	K1133	I1027	R915	
		Y1240	D1134	R915	N916	L809
	P1349	S1246	I1135	Q1034		D810
	GLU		E1136	L1035		L811
E1476	THR	A1266	E1137	R923	R923	R812
D1477	LVS		L1143	Q1039	T924	L813
K1478		A1264	P1144	S1040	L925	
K1479	ARG	P1265	I1147	SER	R932	R819
	PRO	D1266		E933	E933	N820
E1494	GLN	A1267		ALA	Q822	E821
M1495	ASP	Q1268	M1157	PHE	V823	Q822
C1496	ALA	E1269	Y1165	ALA	E924	E824
F1497	K1359	L1270	W1166	A1046	K937	
I1498	N1360	L1271		F1047	T940	L829
Q1499	T1361			V1048		
		P1279	Y1172	K1049	A943	R833
A1500		S1280	A1173	R1050	D944	Q834
S1501	L1364	R1281		A1051	L945	N835
D1502		Y1370	M1177			Q836
		R1371				R837
T1506		C1372				



• Molecule 2: COMPLEMENT C3B ALPHA' CHAIN

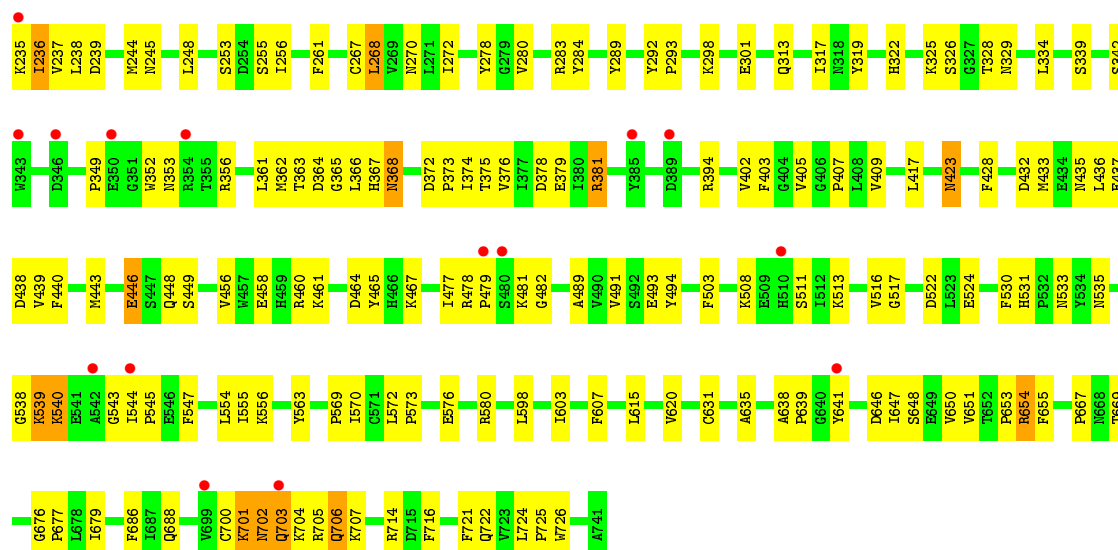


• Molecule 3: COMPLEMENT FACTOR B

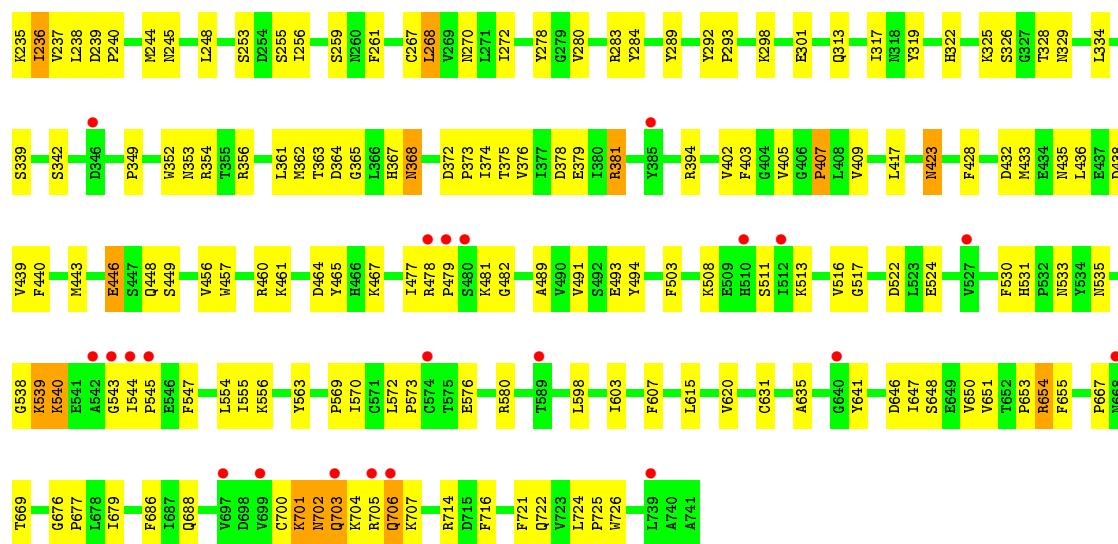




• Molecule 3: COMPLEMENT FACTOR B

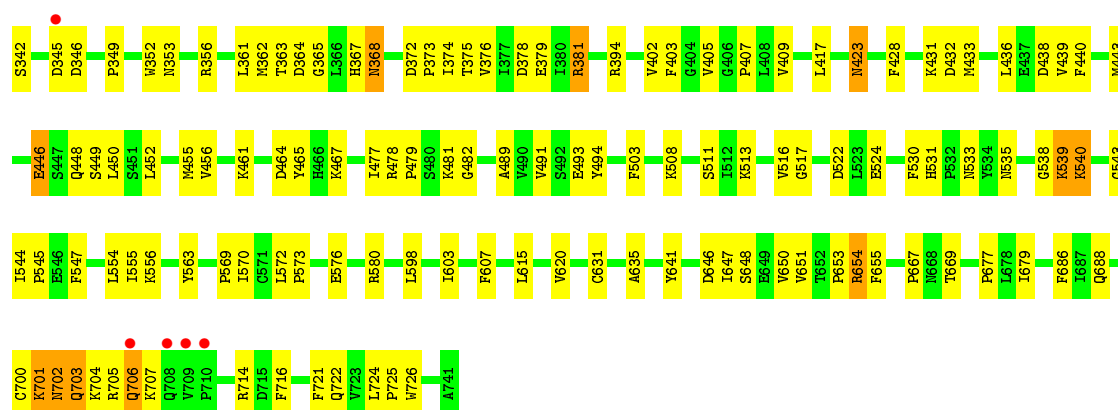


• Molecule 3: COMPLEMENT FACTOR B

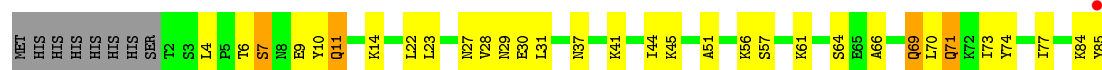


• Molecule 3: COMPLEMENT FACTOR B





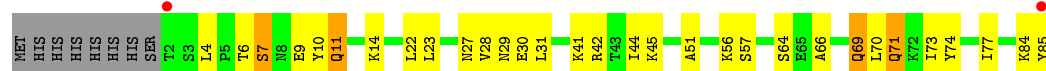
• Molecule 4: STAPHYLOCOCCAL COMPLEMENT INHIBITOR



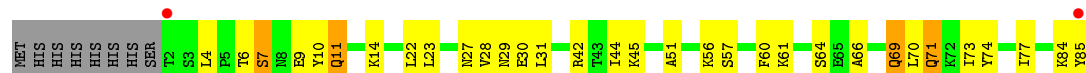
• Molecule 4: STAPHYLOCOCCAL COMPLEMENT INHIBITOR



• Molecule 4: STAPHYLOCOCCAL COMPLEMENT INHIBITOR



• Molecule 4: STAPHYLOCOCCAL COMPLEMENT INHIBITOR



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	228.63Å 121.49Å 280.78Å 90.00° 91.64° 90.00°	Depositor
Resolution (Å)	39.67 – 3.90 39.68 – 3.90	Depositor EDS
% Data completeness (in resolution range)	97.6 (39.67-3.90) 97.6 (39.68-3.90)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.95 (at 3.87Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.253 , 0.268 0.244 , 0.259	Depositor DCC
R_{free} test set	2089 reflections (1.52%)	DCC
Wilson B-factor (Å ²)	125.3	Xtriage
Anisotropy	0.223	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 71.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.41$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.128 for h,-k,-l	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	67989	wwPDB-VP
Average B, all atoms (Å ²)	158.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, BMA, NAG, NDG, MAN

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	0.20	0/5056	0.37	0/6870
1	C	0.20	0/5056	0.37	0/6870
1	E	0.20	0/5056	0.37	0/6870
1	G	0.21	0/5056	0.38	0/6870
2	B	0.21	0/7317	0.36	0/9907
2	D	0.21	0/7306	0.36	0/9894
2	F	0.21	0/7314	0.36	0/9905
2	H	0.22	0/7315	0.36	0/9902
3	I	0.20	0/4092	0.37	0/5543
3	J	0.20	0/4092	0.37	0/5543
3	K	0.20	0/4092	0.37	0/5543
3	L	0.20	0/4092	0.37	0/5543
4	M	0.21	0/690	0.33	0/923
4	N	0.21	0/690	0.32	0/923
4	P	0.21	0/690	0.33	0/923
4	Q	0.21	0/690	0.33	0/923
All	All	0.21	0/68604	0.36	0/92952

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	4958	0	5017	127	0
1	C	4958	0	5017	129	0
1	E	4958	0	5017	132	0
1	G	4958	0	5016	145	0
2	B	7177	0	7085	201	0
2	D	7166	0	7062	193	0
2	F	7172	0	7080	220	0
2	H	7175	0	7087	195	0
3	I	4004	0	3966	129	0
3	J	4004	0	3967	129	0
3	K	4004	0	3965	128	0
3	L	4004	0	3966	126	0
4	M	682	0	697	35	0
4	N	682	0	697	38	0
4	P	682	0	697	33	0
4	Q	682	0	697	38	0
5	A	14	0	12	1	0
5	B	14	0	11	1	0
5	C	14	0	12	2	0
5	D	14	0	12	1	0
5	E	14	0	12	4	0
5	F	14	0	12	0	0
5	G	14	0	12	2	0
5	H	14	0	12	0	0
5	I	28	0	24	2	0
5	J	14	0	12	1	0
5	K	28	0	25	7	0
5	L	28	0	25	0	0
6	A	14	0	12	1	0
6	B	14	0	12	0	0
6	C	14	0	12	1	0
6	D	14	0	12	1	0
6	E	14	0	12	1	0
6	F	14	0	12	0	0
6	G	14	0	12	3	0
6	H	14	0	12	1	0
6	I	28	0	25	2	0
6	J	14	0	12	2	0
6	K	14	0	12	1	0
6	L	14	0	12	0	0
7	A	22	0	19	0	0
7	B	33	0	29	0	0
7	C	33	0	28	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
7	D	22	0	19	0	0
7	E	22	0	19	1	0
7	F	44	0	37	2	0
7	G	33	0	28	4	0
7	K	11	0	10	0	0
7	L	11	0	10	0	0
8	G	11	0	10	1	0
8	H	22	0	19	1	0
8	I	11	0	10	0	0
8	J	11	0	10	0	0
8	K	33	0	28	2	0
9	I	1	0	0	0	0
9	J	1	0	0	0	0
9	K	1	0	0	0	0
9	L	1	0	0	0	0
10	B	1	0	0	0	0
10	I	2	0	0	0	0
10	J	2	0	0	1	0
10	K	2	0	0	0	0
10	L	1	0	0	0	0
All	All	67989	0	67647	1876	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 14.

All (1876) 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:G:426:THR:HG21	1:G:432:ASN:H	1.20	1.07
2:H:1494:GLU:HB3	2:H:1602:LYS:HB3	1.36	1.04
2:D:1569:ARG:HB2	2:D:1569:ARG:HH11	1.32	0.94
2:F:1569:ARG:HB2	2:F:1569:ARG:HH11	1.32	0.94
2:H:1569:ARG:HB2	2:H:1569:ARG:HH11	1.32	0.94
2:B:1569:ARG:HH11	2:B:1569:ARG:HB2	1.32	0.94
2:H:1268:GLN:HG3	2:H:1269:GLU:H	1.34	0.92
1:G:505:PRO:HG3	1:G:595:TRP:CE3	2.08	0.88
3:L:267:CYS:HB2	3:L:433:MET:HE1	1.54	0.87
2:F:1359:LYS:HD2	4:M:4:LEU:HD11	1.58	0.86
1:A:549:GLU:HG2	1:A:550:ASP:H	1.44	0.83
1:G:477:ARG:HH11	1:G:477:ARG:HG2	1.44	0.83
1:C:549:GLU:HG2	1:C:550:ASP:H	1.44	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:477:ARG:HH11	1:E:477:ARG:HG2	1.44	0.82
2:H:1497:PHE:HE2	2:H:1571:ALA:HB1	1.43	0.82
1:E:547:GLN:HE22	1:E:559:MET:HA	1.44	0.82
1:G:549:GLU:HG2	1:G:550:ASP:H	1.44	0.82
3:J:381:ARG:HH21	3:J:381:ARG:HG2	1.45	0.82
1:E:549:GLU:HG2	1:E:550:ASP:H	1.44	0.82
4:Q:6:THR:H	4:Q:9:GLU:HB3	1.45	0.82
4:N:6:THR:H	4:N:9:GLU:HB3	1.45	0.81
4:P:6:THR:H	4:P:9:GLU:HB3	1.45	0.81
1:A:547:GLN:HE22	1:A:559:MET:HA	1.44	0.81
2:H:1485:ARG:HD3	2:H:1536:PHE:CZ	2.16	0.81
1:G:547:GLN:HE22	1:G:559:MET:HA	1.44	0.81
3:K:381:ARG:HG2	3:K:381:ARG:HH21	1.45	0.81
1:C:547:GLN:HE22	1:C:559:MET:HA	1.44	0.81
4:M:6:THR:H	4:M:9:GLU:HB3	1.45	0.81
1:A:477:ARG:HG2	1:A:477:ARG:HH11	1.44	0.80
1:C:477:ARG:HH11	1:C:477:ARG:HG2	1.44	0.80
1:G:508:ARG:CZ	1:G:604:GLY:HA3	2.12	0.80
3:L:381:ARG:HG2	3:L:381:ARG:HH21	1.45	0.80
2:B:819:ARG:HG2	2:B:819:ARG:HH11	1.46	0.80
1:G:481:ALA:H	5:G:1646:NDG:H8C3	1.46	0.80
2:D:819:ARG:HG2	2:D:819:ARG:HH11	1.46	0.80
3:I:381:ARG:HH21	3:I:381:ARG:HG2	1.45	0.80
1:C:45:LEU:HD11	1:C:48:SER:HB3	1.64	0.79
2:H:833:ARG:HH11	2:H:833:ARG:HG2	1.48	0.79
2:D:833:ARG:HG2	2:D:833:ARG:HH11	1.48	0.79
2:H:1488:LEU:HG	2:H:1590:TRP:HH2	1.47	0.79
2:F:819:ARG:HH11	2:F:819:ARG:HG2	1.46	0.79
2:H:819:ARG:HG2	2:H:819:ARG:HH11	1.46	0.79
2:D:1532:LEU:HD11	2:D:1569:ARG:HD3	1.65	0.78
3:I:244:MET:HG3	3:I:356:ARG:HB2	1.65	0.78
1:G:45:LEU:HD11	1:G:48:SER:HB3	1.64	0.78
2:H:1532:LEU:HD11	2:H:1569:ARG:HD3	1.65	0.78
2:F:1532:LEU:HD11	2:F:1569:ARG:HD3	1.65	0.78
1:E:45:LEU:HD11	1:E:48:SER:HB3	1.64	0.78
1:A:45:LEU:HD11	1:A:48:SER:HB3	1.64	0.78
2:B:1532:LEU:HD11	2:B:1569:ARG:HD3	1.65	0.78
2:F:833:ARG:HG2	2:F:833:ARG:HH11	1.48	0.78
2:H:966:ALA:O	2:H:967:GLN:HB2	1.83	0.78
2:F:738:ASN:HD22	4:P:45:LYS:HE2	1.47	0.78
2:B:833:ARG:HG2	2:B:833:ARG:HH11	1.48	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:738:ASN:HD22	4:Q:45:LYS:HE2	1.49	0.77
2:F:932:ARG:NH1	3:L:339:SER:HB2	1.99	0.77
2:F:841:ARG:HH11	2:F:841:ARG:HG2	1.50	0.77
3:J:244:MET:HG3	3:J:356:ARG:HB2	1.65	0.77
3:K:244:MET:HG3	3:K:356:ARG:HB2	1.65	0.77
3:L:244:MET:HG3	3:L:356:ARG:HB2	1.65	0.77
2:F:742:ARG:HB3	2:F:775:ASP:HB3	1.67	0.77
1:G:506:SER:HB2	1:G:530:TRP:HE1	1.50	0.77
2:B:841:ARG:HG2	2:B:841:ARG:HH11	1.50	0.76
2:F:740:VAL:HB	4:P:42:ARG:HB2	1.68	0.76
1:A:506:SER:HB2	1:A:530:TRP:HE1	1.50	0.76
1:E:506:SER:HB2	1:E:530:TRP:HE1	1.50	0.76
3:I:705:ARG:O	3:I:706:GLN:HB2	1.86	0.75
3:L:705:ARG:O	3:L:706:GLN:HB2	1.86	0.75
2:D:841:ARG:HH11	2:D:841:ARG:HG2	1.50	0.75
2:H:1498:ILE:HD12	2:H:1605:TRP:HA	1.65	0.75
3:J:705:ARG:O	3:J:706:GLN:HB2	1.86	0.75
2:F:1569:ARG:CB	2:F:1569:ARG:HH11	2.00	0.75
2:H:841:ARG:HG2	2:H:841:ARG:HH11	1.50	0.75
1:C:440:ARG:HG3	1:C:440:ARG:O	1.85	0.75
1:C:506:SER:HB2	1:C:530:TRP:HE1	1.50	0.75
3:L:446:GLU:O	3:L:450:LEU:HG	1.86	0.74
2:B:1569:ARG:HH11	2:B:1569:ARG:CB	2.00	0.74
1:C:404:THR:HG23	1:C:414:GLN:HE21	1.53	0.74
3:L:489:ALA:HB2	3:L:677:PRO:HG3	1.70	0.74
1:E:440:ARG:HG3	1:E:440:ARG:O	1.85	0.74
3:K:705:ARG:O	3:K:706:GLN:HB2	1.86	0.74
2:H:1569:ARG:HH11	2:H:1569:ARG:CB	2.00	0.74
3:I:464:ASP:HB3	3:I:615:LEU:HB2	1.70	0.74
1:A:440:ARG:O	1:A:440:ARG:HG3	1.86	0.74
1:G:440:ARG:O	1:G:440:ARG:HG3	1.85	0.74
2:H:877:VAL:HG22	2:H:1451:GLN:HE21	1.53	0.74
3:K:464:ASP:HB3	3:K:615:LEU:HB2	1.70	0.74
1:A:404:THR:HG23	1:A:414:GLN:HE21	1.53	0.74
1:E:223:ILE:HD12	1:E:223:ILE:H	1.53	0.74
2:H:740:VAL:HB	4:Q:42:ARG:HB2	1.69	0.74
2:F:834:GLN:NE2	2:F:835:ASN:H	1.86	0.73
2:D:1569:ARG:HH11	2:D:1569:ARG:CB	2.00	0.73
1:G:223:ILE:HD12	1:G:223:ILE:H	1.53	0.73
3:I:248:LEU:HD22	3:I:268:LEU:HD22	1.71	0.73
2:B:834:GLN:NE2	2:B:835:ASN:H	1.86	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:404:THR:HG23	1:E:414:GLN:HE21	1.53	0.73
2:H:742:ARG:HB3	2:H:775:ASP:HB3	1.71	0.73
1:C:223:ILE:H	1:C:223:ILE:HD12	1.53	0.73
1:G:404:THR:HG23	1:G:414:GLN:HE21	1.52	0.73
1:A:223:ILE:H	1:A:223:ILE:HD12	1.53	0.73
3:L:248:LEU:HD22	3:L:268:LEU:HD22	1.71	0.73
2:B:966:ALA:O	2:B:967:GLN:HB2	1.88	0.73
3:I:489:ALA:HB2	3:I:677:PRO:HG3	1.70	0.73
2:D:834:GLN:NE2	2:D:835:ASN:H	1.86	0.73
2:F:966:ALA:O	2:F:967:GLN:HB2	1.89	0.73
2:D:966:ALA:O	2:D:967:GLN:HB2	1.88	0.73
2:D:742:ARG:HB3	2:D:775:ASP:HB3	1.71	0.72
3:L:464:ASP:HB3	3:L:615:LEU:HB2	1.70	0.72
1:G:424:TYR:O	1:G:433:TYR:HE1	1.73	0.72
3:K:407:PRO:HD3	5:K:1743:NDG:H8C1	1.71	0.72
2:F:1269:GLU:HG3	2:F:1315:LYS:HB3	1.70	0.72
2:H:1497:PHE:CE2	2:H:1571:ALA:HB1	2.24	0.72
3:K:489:ALA:HB2	3:K:677:PRO:HG3	1.70	0.72
2:F:937:LYS:HG2	3:L:345:ASP:OD1	1.88	0.72
3:J:489:ALA:HB2	3:J:677:PRO:HG3	1.70	0.72
1:G:426:THR:HG21	1:G:432:ASN:N	2.02	0.72
3:K:635:ALA:HB3	3:K:647:ILE:HD11	1.71	0.72
3:J:248:LEU:HD22	3:J:268:LEU:HD22	1.70	0.72
3:J:464:ASP:HB3	3:J:615:LEU:HB2	1.70	0.72
3:J:653:PRO:HD2	3:J:654:ARG:HH12	1.55	0.72
2:H:834:GLN:NE2	2:H:835:ASN:H	1.86	0.72
1:C:6:ILE:HD13	1:C:22:LEU:HD23	1.72	0.71
1:G:6:ILE:HD13	1:G:22:LEU:HD23	1.72	0.71
3:L:461:LYS:HE2	3:L:461:LYS:HA	1.73	0.71
3:J:539:LYS:HG2	3:J:544:ILE:HD12	1.73	0.71
3:J:576:GLU:HB3	3:J:580:ARG:HH22	1.55	0.71
3:K:539:LYS:HG2	3:K:544:ILE:HD12	1.73	0.71
1:C:13:ARG:HH22	1:C:476:GLY:HA3	1.54	0.71
3:J:635:ALA:HB3	3:J:647:ILE:HD11	1.71	0.71
3:K:461:LYS:HE2	3:K:461:LYS:HA	1.73	0.71
3:I:461:LYS:HE2	3:I:461:LYS:HA	1.73	0.71
3:I:653:PRO:HD2	3:I:654:ARG:HH12	1.55	0.71
3:J:461:LYS:HA	3:J:461:LYS:HE2	1.73	0.71
3:K:576:GLU:HB3	3:K:580:ARG:HH22	1.55	0.71
1:C:439:LEU:HG	1:E:439:LEU:HG	1.71	0.71
3:I:635:ALA:HB3	3:I:647:ILE:HD11	1.71	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:248:LEU:HD22	3:K:268:LEU:HD22	1.70	0.71
3:L:635:ALA:HB3	3:L:647:ILE:HD11	1.71	0.70
1:E:6:ILE:HD13	1:E:22:LEU:HD23	1.72	0.70
1:C:98:VAL:HG11	2:D:1017:LEU:HD13	1.73	0.70
3:K:653:PRO:HD2	3:K:654:ARG:HH12	1.55	0.70
4:Q:71:GLN:HE21	4:Q:71:GLN:HA	1.57	0.70
3:I:539:LYS:HG2	3:I:544:ILE:HD12	1.73	0.70
3:L:576:GLU:HB3	3:L:580:ARG:HH22	1.55	0.70
2:H:1446:ASN:HB2	4:N:4:LEU:HD13	1.74	0.70
4:P:71:GLN:HE21	4:P:71:GLN:HA	1.57	0.70
3:I:576:GLU:HB3	3:I:580:ARG:HH22	1.55	0.70
2:B:742:ARG:HB3	2:B:775:ASP:HB3	1.74	0.70
3:L:539:LYS:HG2	3:L:544:ILE:HD12	1.73	0.69
1:A:6:ILE:HD13	1:A:22:LEU:HD23	1.72	0.69
2:D:1416:PHE:HZ	2:D:1442:HIS:HB2	1.57	0.69
3:I:381:ARG:HH21	3:I:381:ARG:CG	2.05	0.69
3:J:238:LEU:HD11	3:J:278:TYR:HB3	1.74	0.69
3:L:373:PRO:HB2	3:L:417:LEU:HD21	1.75	0.69
3:I:238:LEU:HD11	3:I:278:TYR:HB3	1.74	0.69
3:K:381:ARG:CG	3:K:381:ARG:HH21	2.06	0.69
3:L:653:PRO:HD2	3:L:654:ARG:HH12	1.55	0.69
2:H:962:GLY:O	2:H:964:PRO:HD3	1.92	0.69
1:E:426:THR:HG21	1:E:432:ASN:H	1.57	0.69
2:F:1387:THR:HG22	2:F:1451:GLN:H	1.58	0.69
3:L:238:LEU:HD11	3:L:278:TYR:HB3	1.74	0.69
2:H:1446:ASN:HB2	4:N:4:LEU:CD1	2.21	0.69
1:G:505:PRO:HG3	1:G:595:TRP:HE3	1.55	0.69
2:H:855:THR:HB	2:H:1602:LYS:HZ3	1.56	0.69
4:N:71:GLN:HE21	4:N:71:GLN:HA	1.56	0.69
3:J:381:ARG:HH21	3:J:381:ARG:CG	2.05	0.69
2:H:1387:THR:HG22	2:H:1451:GLN:H	1.58	0.69
2:D:962:GLY:O	2:D:964:PRO:HD3	1.93	0.69
3:L:381:ARG:CG	3:L:381:ARG:HH21	2.05	0.69
2:B:1416:PHE:HZ	2:B:1442:HIS:HB2	1.57	0.68
3:J:705:ARG:HG3	3:J:705:ARG:O	1.93	0.68
2:B:1488:LEU:HG	2:B:1590:TRP:CZ2	2.27	0.68
2:B:841:ARG:NH1	2:B:841:ARG:HG2	2.08	0.68
2:F:841:ARG:NH1	2:F:841:ARG:HG2	2.08	0.68
2:D:1488:LEU:HG	2:D:1590:TRP:CZ2	2.27	0.68
4:M:71:GLN:HA	4:M:71:GLN:HE21	1.56	0.68
2:F:733:ILE:HG12	2:F:734:ILE:H	1.58	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:373:PRO:HB2	3:I:417:LEU:HD21	1.75	0.68
3:J:373:PRO:HB2	3:J:417:LEU:HD21	1.75	0.68
3:K:373:PRO:HB2	3:K:417:LEU:HD21	1.75	0.68
3:J:435:ASN:ND2	3:J:460:ARG:HH21	1.90	0.68
1:G:100:LEU:HD21	1:G:638:LEU:HD23	1.76	0.68
1:G:567:HIS:ND1	2:H:760:PRO:HG3	2.09	0.68
1:C:606:THR:HG22	1:C:608:GLY:H	1.59	0.68
2:D:1445:PHE:CZ	4:P:7:SER:HA	2.28	0.68
2:H:733:ILE:HG12	2:H:734:ILE:H	1.58	0.68
3:J:432:ASP:HA	4:Q:27:ASN:HD21	1.57	0.67
1:C:372:GLU:O	1:C:375:VAL:HG12	1.95	0.67
3:K:354:ARG:HB2	5:K:1749:NDG:H8C2	1.74	0.67
3:K:446:GLU:HB3	3:K:449:SER:HB2	1.77	0.67
2:D:1518:GLY:HA3	2:D:1585:LEU:HD22	1.77	0.67
2:D:733:ILE:HG12	2:D:734:ILE:H	1.58	0.67
3:K:705:ARG:HG3	3:K:705:ARG:O	1.93	0.67
2:H:841:ARG:HG2	2:H:841:ARG:NH1	2.08	0.67
3:K:238:LEU:HD11	3:K:278:TYR:HB3	1.74	0.67
2:B:733:ILE:HG12	2:B:734:ILE:H	1.58	0.67
3:I:705:ARG:HG3	3:I:705:ARG:O	1.94	0.67
2:B:1518:GLY:HA3	2:B:1585:LEU:HD22	1.77	0.67
1:G:351:MET:SD	1:G:440:ARG:HD2	2.35	0.67
2:H:1268:GLN:CG	2:H:1269:GLU:H	2.00	0.67
3:L:705:ARG:O	3:L:705:ARG:HG3	1.94	0.67
2:H:1359:LYS:HD2	4:N:4:LEU:HD11	1.75	0.67
2:D:876:TYR:HA	2:D:1451:GLN:HE22	1.60	0.66
2:F:962:GLY:O	2:F:964:PRO:HD3	1.95	0.66
2:H:1518:GLY:HA3	2:H:1585:LEU:HD22	1.77	0.66
2:D:1337:ASN:O	2:D:1338:LYS:HB2	1.95	0.66
2:H:1499:GLN:HG2	2:H:1500:LYS:HG3	1.77	0.66
1:G:606:THR:HG22	1:G:608:GLY:H	1.59	0.66
1:G:55:THR:HG22	1:G:57:ALA:H	1.61	0.66
1:A:473:MET:HB2	1:A:508:ARG:HB2	1.78	0.66
1:A:606:THR:HG22	1:A:608:GLY:H	1.59	0.66
2:B:877:VAL:HG22	2:B:1451:GLN:HE21	1.59	0.66
2:D:841:ARG:NH1	2:D:841:ARG:HG2	2.08	0.66
2:H:1498:ILE:HG12	2:H:1499:GLN:H	1.60	0.66
1:E:606:THR:HG22	1:E:608:GLY:H	1.59	0.66
2:B:1387:THR:HG22	2:B:1451:GLN:H	1.60	0.66
3:J:446:GLU:HB3	3:J:449:SER:HB2	1.77	0.66
1:G:510:VAL:HG21	1:G:622:LEU:CD1	2.26	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:896:HIS:HB3	4:N:61:LYS:HD3	1.78	0.65
2:B:962:GLY:O	2:B:964:PRO:HD3	1.96	0.65
1:E:473:MET:HB2	1:E:508:ARG:HB2	1.78	0.65
1:A:55:THR:HG22	1:A:57:ALA:H	1.61	0.65
3:I:446:GLU:HB3	3:I:449:SER:HB2	1.79	0.65
3:I:478:ARG:HG3	3:I:479:PRO:HD2	1.79	0.65
2:B:1417:SER:HB2	4:Q:14:LYS:NZ	2.11	0.65
2:F:1518:GLY:HA3	2:F:1585:LEU:HD22	1.77	0.65
1:C:473:MET:HB2	1:C:508:ARG:HB2	1.78	0.65
2:F:1126:LEU:HG	2:F:1130:GLN:HE21	1.61	0.65
2:F:829:LEU:HD23	2:F:840:VAL:HG11	1.78	0.65
2:B:829:LEU:HD23	2:B:840:VAL:HG11	1.78	0.65
2:H:829:LEU:HD23	2:H:840:VAL:HG11	1.78	0.65
1:G:549:GLU:HG2	1:G:550:ASP:N	2.12	0.65
2:B:1337:ASN:O	2:B:1338:LYS:HB2	1.94	0.65
2:B:1126:LEU:HG	2:B:1130:GLN:HE21	1.61	0.64
2:D:829:LEU:HD23	2:D:840:VAL:HG11	1.78	0.64
1:C:55:THR:HG22	1:C:57:ALA:H	1.61	0.64
2:F:1265:PRO:O	2:F:1266:ASP:HB2	1.96	0.64
3:I:446:GLU:O	3:I:450:LEU:HG	1.97	0.64
2:B:1265:PRO:O	2:B:1266:ASP:HB2	1.97	0.64
2:D:1387:THR:HG22	2:D:1451:GLN:H	1.60	0.64
1:E:55:THR:HG22	1:E:57:ALA:H	1.61	0.64
2:D:1126:LEU:HG	2:D:1130:GLN:HE21	1.61	0.64
1:G:473:MET:HB2	1:G:508:ARG:HB2	1.78	0.64
3:J:478:ARG:HG3	3:J:479:PRO:HD2	1.79	0.64
2:F:1268:GLN:O	2:F:1269:GLU:HG2	1.97	0.64
3:K:478:ARG:HG3	3:K:479:PRO:HD2	1.79	0.64
3:L:446:GLU:HB3	3:L:449:SER:HB2	1.79	0.64
2:D:1265:PRO:O	2:D:1266:ASP:HB2	1.98	0.64
2:F:1337:ASN:O	2:F:1338:LYS:HB2	1.97	0.64
2:H:1338:LYS:HA	2:H:1371:ARG:HB2	1.80	0.64
2:B:837:GLU:HG2	4:Q:64:SER:OG	1.97	0.64
1:C:549:GLU:HG2	1:C:550:ASP:N	2.12	0.63
2:D:1527:LEU:HD13	2:D:1541:MET:HG2	1.80	0.63
1:A:551:ARG:N	1:A:551:ARG:HD2	2.13	0.63
2:D:1416:PHE:CZ	2:D:1442:HIS:HB2	2.34	0.63
3:K:513:LYS:HB3	3:K:522:ASP:HB3	1.81	0.63
2:H:837:GLU:HG2	4:N:64:SER:OG	1.98	0.63
3:K:460:ARG:HE	4:P:28:VAL:HG21	1.63	0.63
1:A:147:ASN:HB2	1:A:148:PRO:HD2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1498:ILE:HG12	2:H:1499:GLN:N	2.13	0.63
1:C:551:ARG:N	1:C:551:ARG:HD2	2.13	0.63
2:F:1498:ILE:HG22	2:F:1499:GLN:N	2.13	0.63
3:L:478:ARG:HG3	3:L:479:PRO:HD2	1.79	0.63
5:C:1646:NDG:H6C1	6:C:1647:NAG:C7	2.29	0.63
1:E:551:ARG:N	1:E:551:ARG:HD2	2.13	0.63
1:E:567:HIS:ND1	2:F:760:PRO:HG3	2.13	0.63
1:G:551:ARG:HD2	1:G:551:ARG:N	2.13	0.63
2:H:1337:ASN:O	2:H:1338:LYS:HB2	1.97	0.63
2:H:876:TYR:HA	2:H:1451:GLN:HE22	1.64	0.63
2:B:1527:LEU:HD13	2:B:1541:MET:HG2	1.80	0.63
1:C:147:ASN:HB2	1:C:148:PRO:HD2	1.80	0.63
1:C:634:GLN:HE22	2:D:1016:GLY:HA2	1.64	0.63
1:A:351:MET:SD	1:A:440:ARG:HD2	2.39	0.63
2:B:1416:PHE:CZ	2:B:1442:HIS:HB2	2.34	0.63
3:J:460:ARG:HE	4:Q:28:VAL:HG21	1.64	0.62
1:E:147:ASN:HB2	1:E:148:PRO:HD2	1.81	0.62
1:G:512:TYR:CZ	1:G:624:PHE:HE1	2.16	0.62
2:H:1527:LEU:HD13	2:H:1541:MET:HG2	1.80	0.62
3:L:513:LYS:HB3	3:L:522:ASP:HB3	1.81	0.62
3:K:432:ASP:HA	4:P:27:ASN:HD21	1.63	0.62
2:B:1295:SER:O	2:B:1297:LEU:HD12	2.00	0.62
2:D:1295:SER:O	2:D:1297:LEU:HD12	2.00	0.62
2:B:876:TYR:HA	2:B:1451:GLN:HE22	1.63	0.62
3:I:513:LYS:HB3	3:I:522:ASP:HB3	1.81	0.62
3:K:433:MET:HE3	3:K:436:LEU:HD21	1.81	0.62
1:G:147:ASN:HB2	1:G:148:PRO:HD2	1.81	0.62
2:F:877:VAL:HG22	2:F:1451:GLN:HE21	1.65	0.62
2:B:1446:ASN:HB2	4:Q:4:LEU:HB2	1.81	0.62
2:H:1498:ILE:HG13	2:H:1605:TRP:CE3	2.34	0.62
1:A:549:GLU:HG2	1:A:550:ASP:N	2.12	0.62
1:A:572:VAL:HG12	2:B:753:VAL:HG22	1.81	0.62
1:C:19:THR:HG21	5:C:1646:NDG:H8C2	1.80	0.62
2:H:855:THR:HB	2:H:1602:LYS:NZ	2.14	0.62
2:H:834:GLN:HE21	2:H:835:ASN:H	1.47	0.62
1:A:222:TYR:CE2	1:A:224:TYR:HB2	2.35	0.62
2:F:1527:LEU:HD13	2:F:1541:MET:HG2	1.80	0.62
3:J:513:LYS:HB3	3:J:522:ASP:HB3	1.81	0.62
3:I:423:ASN:HD22	3:I:423:ASN:N	1.98	0.61
1:G:19:THR:HB	1:G:478:LEU:HB2	1.81	0.61
2:B:834:GLN:HE21	2:B:835:ASN:H	1.47	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:222:TYR:CE2	1:E:224:TYR:HB2	2.35	0.61
2:F:1295:SER:O	2:F:1297:LEU:HD12	2.00	0.61
2:H:1611:GLU:HG3	2:H:1612:GLU:H	1.66	0.61
3:I:650:VAL:HG23	3:I:651:VAL:HG23	1.83	0.61
1:C:13:ARG:NH2	1:C:476:GLY:HA3	2.15	0.61
2:H:1497:PHE:HB2	2:H:1498:ILE:HD13	1.82	0.61
3:I:267:CYS:HB2	3:I:433:MET:HE1	1.82	0.61
3:K:423:ASN:N	3:K:423:ASN:HD22	1.98	0.61
3:L:461:LYS:HG2	4:N:28:VAL:HG12	1.81	0.61
2:B:1490:ARG:HB3	2:B:1590:TRP:CH2	2.36	0.61
1:E:372:GLU:O	1:E:375:VAL:HG12	1.99	0.61
1:G:372:GLU:O	1:G:375:VAL:HG12	2.01	0.61
1:G:222:TYR:CE2	1:G:224:TYR:HB2	2.35	0.61
3:I:461:LYS:HG2	4:M:28:VAL:HG12	1.82	0.61
3:K:478:ARG:HE	3:K:481:LYS:HD2	1.65	0.61
2:B:1291:TRP:CG	2:B:1292:GLU:N	2.69	0.61
3:L:650:VAL:HG23	3:L:651:VAL:HG23	1.83	0.61
1:C:20:MET:HB3	1:C:64:VAL:HG23	1.83	0.61
2:D:1490:ARG:HB3	2:D:1590:TRP:CH2	2.36	0.61
2:H:1498:ILE:CG1	2:H:1499:GLN:H	2.12	0.61
3:J:423:ASN:HD22	3:J:423:ASN:N	1.98	0.61
1:C:222:TYR:CE2	1:C:224:TYR:HB2	2.35	0.61
2:H:923:ARG:HH22	2:H:940:ILE:HG12	1.66	0.61
2:F:1338:LYS:HA	2:F:1371:ARG:HB2	1.81	0.61
2:F:1527:LEU:HD21	2:F:1530:VAL:HG22	1.83	0.61
2:F:834:GLN:HE21	2:F:835:ASN:H	1.47	0.61
3:K:650:VAL:HG23	3:K:651:VAL:HG23	1.83	0.61
2:B:1527:LEU:HD21	2:B:1530:VAL:HG22	1.83	0.60
2:F:1611:GLU:HG3	2:F:1612:GLU:H	1.66	0.60
3:I:478:ARG:HE	3:I:481:LYS:HD2	1.65	0.60
1:A:372:GLU:O	1:A:375:VAL:HG12	2.01	0.60
2:D:1611:GLU:HG3	2:D:1612:GLU:H	1.66	0.60
2:F:923:ARG:HH22	2:F:940:ILE:HG12	1.66	0.60
3:J:478:ARG:HE	3:J:481:LYS:HD2	1.65	0.60
2:D:1291:TRP:CG	2:D:1292:GLU:N	2.69	0.60
2:F:837:GLU:HG2	4:M:64:SER:OG	2.00	0.60
1:G:20:MET:HB3	1:G:64:VAL:HG23	1.83	0.60
1:C:426:THR:HG21	1:C:432:ASN:H	1.65	0.60
2:H:1295:SER:O	2:H:1297:LEU:HD12	2.00	0.60
3:L:449:SER:HA	3:L:452:LEU:HD13	1.84	0.60
3:L:478:ARG:HE	3:L:481:LYS:HD2	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:84:LYS:O	4:P:85:TYR:HB2	2.02	0.60
2:B:973:VAL:HG11	2:B:978:LEU:HD12	1.83	0.60
1:C:572:VAL:HG12	2:D:753:VAL:HG22	1.82	0.60
2:D:973:VAL:HG11	2:D:978:LEU:HD12	1.83	0.60
2:D:772:PHE:HD1	4:M:37:ASN:ND2	1.99	0.60
1:A:20:MET:HB3	1:A:64:VAL:HG23	1.83	0.60
2:B:1532:LEU:HD11	2:B:1569:ARG:CD	2.32	0.60
4:M:84:LYS:O	4:M:85:TYR:HB2	2.02	0.60
2:B:1039:GLN:HB3	2:B:1040:PRO:HD2	1.83	0.60
1:C:10:ASN:HB2	1:C:621:GLY:C	2.21	0.60
3:J:650:VAL:HG23	3:J:651:VAL:HG23	1.83	0.60
3:L:374:ILE:HD13	3:L:417:LEU:HD23	1.84	0.60
2:D:834:GLN:HE21	2:D:835:ASN:H	1.47	0.60
1:E:20:MET:HB3	1:E:64:VAL:HG23	1.83	0.60
2:F:1291:TRP:CD1	2:F:1292:GLU:N	2.70	0.60
2:F:1446:ASN:HB2	4:M:4:LEU:CD1	2.32	0.60
3:J:460:ARG:NE	4:Q:28:VAL:HG21	2.16	0.60
2:D:1532:LEU:HD11	2:D:1569:ARG:CD	2.32	0.59
1:E:220:PHE:CZ	1:E:330:PRO:HB3	2.37	0.59
2:F:1039:GLN:HB3	2:F:1040:PRO:HD2	1.83	0.59
2:F:876:TYR:HA	2:F:1451:GLN:HE22	1.67	0.59
2:D:1039:GLN:HB3	2:D:1040:PRO:HD2	1.83	0.59
2:D:877:VAL:HG22	2:D:1451:GLN:HE21	1.67	0.59
3:J:570:ILE:HD13	3:J:688:GLN:HB2	1.84	0.59
3:K:436:LEU:HB3	3:K:440:PHE:CE2	2.37	0.59
3:L:423:ASN:HD22	3:L:423:ASN:N	1.98	0.59
2:B:1611:GLU:HG3	2:B:1612:GLU:H	1.66	0.59
2:D:1527:LEU:HD21	2:D:1530:VAL:HG22	1.83	0.59
1:E:549:GLU:HG2	1:E:550:ASP:N	2.12	0.59
1:G:13:ARG:NH2	1:G:476:GLY:HA3	2.18	0.59
2:H:833:ARG:CG	2:H:833:ARG:HH11	2.15	0.59
3:I:563:TYR:CE2	3:I:569:PRO:HG3	2.38	0.59
3:I:570:ILE:HD13	3:I:688:GLN:HB2	1.84	0.59
1:G:555:PRO:HB3	2:H:775:ASP:HA	1.83	0.59
2:D:1337:ASN:O	2:D:1338:LYS:CB	2.51	0.59
2:H:1527:LEU:HD21	2:H:1530:VAL:HG22	1.83	0.59
3:L:570:ILE:HD13	3:L:688:GLN:HB2	1.84	0.59
4:N:84:LYS:O	4:N:85:TYR:HB2	2.02	0.59
3:K:563:TYR:CE2	3:K:569:PRO:HG3	2.38	0.59
1:C:558:GLN:HB3	2:D:770:ASN:HD21	1.68	0.59
1:G:350:LEU:HD21	1:G:400:ILE:HG21	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:436:LEU:HB3	3:J:440:PHE:CE2	2.37	0.59
3:J:563:TYR:CE2	3:J:569:PRO:HG3	2.38	0.59
3:L:508:LYS:HE2	3:L:508:LYS:HA	1.85	0.59
4:N:22:LEU:HB3	4:N:74:TYR:HE2	1.68	0.59
4:Q:84:LYS:O	4:Q:85:TYR:HB2	2.02	0.59
3:L:563:TYR:CE2	3:L:569:PRO:HG3	2.38	0.59
2:F:973:VAL:HG11	2:F:978:LEU:HD12	1.84	0.58
3:I:374:ILE:HD13	3:I:417:LEU:HD23	1.84	0.58
2:D:833:ARG:CG	2:D:833:ARG:HH11	2.15	0.58
1:E:477:ARG:HH11	1:E:477:ARG:CG	2.16	0.58
2:F:1215:LEU:HD23	2:F:1256:ALA:HB1	1.85	0.58
3:L:436:LEU:HB3	3:L:440:PHE:CE2	2.37	0.58
3:I:436:LEU:HB3	3:I:440:PHE:CE2	2.37	0.58
3:K:374:ILE:HD13	3:K:417:LEU:HD23	1.84	0.58
1:C:40:PHE:CE2	2:D:1017:LEU:HD22	2.38	0.58
2:F:1291:TRP:CG	2:F:1292:GLU:N	2.70	0.58
2:F:1532:LEU:HD11	2:F:1569:ARG:CD	2.34	0.58
3:J:374:ILE:HD13	3:J:417:LEU:HD23	1.84	0.58
4:P:22:LEU:HB3	4:P:74:TYR:HE2	1.68	0.58
2:H:1535:ASP:O	2:H:1536:PHE:HB3	2.04	0.58
4:M:22:LEU:HB3	4:M:74:TYR:HE2	1.68	0.58
3:I:508:LYS:HE2	3:I:508:LYS:HA	1.85	0.58
3:J:508:LYS:HA	3:J:508:LYS:HE2	1.85	0.58
3:K:570:ILE:HD13	3:K:688:GLN:HB2	1.84	0.58
2:H:877:VAL:H	2:H:1451:GLN:NE2	2.01	0.58
3:L:477:ILE:O	3:L:511:SER:HB2	2.04	0.58
2:B:1215:LEU:HD23	2:B:1256:ALA:HB1	1.85	0.58
2:B:833:ARG:CG	2:B:833:ARG:HH11	2.15	0.58
2:H:1532:LEU:HD11	2:H:1569:ARG:CD	2.34	0.58
3:J:477:ILE:O	3:J:511:SER:HB2	2.04	0.58
2:F:1359:LYS:HD2	4:M:4:LEU:CD1	2.32	0.58
2:D:1470:PHE:HB2	2:D:1478:GLY:HA3	1.86	0.57
1:G:527:ASP:N	1:G:616:VAL:HG11	2.19	0.57
4:Q:6:THR:H	4:Q:9:GLU:CB	2.16	0.57
1:E:350:LEU:HD21	1:E:400:ILE:HG21	1.86	0.57
1:G:510:VAL:HG11	1:G:622:LEU:HD12	1.86	0.57
2:H:1291:TRP:CD1	2:H:1292:GLU:N	2.70	0.57
2:H:1497:PHE:CZ	2:H:1572:LEU:HD23	2.39	0.57
3:I:477:ILE:O	3:I:511:SER:HB2	2.04	0.57
3:K:477:ILE:O	3:K:511:SER:HB2	2.04	0.57
2:B:1445:PHE:CZ	4:Q:7:SER:HA	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1133:LYS:O	2:F:1137:GLU:HG3	2.04	0.57
2:H:1291:TRP:CG	2:H:1292:GLU:N	2.70	0.57
1:A:614:ALA:HB1	1:A:632:THR:HA	1.86	0.57
2:D:1215:LEU:HD23	2:D:1256:ALA:HB1	1.85	0.57
2:D:809:ILE:HD11	2:D:892:ALA:HB3	1.87	0.57
1:G:13:ARG:HH22	1:G:476:GLY:HA3	1.69	0.57
4:Q:22:LEU:HB3	4:Q:74:TYR:HE2	1.68	0.57
2:B:1133:LYS:O	2:B:1137:GLU:HG3	2.04	0.57
2:B:1337:ASN:O	2:B:1338:LYS:CB	2.51	0.57
2:F:1535:ASP:O	2:F:1536:PHE:HB3	2.03	0.57
2:B:809:ILE:HD11	2:B:892:ALA:HB3	1.87	0.57
2:D:962:GLY:C	2:D:964:PRO:HD3	2.24	0.57
2:F:1269:GLU:HG3	2:F:1315:LYS:CB	2.35	0.57
2:F:1446:ASN:HB2	4:M:4:LEU:HD13	1.85	0.57
1:C:567:HIS:ND1	2:D:760:PRO:HG3	2.19	0.57
3:K:460:ARG:NE	4:P:28:VAL:HG21	2.19	0.57
3:K:508:LYS:HA	3:K:508:LYS:HE2	1.85	0.57
2:B:836:GLN:HG2	2:B:897:HIS:HE1	1.70	0.57
1:E:614:ALA:HB1	1:E:632:THR:HA	1.86	0.57
2:B:1470:PHE:HB2	2:B:1478:GLY:HA3	1.86	0.57
2:D:1462:ASN:HD22	2:D:1463:LEU:N	2.03	0.57
2:H:1582:MET:HA	2:H:1605:TRP:O	2.05	0.57
2:H:923:ARG:NH2	2:H:940:ILE:HG12	2.19	0.57
2:F:1055:TRP:CZ2	2:F:1108:ILE:HA	2.40	0.57
2:H:1462:ASN:HD22	2:H:1463:LEU:N	2.03	0.57
2:H:819:ARG:HG2	2:H:819:ARG:NH1	2.19	0.57
2:B:1143:LEU:HB3	2:B:1144:PRO:HD3	1.86	0.56
2:B:965:VAL:O	2:B:1267:HIS:HD2	1.88	0.56
1:C:268:ARG:HD3	2:D:1378:MET:SD	2.44	0.56
2:D:1055:TRP:CZ2	2:D:1108:ILE:HA	2.40	0.56
2:D:1143:LEU:HB3	2:D:1144:PRO:HD3	1.86	0.56
3:L:253:SER:HB2	3:L:326:SER:O	2.05	0.56
2:F:1582:MET:HA	2:F:1605:TRP:O	2.05	0.56
2:F:809:ILE:HD11	2:F:892:ALA:HB3	1.87	0.56
2:F:833:ARG:HH11	2:F:833:ARG:CG	2.15	0.56
1:G:481:ALA:N	5:G:1646:NDG:H8C3	2.17	0.56
1:G:614:ALA:HB1	1:G:632:THR:HA	1.86	0.56
2:H:1494:GLU:HG2	2:H:1602:LYS:HD3	1.87	0.56
5:J:1743:NDG:H6C1	6:J:1744:NAG:C7	2.35	0.56
3:L:461:LYS:HD2	4:N:29:ASN:OD1	2.05	0.56
2:B:1462:ASN:HD22	2:B:1463:LEU:N	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:923:ARG:HH22	2:B:940:ILE:HG12	1.70	0.56
2:D:925:LEU:HD11	2:D:1320:LEU:HD22	1.86	0.56
2:D:1535:ASP:O	2:D:1536:PHE:HB3	2.05	0.56
2:H:1337:ASN:O	2:H:1338:LYS:CB	2.53	0.56
1:A:558:GLN:HB3	2:B:770:ASN:HD21	1.70	0.56
2:B:1516:GLU:HB3	2:B:1517:PRO:HD2	1.88	0.56
2:B:925:LEU:HD11	2:B:1320:LEU:HD22	1.87	0.56
1:C:614:ALA:HB1	1:C:632:THR:HA	1.86	0.56
2:D:1133:LYS:O	2:D:1137:GLU:HG3	2.05	0.56
2:F:1462:ASN:HD22	2:F:1463:LEU:N	2.03	0.56
1:E:572:VAL:HG12	2:F:753:VAL:HG22	1.87	0.56
2:H:1566:ILE:O	2:H:1569:ARG:HG3	2.06	0.56
3:K:364:ASP:O	3:K:409:VAL:HG23	2.06	0.56
2:F:836:GLN:HG2	2:F:897:HIS:HE1	1.70	0.56
2:H:925:LEU:HD11	2:H:1320:LEU:HD22	1.88	0.56
3:I:353:ASN:HB2	3:I:394:ARG:NH1	2.20	0.56
3:K:253:SER:HB2	3:K:326:SER:O	2.05	0.56
3:L:364:ASP:O	3:L:409:VAL:HG23	2.06	0.56
2:B:1055:TRP:CZ2	2:B:1108:ILE:HA	2.40	0.56
2:B:1180:LEU:HD23	2:B:1221:LEU:HD11	1.88	0.56
2:F:923:ARG:NH2	2:F:940:ILE:HG12	2.19	0.56
2:B:1535:ASP:O	2:B:1536:PHE:HB3	2.05	0.56
1:E:116:ILE:HD11	1:E:203:LYS:HB3	1.88	0.56
1:C:441:THR:HG21	1:E:441:THR:HG21	1.88	0.56
1:G:477:ARG:HH11	1:G:477:ARG:CG	2.16	0.56
2:H:836:GLN:HG2	2:H:897:HIS:HE1	1.70	0.56
3:I:253:SER:HB2	3:I:326:SER:O	2.05	0.56
1:A:10:ASN:HB2	1:A:621:GLY:C	2.25	0.56
2:D:1180:LEU:HD23	2:D:1221:LEU:HD11	1.88	0.56
3:J:253:SER:HB2	3:J:326:SER:O	2.06	0.56
3:J:438:ASP:OD2	4:Q:28:VAL:HG13	2.05	0.56
2:D:1279:PRO:HG2	2:D:1306:GLU:HB3	1.88	0.56
2:D:923:ARG:HH22	2:D:940:ILE:HG12	1.70	0.56
2:F:1337:ASN:O	2:F:1338:LYS:CB	2.53	0.56
3:I:364:ASP:O	3:I:409:VAL:HG23	2.06	0.56
3:L:381:ARG:CG	3:L:381:ARG:NH2	2.68	0.56
2:D:1291:TRP:O	2:D:1292:GLU:C	2.45	0.56
2:F:1143:LEU:HB3	2:F:1144:PRO:HD3	1.86	0.56
2:H:964:PRO:HG3	2:H:1270:LEU:HD11	1.88	0.56
2:H:809:ILE:HD11	2:H:892:ALA:HB3	1.87	0.56
3:J:364:ASP:O	3:J:409:VAL:HG23	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:353:ASN:HB2	3:L:394:ARG:NH1	2.20	0.56
3:L:513:LYS:HZ2	3:L:524:GLU:HG2	1.71	0.56
4:N:6:THR:H	4:N:9:GLU:CB	2.16	0.56
1:A:477:ARG:HH11	1:A:477:ARG:CG	2.16	0.56
2:F:1012:TRP:HB3	2:F:1017:LEU:HD23	1.88	0.56
4:P:6:THR:H	4:P:9:GLU:CB	2.16	0.56
2:B:966:ALA:O	2:B:967:GLN:CB	2.54	0.55
2:F:1566:ILE:O	2:F:1569:ARG:HG3	2.06	0.55
3:I:461:LYS:HG2	4:M:28:VAL:CG1	2.36	0.55
3:K:267:CYS:HB2	3:K:433:MET:HE1	1.87	0.55
1:A:350:LEU:HD21	1:A:400:ILE:HG21	1.88	0.55
2:D:1291:TRP:CD1	2:D:1292:GLU:N	2.75	0.55
2:D:1516:GLU:HB3	2:D:1517:PRO:HD2	1.88	0.55
2:F:804:MET:HG2	2:F:805:GLN:H	1.72	0.55
2:F:925:LEU:HD11	2:F:1320:LEU:HD22	1.88	0.55
2:B:1338:LYS:HA	2:B:1371:ARG:HB2	1.88	0.55
2:B:1563:ILE:HB	2:B:1599:ILE:HD13	1.88	0.55
1:A:569:ALA:HB2	2:B:788:SER:HB2	1.88	0.55
2:F:1516:GLU:HB3	2:F:1517:PRO:HD2	1.88	0.55
2:F:1640:PRO:O	2:F:1641:ASN:HB2	2.07	0.55
1:G:143:VAL:C	1:G:144:ASN:HD22	2.10	0.55
2:H:839:LYS:HE2	4:N:60:PHE:CD1	2.41	0.55
1:A:143:VAL:C	1:A:144:ASN:HD22	2.09	0.55
2:B:804:MET:HG2	2:B:805:GLN:H	1.71	0.55
1:C:465:ILE:HD11	1:C:515:LEU:HD22	1.89	0.55
1:C:477:ARG:CG	1:C:477:ARG:HH11	2.16	0.55
1:G:116:ILE:HD11	1:G:203:LYS:HB3	1.88	0.55
2:H:1525:THR:HG22	2:H:1543:ILE:HA	1.88	0.55
2:H:1563:ILE:HB	2:H:1599:ILE:HD13	1.89	0.55
2:F:738:ASN:ND2	4:P:45:LYS:HE2	2.19	0.55
2:B:1566:ILE:O	2:B:1569:ARG:HG3	2.07	0.55
1:C:350:LEU:HD21	1:C:400:ILE:HG21	1.88	0.55
2:D:836:GLN:HG2	2:D:897:HIS:HE1	1.70	0.55
1:E:13:ARG:HH22	1:E:476:GLY:HA3	1.71	0.55
1:E:143:VAL:C	1:E:144:ASN:HD22	2.10	0.55
2:F:1498:ILE:HD12	2:F:1498:ILE:N	2.21	0.55
2:H:1338:LYS:CA	2:H:1371:ARG:HB2	2.36	0.55
3:K:353:ASN:HB2	3:K:394:ARG:NH1	2.21	0.55
2:F:740:VAL:O	4:P:42:ARG:HD3	2.06	0.55
2:B:1291:TRP:CD1	2:B:1292:GLU:N	2.75	0.55
1:C:252:GLY:HA2	1:C:262:LEU:HG	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1012:TRP:HB3	2:D:1017:LEU:HD23	1.88	0.55
2:F:1525:THR:HG22	2:F:1543:ILE:HA	1.88	0.55
2:F:776:SER:HB2	2:F:780:TRP:CZ2	2.42	0.55
2:B:1012:TRP:HB3	2:B:1017:LEU:HD23	1.88	0.55
2:B:877:VAL:H	2:B:1451:GLN:NE2	2.03	0.55
1:G:252:GLY:HA2	1:G:262:LEU:HG	1.89	0.55
2:H:1498:ILE:CD1	2:H:1605:TRP:HA	2.35	0.55
2:F:896:HIS:HB3	4:M:61:LYS:HD3	1.88	0.55
1:G:386:LYS:HD3	1:G:440:ARG:HG2	1.87	0.55
1:G:465:ILE:HD11	1:G:515:LEU:HD22	1.89	0.55
1:G:473:MET:CE	1:G:603:ILE:HD11	2.37	0.55
2:H:1516:GLU:HB3	2:H:1517:PRO:HD2	1.88	0.55
2:B:1417:SER:HB2	4:Q:14:LYS:HZ3	1.71	0.55
1:A:116:ILE:HD11	1:A:203:LYS:HB3	1.88	0.55
2:D:1338:LYS:HA	2:D:1371:ARG:HB2	1.89	0.55
2:F:1084:TRP:CD1	2:F:1088:GLU:HG3	2.42	0.55
2:F:1268:GLN:O	2:F:1269:GLU:CG	2.55	0.55
2:F:1291:TRP:O	2:F:1292:GLU:C	2.44	0.55
1:C:116:ILE:HD11	1:C:203:LYS:HB3	1.88	0.55
2:F:1338:LYS:CA	2:F:1371:ARG:HB2	2.37	0.55
2:H:1641:ASN:HD21	3:J:366:LEU:HB3	1.72	0.55
3:J:353:ASN:HB2	3:J:394:ARG:NH1	2.21	0.55
2:D:776:SER:HB2	2:D:780:TRP:CZ2	2.42	0.54
1:E:10:ASN:HA	1:E:623:THR:HG23	1.89	0.54
2:F:1180:LEU:HD23	2:F:1221:LEU:HD11	1.88	0.54
2:F:1279:PRO:HG2	2:F:1306:GLU:HB3	1.88	0.54
1:G:508:ARG:NH1	1:G:604:GLY:HA3	2.22	0.54
2:D:1525:THR:HG22	2:D:1543:ILE:HA	1.89	0.54
2:H:1279:PRO:HG2	2:H:1306:GLU:HB3	1.88	0.54
2:H:744:GLU:C	2:H:746:PRO:HD3	2.28	0.54
3:L:461:LYS:HG2	4:N:28:VAL:CG1	2.37	0.54
2:B:776:SER:HB2	2:B:780:TRP:CZ2	2.42	0.54
1:C:143:VAL:C	1:C:144:ASN:HD22	2.10	0.54
2:H:1291:TRP:O	2:H:1292:GLU:C	2.45	0.54
2:H:1445:PHE:CE2	4:N:7:SER:HA	2.43	0.54
2:B:1291:TRP:O	2:B:1292:GLU:C	2.45	0.54
1:E:478:LEU:HD21	1:E:622:LEU:HD21	1.88	0.54
2:H:1289:ILE:HD13	2:H:1298:ARG:HE	1.73	0.54
3:J:368:ASN:ND2	3:J:368:ASN:H	2.06	0.54
1:A:465:ILE:HD11	1:A:515:LEU:HD22	1.89	0.54
1:E:252:GLY:HA2	1:E:262:LEU:HG	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:535:ASN:O	3:I:547:PHE:HB3	2.07	0.54
3:L:535:ASN:O	3:L:547:PHE:HB3	2.07	0.54
2:D:804:MET:HG2	2:D:805:GLN:H	1.71	0.54
2:H:804:MET:HG2	2:H:805:GLN:H	1.72	0.54
3:K:535:ASN:O	3:K:547:PHE:HB3	2.07	0.54
2:B:1084:TRP:CD1	2:B:1088:GLU:HG3	2.42	0.54
2:D:1566:ILE:O	2:D:1569:ARG:HG3	2.07	0.54
2:D:966:ALA:O	2:D:967:GLN:CB	2.54	0.54
1:E:396:LYS:HG3	1:E:397:PRO:HD2	1.90	0.54
1:E:555:PRO:HB3	2:F:775:ASP:HA	1.90	0.54
2:H:1268:GLN:CG	2:H:1269:GLU:N	2.70	0.54
1:A:269:ILE:HD13	1:A:278:VAL:HB	1.90	0.54
2:B:1525:THR:HG22	2:B:1543:ILE:HA	1.89	0.54
2:D:1563:ILE:HB	2:D:1599:ILE:HD13	1.88	0.54
2:D:837:GLU:HG2	4:P:64:SER:OG	2.07	0.54
2:F:1289:ILE:HD13	2:F:1298:ARG:HE	1.73	0.54
1:G:534:LYS:HD2	1:G:535:ASP:H	1.72	0.54
3:J:631:CYS:SG	3:J:714:ARG:HD2	2.48	0.54
3:K:631:CYS:SG	3:K:714:ARG:HD2	2.48	0.54
3:L:478:ARG:NE	3:L:481:LYS:HD2	2.23	0.54
1:E:481:ALA:N	5:E:1646:NDG:H8C3	2.23	0.54
2:F:1563:ILE:HB	2:F:1599:ILE:HD13	1.89	0.54
1:G:396:LYS:HG3	1:G:397:PRO:HD2	1.90	0.54
3:K:478:ARG:NE	3:K:481:LYS:HD2	2.23	0.54
2:B:1582:MET:HA	2:B:1605:TRP:O	2.08	0.53
2:B:819:ARG:HG2	2:B:819:ARG:NH1	2.19	0.53
2:D:1084:TRP:CD1	2:D:1088:GLU:HG3	2.41	0.53
3:K:381:ARG:CG	3:K:381:ARG:NH2	2.68	0.53
3:L:436:LEU:HB3	3:L:440:PHE:HE2	1.73	0.53
1:A:13:ARG:HH22	1:A:476:GLY:HA3	1.73	0.53
2:B:1279:PRO:HG2	2:B:1306:GLU:HB3	1.88	0.53
2:B:923:ARG:NH2	2:B:940:ILE:HG12	2.23	0.53
1:C:436:LEU:HD11	1:C:511:ALA:HB3	1.90	0.53
1:C:505:PRO:HG3	1:C:595:TRP:CE3	2.42	0.53
2:D:997:THR:N	2:D:998:PRO:HD2	2.24	0.53
1:E:568:GLY:HA2	2:F:757:LYS:HE2	1.89	0.53
2:F:804:MET:HG2	2:F:805:GLN:N	2.23	0.53
1:G:451:VAL:HB	1:G:495:LEU:HB3	1.91	0.53
1:A:472:ILE:HD13	1:A:509:LEU:HD23	1.90	0.53
2:D:804:MET:HG2	2:D:805:GLN:N	2.23	0.53
3:J:535:ASN:O	3:J:547:PHE:HB3	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:744:GLU:C	2:F:746:PRO:HD3	2.29	0.53
3:K:435:ASN:ND2	3:K:460:ARG:HH21	2.06	0.53
3:L:631:CYS:SG	3:L:714:ARG:HD2	2.48	0.53
1:A:252:GLY:HA2	1:A:262:LEU:HG	1.89	0.53
1:A:436:LEU:HD11	1:A:511:ALA:HB3	1.90	0.53
1:E:465:ILE:HD11	1:E:515:LEU:HD22	1.89	0.53
2:F:940:ILE:HD12	2:F:1308:PHE:CE1	2.44	0.53
2:D:1289:ILE:HD13	2:D:1298:ARG:HE	1.74	0.53
2:D:1582:MET:HA	2:D:1605:TRP:O	2.08	0.53
1:E:219:LYS:NZ	1:E:356:ASN:HD22	2.07	0.53
1:G:269:ILE:HD13	1:G:278:VAL:HB	1.90	0.53
3:J:478:ARG:NE	3:J:481:LYS:HD2	2.23	0.53
1:A:451:VAL:HB	1:A:495:LEU:HB3	1.91	0.53
2:B:997:THR:N	2:B:998:PRO:HD2	2.24	0.53
1:C:269:ILE:HD13	1:C:278:VAL:HB	1.90	0.53
2:D:923:ARG:NH2	2:D:940:ILE:HG12	2.23	0.53
2:D:967:GLN:O	2:D:968:MET:HB2	2.08	0.53
2:H:940:ILE:HD12	2:H:1308:PHE:CE1	2.43	0.53
2:B:804:MET:HG2	2:B:805:GLN:N	2.23	0.53
1:E:477:ARG:HG2	1:E:477:ARG:NH1	2.21	0.53
2:H:1521:TYR:HB2	2:H:1523:TYR:CE2	2.44	0.53
3:I:478:ARG:NE	3:I:481:LYS:HD2	2.23	0.53
3:K:456:VAL:HG13	3:K:467:LYS:HA	1.91	0.53
1:A:506:SER:CB	1:A:530:TRP:HE1	2.21	0.53
2:F:937:LYS:HD2	2:F:937:LYS:O	2.09	0.53
2:H:776:SER:HB2	2:H:780:TRP:CZ2	2.42	0.53
3:I:456:VAL:HG13	3:I:467:LYS:HA	1.91	0.53
3:J:456:VAL:HG13	3:J:467:LYS:HA	1.91	0.53
4:M:6:THR:H	4:M:9:GLU:CB	2.16	0.53
3:L:438:ASP:OD2	4:N:28:VAL:HG13	2.09	0.53
2:D:877:VAL:H	2:D:1451:GLN:NE2	2.07	0.53
2:D:1470:PHE:CB	2:D:1478:GLY:HA3	2.39	0.53
2:D:865:THR:OG1	4:P:11:GLN:HG2	2.08	0.53
1:E:505:PRO:HG3	1:E:595:TRP:CE3	2.44	0.53
2:F:1387:THR:CG2	2:F:1451:GLN:H	2.21	0.53
2:F:822:GLN:OE1	2:F:1479:LYS:HA	2.09	0.53
2:F:973:VAL:HG12	2:F:975:ALA:H	1.73	0.53
2:F:997:THR:N	2:F:998:PRO:HD2	2.24	0.53
3:I:631:CYS:SG	3:I:714:ARG:HD2	2.48	0.53
3:J:436:LEU:HB3	3:J:440:PHE:HE2	1.73	0.53
3:K:436:LEU:HB3	3:K:440:PHE:HE2	1.73	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1289:ILE:HD13	2:B:1298:ARG:HE	1.73	0.52
1:C:439:LEU:HD12	1:C:439:LEU:H	1.74	0.52
1:E:590:THR:HG22	1:E:592:SER:H	1.75	0.52
2:H:740:VAL:O	4:Q:42:ARG:HD3	2.09	0.52
1:G:569:ALA:HB2	2:H:788:SER:HB2	1.90	0.52
2:B:962:GLY:C	2:B:964:PRO:HD3	2.29	0.52
2:D:1196:ASN:HD22	2:D:1196:ASN:N	2.07	0.52
2:F:978:LEU:HG	2:F:1240:TYR:HB3	1.91	0.52
1:G:342:PHE:CE1	1:G:391:THR:HG21	2.45	0.52
1:G:472:ILE:HD13	1:G:509:LEU:HD23	1.90	0.52
3:K:438:ASP:OD2	4:P:28:VAL:HG13	2.09	0.52
3:K:654:ARG:HA	3:K:722:GLN:HG3	1.91	0.52
3:L:368:ASN:ND2	3:L:368:ASN:H	2.08	0.52
2:B:1387:THR:CG2	2:B:1451:GLN:H	2.22	0.52
2:B:1470:PHE:CB	2:B:1478:GLY:HA3	2.39	0.52
1:C:19:THR:HB	1:C:478:LEU:HB2	1.91	0.52
1:C:396:LYS:HG3	1:C:397:PRO:HD2	1.90	0.52
1:C:569:ALA:HB2	2:D:788:SER:HB2	1.89	0.52
2:D:1387:THR:CG2	2:D:1451:GLN:H	2.22	0.52
1:E:439:LEU:H	1:E:439:LEU:HD12	1.74	0.52
1:G:527:ASP:CA	1:G:616:VAL:HG11	2.40	0.52
2:H:804:MET:HG2	2:H:805:GLN:N	2.23	0.52
3:K:598:LEU:HA	3:K:603:ILE:HD13	1.91	0.52
3:K:461:LYS:HD2	4:P:29:ASN:OD1	2.10	0.52
2:B:1446:ASN:CB	4:Q:4:LEU:HB2	2.40	0.52
2:B:978:LEU:HG	2:B:1240:TYR:HB3	1.91	0.52
2:B:973:VAL:HG12	2:B:975:ALA:H	1.73	0.52
2:D:1360:ASN:O	2:D:1361:THR:C	2.48	0.52
1:E:451:VAL:HB	1:E:495:LEU:HB3	1.91	0.52
3:J:654:ARG:HA	3:J:722:GLN:HG3	1.91	0.52
2:B:1344:THR:HG21	2:B:1346:LYS:HE2	1.92	0.52
2:D:973:VAL:HG12	2:D:975:ALA:H	1.73	0.52
2:F:932:ARG:HH11	3:L:339:SER:HB2	1.73	0.52
3:I:461:LYS:HD2	4:M:29:ASN:OD1	2.09	0.52
1:A:344:PRO:HD2	1:A:433:TYR:CE1	2.44	0.52
1:A:434:LEU:HB2	1:A:513:TYR:HE2	1.75	0.52
1:C:451:VAL:HB	1:C:495:LEU:HB3	1.91	0.52
2:D:1521:TYR:HB2	2:D:1523:TYR:CE2	2.44	0.52
1:E:434:LEU:HB2	1:E:513:TYR:HE2	1.75	0.52
1:G:436:LEU:HD11	1:G:511:ALA:HB3	1.90	0.52
1:G:339:PRO:HB3	1:G:608:GLY:O	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1578:LYS:HD3	2:H:1608:HIS:HE1	1.74	0.52
6:H:2643:NAG:H82	6:H:2643:NAG:O3	2.10	0.52
3:J:598:LEU:HA	3:J:603:ILE:HD13	1.91	0.52
3:K:531:HIS:CD2	3:K:533:ASN:H	2.27	0.52
1:C:434:LEU:HB2	1:C:513:TYR:HE2	1.75	0.52
1:E:472:ILE:HD13	1:E:509:LEU:HD23	1.90	0.52
2:F:1196:ASN:N	2:F:1196:ASN:HD22	2.07	0.52
2:F:1521:TYR:HB2	2:F:1523:TYR:CE2	2.44	0.52
2:H:1470:PHE:HB2	2:H:1478:GLY:HA3	1.92	0.52
3:I:313:GLN:O	3:I:317:ILE:HG13	2.10	0.52
3:I:513:LYS:HZ2	3:I:524:GLU:HG2	1.75	0.52
3:I:531:HIS:CD2	3:I:533:ASN:H	2.27	0.52
3:L:256:ILE:HD12	3:L:405:VAL:HG23	1.92	0.52
1:A:214:VAL:HG23	1:A:321:ARG:HB2	1.92	0.52
1:C:472:ILE:HD13	1:C:509:LEU:HD23	1.90	0.52
3:I:292:TYR:HD1	3:I:325:LYS:HD3	1.74	0.52
3:I:368:ASN:H	3:I:368:ASN:ND2	2.08	0.52
3:I:654:ARG:HA	3:I:722:GLN:HG3	1.91	0.52
3:J:531:HIS:CD2	3:J:533:ASN:H	2.27	0.52
3:L:292:TYR:HD1	3:L:325:LYS:HD3	1.74	0.52
2:B:1521:TYR:HB2	2:B:1523:TYR:CE2	2.44	0.52
2:D:978:LEU:HG	2:D:1240:TYR:HB3	1.91	0.52
2:F:1470:PHE:HB2	2:F:1478:GLY:HA3	1.92	0.52
1:G:214:VAL:HG23	1:G:321:ARG:HB2	1.92	0.52
1:G:506:SER:CB	1:G:530:TRP:HE1	2.21	0.52
2:H:1359:LYS:HD2	4:N:4:LEU:CD1	2.40	0.52
2:H:1387:THR:CG2	2:H:1451:GLN:H	2.21	0.52
2:H:1641:ASN:O	3:J:368:ASN:ND2	2.43	0.52
3:J:239:ASP:HB3	3:J:448:GLN:HB2	1.92	0.52
3:J:256:ILE:HD12	3:J:405:VAL:HG23	1.92	0.52
3:J:381:ARG:CG	3:J:381:ARG:NH2	2.68	0.52
3:L:598:LEU:HA	3:L:603:ILE:HD13	1.91	0.52
1:A:396:LYS:HG3	1:A:397:PRO:HD2	1.90	0.52
1:A:404:THR:HG23	1:A:414:GLN:HB3	1.92	0.52
1:E:269:ILE:HD13	1:E:278:VAL:HB	1.90	0.52
1:E:436:LEU:HD11	1:E:511:ALA:HB3	1.90	0.52
1:G:424:TYR:O	1:G:433:TYR:CE1	2.59	0.52
3:I:436:LEU:HB3	3:I:440:PHE:HE2	1.73	0.52
3:L:654:ARG:HA	3:L:722:GLN:HG3	1.91	0.52
4:P:30:GLU:HA	4:P:44:ILE:HD13	1.92	0.52
2:B:1196:ASN:N	2:B:1196:ASN:HD22	2.07	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1228:PRO:HB2	2:F:1229:PRO:HD3	1.92	0.51
3:L:239:ASP:HB3	3:L:448:GLN:HB2	1.92	0.51
1:A:439:LEU:HD12	1:A:439:LEU:H	1.74	0.51
2:B:1360:ASN:O	2:B:1361:THR:C	2.48	0.51
2:H:860:HIS:CE1	2:H:862:GLN:HE22	2.29	0.51
3:K:313:GLN:O	3:K:317:ILE:HG13	2.10	0.51
3:K:368:ASN:H	3:K:368:ASN:ND2	2.07	0.51
3:L:531:HIS:CD2	3:L:533:ASN:H	2.27	0.51
4:N:30:GLU:HA	4:N:44:ILE:HD13	1.92	0.51
1:C:126:ARG:HG2	1:C:168:PRO:HA	1.93	0.51
1:E:214:VAL:HG23	1:E:321:ARG:HB2	1.92	0.51
1:A:590:THR:HG22	1:A:592:SER:H	1.75	0.51
2:D:1228:PRO:HB2	2:D:1229:PRO:HD3	1.92	0.51
2:D:1344:THR:HG21	2:D:1346:LYS:HE2	1.92	0.51
2:D:972:ALA:HB1	2:D:1005:TYR:OH	2.10	0.51
1:E:410:SER:O	1:E:414:GLN:HG2	2.11	0.51
2:F:754:GLU:HG3	2:F:769:MET:SD	2.51	0.51
3:I:598:LEU:HA	3:I:603:ILE:HD13	1.91	0.51
3:J:292:TYR:HD1	3:J:325:LYS:HD3	1.74	0.51
3:L:313:GLN:O	3:L:317:ILE:HG13	2.10	0.51
1:C:568:GLY:HA2	2:D:757:LYS:HE2	1.93	0.51
2:D:1381:LEU:HD23	2:D:1457:VAL:HG12	1.92	0.51
2:F:972:ALA:HB1	2:F:1005:TYR:OH	2.09	0.51
2:F:1578:LYS:HD3	2:F:1608:HIS:HE1	1.74	0.51
3:K:256:ILE:HD12	3:K:405:VAL:HG23	1.92	0.51
4:M:70:LEU:HG	4:M:74:TYR:CE2	2.46	0.51
2:B:972:ALA:HB1	2:B:1005:TYR:OH	2.10	0.51
1:C:478:LEU:HD21	1:C:622:LEU:HD21	1.91	0.51
2:D:754:GLU:HG3	2:D:769:MET:SD	2.51	0.51
3:J:461:LYS:HD2	4:Q:29:ASN:OD1	2.10	0.51
3:K:292:TYR:HD1	3:K:325:LYS:HD3	1.74	0.51
1:A:640:CYS:HB3	1:A:641:PRO:HD2	1.93	0.51
2:B:1126:LEU:HD23	2:B:1173:ALA:HB1	1.93	0.51
2:B:1381:LEU:HD23	2:B:1457:VAL:HG12	1.92	0.51
2:B:754:GLU:HG3	2:B:769:MET:SD	2.51	0.51
2:D:1233:TRP:O	2:D:1237:GLN:HG2	2.11	0.51
1:E:19:THR:HB	1:E:478:LEU:HB2	1.93	0.51
1:E:506:SER:CB	1:E:530:TRP:HE1	2.21	0.51
1:G:439:LEU:HD12	1:G:439:LEU:H	1.74	0.51
1:G:36:THR:HG23	1:G:48:SER:HA	1.93	0.51
1:G:590:THR:HG22	1:G:592:SER:H	1.74	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:937:LYS:HD2	2:H:937:LYS:O	2.10	0.51
3:L:235:LYS:O	3:L:236:ILE:HB	2.11	0.51
3:L:456:VAL:HG13	3:L:467:LYS:HA	1.91	0.51
1:A:410:SER:O	1:A:414:GLN:HG2	2.11	0.51
1:A:36:THR:HG23	1:A:48:SER:HA	1.93	0.51
2:B:1228:PRO:HB2	2:B:1229:PRO:HD3	1.91	0.51
2:B:860:HIS:CE1	2:B:862:GLN:HE22	2.29	0.51
1:C:214:VAL:HG23	1:C:321:ARG:HB2	1.93	0.51
2:D:1126:LEU:HD23	2:D:1173:ALA:HB1	1.93	0.51
2:D:1480:LEU:HB3	2:D:1493:GLU:OE2	2.10	0.51
1:G:404:THR:HG23	1:G:414:GLN:HB3	1.92	0.51
1:G:640:CYS:HB3	1:G:641:PRO:HD2	1.93	0.51
1:C:590:THR:HG22	1:C:592:SER:H	1.75	0.51
2:D:819:ARG:HG2	2:D:819:ARG:NH1	2.19	0.51
1:G:126:ARG:HG2	1:G:168:PRO:HA	1.93	0.51
4:Q:30:GLU:HA	4:Q:44:ILE:HD13	1.92	0.51
2:B:839:LYS:HE2	4:Q:60:PHE:CD1	2.46	0.51
4:Q:70:LEU:HG	4:Q:74:TYR:CE2	2.46	0.51
2:B:1578:LYS:HD3	2:B:1608:HIS:HE1	1.75	0.51
1:C:640:CYS:HB3	1:C:641:PRO:HD2	1.93	0.51
2:D:772:PHE:CD1	4:M:37:ASN:ND2	2.78	0.51
2:F:1126:LEU:HD23	2:F:1173:ALA:HB1	1.93	0.51
2:F:1233:TRP:O	2:F:1237:GLN:HG2	2.11	0.51
2:F:860:HIS:CE1	2:F:862:GLN:HE22	2.29	0.51
2:F:966:ALA:O	2:F:967:GLN:CB	2.57	0.51
1:G:434:LEU:HB2	1:G:513:TYR:HE2	1.75	0.51
2:H:754:GLU:HG3	2:H:769:MET:SD	2.51	0.51
3:I:334:LEU:HB3	3:I:376:VAL:HG11	1.93	0.51
3:I:381:ARG:CG	3:I:381:ARG:NH2	2.68	0.51
3:L:339:SER:HA	3:L:342:SER:HB3	1.93	0.51
3:L:724:LEU:HB3	3:L:725:PRO:HD3	1.92	0.51
2:H:738:ASN:ND2	4:Q:45:LYS:HE2	2.22	0.51
1:E:36:THR:HG23	1:E:48:SER:HA	1.93	0.50
3:I:256:ILE:HD12	3:I:405:VAL:HG23	1.92	0.50
3:J:563:TYR:CZ	3:J:569:PRO:HG3	2.47	0.50
3:K:724:LEU:HB3	3:K:725:PRO:HD3	1.92	0.50
4:P:70:LEU:HG	4:P:74:TYR:CE2	2.46	0.50
1:C:36:THR:HG23	1:C:48:SER:HA	1.93	0.50
2:D:1593:LYS:HG2	2:D:1596:LEU:HD11	1.94	0.50
1:E:404:THR:HG23	1:E:414:GLN:HB3	1.92	0.50
1:E:640:CYS:HB3	1:E:641:PRO:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:882:LYS:HG3	2:F:886:GLN:NE2	2.27	0.50
2:H:1381:LEU:HD23	2:H:1457:VAL:HG12	1.93	0.50
3:I:724:LEU:HB3	3:I:725:PRO:HD3	1.92	0.50
3:L:334:LEU:HB3	3:L:376:VAL:HG11	1.93	0.50
2:B:1233:TRP:O	2:B:1237:GLN:HG2	2.11	0.50
1:C:410:SER:O	1:C:414:GLN:HG2	2.11	0.50
2:F:1344:THR:HG21	2:F:1346:LYS:HE2	1.93	0.50
3:J:313:GLN:O	3:J:317:ILE:HG13	2.10	0.50
3:K:239:ASP:HB3	3:K:448:GLN:HB2	1.92	0.50
3:L:439:VAL:HG22	4:N:31:LEU:HD21	1.91	0.50
2:B:772:PHE:HD1	4:N:37:ASN:ND2	2.10	0.50
1:G:554:VAL:HG13	1:G:555:PRO:HD2	1.94	0.50
3:I:239:ASP:HB3	3:I:448:GLN:HB2	1.92	0.50
3:J:334:LEU:HB3	3:J:376:VAL:HG11	1.93	0.50
3:L:278:TYR:HA	3:L:455:MET:HE1	1.92	0.50
3:L:465:TYR:CD1	3:L:517:GLY:HA2	2.46	0.50
3:L:641:TYR:HE2	3:L:650:VAL:HB	1.77	0.50
2:B:964:PRO:HG3	2:B:1270:LEU:HD11	1.92	0.50
2:B:940:ILE:HD12	2:B:1308:PHE:CE1	2.47	0.50
2:B:1569:ARG:CG	2:B:1569:ARG:HH11	2.25	0.50
1:C:404:THR:HG23	1:C:414:GLN:HB3	1.92	0.50
2:D:1578:LYS:HD3	2:D:1608:HIS:HE1	1.75	0.50
2:D:860:HIS:CE1	2:D:862:GLN:HE22	2.29	0.50
2:F:819:ARG:HH11	2:F:819:ARG:CG	2.22	0.50
1:G:369:VAL:HG12	1:G:370:GLN:H	1.77	0.50
1:G:410:SER:O	1:G:414:GLN:HG2	2.11	0.50
2:H:882:LYS:HG3	2:H:886:GLN:NE2	2.27	0.50
3:I:563:TYR:CZ	3:I:569:PRO:HG3	2.46	0.50
3:I:641:TYR:HE2	3:I:650:VAL:HB	1.77	0.50
3:J:235:LYS:O	3:J:236:ILE:HB	2.11	0.50
3:J:724:LEU:HB3	3:J:725:PRO:HD3	1.92	0.50
2:B:1593:LYS:HG2	2:B:1596:LEU:HD11	1.94	0.50
2:B:882:LYS:HG3	2:B:886:GLN:NE2	2.27	0.50
3:J:339:SER:HA	3:J:342:SER:HB3	1.93	0.50
3:J:465:TYR:CD1	3:J:517:GLY:HA2	2.46	0.50
3:K:641:TYR:HE2	3:K:650:VAL:HB	1.77	0.50
3:L:513:LYS:NZ	3:L:524:GLU:HG2	2.27	0.50
4:M:30:GLU:HA	4:M:44:ILE:HD13	1.92	0.50
1:A:126:ARG:HG2	1:A:168:PRO:HA	1.93	0.50
1:E:126:ARG:HG2	1:E:168:PRO:HA	1.93	0.50
1:E:268:ARG:HD3	2:F:1378:MET:SD	2.51	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:964:PRO:HG3	2:F:1270:LEU:HD11	1.93	0.50
2:H:1617:ASP:O	2:H:1621:GLN:HG3	2.12	0.50
3:K:339:SER:HA	3:K:342:SER:HB3	1.93	0.50
1:A:554:VAL:HG13	1:A:555:PRO:HD2	1.94	0.50
2:D:907:LEU:H	2:D:907:LEU:HD23	1.77	0.50
2:F:1617:ASP:O	2:F:1621:GLN:HG3	2.12	0.50
2:F:855:THR:HB	2:F:1602:LYS:HZ3	1.76	0.50
2:H:907:LEU:HD23	2:H:907:LEU:H	1.77	0.50
2:H:962:GLY:C	2:H:964:PRO:HD3	2.31	0.50
3:I:339:SER:HA	3:I:342:SER:HB3	1.93	0.50
3:J:478:ARG:CG	3:J:479:PRO:HD2	2.42	0.50
2:H:839:LYS:HE2	4:N:60:PHE:CE1	2.47	0.50
1:C:222:TYR:HB3	1:C:225:ASN:HB2	1.94	0.50
1:C:10:ASN:HA	1:C:623:THR:HG23	1.93	0.50
1:E:222:TYR:HB3	1:E:225:ASN:HB2	1.94	0.50
2:F:1268:GLN:O	2:F:1269:GLU:CB	2.59	0.50
3:K:334:LEU:HB3	3:K:376:VAL:HG11	1.93	0.50
3:K:563:TYR:CZ	3:K:569:PRO:HG3	2.47	0.50
3:L:431:LYS:HG3	4:N:27:ASN:ND2	2.27	0.50
1:A:103:LEU:HB3	1:A:193:GLN:HE21	1.77	0.49
2:B:1617:ASP:O	2:B:1621:GLN:HG3	2.12	0.49
1:A:568:GLY:HA2	2:B:757:LYS:HE2	1.94	0.49
2:H:1488:LEU:HG	2:H:1590:TRP:CH2	2.35	0.49
3:J:267:CYS:HB2	3:J:433:MET:HE1	1.94	0.49
3:J:641:TYR:HE2	3:J:650:VAL:HB	1.77	0.49
1:A:426:THR:HG21	1:A:432:ASN:H	1.77	0.49
2:D:733:ILE:HG12	2:D:734:ILE:N	2.26	0.49
2:F:1593:LYS:HG2	2:F:1596:LEU:HD11	1.94	0.49
3:I:465:TYR:CD1	3:I:517:GLY:HA2	2.46	0.49
3:K:465:TYR:CD1	3:K:517:GLY:HA2	2.46	0.49
1:C:351:MET:SD	1:C:440:ARG:HD2	2.53	0.49
2:D:940:ILE:HD12	2:D:1308:PHE:CE1	2.47	0.49
2:D:1617:ASP:O	2:D:1621:GLN:HG3	2.12	0.49
2:D:841:ARG:HH11	2:D:841:ARG:CG	2.23	0.49
2:D:882:LYS:HG3	2:D:886:GLN:NE2	2.27	0.49
1:G:572:VAL:CG2	2:H:785:VAL:HB	2.42	0.49
3:J:435:ASN:HD21	3:J:460:ARG:HH21	1.57	0.49
3:I:438:ASP:OD2	4:M:28:VAL:HG13	2.12	0.49
2:B:1505:VAL:HG23	2:B:1505:VAL:O	2.12	0.49
2:D:1505:VAL:HG23	2:D:1505:VAL:O	2.12	0.49
1:E:554:VAL:HG13	1:E:555:PRO:HD2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:1495:ASN:O	2:F:1602:LYS:HA	2.13	0.49
3:I:328:THR:HB	3:I:367:HIS:HA	1.94	0.49
3:K:235:LYS:O	3:K:236:ILE:HB	2.11	0.49
3:L:478:ARG:CG	3:L:479:PRO:HD2	2.42	0.49
4:N:70:LEU:HG	4:N:74:TYR:CE2	2.46	0.49
2:B:1239:TYR:OH	2:B:1246:SER:HB2	2.13	0.49
2:F:1569:ARG:HH11	2:F:1569:ARG:CG	2.26	0.49
2:F:841:ARG:CG	2:F:841:ARG:HH11	2.23	0.49
1:G:439:LEU:HD12	1:G:439:LEU:N	2.28	0.49
2:H:1593:LYS:HG2	2:H:1596:LEU:HD11	1.94	0.49
2:H:733:ILE:HG12	2:H:734:ILE:N	2.26	0.49
3:J:513:LYS:NZ	3:J:524:GLU:HG2	2.27	0.49
3:L:328:THR:HB	3:L:367:HIS:HA	1.94	0.49
2:H:1344:THR:HG21	2:H:1346:LYS:HE2	1.93	0.49
2:H:1635:VAL:HG23	2:H:1636:VAL:H	1.78	0.49
2:D:1485:ARG:HD3	2:D:1536:PHE:HZ	1.78	0.49
1:E:108:LEU:HB2	1:E:196:PHE:CD1	2.48	0.49
2:F:1381:LEU:HD23	2:F:1457:VAL:HG12	1.93	0.49
3:I:573:PRO:HB3	3:I:721:PHE:CZ	2.48	0.49
3:K:328:THR:HB	3:K:367:HIS:HA	1.95	0.49
3:L:563:TYR:CZ	3:L:569:PRO:HG3	2.47	0.49
1:A:108:LEU:HB2	1:A:196:PHE:CD1	2.48	0.49
1:C:554:VAL:HG13	1:C:555:PRO:HD2	1.94	0.49
2:D:1569:ARG:HH11	2:D:1569:ARG:CG	2.24	0.49
2:F:907:LEU:HD23	2:F:907:LEU:H	1.77	0.49
1:G:369:VAL:HG12	1:G:370:GLN:N	2.28	0.49
3:L:268:LEU:O	3:L:272:ILE:HG13	2.13	0.49
1:A:222:TYR:HB3	1:A:225:ASN:HB2	1.94	0.49
1:A:567:HIS:ND1	2:B:760:PRO:HG3	2.27	0.49
1:A:505:PRO:HG3	1:A:595:TRP:CE3	2.48	0.49
2:B:813:LEU:HD23	2:B:907:LEU:HB3	1.95	0.49
3:I:235:LYS:O	3:I:236:ILE:HB	2.11	0.49
2:B:738:ASN:HD22	4:N:45:LYS:HE2	1.78	0.49
1:A:477:ARG:NH1	1:A:477:ARG:CG	2.76	0.48
2:B:907:LEU:HD23	2:B:907:LEU:H	1.77	0.48
2:D:1239:TYR:OH	2:D:1246:SER:HB2	2.13	0.48
2:D:1417:SER:HB2	4:P:14:LYS:NZ	2.27	0.48
2:D:833:ARG:CG	2:D:833:ARG:NH1	2.76	0.48
2:D:813:LEU:HD23	2:D:907:LEU:HB3	1.95	0.48
1:G:477:ARG:CG	1:G:477:ARG:NH1	2.76	0.48
1:G:454:LEU:HA	1:G:491:ASP:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:813:LEU:HD23	2:H:907:LEU:HB3	1.95	0.48
3:J:268:LEU:O	3:J:272:ILE:HG13	2.13	0.48
3:J:573:PRO:HB3	3:J:721:PHE:CZ	2.48	0.48
3:L:372:ASP:O	3:L:375:THR:HG22	2.13	0.48
3:L:573:PRO:HB3	3:L:721:PHE:CZ	2.48	0.48
1:C:477:ARG:CG	1:C:477:ARG:NH1	2.76	0.48
2:H:1446:ASN:HB2	4:N:4:LEU:HB2	1.94	0.48
2:H:1492:ALA:O	2:H:1494:GLU:N	2.46	0.48
3:I:620:VAL:HG12	3:I:667:PRO:HD2	1.95	0.48
3:K:372:ASP:O	3:K:375:THR:HG22	2.13	0.48
3:K:513:LYS:NZ	3:K:524:GLU:HG2	2.27	0.48
3:L:620:VAL:HG12	3:L:667:PRO:HD2	1.95	0.48
2:F:1635:VAL:HG23	2:F:1636:VAL:H	1.78	0.48
2:H:1338:LYS:H	2:H:1371:ARG:HD2	1.78	0.48
2:H:1499:GLN:HG2	2:H:1500:LYS:N	2.27	0.48
3:I:372:ASP:O	3:I:375:THR:HG22	2.13	0.48
3:I:513:LYS:NZ	3:I:524:GLU:HG2	2.27	0.48
3:J:328:THR:HB	3:J:367:HIS:HA	1.95	0.48
3:J:372:ASP:O	3:J:375:THR:HG22	2.13	0.48
3:K:268:LEU:O	3:K:272:ILE:HG13	2.13	0.48
3:K:478:ARG:CG	3:K:479:PRO:HD2	2.42	0.48
1:A:439:LEU:HD12	1:A:439:LEU:N	2.28	0.48
1:C:108:LEU:HB2	1:C:196:PHE:CD1	2.48	0.48
5:E:1646:NDG:H6C1	6:E:1647:NAG:H83	1.94	0.48
3:I:268:LEU:O	3:I:272:ILE:HG13	2.13	0.48
3:I:270:ASN:HD22	3:I:270:ASN:N	2.12	0.48
3:J:493:GLU:HG3	3:J:563:TYR:OH	2.14	0.48
3:J:620:VAL:HG12	3:J:667:PRO:HD2	1.95	0.48
2:D:744:GLU:C	2:D:746:PRO:HD3	2.34	0.48
2:F:1239:TYR:OH	2:F:1246:SER:HB2	2.13	0.48
2:F:1445:PHE:CE2	4:M:7:SER:HA	2.48	0.48
1:G:108:LEU:HB2	1:G:196:PHE:CD1	2.48	0.48
2:H:1569:ARG:CG	2:H:1569:ARG:HH11	2.26	0.48
3:I:478:ARG:CG	3:I:479:PRO:HD2	2.42	0.48
2:B:1485:ARG:HD3	2:B:1536:PHE:HZ	1.78	0.48
3:J:270:ASN:N	3:J:270:ASN:HD22	2.11	0.48
3:K:362:MET:HG2	3:K:403:PHE:HB2	1.95	0.48
3:K:267:CYS:HB2	3:K:433:MET:CE	2.44	0.48
4:N:11:GLN:NE2	4:N:11:GLN:H	2.11	0.48
3:L:493:GLU:HG3	3:L:563:TYR:OH	2.14	0.48
2:D:738:ASN:HD22	4:M:45:LYS:HE2	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:P:11:GLN:H	4:P:11:GLN:NE2	2.11	0.48
4:Q:11:GLN:NE2	4:Q:11:GLN:H	2.11	0.48
1:C:506:SER:CB	1:C:530:TRP:HE1	2.21	0.48
1:E:369:VAL:HG12	1:E:370:GLN:H	1.78	0.48
1:G:222:TYR:HB3	1:G:225:ASN:HB2	1.94	0.48
3:I:465:TYR:CE1	3:I:517:GLY:HA2	2.49	0.48
3:I:493:GLU:HG3	3:I:563:TYR:OH	2.14	0.48
3:K:378:ASP:HA	3:K:381:ARG:HB2	1.96	0.48
3:K:573:PRO:HB3	3:K:721:PHE:CZ	2.48	0.48
3:I:439:VAL:HG22	4:M:31:LEU:HD21	1.95	0.48
2:D:1291:TRP:O	2:D:1294:ALA:N	2.47	0.48
2:D:1361:THR:HA	2:D:1441:VAL:O	2.14	0.48
1:G:624:PHE:HB3	1:G:632:THR:HG23	1.96	0.48
3:J:465:TYR:CE1	3:J:517:GLY:HA2	2.49	0.48
3:K:465:TYR:CE1	3:K:517:GLY:HA2	2.49	0.48
3:L:328:THR:O	3:L:367:HIS:HB2	2.14	0.48
3:L:544:ILE:HD13	3:L:650:VAL:HG12	1.96	0.48
4:M:11:GLN:NE2	4:M:11:GLN:H	2.11	0.48
1:A:624:PHE:HB3	1:A:632:THR:HG23	1.96	0.48
1:C:439:LEU:HD12	1:C:439:LEU:N	2.28	0.48
1:E:606:THR:HB	1:E:619:ASP:HB3	1.96	0.48
2:F:819:ARG:HG2	2:F:819:ARG:NH1	2.19	0.48
1:G:528:SER:N	1:G:616:VAL:HG13	2.29	0.48
2:H:932:ARG:O	2:H:934:GLY:N	2.47	0.48
3:K:493:GLU:HG3	3:K:563:TYR:OH	2.14	0.48
2:B:865:THR:OG1	4:Q:11:GLN:HG2	2.14	0.48
1:A:470:TYR:HA	1:A:510:VAL:O	2.14	0.47
2:B:1361:THR:HA	2:B:1441:VAL:O	2.14	0.47
2:D:964:PRO:HB3	2:D:1270:LEU:HD11	1.95	0.47
1:E:439:LEU:N	1:E:439:LEU:HD12	2.28	0.47
2:F:733:ILE:HG12	2:F:734:ILE:N	2.26	0.47
1:G:35:VAL:HG21	1:G:64:VAL:HG21	1.96	0.47
3:J:267:CYS:HB2	3:J:433:MET:CE	2.44	0.47
3:J:539:LYS:HD2	3:J:539:LYS:N	2.30	0.47
3:K:328:THR:O	3:K:367:HIS:HB2	2.14	0.47
3:L:361:LEU:O	3:L:402:VAL:HA	2.14	0.47
3:L:465:TYR:CE1	3:L:517:GLY:HA2	2.49	0.47
5:A:1646:NDG:H4	6:A:1647:NAG:H2	1.61	0.47
1:A:382:ASP:OD2	1:A:440:ARG:NH2	2.47	0.47
1:C:35:VAL:HG21	1:C:64:VAL:HG21	1.96	0.47
2:F:1338:LYS:H	2:F:1371:ARG:HD2	1.79	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:877:VAL:H	2:F:1451:GLN:NE2	2.12	0.47
1:G:510:VAL:HG21	1:G:622:LEU:HD12	1.96	0.47
1:G:470:TYR:HA	1:G:510:VAL:O	2.14	0.47
3:I:278:TYR:HA	3:I:455:MET:HE1	1.97	0.47
1:A:6:ILE:HD12	1:A:21:VAL:O	2.15	0.47
2:D:1521:TYR:HB2	2:D:1523:TYR:CZ	2.50	0.47
1:G:345:GLY:HA2	1:G:391:THR:O	2.14	0.47
3:I:544:ILE:HD13	3:I:650:VAL:HG12	1.96	0.47
3:K:620:VAL:HG12	3:K:667:PRO:HD2	1.95	0.47
2:B:1291:TRP:O	2:B:1294:ALA:N	2.47	0.47
2:D:965:VAL:O	2:D:1267:HIS:HD2	1.97	0.47
1:C:555:PRO:HB3	2:D:775:ASP:HA	1.96	0.47
2:F:813:LEU:HD23	2:F:907:LEU:HB3	1.95	0.47
3:J:378:ASP:HA	3:J:381:ARG:HB2	1.96	0.47
3:J:362:MET:HG2	3:J:403:PHE:HB2	1.95	0.47
3:L:334:LEU:HD12	3:L:373:PRO:HB3	1.97	0.47
4:N:10:TYR:HE2	4:N:14:LYS:HE3	1.80	0.47
2:B:1521:TYR:HB2	2:B:1523:TYR:CZ	2.50	0.47
1:C:624:PHE:HB3	1:C:632:THR:HG23	1.96	0.47
1:E:13:ARG:NH2	1:E:476:GLY:HA3	2.28	0.47
1:E:369:VAL:HG12	1:E:370:GLN:N	2.29	0.47
1:E:624:PHE:HB3	1:E:632:THR:HG23	1.96	0.47
2:H:1270:LEU:O	2:H:1290:HIS:HA	2.15	0.47
3:I:378:ASP:HA	3:I:381:ARG:HB2	1.96	0.47
3:I:538:GLY:C	3:I:539:LYS:HD2	2.35	0.47
3:K:334:LEU:HD12	3:K:373:PRO:HB3	1.97	0.47
4:M:10:TYR:HE2	4:M:14:LYS:HE3	1.79	0.47
1:C:166:VAL:O	1:C:168:PRO:HD3	2.15	0.47
1:E:35:VAL:HG21	1:E:64:VAL:HG21	1.96	0.47
2:F:932:ARG:O	2:F:934:GLY:N	2.47	0.47
1:G:606:THR:HB	1:G:619:ASP:HB3	1.96	0.47
3:I:349:PRO:O	3:I:352:TRP:HD1	1.98	0.47
3:I:362:MET:HG2	3:I:403:PHE:HB2	1.95	0.47
3:I:334:LEU:HD12	3:I:373:PRO:HB3	1.97	0.47
3:I:361:LEU:O	3:I:402:VAL:HA	2.14	0.47
3:J:349:PRO:O	3:J:352:TRP:HD1	1.98	0.47
3:J:538:GLY:C	3:J:539:LYS:HD2	2.35	0.47
1:C:10:ASN:HB2	1:C:621:GLY:HA2	1.95	0.47
2:F:1269:GLU:HG3	2:F:1269:GLU:O	2.15	0.47
3:J:236:ILE:HG21	3:J:443:MET:O	2.15	0.47
3:J:513:LYS:HZ2	3:J:524:GLU:HG2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:544:ILE:HD13	3:K:650:VAL:HG12	1.96	0.47
3:L:362:MET:HG2	3:L:403:PHE:HB2	1.95	0.47
3:L:539:LYS:N	3:L:539:LYS:HD2	2.30	0.47
1:A:35:VAL:HG21	1:A:64:VAL:HG21	1.96	0.47
1:C:470:TYR:HA	1:C:510:VAL:O	2.14	0.47
2:F:1270:LEU:O	2:F:1290:HIS:HA	2.15	0.47
2:H:1521:TYR:HB2	2:H:1523:TYR:CZ	2.49	0.47
2:H:1359:LYS:HD2	4:N:4:LEU:CG	2.45	0.47
1:A:606:THR:HB	1:A:619:ASP:HB3	1.96	0.47
2:B:967:GLN:O	2:B:968:MET:HB2	2.13	0.47
3:I:236:ILE:O	3:I:236:ILE:HG23	2.15	0.47
3:J:328:THR:O	3:J:367:HIS:HB2	2.15	0.47
3:J:544:ILE:HD13	3:J:650:VAL:HG12	1.96	0.47
3:K:363:THR:HG23	3:K:365:GLY:H	1.80	0.47
3:K:538:GLY:C	3:K:539:LYS:HD2	2.35	0.47
2:H:1446:ASN:CB	4:N:4:LEU:HB2	2.44	0.47
1:A:541:LEU:HD22	2:B:786:SER:HB3	1.97	0.47
1:C:510:VAL:HG12	1:C:528:SER:HB3	1.97	0.47
1:E:219:LYS:HZ2	1:E:356:ASN:HD22	1.63	0.47
1:E:6:ILE:HG22	1:E:625:THR:O	2.14	0.47
2:F:1521:TYR:HB2	2:F:1523:TYR:CZ	2.49	0.47
1:G:522:ARG:HG2	1:G:628:SER:CB	2.44	0.47
2:H:1291:TRP:O	2:H:1294:ALA:N	2.48	0.47
2:H:1498:ILE:HG13	2:H:1605:TRP:CZ3	2.50	0.47
3:K:236:ILE:HG21	3:K:443:MET:O	2.15	0.47
3:K:354:ARG:HB2	5:K:1749:NDG:C8	2.42	0.47
1:C:325:PRO:HG2	1:C:357:PRO:HB2	1.97	0.47
1:E:470:TYR:HA	1:E:510:VAL:O	2.14	0.47
3:K:270:ASN:N	3:K:270:ASN:HD22	2.12	0.47
3:K:539:LYS:N	3:K:539:LYS:HD2	2.30	0.47
3:L:236:ILE:HG23	3:L:236:ILE:O	2.15	0.47
2:B:733:ILE:HD13	2:B:841:ARG:HD3	1.98	0.46
2:D:1524:LYS:HB3	2:D:1545:GLN:HG2	1.97	0.46
1:C:541:LEU:HD22	2:D:786:SER:HB3	1.96	0.46
1:E:34:THR:HG22	1:E:51:LYS:HE3	1.97	0.46
1:C:378:LEU:HD13	1:E:446:GLY:O	2.16	0.46
2:F:1269:GLU:CG	2:F:1315:LYS:HB3	2.40	0.46
2:F:1524:LYS:HB3	2:F:1545:GLN:HG2	1.97	0.46
3:L:236:ILE:HG21	3:L:443:MET:O	2.15	0.46
2:B:1640:PRO:HA	3:L:326:SER:OG	2.14	0.46
1:A:166:VAL:O	1:A:168:PRO:HD3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:ILE:HG22	1:A:215:GLU:HG3	1.97	0.46
2:B:1524:LYS:HB3	2:B:1545:GLN:HG2	1.97	0.46
1:C:369:VAL:HG12	1:C:370:GLN:N	2.31	0.46
1:C:6:ILE:HD12	1:C:21:VAL:O	2.14	0.46
2:D:1172:TYR:CE1	2:D:1216:LEU:HB3	2.51	0.46
2:D:990:GLU:O	2:D:994:ILE:HG13	2.16	0.46
1:E:481:ALA:H	5:E:1646:NDG:H8C3	1.80	0.46
2:F:1265:PRO:O	2:F:1266:ASP:CB	2.64	0.46
2:F:733:ILE:HD13	2:F:841:ARG:HD3	1.97	0.46
3:I:328:THR:O	3:I:367:HIS:HB2	2.14	0.46
3:L:270:ASN:HD22	3:L:270:ASN:N	2.11	0.46
2:B:1172:TYR:CE1	2:B:1216:LEU:HB3	2.51	0.46
1:E:207:LEU:HA	1:E:208:PRO:HD2	1.82	0.46
1:E:6:ILE:HD12	1:E:21:VAL:O	2.14	0.46
2:F:1291:TRP:O	2:F:1294:ALA:N	2.48	0.46
2:F:990:GLU:O	2:F:994:ILE:HG13	2.16	0.46
1:G:477:ARG:NH1	1:G:477:ARG:HG2	2.21	0.46
1:G:34:THR:HG22	1:G:51:LYS:HE3	1.97	0.46
2:H:1444:TYR:HB2	4:N:10:TYR:CE1	2.50	0.46
3:I:700:CYS:O	3:I:701:LYS:C	2.53	0.46
3:J:361:LEU:O	3:J:402:VAL:HA	2.14	0.46
8:K:1745:MAN:O3	8:K:1748:MAN:H61	2.16	0.46
3:L:538:GLY:C	3:L:539:LYS:HD2	2.35	0.46
3:L:679:ILE:HG21	3:L:686:PHE:HB3	1.97	0.46
3:L:700:CYS:O	3:L:701:LYS:C	2.53	0.46
1:A:34:THR:HG22	1:A:51:LYS:HE3	1.97	0.46
2:B:733:ILE:HG12	2:B:734:ILE:N	2.26	0.46
2:B:990:GLU:O	2:B:994:ILE:HG13	2.16	0.46
1:E:166:VAL:O	1:E:168:PRO:HD3	2.15	0.46
1:E:80:ARG:HD2	2:F:1010:GLU:HG3	1.97	0.46
3:K:361:LEU:O	3:K:402:VAL:HA	2.14	0.46
3:K:700:CYS:O	3:K:701:LYS:C	2.53	0.46
3:L:378:ASP:HA	3:L:381:ARG:HB2	1.96	0.46
4:Q:10:TYR:HE2	4:Q:14:LYS:HE3	1.79	0.46
4:Q:73:ILE:O	4:Q:77:ILE:HG13	2.16	0.46
1:G:154:LYS:HD2	1:G:171:TRP:CD1	2.51	0.46
2:H:833:ARG:CG	2:H:833:ARG:NH1	2.75	0.46
3:I:363:THR:HG23	3:I:365:GLY:H	1.80	0.46
3:I:236:ILE:HG21	3:I:443:MET:O	2.15	0.46
3:I:539:LYS:HD2	3:I:539:LYS:N	2.30	0.46
3:J:236:ILE:O	3:J:236:ILE:HG23	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:700:CYS:O	3:J:701:LYS:C	2.53	0.46
3:K:349:PRO:O	3:K:352:TRP:HD1	1.98	0.46
3:L:349:PRO:O	3:L:352:TRP:HD1	1.98	0.46
2:F:740:VAL:CB	4:P:42:ARG:HB2	2.43	0.46
1:A:154:LYS:HD2	1:A:171:TRP:CD1	2.51	0.46
1:C:213:ILE:HG22	1:C:215:GLU:HG3	1.97	0.46
1:C:639:GLN:NE2	1:C:639:GLN:H	2.14	0.46
2:F:1172:TYR:CE1	2:F:1216:LEU:HB3	2.51	0.46
1:G:6:ILE:HD12	1:G:21:VAL:O	2.15	0.46
8:H:2644:MAN:H62	8:H:2645:MAN:H2	1.43	0.46
3:I:531:HIS:HD2	3:I:533:ASN:H	1.64	0.46
3:K:236:ILE:HG23	3:K:236:ILE:O	2.15	0.46
4:M:73:ILE:O	4:M:77:ILE:HG13	2.16	0.46
1:C:606:THR:HB	1:C:619:ASP:HB3	1.96	0.46
1:E:342:PHE:CE1	1:E:391:THR:HG21	2.50	0.46
2:F:1494:GLU:HB2	2:F:1602:LYS:HB3	1.97	0.46
1:G:247:ALA:HB2	1:G:308:VAL:HG22	1.97	0.46
2:H:837:GLU:HB3	2:H:868:PRO:HD3	1.97	0.46
3:J:531:HIS:HD2	3:J:533:ASN:H	1.64	0.46
3:K:292:TYR:CD1	3:K:325:LYS:HD3	2.51	0.46
3:L:363:THR:HG23	3:L:365:GLY:H	1.80	0.46
1:A:47:LEU:HD13	1:A:66:PHE:HB2	1.97	0.46
2:B:1393:THR:O	2:B:1397:LYS:HD3	2.16	0.46
2:B:744:GLU:C	2:B:746:PRO:HD3	2.35	0.46
1:C:154:LYS:HD2	1:C:171:TRP:CD1	2.51	0.46
1:C:47:LEU:HD13	1:C:66:PHE:HB2	1.97	0.46
2:D:1393:THR:O	2:D:1397:LYS:HD3	2.16	0.46
1:G:354:VAL:HG11	1:G:365:VAL:HG11	1.98	0.46
3:J:363:THR:HG23	3:J:365:GLY:H	1.80	0.46
3:K:261:PHE:HB3	3:K:319:TYR:HD1	1.81	0.46
3:K:679:ILE:HG21	3:K:686:PHE:HB3	1.97	0.46
3:L:345:ASP:HB3	3:L:346:ASP:H	1.49	0.46
3:L:531:HIS:HD2	3:L:533:ASN:H	1.64	0.46
4:N:73:ILE:O	4:N:77:ILE:HG13	2.15	0.46
1:A:639:GLN:NE2	1:A:639:GLN:H	2.14	0.46
1:C:6:ILE:HG22	1:C:625:THR:O	2.16	0.46
1:E:10:ASN:HB2	1:E:621:GLY:C	2.36	0.46
2:F:1290:HIS:O	2:F:1291:TRP:O	2.34	0.46
7:F:2645:BMA:H62	7:F:2647:BMA:H2	1.36	0.46
2:F:811:LEU:HG	2:F:813:LEU:HD13	1.98	0.46
3:I:700:CYS:HA	3:I:704:LYS:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:334:LEU:HD12	3:J:373:PRO:HB3	1.97	0.46
5:K:1743:NDG:H6C1	6:K:1744:NAG:C7	2.45	0.46
3:L:261:PHE:HB3	3:L:319:TYR:HD1	1.81	0.46
4:P:73:ILE:O	4:P:77:ILE:HG13	2.16	0.46
1:E:147:ASN:HB2	1:E:148:PRO:CD	2.46	0.46
1:E:354:VAL:HG11	1:E:365:VAL:HG11	1.98	0.46
1:G:144:ASN:HD22	1:G:144:ASN:N	2.14	0.46
1:G:166:VAL:O	1:G:168:PRO:HD3	2.15	0.46
1:G:47:LEU:HD13	1:G:66:PHE:HB2	1.97	0.46
3:I:267:CYS:HB2	3:I:433:MET:CE	2.44	0.46
4:M:66:ALA:HA	4:M:69:GLN:HB2	1.98	0.46
2:B:819:ARG:HH11	2:B:819:ARG:CG	2.22	0.45
1:C:34:THR:HG22	1:C:51:LYS:HE3	1.97	0.45
1:G:213:ILE:HG22	1:G:215:GLU:HG3	1.97	0.45
3:J:679:ILE:HG21	3:J:686:PHE:HB3	1.97	0.45
3:K:646:ASP:OD2	3:K:648:SER:HB3	2.17	0.45
4:N:66:ALA:HA	4:N:69:GLN:HB2	1.98	0.45
4:P:10:TYR:HE2	4:P:14:LYS:HE3	1.79	0.45
1:A:369:VAL:HG12	1:A:370:GLN:N	2.31	0.45
1:A:426:THR:HG22	1:A:427:VAL:N	2.31	0.45
3:I:646:ASP:OD2	3:I:648:SER:HB3	2.16	0.45
3:L:653:PRO:CD	3:L:654:ARG:HH12	2.27	0.45
1:A:144:ASN:HD22	1:A:144:ASN:N	2.14	0.45
1:A:427:VAL:HB	1:A:523:GLU:HG3	1.99	0.45
1:A:538:VAL:HB	2:B:791:LYS:O	2.16	0.45
1:E:351:MET:SD	1:E:440:ARG:HD2	2.57	0.45
1:E:47:LEU:HD13	1:E:66:PHE:HB2	1.97	0.45
1:G:639:GLN:H	1:G:639:GLN:NE2	2.14	0.45
2:H:1524:LYS:HB3	2:H:1545:GLN:HG2	1.97	0.45
3:I:261:PHE:HB3	3:I:319:TYR:HD1	1.81	0.45
3:J:700:CYS:HA	3:J:704:LYS:O	2.16	0.45
3:L:292:TYR:CD1	3:L:325:LYS:HD3	2.51	0.45
2:B:819:ARG:O	2:B:820:ASN:HB2	2.17	0.45
2:B:837:GLU:HB3	2:B:868:PRO:HD3	1.97	0.45
1:E:154:LYS:HD2	1:E:171:TRP:CD1	2.51	0.45
2:F:837:GLU:HB3	2:F:868:PRO:HD3	1.97	0.45
1:G:473:MET:HE2	1:G:603:ILE:HD11	1.98	0.45
2:H:733:ILE:HD13	2:H:841:ARG:HD3	1.98	0.45
3:K:239:ASP:HA	3:K:240:PRO:HD3	1.86	0.45
3:K:702:ASN:O	3:K:703:GLN:HG3	2.17	0.45
3:L:702:ASN:O	3:L:703:GLN:HG3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1264:ALA:HA	2:B:1265:PRO:HD3	1.73	0.45
2:D:1223:ASP:O	2:D:1227:VAL:HG23	2.17	0.45
2:D:1280:SER:O	2:D:1281:ARG:C	2.55	0.45
2:D:1288:ARG:HD3	2:D:1290:HIS:NE2	2.32	0.45
2:D:1364:LEU:HD23	2:D:1439:PHE:CZ	2.52	0.45
5:D:2642:NDG:H6C1	6:D:2643:NAG:C7	2.46	0.45
1:E:569:ALA:HB2	2:F:788:SER:HB2	1.99	0.45
1:G:100:LEU:HD21	1:G:638:LEU:CD2	2.44	0.45
1:G:567:HIS:CG	2:H:760:PRO:HG3	2.52	0.45
3:I:679:ILE:HG21	3:I:686:PHE:HB3	1.97	0.45
3:J:646:ASP:OD2	3:J:648:SER:HB3	2.17	0.45
3:J:705:ARG:O	3:J:706:GLN:CB	2.60	0.45
2:B:1123:ALA:O	2:B:1127:ILE:HG13	2.17	0.45
2:B:1288:ARG:HD3	2:B:1290:HIS:NE2	2.32	0.45
1:C:342:PHE:CE1	1:C:391:THR:HG21	2.52	0.45
1:C:427:VAL:HB	1:C:523:GLU:HG3	1.99	0.45
2:D:1192:ALA:HB2	2:D:1198:TRP:CZ2	2.52	0.45
1:E:510:VAL:HG12	1:E:528:SER:HB3	1.97	0.45
1:G:424:TYR:OH	1:G:613:TYR:HB3	2.16	0.45
2:H:1492:ALA:O	2:H:1493:GLU:C	2.55	0.45
2:H:1495:ASN:O	2:H:1496:CYS:C	2.54	0.45
3:I:292:TYR:CD1	3:I:325:LYS:HD3	2.51	0.45
3:J:261:PHE:HB3	3:J:319:TYR:HD1	1.81	0.45
3:L:646:ASP:OD2	3:L:648:SER:HB3	2.16	0.45
2:B:1192:ALA:HB2	2:B:1198:TRP:CZ2	2.52	0.45
2:B:1203:LYS:HD2	2:B:1206:TYR:CE2	2.52	0.45
2:F:1470:PHE:CB	2:F:1478:GLY:HA3	2.47	0.45
2:H:819:ARG:O	2:H:820:ASN:HB2	2.17	0.45
3:I:653:PRO:CD	3:I:654:ARG:HH12	2.27	0.45
3:K:653:PRO:CD	3:K:654:ARG:HH12	2.27	0.45
3:K:428:PHE:CE1	4:P:31:LEU:HD11	2.52	0.45
4:P:66:ALA:HA	4:P:69:GLN:HB2	1.98	0.45
1:A:354:VAL:HG11	1:A:365:VAL:HG11	1.98	0.45
1:A:510:VAL:HG12	1:A:528:SER:HB3	1.98	0.45
2:B:1280:SER:O	2:B:1281:ARG:C	2.55	0.45
2:B:729:LEU:O	2:B:729:LEU:HD22	2.17	0.45
2:B:851:CYS:HB2	2:B:1491:CYS:HB2	1.90	0.45
2:D:1123:ALA:O	2:D:1127:ILE:HG13	2.17	0.45
2:D:811:LEU:HG	2:D:813:LEU:HD13	1.98	0.45
2:D:837:GLU:HB3	2:D:868:PRO:HD3	1.97	0.45
2:F:1182:GLY:HA3	2:F:1183:PRO:HD2	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:516:ILE:N	1:G:516:ILE:HD12	2.32	0.45
2:H:1497:PHE:C	2:H:1498:ILE:HD13	2.37	0.45
3:J:292:TYR:CD1	3:J:325:LYS:HD3	2.51	0.45
2:D:937:LYS:HD2	2:D:937:LYS:O	2.17	0.45
1:E:213:ILE:HG22	1:E:215:GLU:HG3	1.97	0.45
1:E:639:GLN:H	1:E:639:GLN:NE2	2.14	0.45
2:F:1203:LYS:HD2	2:F:1206:TYR:CE2	2.52	0.45
2:F:1280:SER:O	2:F:1281:ARG:C	2.55	0.45
2:F:1288:ARG:HD3	2:F:1290:HIS:NE2	2.32	0.45
2:F:1364:LEU:HD23	2:F:1439:PHE:CZ	2.52	0.45
2:F:962:GLY:C	2:F:964:PRO:HD3	2.37	0.45
7:G:1648:BMA:H3	8:G:1651:MAN:C1	2.46	0.45
2:H:811:LEU:HG	2:H:813:LEU:HD13	1.98	0.45
1:A:369:VAL:HG12	1:A:370:GLN:H	1.82	0.45
2:D:1126:LEU:HD21	2:D:1177:MET:HE3	1.99	0.45
2:D:733:ILE:HD13	2:D:841:ARG:HD3	1.98	0.45
2:F:1506:THR:OG1	2:F:1509:GLU:HG2	2.17	0.45
2:H:1498:ILE:HD13	2:H:1498:ILE:N	2.32	0.45
2:H:734:ILE:N	2:H:734:ILE:HD12	2.32	0.45
3:J:702:ASN:O	3:J:703:GLN:HG3	2.17	0.45
3:K:554:LEU:H	3:K:726:TRP:HH2	1.65	0.45
3:L:272:ILE:HG12	3:L:284:TYR:CE1	2.52	0.45
3:L:432:ASP:HA	4:N:27:ASN:HD21	1.82	0.45
2:D:1444:TYR:HB2	4:P:10:TYR:CE1	2.52	0.45
2:B:1126:LEU:HD21	2:B:1177:MET:HE3	1.99	0.44
2:B:1223:ASP:O	2:B:1227:VAL:HG23	2.17	0.44
1:C:354:VAL:HG11	1:C:365:VAL:HG11	1.98	0.44
1:C:344:PRO:HD2	1:C:433:TYR:CE1	2.51	0.44
1:E:477:ARG:NH1	1:E:477:ARG:CG	2.76	0.44
2:F:1192:ALA:HB2	2:F:1198:TRP:CZ2	2.52	0.44
2:H:1290:HIS:O	2:H:1291:TRP:O	2.34	0.44
3:K:238:LEU:HD22	3:K:280:VAL:HG21	1.99	0.44
3:K:531:HIS:HD2	3:K:533:ASN:H	1.64	0.44
3:L:700:CYS:HA	3:L:704:LYS:O	2.16	0.44
3:L:705:ARG:O	3:L:706:GLN:CB	2.60	0.44
1:A:147:ASN:HB2	1:A:148:PRO:CD	2.46	0.44
1:A:516:ILE:HD12	1:A:516:ILE:N	2.32	0.44
1:C:369:VAL:HG12	1:C:370:GLN:H	1.82	0.44
2:F:1126:LEU:O	2:F:1130:GLN:HG3	2.17	0.44
2:F:1223:ASP:O	2:F:1227:VAL:HG23	2.17	0.44
1:G:526:ALA:HB2	1:G:617:PHE:CE2	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:1497:PHE:O	2:H:1498:ILE:C	2.56	0.44
3:J:272:ILE:HG12	3:J:284:TYR:CE1	2.52	0.44
3:J:554:LEU:H	3:J:726:TRP:HH2	1.65	0.44
3:K:491:VAL:HB	3:K:572:LEU:HD11	1.99	0.44
3:L:554:LEU:H	3:L:726:TRP:HH2	1.65	0.44
1:A:100:LEU:HD21	1:A:638:LEU:HD23	2.00	0.44
2:B:1126:LEU:O	2:B:1130:GLN:HG3	2.17	0.44
2:B:1283:SER:O	2:B:1284:LYS:HG2	2.18	0.44
2:B:734:ILE:N	2:B:734:ILE:HD12	2.33	0.44
2:D:1203:LYS:HD2	2:D:1206:TYR:CE2	2.52	0.44
2:D:819:ARG:O	2:D:820:ASN:HB2	2.17	0.44
2:F:1360:ASN:O	2:F:1361:THR:O	2.36	0.44
6:G:1647:NAG:H3	7:G:1649:BMA:O3	2.17	0.44
2:H:1470:PHE:CB	2:H:1478:GLY:HA3	2.47	0.44
3:I:433:MET:HE3	3:I:433:MET:HB3	1.83	0.44
3:K:489:ALA:HB2	3:K:677:PRO:CG	2.45	0.44
1:A:459:ARG:HH21	1:G:459:ARG:HE	1.66	0.44
2:B:847:ASN:HA	2:B:848:PRO:HD2	1.83	0.44
1:C:250:ILE:HG22	1:C:305:SER:HB3	2.00	0.44
1:E:144:ASN:N	1:E:144:ASN:HD22	2.14	0.44
1:E:247:ALA:HB2	1:E:308:VAL:HG22	1.98	0.44
1:E:427:VAL:HB	1:E:523:GLU:HG3	1.99	0.44
2:F:943:ALA:O	2:F:1305:ASN:ND2	2.49	0.44
2:F:734:ILE:HD12	2:F:734:ILE:N	2.33	0.44
2:H:1288:ARG:HD3	2:H:1290:HIS:NE2	2.32	0.44
2:H:943:ALA:O	2:H:1305:ASN:ND2	2.49	0.44
2:H:1360:ASN:O	2:H:1361:THR:O	2.36	0.44
2:H:1364:LEU:HD23	2:H:1439:PHE:CZ	2.52	0.44
1:A:342:PHE:CE1	1:A:391:THR:HG21	2.53	0.44
1:A:555:PRO:HB3	2:B:775:ASP:HA	1.98	0.44
2:B:1364:LEU:HD23	2:B:1439:PHE:CZ	2.52	0.44
2:H:1280:SER:O	2:H:1281:ARG:C	2.55	0.44
2:H:847:ASN:HA	2:H:848:PRO:HD2	1.83	0.44
3:I:272:ILE:HG12	3:I:284:TYR:CE1	2.52	0.44
3:I:554:LEU:H	3:I:726:TRP:HH2	1.65	0.44
3:K:238:LEU:HD11	3:K:278:TYR:CB	2.46	0.44
2:B:1639:CYS:HB2	3:L:368:ASN:OD1	2.18	0.44
3:L:491:VAL:HB	3:L:572:LEU:HD11	1.99	0.44
2:B:811:LEU:HG	2:B:813:LEU:HD13	1.98	0.44
2:D:1265:PRO:O	2:D:1266:ASP:CB	2.65	0.44
2:D:1292:GLU:HG2	2:D:1293:SER:H	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:847:ASN:HA	2:F:848:PRO:HD2	1.83	0.44
2:D:1639:CYS:HB2	3:I:368:ASN:OD1	2.18	0.44
3:I:375:THR:O	3:I:379:GLU:HG3	2.18	0.44
3:K:446:GLU:OE2	3:K:457:TRP:NE1	2.50	0.44
3:L:375:THR:O	3:L:379:GLU:HG3	2.18	0.44
4:Q:66:ALA:HA	4:Q:69:GLN:HB2	1.98	0.44
2:B:840:VAL:HG22	2:B:894:VAL:HG12	2.00	0.44
2:B:937:LYS:O	2:B:937:LYS:HD2	2.17	0.44
1:C:22:LEU:HD13	1:C:33:VAL:HG11	2.00	0.44
1:E:516:ILE:N	1:E:516:ILE:HD12	2.32	0.44
1:E:558:GLN:HB3	2:F:770:ASN:HD21	1.82	0.44
1:E:567:HIS:CG	2:F:760:PRO:HG3	2.53	0.44
2:F:1370:TYR:CD1	2:F:1376:ALA:HB2	2.52	0.44
1:G:147:ASN:HB2	1:G:148:PRO:CD	2.46	0.44
1:A:459:ARG:HE	1:G:459:ARG:NH2	2.16	0.44
3:J:375:THR:O	3:J:379:GLU:HG3	2.18	0.44
2:D:1446:ASN:HB2	4:P:4:LEU:HB2	1.99	0.44
1:A:329:SER:HA	1:A:330:PRO:HD3	1.78	0.44
2:B:1462:ASN:C	2:B:1462:ASN:HD22	2.21	0.44
2:D:1283:SER:O	2:D:1284:LYS:HG2	2.18	0.44
2:F:1126:LEU:HD21	2:F:1177:MET:HE3	1.99	0.44
2:F:1264:ALA:HA	2:F:1265:PRO:HD3	1.74	0.44
2:F:1375:ASP:OD1	2:F:1431:HIS:HD2	2.01	0.44
2:H:1283:SER:O	2:H:1284:LYS:HG2	2.18	0.44
2:H:1375:ASP:OD1	2:H:1431:HIS:HD2	2.01	0.44
3:I:543:GLY:O	3:I:545:PRO:HD3	2.18	0.44
3:J:366:LEU:HB2	10:J:2002:HOH:O	2.18	0.44
3:J:433:MET:HE1	3:J:436:LEU:HD21	1.99	0.44
3:K:245:ASN:OD1	3:K:283:ARG:HB2	2.18	0.44
1:A:407:GLN:C	1:A:409:LEU:H	2.21	0.44
1:C:10:ASN:HB2	1:C:621:GLY:CA	2.48	0.44
2:D:1338:LYS:H	2:D:1371:ARG:HD2	1.83	0.44
2:D:1375:ASP:OD1	2:D:1431:HIS:HD2	2.01	0.44
2:D:1462:ASN:HD21	2:D:1464:GLU:HB2	1.83	0.44
2:D:734:ILE:N	2:D:734:ILE:HD12	2.33	0.44
2:F:1123:ALA:O	2:F:1127:ILE:HG13	2.17	0.44
1:G:407:GLN:C	1:G:409:LEU:H	2.21	0.44
1:G:510:VAL:HG12	1:G:528:SER:HB3	1.99	0.44
2:H:1292:GLU:HG2	2:H:1293:SER:H	1.83	0.44
3:I:702:ASN:O	3:I:703:GLN:HG3	2.17	0.44
3:J:238:LEU:HD22	3:J:280:VAL:HG21	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:491:VAL:HB	3:J:572:LEU:HD11	1.99	0.44
3:J:654:ARG:HG3	3:J:722:GLN:CB	2.48	0.44
3:K:272:ILE:HG12	3:K:284:TYR:CE1	2.52	0.44
3:K:375:THR:O	3:K:379:GLU:HG3	2.18	0.44
1:A:207:LEU:HA	1:A:208:PRO:HD2	1.81	0.43
2:B:1056:LEU:O	2:B:1060:VAL:HG23	2.18	0.43
1:C:144:ASN:N	1:C:144:ASN:HD22	2.14	0.43
2:D:1126:LEU:O	2:D:1130:GLN:HG3	2.17	0.43
1:E:407:GLN:C	1:E:409:LEU:H	2.21	0.43
2:F:1497:PHE:CZ	2:F:1572:LEU:HD23	2.52	0.43
2:F:819:ARG:O	2:F:820:ASN:HB2	2.17	0.43
3:I:263:GLY:HA3	5:I:1743:NDG:H8C1	2.00	0.43
3:I:491:VAL:HB	3:I:572:LEU:HD11	1.99	0.43
3:K:700:CYS:HA	3:K:704:LYS:O	2.16	0.43
3:K:654:ARG:HG3	3:K:722:GLN:CB	2.48	0.43
1:A:19:THR:HB	1:A:478:LEU:HB2	1.99	0.43
1:A:247:ALA:HB2	1:A:308:VAL:HG22	1.99	0.43
2:B:1038:ARG:NH1	2:B:1077:VAL:HG22	2.33	0.43
1:E:343:LYS:HB2	1:E:346:MET:HB2	2.00	0.43
2:F:1283:SER:O	2:F:1284:LYS:HG2	2.18	0.43
2:F:1359:LYS:HB2	4:M:4:LEU:HD21	2.00	0.43
2:F:1462:ASN:HD21	2:F:1464:GLU:HB2	1.84	0.43
2:H:1370:TYR:CD1	2:H:1376:ALA:HB2	2.52	0.43
2:H:840:VAL:HG22	2:H:894:VAL:HG12	2.00	0.43
5:I:1743:NDG:H6C1	6:I:1744:NAG:C7	2.48	0.43
2:D:1056:LEU:O	2:D:1060:VAL:HG23	2.19	0.43
2:D:887:GLU:OE2	2:D:904:ARG:HD2	2.19	0.43
2:F:1038:ARG:NH1	2:F:1077:VAL:HG22	2.33	0.43
1:G:343:LYS:N	1:G:343:LYS:HD2	2.33	0.43
2:H:887:GLU:OE2	2:H:904:ARG:HD2	2.18	0.43
3:J:543:GLY:O	3:J:545:PRO:HD3	2.18	0.43
3:J:653:PRO:CD	3:J:654:ARG:HH12	2.27	0.43
3:K:513:LYS:HZ2	3:K:524:GLU:HG2	1.82	0.43
3:L:654:ARG:HG3	3:L:722:GLN:CB	2.48	0.43
1:A:126:ARG:HG3	2:B:751:TRP:CZ2	2.54	0.43
1:E:208:PRO:CD	1:E:583:LEU:HD11	2.48	0.43
2:F:1639:CYS:HA	2:F:1640:PRO:HD3	1.69	0.43
2:F:833:ARG:NH1	2:F:833:ARG:CG	2.75	0.43
6:G:1647:NAG:H61	7:G:1648:BMA:H2	1.99	0.43
1:G:341:TYR:CE1	1:G:611:LYS:HB3	2.53	0.43
1:G:427:VAL:HB	1:G:523:GLU:HG3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:473:MET:HE1	1:G:603:ILE:HD11	1.99	0.43
3:I:245:ASN:OD1	3:I:283:ARG:HB2	2.18	0.43
1:A:22:LEU:HD13	1:A:33:VAL:HG11	2.00	0.43
2:B:1338:LYS:H	2:B:1371:ARG:HD2	1.83	0.43
2:B:1482:LYS:HA	2:B:1492:ALA:HB3	2.00	0.43
1:C:407:GLN:C	1:C:409:LEU:H	2.21	0.43
1:C:516:ILE:HD12	1:C:516:ILE:N	2.32	0.43
1:E:250:ILE:HG12	1:E:251:PHE:H	1.84	0.43
1:E:22:LEU:HD13	1:E:33:VAL:HG11	2.00	0.43
1:E:343:LYS:HD2	1:E:343:LYS:N	2.33	0.43
2:F:1462:ASN:HD22	2:F:1462:ASN:C	2.21	0.43
3:L:238:LEU:HD22	3:L:280:VAL:HG21	1.99	0.43
2:B:1290:HIS:O	2:B:1291:TRP:O	2.37	0.43
2:B:1336:CYS:O	2:B:1337:ASN:O	2.37	0.43
2:B:1375:ASP:OD1	2:B:1431:HIS:HD2	2.01	0.43
2:D:1336:CYS:O	2:D:1337:ASN:O	2.36	0.43
2:D:840:VAL:HG22	2:D:894:VAL:HG12	2.00	0.43
1:G:2:PRO:HA	1:G:25:HIS:O	2.19	0.43
2:H:1506:THR:OG1	2:H:1509:GLU:HG2	2.17	0.43
3:I:654:ARG:HG3	3:I:722:GLN:CB	2.48	0.43
3:J:245:ASN:OD1	3:J:283:ARG:HB2	2.18	0.43
2:B:944:ASP:O	2:B:945:LEU:C	2.57	0.43
1:C:343:LYS:HD2	1:C:343:LYS:N	2.33	0.43
2:D:944:ASP:O	2:D:945:LEU:C	2.57	0.43
1:E:282:ARG:CZ	1:E:286:LEU:HD11	2.49	0.43
2:F:1078:LEU:HD23	2:F:1135:ILE:HG21	2.01	0.43
2:F:840:VAL:HG22	2:F:894:VAL:HG12	2.00	0.43
1:G:572:VAL:HG23	2:H:785:VAL:HB	2.01	0.43
3:I:238:LEU:HD22	3:I:280:VAL:HG21	1.99	0.43
3:K:543:GLY:O	3:K:545:PRO:HD3	2.18	0.43
3:K:655:PHE:HD2	3:K:716:PHE:HB3	1.84	0.43
3:L:543:GLY:O	3:L:545:PRO:HD3	2.18	0.43
1:A:343:LYS:HD2	1:A:343:LYS:N	2.33	0.43
1:C:2:PRO:HA	1:C:25:HIS:O	2.19	0.43
1:E:251:PHE:CG	1:E:280:LEU:HD22	2.54	0.43
1:E:2:PRO:HA	1:E:25:HIS:O	2.19	0.43
1:G:526:ALA:O	1:G:616:VAL:HG21	2.19	0.43
3:I:655:PHE:HD2	3:I:716:PHE:HB3	1.84	0.43
1:C:282:ARG:CZ	1:C:286:LEU:HD11	2.49	0.43
1:C:503:PHE:HD1	1:C:507:PHE:CG	2.37	0.43
1:G:250:ILE:HG12	1:G:251:PHE:H	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:343:LYS:HB2	1:G:346:MET:HB2	2.00	0.43
2:H:1528:VAL:HG21	2:H:1559:GLN:HE21	1.84	0.43
3:I:431:LYS:HG3	4:M:27:ASN:ND2	2.34	0.43
3:I:446:GLU:H	3:I:446:GLU:HG3	1.66	0.43
2:B:1386:MET:O	2:B:1387:THR:C	2.57	0.43
2:B:1462:ASN:HD21	2:B:1464:GLU:HB2	1.83	0.43
2:B:1523:TYR:HB3	2:B:1543:ILE:HG23	2.01	0.43
2:B:824:GLU:OE2	2:B:875:PRO:HB3	2.19	0.43
2:B:896:HIS:HB3	4:Q:61:LYS:HD3	2.00	0.43
2:B:887:GLU:OE2	2:B:904:ARG:HD2	2.18	0.43
1:C:506:SER:HB2	1:C:530:TRP:NE1	2.27	0.43
2:D:1038:ARG:NH1	2:D:1077:VAL:HG22	2.33	0.43
2:D:1523:TYR:HB3	2:D:1543:ILE:HG23	2.01	0.43
1:E:481:ALA:HB3	5:E:1646:NDG:H8C3	1.99	0.43
2:F:1056:LEU:O	2:F:1060:VAL:HG23	2.19	0.43
2:F:1227:VAL:HB	2:F:1228:PRO:HD3	2.01	0.43
2:H:1376:ALA:HB3	2:H:1429:VAL:CG2	2.49	0.43
3:L:238:LEU:HD11	3:L:278:TYR:CB	2.46	0.43
1:A:251:PHE:CG	1:A:280:LEU:HD22	2.54	0.42
2:B:1334:LEU:HD13	2:B:1334:LEU:HA	1.80	0.42
1:A:577:ASP:CG	2:B:778:THR:HG21	2.40	0.42
1:C:251:PHE:CG	1:C:280:LEU:HD22	2.54	0.42
1:C:538:VAL:HB	2:D:791:LYS:O	2.18	0.42
1:G:282:ARG:CZ	1:G:286:LEU:HD11	2.49	0.42
2:H:1462:ASN:HD21	2:H:1464:GLU:HB2	1.84	0.42
2:H:851:CYS:HB2	2:H:1491:CYS:HB2	1.81	0.42
3:J:607:PHE:CE1	3:J:669:THR:HG22	2.54	0.42
3:K:407:PRO:CD	5:K:1743:NDG:H8C1	2.46	0.42
3:K:503:PHE:HB2	3:K:530:PHE:CZ	2.54	0.42
3:K:607:PHE:CE1	3:K:669:THR:HG22	2.54	0.42
2:B:1215:LEU:O	2:B:1219:LEU:HG	2.19	0.42
1:C:247:ALA:HB2	1:C:308:VAL:HG22	2.02	0.42
2:D:819:ARG:NH1	2:D:819:ARG:CG	2.80	0.42
2:F:1292:GLU:HG2	2:F:1293:SER:H	1.83	0.42
2:F:745:PHE:N	2:F:746:PRO:HD3	2.32	0.42
2:H:824:GLU:OE2	2:H:875:PRO:HB3	2.19	0.42
3:I:238:LEU:HD11	3:I:278:TYR:CB	2.46	0.42
3:J:446:GLU:HG3	3:J:446:GLU:H	1.66	0.42
3:L:245:ASN:OD1	3:L:283:ARG:HB2	2.18	0.42
2:B:772:PHE:CD1	4:N:37:ASN:ND2	2.87	0.42
1:A:439:LEU:CD1	1:A:439:LEU:H	2.32	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1265:PRO:O	2:B:1266:ASP:CB	2.64	0.42
2:B:1292:GLU:HG2	2:B:1293:SER:H	1.83	0.42
2:B:932:ARG:O	2:B:933:GLU:C	2.57	0.42
1:C:343:LYS:HB2	1:C:346:MET:HB2	2.00	0.42
2:D:1482:LYS:HA	2:D:1492:ALA:HB3	2.01	0.42
2:D:824:GLU:OE2	2:D:875:PRO:HB3	2.19	0.42
1:E:111:GLN:O	1:E:125:TYR:HA	2.20	0.42
6:G:1647:NAG:N2	7:G:1649:BMA:O3	2.52	0.42
1:G:22:LEU:HD13	1:G:33:VAL:HG11	2.00	0.42
2:H:1500:LYS:NZ	2:H:1504:LYS:HB2	2.34	0.42
3:I:449:SER:HA	3:I:452:LEU:HD13	2.01	0.42
3:J:437:GLU:CD	3:J:458:GLU:HB2	2.40	0.42
3:J:655:PHE:HD2	3:J:716:PHE:HB3	1.84	0.42
3:L:655:PHE:HD2	3:L:716:PHE:HB3	1.84	0.42
1:A:503:PHE:HD1	1:A:507:PHE:CG	2.37	0.42
1:A:549:GLU:O	1:A:550:ASP:HB2	2.20	0.42
2:B:1446:ASN:HB2	4:Q:4:LEU:CD1	2.49	0.42
2:D:932:ARG:O	2:D:933:GLU:C	2.57	0.42
1:G:127:ILE:N	1:G:127:ILE:HD12	2.35	0.42
3:I:607:PHE:CE1	3:I:669:THR:HG22	2.55	0.42
3:L:607:PHE:CE1	3:L:669:THR:HG22	2.54	0.42
1:A:10:ASN:HB2	1:A:621:GLY:HA2	2.01	0.42
1:A:127:ILE:HD12	1:A:127:ILE:N	2.35	0.42
1:A:282:ARG:CZ	1:A:286:LEU:HD11	2.49	0.42
1:C:111:GLN:O	1:C:125:TYR:HA	2.20	0.42
2:D:1082:VAL:HG13	2:D:1129:LEU:HD22	2.01	0.42
2:D:1078:LEU:HD23	2:D:1135:ILE:HG21	2.01	0.42
2:F:1528:VAL:HG21	2:F:1559:GLN:HE21	1.84	0.42
2:F:969:THR:O	2:F:970:GLU:C	2.57	0.42
2:H:745:PHE:N	2:H:746:PRO:HD3	2.35	0.42
6:I:1744:NAG:H82	6:I:1744:NAG:H2	1.91	0.42
3:I:432:ASP:HA	4:M:27:ASN:HD21	1.84	0.42
3:I:709:VAL:HA	3:I:710:PRO:HD3	1.92	0.42
1:A:40:PHE:HA	1:A:41:PRO:HA	1.84	0.42
2:B:1506:THR:OG1	2:B:1509:GLU:HG2	2.20	0.42
2:D:1215:LEU:O	2:D:1219:LEU:HG	2.19	0.42
2:D:1290:HIS:O	2:D:1291:TRP:O	2.37	0.42
2:D:1506:THR:OG1	2:D:1509:GLU:HG2	2.20	0.42
1:E:454:LEU:HA	1:E:491:ASP:O	2.19	0.42
1:G:251:PHE:CG	1:G:280:LEU:HD22	2.54	0.42
3:I:289:TYR:HA	3:I:293:PRO:HA	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:353:ASN:OD1	5:K:1749:NDG:C7	2.67	0.42
3:L:489:ALA:HB2	3:L:677:PRO:CG	2.45	0.42
2:B:1227:VAL:HB	2:B:1228:PRO:HD3	2.01	0.42
1:C:147:ASN:HB2	1:C:148:PRO:CD	2.46	0.42
1:C:218:GLU:C	1:C:220:PHE:H	2.23	0.42
1:E:127:ILE:HD12	1:E:127:ILE:N	2.35	0.42
1:G:439:LEU:H	1:G:439:LEU:CD1	2.32	0.42
2:H:1485:ARG:HH21	2:H:1590:TRP:HE1	1.67	0.42
2:H:1516:GLU:HB3	2:H:1517:PRO:CD	2.50	0.42
3:J:531:HIS:CD2	3:J:533:ASN:HB2	2.55	0.42
1:A:218:GLU:C	1:A:220:PHE:H	2.23	0.42
2:B:1078:LEU:HD23	2:B:1135:ILE:HG21	2.01	0.42
1:C:127:ILE:N	1:C:127:ILE:HD12	2.35	0.42
2:D:943:ALA:O	2:D:1305:ASN:ND2	2.53	0.42
1:E:6:ILE:HD11	1:E:20:MET:CG	2.50	0.42
1:E:219:LYS:NZ	1:E:356:ASN:ND2	2.68	0.42
2:F:1215:LEU:O	2:F:1219:LEU:HG	2.19	0.42
2:F:1216:LEU:HD21	2:F:1256:ALA:HA	2.02	0.42
2:F:887:GLU:OE2	2:F:904:ARG:HD2	2.19	0.42
2:F:944:ASP:O	2:F:945:LEU:C	2.57	0.42
1:G:512:TYR:CE1	1:G:624:PHE:HE1	2.37	0.42
2:H:1386:MET:O	2:H:1387:THR:C	2.58	0.42
2:H:944:ASP:O	2:H:945:LEU:C	2.57	0.42
3:I:531:HIS:CD2	3:I:533:ASN:HB2	2.55	0.42
3:L:289:TYR:HA	3:L:293:PRO:HA	2.02	0.42
3:L:503:PHE:HB2	3:L:530:PHE:CZ	2.54	0.42
3:L:531:HIS:CD2	3:L:533:ASN:HB2	2.55	0.42
1:A:250:ILE:HG22	1:A:305:SER:HB3	2.01	0.42
2:B:1376:ALA:HB3	2:B:1429:VAL:CG2	2.49	0.42
1:C:330:PRO:HG2	1:C:409:LEU:HD21	2.01	0.42
2:D:1386:MET:O	2:D:1387:THR:C	2.58	0.42
1:G:111:GLN:O	1:G:125:TYR:HA	2.20	0.42
1:G:574:VAL:HG13	2:H:783:LEU:HB3	2.01	0.42
2:H:1334:LEU:HD13	2:H:1334:LEU:HA	1.80	0.42
3:I:676:GLY:HA2	3:I:677:PRO:HD3	1.83	0.42
3:I:705:ARG:O	3:I:706:GLN:CB	2.60	0.42
3:J:443:MET:HB3	3:J:443:MET:HE2	1.86	0.42
3:K:244:MET:HG2	3:K:245:ASN:N	2.35	0.42
4:Q:84:LYS:O	4:Q:84:LYS:HG3	2.20	0.42
1:C:250:ILE:HG12	1:C:251:PHE:H	1.84	0.42
2:D:1009:THR:HB	2:D:1011:GLN:HE21	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1462:ASN:HD22	2:D:1462:ASN:C	2.21	0.42
2:D:1518:GLY:CA	2:D:1585:LEU:HD22	2.48	0.42
2:F:1009:THR:HB	2:F:1011:GLN:HE21	1.85	0.42
2:F:1269:GLU:O	2:F:1271:ASN:N	2.52	0.42
2:F:1522:VAL:HG22	2:F:1583:TRP:HB3	2.02	0.42
1:G:19:THR:HG22	1:G:20:MET:N	2.35	0.42
1:G:503:PHE:HD1	1:G:507:PHE:CG	2.37	0.42
3:I:503:PHE:HB2	3:I:530:PHE:CZ	2.54	0.42
3:J:503:PHE:HB2	3:J:530:PHE:CZ	2.54	0.42
3:L:298:LYS:HB2	3:L:301:GLU:HG3	2.02	0.42
3:L:443:MET:HE2	3:L:443:MET:HB3	1.87	0.42
2:B:1082:VAL:HG13	2:B:1129:LEU:HD22	2.02	0.41
1:C:439:LEU:CD1	1:C:439:LEU:H	2.32	0.41
1:C:6:ILE:HD11	1:C:20:MET:CG	2.50	0.41
2:D:1227:VAL:HB	2:D:1228:PRO:HD3	2.01	0.41
2:F:1336:CYS:O	2:F:1337:ASN:C	2.59	0.41
2:F:1390:ALA:HA	2:F:1391:PRO:HD3	1.91	0.41
1:G:526:ALA:CB	1:G:617:PHE:CE2	3.03	0.41
1:G:6:ILE:HD11	1:G:20:MET:CG	2.50	0.41
2:H:1338:LYS:N	2:H:1371:ARG:HB2	2.34	0.41
2:H:841:ARG:CG	2:H:841:ARG:HH11	2.23	0.41
2:H:854:ALA:HB2	2:H:860:HIS:HB3	2.02	0.41
2:H:877:VAL:H	2:H:1451:GLN:HE21	1.68	0.41
4:M:23:LEU:HD21	4:M:51:ALA:HB3	2.02	0.41
4:N:56:LYS:HG3	4:N:57:SER:N	2.34	0.41
1:A:330:PRO:HG2	1:A:409:LEU:HD21	2.00	0.41
1:A:80:ARG:HD2	2:B:1010:GLU:HG3	2.01	0.41
2:B:1165:TYR:HD1	2:B:1210:ALA:HB2	1.85	0.41
2:B:943:ALA:O	2:B:1305:ASN:ND2	2.53	0.41
2:B:932:ARG:O	2:B:934:GLY:N	2.53	0.41
2:D:1528:VAL:HG21	2:D:1559:GLN:HE21	1.84	0.41
2:D:932:ARG:O	2:D:934:GLY:N	2.53	0.41
1:G:350:LEU:CD2	1:G:400:ILE:HG21	2.50	0.41
3:J:489:ALA:HB2	3:J:677:PRO:CG	2.45	0.41
3:K:540:LYS:HB2	3:K:540:LYS:NZ	2.36	0.41
3:L:239:ASP:HA	3:L:240:PRO:HD3	1.86	0.41
4:M:56:LYS:HG3	4:M:57:SER:N	2.34	0.41
4:Q:23:LEU:HD21	4:Q:51:ALA:HB3	2.02	0.41
1:A:111:GLN:O	1:A:125:TYR:HA	2.20	0.41
1:A:249:VAL:HG13	1:A:267:LYS:HB2	2.02	0.41
2:B:1009:THR:HB	2:B:1011:GLN:HE21	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1541:MET:HE3	2:B:1541:MET:HB2	1.96	0.41
2:B:1528:VAL:HG21	2:B:1559:GLN:HE21	1.84	0.41
1:C:19:THR:HG22	1:C:20:MET:N	2.35	0.41
2:D:1370:TYR:CG	2:D:1376:ALA:HB2	2.55	0.41
2:D:1376:ALA:HB3	2:D:1429:VAL:CG2	2.49	0.41
1:E:126:ARG:CZ	1:E:572:VAL:HB	2.50	0.41
1:E:365:VAL:HA	1:E:366:PRO:HD2	1.80	0.41
1:E:386:LYS:HD3	1:E:440:ARG:HG2	2.02	0.41
2:F:1165:TYR:HD1	2:F:1210:ALA:HB2	1.85	0.41
2:F:1472:HIS:HA	2:F:1473:PRO:HD3	1.94	0.41
7:F:2644:BMA:H5	7:F:2645:BMA:H2	2.01	0.41
2:F:915:ARG:O	2:F:916:MET:HG3	2.21	0.41
1:G:341:TYR:CD2	1:G:610:GLY:HA2	2.56	0.41
2:H:1611:GLU:HG3	2:H:1612:GLU:N	2.34	0.41
3:I:666:ASP:HA	3:I:667:PRO:HD3	1.95	0.41
3:J:244:MET:HG2	3:J:245:ASN:N	2.35	0.41
3:J:298:LYS:HB2	3:J:301:GLU:HG3	2.02	0.41
3:J:433:MET:HE3	3:J:433:MET:HB3	1.82	0.41
3:K:443:MET:HE2	3:K:443:MET:HB3	1.87	0.41
3:K:531:HIS:CD2	3:K:533:ASN:HB2	2.55	0.41
3:L:503:PHE:CZ	3:L:555:ILE:HD11	2.55	0.41
3:L:540:LYS:NZ	3:L:540:LYS:HB2	2.36	0.41
3:L:494:TYR:O	3:L:556:LYS:HA	2.21	0.41
4:N:84:LYS:O	4:N:84:LYS:HG3	2.20	0.41
4:Q:56:LYS:HG3	4:Q:57:SER:N	2.34	0.41
1:A:343:LYS:HB2	1:A:346:MET:HB2	2.00	0.41
1:A:454:LEU:HA	1:A:491:ASP:O	2.21	0.41
2:B:1055:TRP:CD1	2:B:1111:LEU:HD22	2.56	0.41
1:C:100:LEU:HD12	1:C:101:VAL:H	1.86	0.41
2:F:1055:TRP:CD1	2:F:1111:LEU:HD22	2.56	0.41
2:F:1518:GLY:CA	2:F:1585:LEU:HD22	2.48	0.41
2:F:932:ARG:HH11	3:L:339:SER:CB	2.34	0.41
1:G:218:GLU:C	1:G:220:PHE:H	2.23	0.41
2:H:1514:ALA:O	2:H:1519:VAL:HG11	2.20	0.41
3:I:503:PHE:CZ	3:I:555:ILE:HD11	2.55	0.41
3:J:494:TYR:O	3:J:556:LYS:HA	2.21	0.41
8:K:1745:MAN:H62	8:K:1746:MAN:H2	1.74	0.41
3:K:259:SER:HB3	5:K:1743:NDG:O7	2.20	0.41
3:L:278:TYR:CE2	3:L:455:MET:SD	3.13	0.41
4:N:41:LYS:O	4:N:45:LYS:HG3	2.21	0.41
4:P:84:LYS:HG3	4:P:84:LYS:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:740:VAL:CB	4:Q:42:ARG:HB2	2.45	0.41
1:A:250:ILE:HG12	1:A:251:PHE:H	1.84	0.41
1:A:2:PRO:HA	1:A:25:HIS:O	2.19	0.41
1:A:13:ARG:NH2	1:A:476:GLY:HA3	2.35	0.41
2:B:1451:GLN:HA	2:B:1452:PRO:HD3	1.94	0.41
2:D:1055:TRP:CD1	2:D:1111:LEU:HD22	2.56	0.41
2:D:1516:GLU:HB3	2:D:1517:PRO:CD	2.50	0.41
2:F:1082:VAL:HG13	2:F:1129:LEU:HD22	2.02	0.41
2:F:759:PRO:HA	2:F:760:PRO:HD3	1.84	0.41
2:F:932:ARG:O	2:F:933:GLU:C	2.58	0.41
2:H:1359:LYS:CB	4:N:4:LEU:HD21	2.50	0.41
2:H:1462:ASN:HD22	2:H:1462:ASN:C	2.21	0.41
3:I:244:MET:HG2	3:I:245:ASN:N	2.35	0.41
3:J:289:TYR:HA	3:J:293:PRO:HA	2.02	0.41
3:J:461:LYS:HG2	4:Q:28:VAL:HG12	2.03	0.41
3:J:676:GLY:HA2	3:J:677:PRO:HD3	1.83	0.41
3:K:446:GLU:H	3:K:446:GLU:HG3	1.66	0.41
3:K:503:PHE:CZ	3:K:555:ILE:HD11	2.55	0.41
2:B:813:LEU:HD23	2:B:907:LEU:HD22	2.02	0.41
1:C:549:GLU:O	1:C:550:ASP:HB2	2.20	0.41
2:D:1357:ASP:C	2:D:1359:LYS:H	2.24	0.41
2:F:1334:LEU:HA	2:F:1334:LEU:HD13	1.80	0.41
2:F:824:GLU:OE2	2:F:875:PRO:HB3	2.19	0.41
1:G:549:GLU:O	1:G:550:ASP:HB2	2.20	0.41
2:H:1500:LYS:HE3	2:H:1504:LYS:O	2.21	0.41
3:J:368:ASN:ND2	3:J:368:ASN:N	2.69	0.41
3:J:540:LYS:NZ	3:J:540:LYS:HB2	2.35	0.41
4:M:84:LYS:O	4:M:84:LYS:HG3	2.20	0.41
4:P:56:LYS:HG3	4:P:57:SER:N	2.34	0.41
1:A:10:ASN:HA	1:A:623:THR:HG23	2.03	0.41
2:B:1522:VAL:HG22	2:B:1583:TRP:HB3	2.02	0.41
2:B:854:ALA:HB2	2:B:860:HIS:HB3	2.02	0.41
2:D:851:CYS:HB2	2:D:1491:CYS:HB2	1.78	0.41
2:D:1522:VAL:HG22	2:D:1583:TRP:HB3	2.02	0.41
2:D:1611:GLU:HG3	2:D:1612:GLU:N	2.34	0.41
1:E:503:PHE:HD1	1:E:507:PHE:CG	2.37	0.41
2:F:1386:MET:O	2:F:1387:THR:C	2.58	0.41
2:F:1514:ALA:O	2:F:1519:VAL:HG11	2.20	0.41
1:A:459:ARG:NH2	1:G:459:ARG:HE	2.19	0.41
1:G:7:ILE:HG21	1:G:471:LEU:HD22	2.02	0.41
2:H:1518:GLY:CA	2:H:1585:LEU:HD22	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:494:TYR:O	3:I:556:LYS:HA	2.21	0.41
3:K:298:LYS:HB2	3:K:301:GLU:HG3	2.02	0.41
1:A:363:TYR:CD2	1:A:381:GLY:HA2	2.56	0.41
1:A:6:ILE:HD11	1:A:20:MET:CG	2.50	0.41
2:B:1216:LEU:HD21	2:B:1256:ALA:HA	2.02	0.41
2:B:1522:VAL:HG12	2:B:1547:ILE:HD12	2.03	0.41
2:B:841:ARG:HH11	2:B:841:ARG:CG	2.23	0.41
1:C:207:LEU:HA	1:C:208:PRO:HD2	1.82	0.41
1:E:549:GLU:O	1:E:550:ASP:HB2	2.20	0.41
2:F:1338:LYS:N	2:F:1371:ARG:HB2	2.36	0.41
1:G:23:GLU:OE1	1:G:469:THR:HG21	2.21	0.41
1:G:249:VAL:HG13	1:G:267:LYS:HB2	2.02	0.41
2:H:1639:CYS:HA	2:H:1640:PRO:HD3	1.76	0.41
2:H:813:LEU:HA	2:H:814:PRO:HD3	1.97	0.41
3:L:428:PHE:CE1	3:L:439:VAL:HG13	2.56	0.41
2:B:1444:TYR:HB2	4:Q:10:TYR:CE1	2.55	0.41
1:A:250:ILE:HG12	1:A:251:PHE:N	2.36	0.41
2:B:1192:ALA:HB2	2:B:1198:TRP:CE2	2.56	0.41
2:B:1370:TYR:CG	2:B:1376:ALA:HB2	2.55	0.41
2:B:1611:GLU:HB3	2:B:1614:GLU:HG3	2.03	0.41
1:C:10:ASN:HB2	1:C:622:LEU:N	2.36	0.41
1:C:454:LEU:HA	1:C:491:ASP:O	2.21	0.41
2:D:1611:GLU:HB3	2:D:1614:GLU:HG3	2.03	0.41
1:E:19:THR:HG22	1:E:20:MET:N	2.35	0.41
1:E:250:ILE:HG22	1:E:305:SER:HB3	2.03	0.41
1:E:640:CYS:HB3	1:E:641:PRO:CD	2.51	0.41
2:H:1522:VAL:HG22	2:H:1583:TRP:HB3	2.02	0.41
3:I:239:ASP:HA	3:I:240:PRO:HD3	1.86	0.41
6:J:1744:NAG:H2	6:J:1744:NAG:H82	1.91	0.41
3:J:428:PHE:CE1	4:Q:31:LEU:HD11	2.55	0.41
3:J:503:PHE:CZ	3:J:555:ILE:HD11	2.55	0.41
3:K:289:TYR:HA	3:K:293:PRO:HA	2.02	0.41
4:P:23:LEU:HD21	4:P:51:ALA:HB3	2.02	0.41
1:A:506:SER:HB2	1:A:530:TRP:NE1	2.27	0.41
1:A:552:GLN:HA	1:A:553:PRO:HD3	1.81	0.41
1:A:24:ALA:HB3	1:A:60:HIS:HB3	2.03	0.41
2:D:1165:TYR:HD1	2:D:1210:ALA:HB2	1.85	0.41
1:E:218:GLU:C	1:E:220:PHE:H	2.23	0.41
1:E:250:ILE:HG12	1:E:251:PHE:N	2.36	0.41
1:E:324:ILE:HA	1:E:325:PRO:HD3	1.89	0.41
2:F:1376:ALA:HB3	2:F:1429:VAL:CG2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:745:PHE:HA	2:F:776:SER:OG	2.21	0.41
1:G:207:LEU:HA	1:G:208:PRO:HD2	1.82	0.41
2:H:1523:TYR:HB3	2:H:1543:ILE:HG23	2.02	0.41
2:H:1541:MET:HB2	2:H:1541:MET:HE3	1.96	0.41
3:J:238:LEU:HD11	3:J:278:TYR:CB	2.46	0.41
3:J:423:ASN:ND2	3:J:423:ASN:N	2.68	0.41
3:J:638:ALA:HA	3:J:639:PRO:HD3	1.98	0.41
3:K:676:GLY:HA2	3:K:677:PRO:HD3	1.83	0.41
4:M:69:GLN:HE21	4:M:69:GLN:HB3	1.68	0.41
1:A:100:LEU:HD12	1:A:101:VAL:H	1.86	0.41
1:A:19:THR:HG22	1:A:20:MET:N	2.35	0.41
2:B:1229:PRO:HA	2:B:1232:ARG:NH1	2.36	0.41
2:B:729:LEU:C	2:B:729:LEU:HD13	2.41	0.41
1:C:477:ARG:HG2	1:C:477:ARG:NH1	2.21	0.41
2:D:1216:LEU:HD21	2:D:1256:ALA:HA	2.02	0.41
2:D:745:PHE:N	2:D:746:PRO:HD3	2.35	0.41
1:E:439:LEU:CD1	1:E:439:LEU:H	2.32	0.41
1:E:438:VAL:HG13	1:E:449:LEU:HD11	2.03	0.41
2:F:1522:VAL:HG12	2:F:1547:ILE:HD12	2.03	0.41
2:F:813:LEU:HD23	2:F:907:LEU:HD22	2.02	0.41
1:G:391:THR:HG22	1:G:392:HIS:N	2.36	0.41
2:H:1635:VAL:HG23	2:H:1636:VAL:N	2.36	0.41
3:I:503:PHE:HB2	3:I:530:PHE:HZ	1.86	0.41
3:J:428:PHE:CE1	3:J:439:VAL:HG13	2.56	0.41
3:K:244:MET:HG2	3:K:245:ASN:H	1.86	0.41
1:A:400:ILE:N	1:A:400:ILE:HD12	2.36	0.40
2:B:917:ASN:OD1	5:B:2642:NDG:O	2.38	0.40
1:C:365:VAL:HA	1:C:366:PRO:HD2	1.81	0.40
2:D:1192:ALA:HB2	2:D:1198:TRP:CE2	2.56	0.40
1:E:249:VAL:HG13	1:E:267:LYS:HB2	2.03	0.40
2:F:1229:PRO:HA	2:F:1232:ARG:NH1	2.36	0.40
2:F:1516:GLU:HB3	2:F:1517:PRO:CD	2.50	0.40
1:E:541:LEU:HD22	2:F:786:SER:HB3	2.02	0.40
2:F:819:ARG:CG	2:F:819:ARG:NH1	2.80	0.40
2:F:854:ALA:HB2	2:F:860:HIS:HB3	2.02	0.40
1:G:400:ILE:N	1:G:400:ILE:HD12	2.36	0.40
2:H:1522:VAL:HG12	2:H:1547:ILE:HD12	2.03	0.40
2:H:915:ARG:O	2:H:916:MET:HG3	2.21	0.40
2:H:965:VAL:HG23	2:H:1268:GLN:OE1	2.22	0.40
3:K:439:VAL:HA	4:P:31:LEU:HD21	2.02	0.40
3:K:428:PHE:CE1	3:K:439:VAL:HG13	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:M:41:LYS:O	4:M:45:LYS:HG3	2.21	0.40
4:P:41:LYS:O	4:P:45:LYS:HG3	2.21	0.40
1:A:344:PRO:HG3	1:A:423:PRO:HB3	2.02	0.40
1:E:24:ALA:HB3	1:E:60:HIS:HB3	2.03	0.40
1:E:391:THR:HG22	1:E:392:HIS:N	2.36	0.40
1:E:552:GLN:HA	1:E:553:PRO:HD3	1.81	0.40
2:F:1000:VAL:HG22	2:F:1027:ILE:HG23	2.04	0.40
2:F:1192:ALA:HB2	2:F:1198:TRP:CE2	2.56	0.40
2:F:1370:TYR:CE2	2:F:1372:GLY:HA3	2.56	0.40
2:F:1611:GLU:HB3	2:F:1614:GLU:HG3	2.03	0.40
2:H:1370:TYR:CG	2:H:1376:ALA:HB2	2.56	0.40
2:H:1503:ASP:O	2:H:1504:LYS:HG3	2.21	0.40
1:G:558:GLN:HB3	2:H:770:ASN:HD21	1.86	0.40
2:H:877:VAL:HG22	2:H:1451:GLN:NE2	2.28	0.40
2:H:813:LEU:HD23	2:H:907:LEU:HD22	2.02	0.40
1:C:109:PHE:CZ	1:C:594:ILE:HG23	2.56	0.40
2:D:813:LEU:HD23	2:D:907:LEU:HD22	2.02	0.40
7:E:1648:BMA:H62	7:E:1649:BMA:H2	1.58	0.40
1:E:480:LYS:HG2	1:E:481:ALA:N	2.36	0.40
2:F:1523:TYR:HB3	2:F:1543:ILE:HG23	2.02	0.40
1:G:480:LYS:HG2	1:G:481:ALA:N	2.37	0.40
1:G:505:PRO:O	1:G:533:VAL:HB	2.21	0.40
1:G:506:SER:HB2	1:G:530:TRP:NE1	2.27	0.40
2:H:1527:LEU:HD22	2:H:1574:LEU:HB3	2.04	0.40
1:G:126:ARG:HG3	2:H:751:TRP:CZ2	2.56	0.40
2:H:809:ILE:HD11	2:H:892:ALA:CB	2.52	0.40
3:I:345:ASP:HB3	3:I:346:ASP:H	1.49	0.40
3:I:654:ARG:HG3	3:I:722:GLN:HB3	2.03	0.40
1:A:342:PHE:CZ	1:A:423:PRO:HG3	2.56	0.40
1:A:363:TYR:HD2	1:A:381:GLY:HA2	1.86	0.40
1:C:391:THR:HG22	1:C:392:HIS:N	2.36	0.40
1:C:392:HIS:C	1:C:394:SER:H	2.25	0.40
1:C:583:LEU:HD12	1:C:583:LEU:N	2.36	0.40
2:D:1229:PRO:HA	2:D:1232:ARG:NH1	2.36	0.40
2:D:776:SER:HB2	2:D:780:TRP:HZ2	1.86	0.40
1:E:100:LEU:HD12	1:E:101:VAL:H	1.86	0.40
1:E:583:LEU:N	1:E:583:LEU:HD12	2.36	0.40
2:H:1370:TYR:CE2	2:H:1372:GLY:HA3	2.56	0.40
2:H:1609:TRP:HD1	2:H:1610:PRO:O	2.04	0.40
3:I:298:LYS:HB2	3:I:301:GLU:HG3	2.02	0.40
3:I:402:VAL:HG11	3:I:414:ILE:HG23	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:428:PHE:CE1	3:I:439:VAL:HG13	2.56	0.40
3:I:540:LYS:HB2	3:I:540:LYS:NZ	2.35	0.40
3:K:328:THR:N	3:K:368:ASN:HD21	2.20	0.40
3:K:494:TYR:O	3:K:556:LYS:HA	2.21	0.40
3:L:244:MET:HG2	3:L:245:ASN:N	2.35	0.40
3:I:461:LYS:CG	4:M:28:VAL:HG12	2.51	0.40
2:B:1446:ASN:HB2	4:Q:4:LEU:HD12	2.03	0.40
2:B:1609:TRP:HD1	2:B:1610:PRO:O	2.04	0.40
1:C:400:ILE:N	1:C:400:ILE:HD12	2.36	0.40
1:C:480:LYS:HG2	1:C:481:ALA:N	2.37	0.40
1:C:199:GLU:HB2	1:C:587:ASN:OD1	2.22	0.40
1:C:24:ALA:HB3	1:C:60:HIS:HB3	2.03	0.40
2:D:1527:LEU:HD22	2:D:1574:LEU:HB3	2.04	0.40
1:E:642:GLN:O	1:E:644:ALA:N	2.54	0.40
2:F:1143:LEU:O	2:F:1147:ILE:HG13	2.22	0.40
2:F:1632:GLU:HA	2:F:1635:VAL:HG22	2.04	0.40
1:G:220:PHE:CZ	1:G:330:PRO:HB3	2.56	0.40
3:J:292:TYR:HA	3:J:293:PRO:HD3	1.95	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	632/645 (98%)	576 (91%)	52 (8%)	4 (1%)	28	70
1	C	632/645 (98%)	576 (91%)	52 (8%)	4 (1%)	28	70
1	E	632/645 (98%)	575 (91%)	53 (8%)	4 (1%)	28	70
1	G	632/645 (98%)	575 (91%)	53 (8%)	4 (1%)	28	70
2	B	893/915 (98%)	785 (88%)	80 (9%)	28 (3%)	5	40
2	D	893/915 (98%)	784 (88%)	82 (9%)	27 (3%)	5	41

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	894/915 (98%)	786 (88%)	78 (9%)	30 (3%)	4	39
2	H	890/915 (97%)	782 (88%)	75 (8%)	33 (4%)	4	36
3	I	505/507 (100%)	446 (88%)	51 (10%)	8 (2%)	11	53
3	J	505/507 (100%)	446 (88%)	51 (10%)	8 (2%)	11	53
3	K	505/507 (100%)	445 (88%)	52 (10%)	8 (2%)	11	53
3	L	505/507 (100%)	446 (88%)	51 (10%)	8 (2%)	11	53
4	M	82/92 (89%)	77 (94%)	4 (5%)	1 (1%)	15	58
4	N	82/92 (89%)	77 (94%)	4 (5%)	1 (1%)	15	58
4	P	82/92 (89%)	77 (94%)	4 (5%)	1 (1%)	15	58
4	Q	82/92 (89%)	77 (94%)	4 (5%)	1 (1%)	15	58
All	All	8446/8636 (98%)	7530 (89%)	746 (9%)	170 (2%)	9	49

All (170) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	933	GLU
2	B	967	GLN
2	B	1269	GLU
2	B	1281	ARG
2	B	1291	TRP
2	B	1292	GLU
2	B	1294	ALA
2	B	1337	ASN
2	B	1338	LYS
2	B	1359	LYS
2	B	1377	THR
2	B	1503	ASP
2	D	933	GLU
2	D	967	GLN
2	D	1281	ARG
2	D	1291	TRP
2	D	1292	GLU
2	D	1294	ALA
2	D	1337	ASN
2	D	1338	LYS
2	D	1359	LYS
2	D	1377	THR
2	D	1503	ASP

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Mol	Chain	Res	Type
2	F	933	GLU
2	F	967	GLN
2	F	1269	GLU
2	F	1281	ARG
2	F	1291	TRP
2	F	1292	GLU
2	F	1337	ASN
2	F	1338	LYS
2	F	1361	THR
2	F	1377	THR
2	F	1417	SER
2	F	1446	ASN
2	H	933	GLU
2	H	968	MET
2	H	1281	ARG
2	H	1291	TRP
2	H	1292	GLU
2	H	1337	ASN
2	H	1338	LYS
2	H	1361	THR
2	H	1377	THR
2	H	1417	SER
2	H	1446	ASN
2	H	1493	GLU
3	I	236	ILE
3	I	407	PRO
3	I	701	LYS
3	I	706	GLN
3	J	236	ILE
3	J	407	PRO
3	J	701	LYS
3	J	706	GLN
3	K	236	ILE
3	K	407	PRO
3	K	701	LYS
3	K	706	GLN
3	L	236	ILE
3	L	407	PRO
3	L	701	LYS
3	L	706	GLN
2	B	911	PRO
2	B	1360	ASN

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Mol	Chain	Res	Type
2	B	1361	THR
2	B	1476	GLU
2	B	1571	ALA
2	D	911	PRO
2	D	1360	ASN
2	D	1361	THR
2	D	1476	GLU
2	D	1480	LEU
2	D	1571	ALA
2	F	911	PRO
2	F	1267	HIS
2	F	1294	ALA
2	F	1476	GLU
2	F	1498	ILE
2	F	1571	ALA
2	H	1266	ASP
2	H	1269	GLU
2	H	1294	ALA
2	H	1476	GLU
2	H	1496	CYS
2	H	1498	ILE
2	H	1571	ALA
1	A	442	GLU
1	A	643	PRO
2	B	1387	THR
2	B	1502	ASP
2	B	1573	LYS
1	C	442	GLU
1	C	643	PRO
2	D	1387	THR
2	D	1502	ASP
2	D	1573	LYS
1	E	442	GLU
1	E	643	PRO
2	F	1387	THR
2	F	1573	LYS
1	G	442	GLU
2	H	911	PRO
2	H	1387	THR
2	H	1573	LYS
3	I	707	LYS
3	J	516	VAL

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Mol	Chain	Res	Type
3	J	707	LYS
3	K	516	VAL
3	K	707	LYS
3	L	707	LYS
1	A	505	PRO
2	B	1196	ASN
2	B	1265	PRO
2	B	1480	LEU
1	C	505	PRO
2	D	1196	ASN
2	D	1265	PRO
2	D	1269	GLU
1	E	505	PRO
2	F	1196	ASN
2	F	1265	PRO
2	F	1268	GLN
2	F	1331	LYS
2	F	1637	PHE
1	G	505	PRO
2	H	967	GLN
2	H	1267	HIS
2	H	1486	ASP
2	H	1495	ASN
2	H	1502	ASP
3	I	516	VAL
3	L	516	VAL
4	M	7	SER
4	N	7	SER
4	P	7	SER
4	Q	7	SER
2	B	834	GLN
2	B	1201	PRO
2	B	1267	HIS
2	B	1536	PHE
2	D	834	GLN
2	D	1201	PRO
2	D	1536	PHE
2	F	834	GLN
2	F	1201	PRO
2	F	1270	LEU
2	F	1536	PHE
1	G	643	PRO

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Mol	Chain	Res	Type
2	H	834	GLN
2	H	1196	ASN
2	H	1201	PRO
2	H	1264	ALA
2	H	1536	PHE
3	I	268	LEU
3	J	268	LEU
3	K	268	LEU
3	L	268	LEU
3	I	482	GLY
3	J	482	GLY
3	K	482	GLY
3	L	482	GLY
2	B	1517	PRO
2	D	1517	PRO
2	F	1517	PRO
2	H	1517	PRO
1	A	208	PRO
1	C	208	PRO
1	E	208	PRO
1	G	208	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	558/567 (98%)	549 (98%)	9 (2%)	68	86
1	C	558/567 (98%)	549 (98%)	9 (2%)	68	86
1	E	558/567 (98%)	549 (98%)	9 (2%)	68	86
1	G	558/567 (98%)	549 (98%)	9 (2%)	68	86
2	B	793/810 (98%)	769 (97%)	24 (3%)	46	75
2	D	790/810 (98%)	766 (97%)	24 (3%)	46	75
2	F	793/810 (98%)	769 (97%)	24 (3%)	46	75
2	H	793/810 (98%)	766 (97%)	27 (3%)	42	73

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	I	442/446 (99%)	429 (97%)	13 (3%)	48	75
3	J	442/446 (99%)	429 (97%)	13 (3%)	48	75
3	K	442/446 (99%)	429 (97%)	13 (3%)	48	75
3	L	442/446 (99%)	429 (97%)	13 (3%)	48	75
4	M	76/84 (90%)	73 (96%)	3 (4%)	37	69
4	N	76/84 (90%)	73 (96%)	3 (4%)	37	69
4	P	76/84 (90%)	73 (96%)	3 (4%)	37	69
4	Q	76/84 (90%)	73 (96%)	3 (4%)	37	69
All	All	7473/7628 (98%)	7274 (97%)	199 (3%)	50	77

All (199) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	81	ASN
1	A	144	ASN
1	A	155	GLN
1	A	289	VAL
1	A	398	LEU
1	A	404	THR
1	A	440	ARG
1	A	551	ARG
2	B	757	LYS
2	B	770	ASN
2	B	833	ARG
2	B	834	GLN
2	B	841	ARG
2	B	937	LYS
2	B	945	LEU
2	B	953	GLU
2	B	1018	GLU
2	B	1196	ASN
2	B	1292	GLU
2	B	1334	LEU
2	B	1335	THR
2	B	1342	LYS
2	B	1361	THR
2	B	1416	PHE
2	B	1433	GLU

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Mol	Chain	Res	Type
2	B	1445	PHE
2	B	1462	ASN
2	B	1520	ASP
2	B	1535	ASP
2	B	1536	PHE
2	B	1569	ARG
2	B	1637	PHE
1	C	10	ASN
1	C	81	ASN
1	C	144	ASN
1	C	155	GLN
1	C	289	VAL
1	C	398	LEU
1	C	404	THR
1	C	440	ARG
1	C	551	ARG
2	D	757	LYS
2	D	770	ASN
2	D	833	ARG
2	D	834	GLN
2	D	841	ARG
2	D	937	LYS
2	D	945	LEU
2	D	953	GLU
2	D	1018	GLU
2	D	1196	ASN
2	D	1292	GLU
2	D	1334	LEU
2	D	1335	THR
2	D	1342	LYS
2	D	1361	THR
2	D	1416	PHE
2	D	1433	GLU
2	D	1445	PHE
2	D	1462	ASN
2	D	1520	ASP
2	D	1535	ASP
2	D	1536	PHE
2	D	1569	ARG
2	D	1637	PHE
1	E	10	ASN
1	E	81	ASN

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Mol	Chain	Res	Type
1	E	144	ASN
1	E	155	GLN
1	E	289	VAL
1	E	398	LEU
1	E	404	THR
1	E	440	ARG
1	E	551	ARG
2	F	757	LYS
2	F	770	ASN
2	F	833	ARG
2	F	834	GLN
2	F	841	ARG
2	F	937	LYS
2	F	945	LEU
2	F	953	GLU
2	F	1018	GLU
2	F	1196	ASN
2	F	1268	GLN
2	F	1292	GLU
2	F	1334	LEU
2	F	1335	THR
2	F	1342	LYS
2	F	1397	LYS
2	F	1433	GLU
2	F	1462	ASN
2	F	1520	ASP
2	F	1535	ASP
2	F	1536	PHE
2	F	1569	ARG
2	F	1572	LEU
2	F	1640	PRO
1	G	10	ASN
1	G	81	ASN
1	G	144	ASN
1	G	155	GLN
1	G	289	VAL
1	G	398	LEU
1	G	404	THR
1	G	440	ARG
1	G	551	ARG
2	H	757	LYS
2	H	770	ASN

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Mol	Chain	Res	Type
2	H	833	ARG
2	H	834	GLN
2	H	841	ARG
2	H	937	LYS
2	H	945	LEU
2	H	953	GLU
2	H	968	MET
2	H	969	THR
2	H	1018	GLU
2	H	1196	ASN
2	H	1267	HIS
2	H	1292	GLU
2	H	1334	LEU
2	H	1335	THR
2	H	1342	LYS
2	H	1397	LYS
2	H	1433	GLU
2	H	1462	ASN
2	H	1498	ILE
2	H	1499	GLN
2	H	1520	ASP
2	H	1535	ASP
2	H	1536	PHE
2	H	1569	ARG
2	H	1572	LEU
3	I	237	VAL
3	I	255	SER
3	I	322	HIS
3	I	329	ASN
3	I	368	ASN
3	I	381	ARG
3	I	423	ASN
3	I	446	GLU
3	I	539	LYS
3	I	540	LYS
3	I	654	ARG
3	I	702	ASN
3	I	703	GLN
3	J	237	VAL
3	J	255	SER
3	J	322	HIS
3	J	329	ASN

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Mol	Chain	Res	Type
3	J	368	ASN
3	J	381	ARG
3	J	423	ASN
3	J	446	GLU
3	J	539	LYS
3	J	540	LYS
3	J	654	ARG
3	J	702	ASN
3	J	703	GLN
3	K	237	VAL
3	K	255	SER
3	K	322	HIS
3	K	329	ASN
3	K	368	ASN
3	K	381	ARG
3	K	423	ASN
3	K	446	GLU
3	K	539	LYS
3	K	540	LYS
3	K	654	ARG
3	K	702	ASN
3	K	703	GLN
3	L	237	VAL
3	L	255	SER
3	L	322	HIS
3	L	329	ASN
3	L	368	ASN
3	L	381	ARG
3	L	423	ASN
3	L	446	GLU
3	L	539	LYS
3	L	540	LYS
3	L	654	ARG
3	L	702	ASN
3	L	703	GLN
4	M	11	GLN
4	M	69	GLN
4	M	71	GLN
4	N	11	GLN
4	N	69	GLN
4	N	71	GLN
4	P	11	GLN

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Mol	Chain	Res	Type
4	P	69	GLN
4	P	71	GLN
4	Q	11	GLN
4	Q	69	GLN
4	Q	71	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (256) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	87	GLN
1	A	104	GLN
1	A	144	ASN
1	A	155	GLN
1	A	161	GLN
1	A	162	ASN
1	A	163	GLN
1	A	370	GLN
1	A	380	GLN
1	A	390	ASN
1	A	414	GLN
1	A	490	GLN
1	A	558	GLN
1	A	567	HIS
1	A	634	GLN
1	A	639	GLN
2	B	738	ASN
2	B	752	ASN
2	B	762	ASN
2	B	770	ASN
2	B	820	ASN
2	B	834	GLN
2	B	860	HIS
2	B	886	GLN
2	B	896	HIS
2	B	897	HIS
2	B	1011	GLN
2	B	1069	ASN
2	B	1076	GLN
2	B	1114	ASN
2	B	1130	GLN
2	B	1141	ASN

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Mol	Chain	Res	Type
2	B	1160	ASN
2	B	1196	ASN
2	B	1204	GLN
2	B	1267	HIS
2	B	1277	GLN
2	B	1333	GLN
2	B	1337	ASN
2	B	1401	ASN
2	B	1431	HIS
2	B	1451	GLN
2	B	1462	ASN
2	B	1559	GLN
2	B	1579	HIS
2	B	1608	HIS
2	B	1620	ASN
1	C	10	ASN
1	C	60	HIS
1	C	87	GLN
1	C	104	GLN
1	C	132	HIS
1	C	144	ASN
1	C	155	GLN
1	C	161	GLN
1	C	162	ASN
1	C	163	GLN
1	C	356	ASN
1	C	370	GLN
1	C	380	GLN
1	C	390	ASN
1	C	414	GLN
1	C	450	ASN
1	C	490	GLN
1	C	558	GLN
1	C	567	HIS
1	C	634	GLN
1	C	639	GLN
2	D	738	ASN
2	D	752	ASN
2	D	762	ASN
2	D	770	ASN
2	D	820	ASN
2	D	834	GLN

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Mol	Chain	Res	Type
2	D	860	HIS
2	D	897	HIS
2	D	1011	GLN
2	D	1069	ASN
2	D	1076	GLN
2	D	1114	ASN
2	D	1130	GLN
2	D	1141	ASN
2	D	1160	ASN
2	D	1196	ASN
2	D	1204	GLN
2	D	1267	HIS
2	D	1277	GLN
2	D	1333	GLN
2	D	1337	ASN
2	D	1401	ASN
2	D	1431	HIS
2	D	1451	GLN
2	D	1462	ASN
2	D	1559	GLN
2	D	1579	HIS
2	D	1608	HIS
2	D	1620	ASN
1	E	60	HIS
1	E	87	GLN
1	E	104	GLN
1	E	132	HIS
1	E	144	ASN
1	E	155	GLN
1	E	161	GLN
1	E	162	ASN
1	E	163	GLN
1	E	356	ASN
1	E	370	GLN
1	E	380	GLN
1	E	390	ASN
1	E	414	GLN
1	E	450	ASN
1	E	490	GLN
1	E	558	GLN
1	E	567	HIS
1	E	639	GLN

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Mol	Chain	Res	Type
2	F	738	ASN
2	F	752	ASN
2	F	762	ASN
2	F	770	ASN
2	F	820	ASN
2	F	834	GLN
2	F	860	HIS
2	F	897	HIS
2	F	1011	GLN
2	F	1069	ASN
2	F	1076	GLN
2	F	1114	ASN
2	F	1130	GLN
2	F	1141	ASN
2	F	1160	ASN
2	F	1196	ASN
2	F	1204	GLN
2	F	1267	HIS
2	F	1277	GLN
2	F	1333	GLN
2	F	1337	ASN
2	F	1401	ASN
2	F	1431	HIS
2	F	1451	GLN
2	F	1462	ASN
2	F	1559	GLN
2	F	1579	HIS
2	F	1608	HIS
2	F	1620	ASN
2	F	1641	ASN
1	G	60	HIS
1	G	87	GLN
1	G	104	GLN
1	G	132	HIS
1	G	144	ASN
1	G	155	GLN
1	G	161	GLN
1	G	162	ASN
1	G	163	GLN
1	G	356	ASN
1	G	370	GLN
1	G	380	GLN

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Mol	Chain	Res	Type
1	G	390	ASN
1	G	414	GLN
1	G	490	GLN
1	G	558	GLN
1	G	587	ASN
1	G	634	GLN
1	G	639	GLN
2	H	738	ASN
2	H	752	ASN
2	H	762	ASN
2	H	770	ASN
2	H	820	ASN
2	H	834	GLN
2	H	860	HIS
2	H	896	HIS
2	H	897	HIS
2	H	1277	GLN
2	H	1333	GLN
2	H	1337	ASN
2	H	1401	ASN
2	H	1431	HIS
2	H	1451	GLN
2	H	1462	ASN
2	H	1559	GLN
2	H	1579	HIS
2	H	1608	HIS
2	H	1620	ASN
3	I	270	ASN
3	I	329	ASN
3	I	368	ASN
3	I	392	ASN
3	I	411	GLN
3	I	413	ASN
3	I	423	ASN
3	I	466	HIS
3	I	531	HIS
3	I	533	ASN
3	I	591	GLN
3	I	703	GLN
3	J	270	ASN
3	J	329	ASN
3	J	368	ASN

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Mol	Chain	Res	Type
3	J	392	ASN
3	J	411	GLN
3	J	413	ASN
3	J	423	ASN
3	J	435	ASN
3	J	466	HIS
3	J	531	HIS
3	J	533	ASN
3	J	591	GLN
3	J	703	GLN
3	K	270	ASN
3	K	329	ASN
3	K	368	ASN
3	K	392	ASN
3	K	411	GLN
3	K	413	ASN
3	K	423	ASN
3	K	435	ASN
3	K	466	HIS
3	K	531	HIS
3	K	533	ASN
3	K	591	GLN
3	K	703	GLN
3	L	270	ASN
3	L	329	ASN
3	L	368	ASN
3	L	392	ASN
3	L	411	GLN
3	L	413	ASN
3	L	423	ASN
3	L	466	HIS
3	L	531	HIS
3	L	533	ASN
3	L	591	GLN
3	L	703	GLN
4	M	11	GLN
4	M	27	ASN
4	M	49	GLN
4	M	69	GLN
4	M	71	GLN
4	N	11	GLN
4	N	27	ASN

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Mol	Chain	Res	Type
4	N	49	GLN
4	N	69	GLN
4	N	71	GLN
4	P	11	GLN
4	P	27	ASN
4	P	49	GLN
4	P	69	GLN
4	P	71	GLN
4	Q	11	GLN
4	Q	27	ASN
4	Q	49	GLN
4	Q	69	GLN
4	Q	71	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 61 ligands modelled in this entry, 4 are monoatomic - leaving 57 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	$\# Z > 2$
5	NDG	A	1646	1,6	14,14,15	0.45	0	15,19,21	0.76	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	NAG	A	1647	5,7	14,14,15	0.63	0	15,19,21	1.89	4 (26%)
7	BMA	A	1648	7,6	11,11,12	0.56	0	13,15,17	1.10	1 (7%)
7	BMA	A	1649	7	11,11,12	0.66	0	13,15,17	1.41	2 (15%)
5	NDG	B	2642	2,6	14,14,15	0.54	0	15,19,21	1.17	2 (13%)
6	NAG	B	2643	5,7	14,14,15	0.53	0	15,19,21	2.31	3 (20%)
7	BMA	B	2644	7,6	11,11,12	0.94	0	13,15,17	1.88	4 (30%)
7	BMA	B	2645	7	11,11,12	0.71	0	13,15,17	0.78	0
7	BMA	B	2646	-	11,11,12	0.72	0	13,15,17	1.46	3 (23%)
5	NDG	C	1646	1,6	14,14,15	0.61	0	15,19,21	1.25	2 (13%)
6	NAG	C	1647	5,7	14,14,15	0.66	0	15,19,21	1.20	2 (13%)
7	BMA	C	1648	7,6	11,11,12	0.66	0	13,15,17	1.09	1 (7%)
7	BMA	C	1649	7	11,11,12	0.75	0	13,15,17	1.66	3 (23%)
7	BMA	C	1650	7	11,11,12	0.66	0	13,15,17	1.81	4 (30%)
5	NDG	D	2642	2,6	14,14,15	0.48	0	15,19,21	0.86	0
6	NAG	D	2643	5,7	14,14,15	0.57	0	15,19,21	1.11	2 (13%)
7	BMA	D	2644	7,6	11,11,12	0.63	0	13,15,17	1.19	1 (7%)
7	BMA	D	2645	7	11,11,12	0.66	0	13,15,17	1.33	2 (15%)
5	NDG	E	1646	1,6	14,14,15	0.55	0	15,19,21	0.95	1 (6%)
6	NAG	E	1647	5,7	14,14,15	0.59	0	15,19,21	1.22	2 (13%)
7	BMA	E	1648	7,6	11,11,12	0.69	0	13,15,17	1.06	1 (7%)
7	BMA	E	1649	7	11,11,12	0.91	1 (9%)	13,15,17	1.78	3 (23%)
5	NDG	F	2642	2,6	14,14,15	0.38	0	15,19,21	1.35	3 (20%)
6	NAG	F	2643	5,7	14,14,15	0.44	0	15,19,21	1.65	3 (20%)
7	BMA	F	2644	7,6	11,11,12	0.59	0	13,15,17	1.58	4 (30%)
7	BMA	F	2645	7	11,11,12	0.98	1 (9%)	13,15,17	1.77	4 (30%)
7	BMA	F	2646	7	11,11,12	0.66	0	13,15,17	1.91	4 (30%)
7	BMA	F	2647	7	11,11,12	0.69	0	13,15,17	1.09	1 (7%)
5	NDG	G	1646	1,6	14,14,15	0.43	0	15,19,21	1.22	1 (6%)
6	NAG	G	1647	5,7	14,14,15	0.51	0	15,19,21	2.29	5 (33%)
7	BMA	G	1648	7,6	11,11,12	0.52	0	13,15,17	2.57	5 (38%)
7	BMA	G	1649	7	11,11,12	0.56	0	13,15,17	4.47	5 (38%)
7	BMA	G	1650	7	11,11,12	0.64	0	13,15,17	1.43	2 (15%)
8	MAN	G	1651	-	11,11,12	0.82	0	13,15,17	1.79	4 (30%)
5	NDG	H	2642	2,6	14,14,15	0.57	0	15,19,21	0.78	0
6	NAG	H	2643	8,5	14,14,15	0.47	0	15,19,21	0.77	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
8	MAN	H	2644	8,6	11,11,12	0.77	0	13,15,17	1.27	1 (7%)
8	MAN	H	2645	8	11,11,12	0.75	0	13,15,17	1.08	2 (15%)
5	NDG	I	1743	3,6	14,14,15	0.55	0	15,19,21	1.06	2 (13%)
6	NAG	I	1744	8,5	14,14,15	0.61	0	15,19,21	1.08	1 (6%)
8	MAN	I	1745	6	11,11,12	0.64	0	13,15,17	0.98	1 (7%)
5	NDG	I	1746	3,6	14,14,15	0.54	0	15,19,21	1.20	2 (13%)
6	NAG	I	1747	5	14,14,15	0.54	0	15,19,21	0.93	1 (6%)
5	NDG	J	1743	3,6	14,14,15	0.51	0	15,19,21	1.07	1 (6%)
6	NAG	J	1744	8,5	14,14,15	0.59	0	15,19,21	1.10	1 (6%)
8	MAN	J	1745	6	11,11,12	0.64	0	13,15,17	0.91	1 (7%)
5	NDG	K	1743	3,6	14,14,15	0.61	0	15,19,21	1.12	2 (13%)
6	NAG	K	1744	8,5	14,14,15	0.69	0	15,19,21	1.46	3 (20%)
8	MAN	K	1745	8,6	11,11,12	0.56	0	13,15,17	1.66	4 (30%)
8	MAN	K	1746	8	11,11,12	0.74	0	13,15,17	1.72	3 (23%)
7	BMA	K	1747	-	11,11,12	0.79	0	13,15,17	1.99	4 (30%)
8	MAN	K	1748	8	11,11,12	0.60	0	13,15,17	1.01	2 (15%)
5	NDG	K	1749	3	14,14,15	0.51	0	15,19,21	2.00	2 (13%)
5	NDG	L	1743	3,6	14,14,15	0.48	0	15,19,21	0.92	0
6	NAG	L	1744	5,7	14,14,15	0.60	0	15,19,21	1.10	1 (6%)
7	BMA	L	1745	6	11,11,12	0.64	0	13,15,17	0.83	1 (7%)
5	NDG	L	1746	3	14,14,15	0.51	0	15,19,21	0.66	0

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
5	NDG	A	1646	1,6	-	0/6/23/26	0/1/1/1
6	NAG	A	1647	5,7	-	0/6/23/26	0/1/1/1
7	BMA	A	1648	7,6	-	0/2/19/22	0/1/1/1
7	BMA	A	1649	7	-	0/2/19/22	0/1/1/1
5	NDG	B	2642	2,6	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	B	2643	5,7	-	0/6/23/26	0/1/1/1
7	BMA	B	2644	7,6	-	0/2/19/22	0/1/1/1
7	BMA	B	2645	7	-	0/2/19/22	0/1/1/1
7	BMA	B	2646	-	-	0/2/19/22	0/1/1/1
5	NDG	C	1646	1,6	1/1/5/7	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	NAG	C	1647	5,7	-	0/6/23/26	0/1/1/1
7	BMA	C	1648	7,6	-	0/2/19/22	0/1/1/1
7	BMA	C	1649	7	-	0/2/19/22	0/1/1/1
7	BMA	C	1650	7	-	0/2/19/22	0/1/1/1
5	NDG	D	2642	2,6	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	D	2643	5,7	-	0/6/23/26	0/1/1/1
7	BMA	D	2644	7,6	-	0/2/19/22	0/1/1/1
7	BMA	D	2645	7	-	0/2/19/22	0/1/1/1
5	NDG	E	1646	1,6	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	E	1647	5,7	-	0/6/23/26	0/1/1/1
7	BMA	E	1648	7,6	-	0/2/19/22	0/1/1/1
7	BMA	E	1649	7	-	0/2/19/22	0/1/1/1
5	NDG	F	2642	2,6	-	0/6/23/26	0/1/1/1
6	NAG	F	2643	5,7	-	0/6/23/26	0/1/1/1
7	BMA	F	2644	7,6	-	0/2/19/22	0/1/1/1
7	BMA	F	2645	7	-	0/2/19/22	0/1/1/1
7	BMA	F	2646	7	-	0/2/19/22	0/1/1/1
7	BMA	F	2647	7	-	0/2/19/22	0/1/1/1
5	NDG	G	1646	1,6	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	G	1647	5,7	-	0/6/23/26	0/1/1/1
7	BMA	G	1648	7,6	-	0/2/19/22	0/1/1/1
7	BMA	G	1649	7	-	0/2/19/22	0/1/1/1
7	BMA	G	1650	7	-	0/2/19/22	0/1/1/1
8	MAN	G	1651	-	-	0/2/19/22	0/1/1/1
5	NDG	H	2642	2,6	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	H	2643	8,5	-	0/6/23/26	0/1/1/1
8	MAN	H	2644	8,6	1/1/4/5	0/2/19/22	0/1/1/1
8	MAN	H	2645	8	1/1/4/5	0/2/19/22	0/1/1/1
5	NDG	I	1743	3,6	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	I	1744	8,5	-	0/6/23/26	0/1/1/1
8	MAN	I	1745	6	1/1/4/5	0/2/19/22	0/1/1/1
5	NDG	I	1746	3,6	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	I	1747	5	-	0/6/23/26	0/1/1/1
5	NDG	J	1743	3,6	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	J	1744	8,5	-	0/6/23/26	0/1/1/1
8	MAN	J	1745	6	1/1/4/5	0/2/19/22	0/1/1/1
5	NDG	K	1743	3,6	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	K	1744	8,5	-	0/6/23/26	0/1/1/1
8	MAN	K	1745	8,6	1/1/4/5	0/2/19/22	0/1/1/1
8	MAN	K	1746	8	1/1/4/5	0/2/19/22	0/1/1/1
7	BMA	K	1747	-	-	0/2/19/22	0/1/1/1
8	MAN	K	1748	8	1/1/4/5	0/2/19/22	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	NDG	K	1749	3	-	0/6/23/26	0/1/1/1
5	NDG	L	1743	3,6	1/1/5/7	0/6/23/26	0/1/1/1
6	NAG	L	1744	5,7	-	0/6/23/26	0/1/1/1
7	BMA	L	1745	6	-	0/2/19/22	0/1/1/1
5	NDG	L	1746	3	1/1/5/7	0/6/23/26	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	E	1649	BMA	O5-C1	-2.28	1.40	1.43
7	F	2645	BMA	O5-C1	-2.16	1.40	1.43

All (119) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	1649	BMA	C1-C2-C3	-10.35	96.54	109.65
7	G	1649	BMA	C3-C4-C5	-7.17	97.58	110.22
7	G	1649	BMA	C1-O5-C5	-6.84	102.74	112.17
5	K	1749	NDG	O-C1-C2	-5.53	103.78	111.47
7	G	1648	BMA	C1-C2-C3	-5.33	102.89	109.65
7	K	1747	BMA	C1-O5-C5	-4.93	105.37	112.17
7	G	1648	BMA	C6-C5-C4	-4.37	102.77	113.00
7	E	1649	BMA	C1-O5-C5	-4.36	106.16	112.17
7	F	2646	BMA	C1-C2-C3	-4.30	104.20	109.65
7	C	1650	BMA	C1-C2-C3	-4.09	104.46	109.65
7	G	1648	BMA	C1-O5-C5	-3.95	106.73	112.17
8	G	1651	MAN	C1-C2-C3	-3.90	104.70	109.65
7	K	1747	BMA	C1-C2-C3	-3.66	105.01	109.65
7	B	2644	BMA	C1-O5-C5	-3.66	107.13	112.17
7	D	2644	BMA	C1-O5-C5	-3.64	107.14	112.17
8	K	1745	MAN	C1-O5-C5	-3.63	107.16	112.17
7	F	2644	BMA	O5-C1-C2	-3.59	105.17	110.79
7	C	1649	BMA	O3-C3-C4	-3.48	102.78	110.36
6	G	1647	NAG	C4-C3-C2	-3.48	105.92	111.02
7	F	2646	BMA	O5-C1-C2	-3.36	105.53	110.79
6	F	2643	NAG	C4-C3-C2	-3.30	106.18	111.02
7	B	2646	BMA	C1-C2-C3	-3.26	105.52	109.65
7	G	1650	BMA	C1-C2-C3	-3.14	105.68	109.65
7	A	1649	BMA	O5-C1-C2	-3.10	105.94	110.79
7	G	1650	BMA	O5-C1-C2	-3.04	106.03	110.79
7	A	1648	BMA	C1-O5-C5	-3.03	107.99	112.17
7	E	1649	BMA	O5-C1-C2	-2.99	106.11	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	F	2642	NDG	O-C1-C2	-2.95	107.37	111.47
7	C	1650	BMA	O5-C1-C2	-2.95	106.17	110.79
7	D	2645	BMA	O5-C1-C2	-2.94	106.19	110.79
8	G	1651	MAN	C1-O5-C5	-2.93	108.12	112.17
8	K	1746	MAN	O5-C1-C2	-2.93	106.21	110.79
7	A	1649	BMA	C1-C2-C3	-2.88	106.00	109.65
8	I	1745	MAN	C1-O5-C5	-2.85	108.24	112.17
7	E	1649	BMA	C1-C2-C3	-2.78	106.13	109.65
7	D	2645	BMA	C1-C2-C3	-2.68	106.25	109.65
8	K	1745	MAN	C1-C2-C3	-2.67	106.26	109.65
7	C	1650	BMA	C1-O5-C5	-2.63	108.54	112.17
7	C	1648	BMA	C1-O5-C5	-2.50	108.72	112.17
8	J	1745	MAN	C1-O5-C5	-2.49	108.73	112.17
7	F	2645	BMA	C1-O5-C5	-2.48	108.75	112.17
6	A	1647	NAG	O4-C4-C3	-2.42	105.10	110.36
7	F	2646	BMA	C1-O5-C5	-2.39	108.87	112.17
7	C	1649	BMA	C1-O5-C5	-2.38	108.88	112.17
7	E	1648	BMA	C1-O5-C5	-2.36	108.92	112.17
7	F	2644	BMA	C2-C3-C4	-2.33	106.81	110.88
8	H	2645	MAN	C1-O5-C5	-2.28	109.03	112.17
7	F	2647	BMA	O5-C1-C2	-2.24	107.29	110.79
8	K	1746	MAN	C6-C5-C4	-2.22	107.81	113.00
7	F	2644	BMA	C1-C2-C3	-2.22	106.84	109.65
5	F	2642	NDG	C4-C3-C2	-2.21	107.77	111.02
6	K	1744	NAG	O4-C4-C3	-2.17	105.62	110.36
8	H	2645	MAN	O5-C1-C2	-2.15	107.43	110.79
7	F	2644	BMA	C6-C5-C4	-2.13	108.03	113.00
7	L	1745	BMA	C1-O5-C5	-2.10	109.27	112.17
7	B	2646	BMA	C1-O5-C5	-2.10	109.28	112.17
8	K	1745	MAN	C2-C3-C4	-2.07	107.26	110.88
6	B	2643	NAG	C6-C5-C4	-2.07	108.15	113.00
5	K	1743	NDG	C4-C3-C2	2.02	113.98	111.02
8	K	1748	MAN	C1-O5-C5	2.03	114.96	112.17
6	D	2643	NAG	C4-C3-C2	2.03	114.00	111.02
5	E	1646	NDG	C3-C4-C5	2.04	113.81	110.22
7	B	2644	BMA	C6-C5-C4	2.05	117.80	113.00
6	G	1647	NAG	O4-C4-C3	2.10	114.92	110.36
8	K	1748	MAN	C3-C4-C5	2.11	113.94	110.22
5	I	1743	NDG	C1-O-C5	2.14	115.11	112.17
5	B	2642	NDG	C3-C4-C5	2.14	113.99	110.22
7	F	2645	BMA	C3-C4-C5	2.16	114.02	110.22
7	K	1747	BMA	C3-C4-C5	2.17	114.03	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	I	1743	NDG	C3-C4-C5	2.21	114.11	110.22
6	C	1647	NAG	O5-C1-C2	2.23	114.58	111.47
5	F	2642	NDG	O4-C4-C5	2.26	114.99	109.28
6	D	2643	NAG	C1-O5-C5	2.27	115.29	112.17
5	C	1646	NDG	C1-O-C5	2.27	115.30	112.17
7	G	1649	BMA	O3-C3-C2	2.30	114.21	110.02
6	C	1647	NAG	C4-C3-C2	2.31	114.41	111.02
7	B	2644	BMA	C2-C3-C4	2.35	114.97	110.88
5	I	1746	NDG	C4-C3-C2	2.43	114.57	111.02
7	C	1650	BMA	C3-C4-C5	2.43	114.50	110.22
6	E	1647	NAG	C1-O5-C5	2.44	115.53	112.17
6	I	1747	NAG	C1-O5-C5	2.44	115.53	112.17
7	G	1648	BMA	O6-C6-C5	2.53	119.86	111.34
6	I	1744	NAG	C4-C3-C2	2.55	114.76	111.02
6	J	1744	NAG	C4-C3-C2	2.58	114.79	111.02
7	B	2646	BMA	O5-C1-C2	2.58	114.83	110.79
5	J	1743	NDG	C1-O-C5	2.59	115.73	112.17
6	E	1647	NAG	O5-C1-C2	2.62	115.11	111.47
7	K	1747	BMA	O5-C1-C2	2.62	114.90	110.79
5	I	1746	NDG	C3-C4-C5	2.62	114.84	110.22
6	A	1647	NAG	C3-C4-C5	2.64	114.87	110.22
6	L	1744	NAG	C4-C3-C2	2.64	114.89	111.02
7	F	2646	BMA	C3-C4-C5	2.65	114.89	110.22
6	G	1647	NAG	O5-C1-C2	2.68	115.21	111.47
8	G	1651	MAN	C3-C4-C5	2.69	114.96	110.22
5	K	1743	NDG	C3-C4-C5	2.74	115.05	110.22
5	G	1646	NDG	C4-C3-C2	2.82	115.15	111.02
6	K	1744	NAG	C3-C4-C5	2.82	115.19	110.22
8	K	1745	MAN	O3-C3-C2	2.87	115.25	110.02
7	F	2645	BMA	C2-C3-C4	2.89	115.91	110.88
5	B	2642	NDG	C1-O-C5	2.90	116.17	112.17
8	G	1651	MAN	O5-C1-C2	2.95	115.41	110.79
6	F	2643	NAG	O4-C4-C3	2.99	116.87	110.36
5	C	1646	NDG	C3-C4-C5	3.02	115.54	110.22
7	C	1649	BMA	C3-C4-C5	3.11	115.70	110.22
6	G	1647	NAG	O4-C4-C5	3.16	117.25	109.28
7	G	1648	BMA	C3-C4-C5	3.20	115.85	110.22
6	A	1647	NAG	C1-O5-C5	3.24	116.63	112.17
6	F	2643	NAG	C1-O5-C5	3.48	116.97	112.17
6	K	1744	NAG	C4-C3-C2	3.67	116.40	111.02
7	F	2645	BMA	C1-C2-C3	3.77	114.44	109.65
8	K	1746	MAN	C3-C4-C5	3.77	116.87	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	H	2644	MAN	C1-C2-C3	3.80	114.46	109.65
5	K	1749	NDG	C1-C2-N2	3.83	117.04	110.49
6	B	2643	NAG	O5-C1-C2	4.17	117.27	111.47
7	B	2644	BMA	C1-C2-C3	4.32	115.13	109.65
6	A	1647	NAG	C4-C3-C2	4.96	118.29	111.02
6	G	1647	NAG	C1-O5-C5	5.87	120.26	112.17
7	G	1649	BMA	O3-C3-C4	6.52	124.55	110.36
6	B	2643	NAG	C1-O5-C5	6.98	121.79	112.17

All (19) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	D	2642	NDG	C1
8	J	1745	MAN	C1
5	L	1746	NDG	C1
5	B	2642	NDG	C1
5	I	1743	NDG	C1
5	K	1743	NDG	C1
5	H	2642	NDG	C1
8	K	1746	MAN	C1
8	I	1745	MAN	C1
5	L	1743	NDG	C1
5	J	1743	NDG	C1
5	C	1646	NDG	C1
5	E	1646	NDG	C1
8	H	2644	MAN	C1
8	K	1748	MAN	C1
8	K	1745	MAN	C1
8	H	2645	MAN	C1
5	I	1746	NDG	C1
5	G	1646	NDG	C1

There are no torsion outliers.

There are no ring outliers.

32 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1646	NDG	1	0
6	A	1647	NAG	1	0
5	B	2642	NDG	1	0
5	C	1646	NDG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	1647	NAG	1	0
5	D	2642	NDG	1	0
6	D	2643	NAG	1	0
5	E	1646	NDG	4	0
6	E	1647	NAG	1	0
7	E	1648	BMA	1	0
7	E	1649	BMA	1	0
7	F	2644	BMA	1	0
7	F	2645	BMA	2	0
7	F	2647	BMA	1	0
5	G	1646	NDG	2	0
6	G	1647	NAG	3	0
7	G	1648	BMA	2	0
7	G	1649	BMA	2	0
8	G	1651	MAN	1	0
6	H	2643	NAG	1	0
8	H	2644	MAN	1	0
8	H	2645	MAN	1	0
5	I	1743	NDG	2	0
6	I	1744	NAG	2	0
5	J	1743	NDG	1	0
6	J	1744	NAG	2	0
5	K	1743	NDG	4	0
6	K	1744	NAG	1	0
8	K	1745	MAN	2	0
8	K	1746	MAN	1	0
8	K	1748	MAN	1	0
5	K	1749	NDG	3	0

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
2	H	2

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	1500:LYS	C	1501:SER	N	3.64
1	H	988:CYS	C	989:GLY	N	2.97

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	638/645 (98%)	0.17	16 (2%) 58 47	87, 142, 190, 237	0
1	C	638/645 (98%)	0.11	13 (2%) 65 56	80, 127, 176, 228	0
1	E	638/645 (98%)	0.11	10 (1%) 72 63	84, 142, 196, 245	0
1	G	638/645 (98%)	0.43	60 (9%) 9 8	93, 180, 241, 267	0
2	B	901/915 (98%)	0.16	26 (2%) 52 42	91, 167, 229, 260	0
2	D	901/915 (98%)	0.17	29 (3%) 48 38	81, 155, 216, 266	0
2	F	900/915 (98%)	0.36	50 (5%) 25 20	96, 179, 284, 329	0
2	H	605/915 (66%)	0.38	37 (6%) 22 16	98, 162, 231, 294	0
3	I	507/507 (100%)	-0.03	2 (0%) 92 88	93, 142, 197, 240	0
3	J	507/507 (100%)	0.13	15 (2%) 51 40	127, 170, 220, 261	0
3	K	507/507 (100%)	0.20	22 (4%) 36 28	132, 183, 230, 284	0
3	L	507/507 (100%)	-0.05	5 (0%) 82 74	101, 144, 194, 239	0
4	M	84/92 (91%)	-0.07	1 (1%) 79 70	87, 110, 186, 221	0
4	N	84/92 (91%)	-0.05	2 (2%) 59 49	97, 116, 189, 227	0
4	P	84/92 (91%)	-0.03	2 (2%) 59 49	100, 124, 176, 211	0
4	Q	84/92 (91%)	-0.11	2 (2%) 59 49	100, 119, 186, 200	0
All	All	8223/8636 (95%)	0.18	292 (3%) 43 34	80, 155, 228, 329	0

All (292) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	645	ALA	9.1
1	G	421	ALA	6.8
2	F	1501	SER	5.7
2	F	1038	ARG	5.6
1	G	399	SER	5.6

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Mol	Chain	Res	Type	RSRZ
1	G	645	ALA	5.2
2	H	1501	SER	5.2
1	A	645	ALA	5.2
2	D	1603	ASP	4.7
2	F	1049	LYS	4.7
2	F	1122	THR	4.6
2	H	1328	ALA	4.6
1	G	398	LEU	4.5
1	G	626	SER	4.4
4	P	2	THR	4.4
1	G	636	ALA	4.4
2	H	967	GLN	4.3
3	L	708	GLN	4.3
2	F	1136	CYS	4.3
3	K	574	CYS	4.3
1	G	400	ILE	4.2
1	G	368	ALA	4.2
2	H	1593	LYS	4.0
2	F	1116	GLU	4.0
2	B	1099	ASP	4.0
1	A	48	SER	4.0
3	K	699	VAL	3.9
1	C	48	SER	3.9
1	G	333	ILE	3.9
1	G	373	ASP	3.9
1	G	420	GLN	3.8
4	N	85	TYR	3.8
2	H	964	PRO	3.7
3	J	703	GLN	3.7
2	F	1329	LYS	3.7
1	G	71	ASN	3.6
2	F	1529	LYS	3.6
3	K	479	PRO	3.6
4	M	85	TYR	3.6
2	H	1316	GLY	3.5
2	F	1593	LYS	3.5
2	F	1328	ALA	3.5
2	H	947	ASP	3.5
2	F	1077	VAL	3.5
2	F	1327	HIS	3.4
2	F	1048	VAL	3.4
1	G	488	PRO	3.4

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Mol	Chain	Res	Type	RSRZ
2	H	935	VAL	3.4
1	C	376	GLN	3.4
2	H	1329	LYS	3.3
2	F	967	GLN	3.3
1	G	28	GLN	3.3
1	G	26	ASP	3.3
3	J	235	LYS	3.3
2	H	1561	THR	3.3
3	J	479	PRO	3.3
2	F	1073	ILE	3.3
1	G	1	SER	3.2
3	J	480	SER	3.2
2	D	1358	ALA	3.2
2	B	1504	LYS	3.2
3	K	668	ASN	3.2
2	F	1594	PRO	3.2
2	B	1622	LYS	3.2
1	G	370	GLN	3.2
2	D	1267	HIS	3.2
3	J	542	ALA	3.2
2	F	1047	PHE	3.2
2	H	1268	GLN	3.2
3	J	510	HIS	3.2
4	Q	2	THR	3.2
1	G	369	VAL	3.2
1	G	643	PRO	3.1
3	K	544	ILE	3.1
1	E	257	GLU	3.1
1	E	83	PHE	3.1
3	K	385	TYR	3.1
3	K	527	VAL	3.1
2	F	1079	CYS	3.1
2	H	1598	TYR	3.1
2	H	1559	GLN	3.1
1	G	644	ALA	3.0
2	H	1594	PRO	3.0
2	D	1269	GLU	3.0
2	H	1283	SER	3.0
1	E	71	ASN	3.0
1	G	609	SER	3.0
2	F	1074	ASP	3.0
1	G	32	PRO	3.0

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Mol	Chain	Res	Type	RSRZ
3	K	542	ALA	3.0
2	D	1293	SER	2.9
1	G	419	MET	2.9
1	G	335	PHE	2.9
2	B	1097	GLN	2.8
3	J	346	ASP	2.8
3	I	708	GLN	2.8
2	H	912	GLU	2.8
2	H	1546	THR	2.8
1	E	101	VAL	2.8
1	E	521	GLN	2.8
1	C	190	ASN	2.8
2	B	1611	GLU	2.8
1	G	100	LEU	2.8
1	G	528	SER	2.8
1	C	314	SER	2.8
2	F	1143	LEU	2.8
1	A	46	VAL	2.7
1	A	437	SER	2.7
2	D	1531	GLN	2.7
2	H	948	GLN	2.7
1	A	20	MET	2.7
1	G	518	ALA	2.7
1	A	100	LEU	2.7
2	D	1618	GLU	2.7
2	B	1180	LEU	2.7
1	G	519	SER	2.7
3	K	703	GLN	2.7
3	K	480	SER	2.6
2	F	1046	ALA	2.6
2	D	928	GLU	2.6
2	F	1181	LYS	2.6
3	J	544	ILE	2.6
4	P	85	TYR	2.6
3	J	699	VAL	2.6
1	G	352	VAL	2.6
1	G	374	THR	2.6
2	B	964	PRO	2.6
2	F	1166	THR	2.6
1	G	41	PRO	2.6
2	B	1623	GLN	2.6
2	F	1119	MET	2.6

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Mol	Chain	Res	Type	RSRZ
3	J	641	TYR	2.6
2	F	987	GLY	2.6
1	G	339	PRO	2.6
2	F	913	GLY	2.5
2	F	1194	ASP	2.5
2	B	1270	LEU	2.5
2	D	1504	LYS	2.5
1	G	20	MET	2.5
3	J	385	TYR	2.5
1	G	340	LYS	2.5
2	F	1094	GLY	2.5
2	F	1035	LEU	2.5
2	H	1502	ASP	2.5
2	H	1531	GLN	2.5
1	G	258	GLN	2.5
2	B	1618	GLU	2.4
2	D	1155	GLU	2.4
2	F	925	LEU	2.4
3	L	709	VAL	2.4
1	C	20	MET	2.4
2	H	1374	GLN	2.4
2	H	1523	TYR	2.4
2	D	1486	ASP	2.4
3	K	512	ILE	2.4
3	K	739	LEU	2.4
1	G	527	ASP	2.4
2	D	1539	TYR	2.4
1	A	101	VAL	2.4
2	D	1314	GLY	2.4
2	B	1621	GLN	2.4
2	H	1325	MET	2.4
2	D	1488	LEU	2.4
1	A	644	ALA	2.4
1	E	636	ALA	2.4
2	F	953	GLU	2.4
3	L	710	PRO	2.4
2	F	1294	ALA	2.4
1	C	450	ASN	2.4
2	F	1534	ASN	2.4
2	B	1488	LEU	2.4
1	G	491	ASP	2.4
1	A	22	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
3	K	640	GLY	2.3
3	K	697	VAL	2.3
2	H	1560	ARG	2.3
2	F	1078	LEU	2.3
2	F	820	ASN	2.3
2	D	1563	ILE	2.3
1	G	102	SER	2.3
3	J	354	ARG	2.3
1	C	644	ALA	2.3
3	K	510	HIS	2.3
3	K	706	GLN	2.3
1	G	637	GLU	2.3
2	H	1327	HIS	2.3
1	E	370	GLN	2.3
2	F	1374	GLN	2.3
2	B	1267	HIS	2.3
2	F	1039	GLN	2.3
1	C	315	ASP	2.3
1	G	72	ARG	2.3
1	G	433	TYR	2.3
3	K	543	GLY	2.3
2	H	921	ALA	2.3
2	B	1614	GLU	2.3
1	G	460	ALA	2.3
2	B	963	THR	2.3
2	F	1051	ALA	2.3
1	G	365	VAL	2.3
3	K	346	ASP	2.3
4	Q	85	TYR	2.3
2	F	1502	ASP	2.2
3	K	478	ARG	2.2
2	D	932	ARG	2.2
3	K	589	THR	2.2
2	F	1135	ILE	2.2
1	C	636	ALA	2.2
2	H	1293	SER	2.2
2	D	1158	TYR	2.2
2	H	1308	PHE	2.2
2	H	1292	GLU	2.2
1	G	99	VAL	2.2
1	G	608	GLY	2.2
1	E	441	THR	2.2

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Mol	Chain	Res	Type	RSRZ
2	F	1118	ASP	2.2
1	E	437	SER	2.2
1	G	564	GLU	2.2
2	B	912	GLU	2.2
1	G	94	VAL	2.2
1	G	256	GLY	2.2
1	G	411	GLU	2.2
2	D	1089	LYS	2.2
2	D	1538	GLU	2.2
1	A	257	GLU	2.2
2	H	916	MET	2.2
2	B	965	VAL	2.2
2	H	1547	ILE	2.2
2	B	1606	VAL	2.2
4	N	83	SER	2.2
2	B	763	GLY	2.1
3	K	545	PRO	2.1
2	B	1365	GLU	2.1
2	B	1539	TYR	2.1
2	D	1537	ASP	2.1
2	F	1093	ASP	2.1
2	F	1076	GLN	2.1
1	A	69	PRO	2.1
2	D	1332	ASP	2.1
1	C	368	ALA	2.1
1	G	98	VAL	2.1
1	E	1	SER	2.1
1	A	190	ASN	2.1
2	D	1534	ASN	2.1
3	L	345	ASP	2.1
2	H	1317	GLN	2.1
1	C	420	GLN	2.1
2	F	912	GLU	2.1
2	D	968	MET	2.1
2	D	1530	VAL	2.1
2	H	1310	VAL	2.1
1	A	389	ILE	2.1
2	F	1559	GLN	2.1
3	L	706	GLN	2.1
1	G	452	ASN	2.1
2	F	1157	ASN	2.1
1	A	421	ALA	2.1

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Mol	Chain	Res	Type	RSRZ
1	G	40	PHE	2.1
2	D	1621	GLN	2.1
2	F	1500	LYS	2.1
1	G	548	SER	2.1
2	B	1594	PRO	2.1
2	D	1184	LEU	2.1
2	H	1324	THR	2.1
1	G	523	GLU	2.1
2	B	1328	ALA	2.1
1	G	81	ASN	2.1
1	G	401	THR	2.1
3	J	343	TRP	2.1
2	H	1540	ILE	2.1
1	A	450	ASN	2.1
1	A	452	ASN	2.1
1	G	50	GLU	2.1
2	D	1510	ARG	2.0
3	K	705	ARG	2.0
1	G	254	GLN	2.0
1	G	27	ALA	2.0
2	F	916	MET	2.0
3	J	389	ASP	2.0
2	F	1034	GLN	2.0
2	H	1562	PHE	2.0
2	F	1514	ALA	2.0
1	G	630	GLN	2.0
3	I	703	GLN	2.0
2	B	1295	SER	2.0
2	B	1269	GLU	2.0
2	H	1269	GLU	2.0
2	D	819	ARG	2.0
2	D	1183	PRO	2.0
2	B	962	GLY	2.0
3	J	350	GLU	2.0
1	C	419	MET	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
5	NDG	L	1743	14/15	0.87	0.36	1.80	122,147,148,148	0
5	NDG	K	1743	14/15	0.87	0.28	0.75	174,204,206,207	0
5	NDG	I	1743	14/15	0.92	0.28	0.68	122,149,151,152	0
9	MG	L	1742	1/1	0.91	0.25	0.53	127,127,127,127	0
5	NDG	J	1743	14/15	0.90	0.27	0.33	158,188,189,189	0
9	MG	I	1742	1/1	0.42	0.17	-0.61	120,120,120,120	0
5	NDG	C	1646	14/15	0.82	0.28	-0.76	163,191,192,193	0
9	MG	K	1742	1/1	0.84	0.11	-0.92	138,138,138,138	0
5	NDG	E	1646	14/15	0.83	0.23	-0.92	174,204,206,206	0
5	NDG	F	2642	14/15	0.86	0.22	-1.27	169,193,194,194	0
9	MG	J	1742	1/1	0.82	0.07	-2.08	148,148,148,148	0
5	NDG	A	1646	14/15	0.88	0.21	-2.67	156,185,187,188	0
7	BMA	E	1648	11/12	0.74	0.43	-	229,230,231,232	0
7	BMA	F	2644	11/12	0.84	0.15	-	232,233,234,234	0
6	NAG	A	1647	14/15	0.82	0.23	-	199,200,201,203	0
8	MAN	G	1651	11/12	0.45	0.54	-	222,225,227,228	0
6	NAG	D	2643	14/15	0.88	0.21	-	200,201,202,203	0
7	BMA	A	1648	11/12	0.80	0.30	-	212,214,215,216	0
6	NAG	K	1744	14/15	0.83	0.27	-	196,199,201,202	0
7	BMA	B	2646	11/12	0.66	0.51	-	198,200,200,201	0
5	NDG	B	2642	14/15	0.91	0.23	-	163,194,194,195	0
6	NAG	J	1744	14/15	0.81	0.33	-	177,179,180,180	0
7	BMA	F	2646	11/12	0.72	0.37	-	221,222,224,224	0
8	MAN	J	1745	11/12	0.61	0.36	-	206,210,211,212	0
7	BMA	F	2647	11/12	0.70	0.50	-	214,215,217,217	0
7	BMA	L	1745	11/12	0.76	0.24	-	197,201,202,202	0
5	NDG	H	2642	14/15	0.90	0.21	-	183,213,214,215	0
8	MAN	K	1746	11/12	0.87	0.52	-	229,230,232,232	0
7	BMA	C	1648	11/12	0.64	0.27	-	219,220,222,223	0
8	MAN	I	1745	11/12	0.79	0.24	-	205,207,208,209	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
7	BMA	G	1648	11/12	0.68	0.54	-	247,249,250,251	0
5	NDG	K	1749	14/15	0.76	0.47	-	184,214,216,217	0
5	NDG	D	2642	14/15	0.89	0.20	-	147,176,178,179	0
7	BMA	F	2645	11/12	0.83	0.23	-	248,249,249,250	0
6	NAG	I	1744	14/15	0.94	0.36	-	178,180,181,182	0
7	BMA	C	1650	11/12	0.70	0.33	-	231,233,235,235	0
7	BMA	K	1747	11/12	0.76	0.52	-	194,195,196,196	0
5	NDG	L	1746	14/15	0.87	0.56	-	176,204,205,205	0
6	NAG	E	1647	14/15	0.83	0.21	-	223,225,227,227	0
6	NAG	C	1647	14/15	0.67	0.27	-	200,202,203,203	0
6	NAG	G	1647	14/15	0.83	0.25	-	213,216,216,217	0
6	NAG	I	1747	14/15	0.63	0.66	-	222,223,224,224	0
7	BMA	D	2645	11/12	0.86	0.28	-	229,232,233,234	0
7	BMA	G	1650	11/12	0.55	0.68	-	229,231,232,232	0
8	MAN	H	2644	11/12	0.64	0.27	-	229,230,231,232	0
7	BMA	B	2645	11/12	0.41	0.37	-	237,239,240,241	0
6	NAG	B	2643	14/15	0.91	0.28	-	193,196,196,197	0
6	NAG	L	1744	14/15	0.85	0.43	-	185,187,189,189	0
6	NAG	F	2643	14/15	0.91	0.21	-	200,202,204,204	0
7	BMA	A	1649	11/12	0.83	0.44	-	226,227,228,228	0
7	BMA	D	2644	11/12	0.67	0.32	-	220,221,223,223	0
7	BMA	G	1649	11/12	0.59	0.37	-	226,228,229,230	0
7	BMA	E	1649	11/12	0.81	0.27	-	209,212,214,215	0
7	BMA	C	1649	11/12	0.65	0.29	-	235,237,239,240	0
8	MAN	K	1748	11/12	0.84	0.36	-	230,232,235,235	0
6	NAG	H	2643	14/15	0.82	0.26	-	221,222,224,225	0
8	MAN	K	1745	11/12	0.73	0.34	-	249,252,253,254	0
7	BMA	B	2644	11/12	0.39	0.35	-	218,220,222,223	0
8	MAN	H	2645	11/12	0.68	0.61	-	234,236,237,238	0
5	NDG	I	1746	14/15	0.79	0.65	-	198,225,227,227	0
5	NDG	G	1646	14/15	0.90	0.16	-	198,201,208,215	0

6.5 Other polymers

There are no such residues in this entry.