



Full wwPDB X-ray Structure Validation Report ⓘ

May 31, 2020 – 05:06 am BST

PDB ID : 4YFN
Title : Escherichia coli RNA polymerase in complex with squaramide compound 14 (N-[3,4-dioxo-2-(4-{[4-(trifluoromethyl)benzyl]amino}piperidin-1-yl)cyclobut-1-en-1-yl]-3,5-dimethyl-1,2-oxazole-4-sulfonamide)
Authors : Molodtsov, V.; Fleming, P.R.; Eyermann, C.J.; Ferguson, A.D.; Foulk, M.A.; McKinney, D.C.; Masse, C.E.; Buurman, E.T.; Murakami, K.S.
Deposited on : 2015-02-25
Resolution : 3.82 Å(reported)

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

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

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

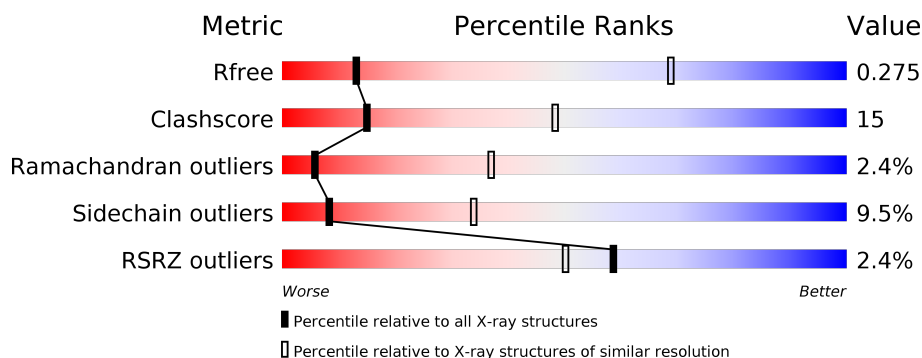
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.82 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}	130704	1231 (4.04-3.60)
Clashscore	141614	1031 (4.02-3.62)
Ramachandran outliers	138981	1261 (4.04-3.60)
Sidechain outliers	138945	1255 (4.04-3.60)
RSRZ outliers	127900	1139 (4.04-3.60)

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 respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	329	<div> <div>43%</div> <div>23%</div> <div>5%</div> <div>29%</div> </div>
1	B	329	<div> <div>47%</div> <div>35%</div> <div>5%</div> <div>12%</div> </div>
1	G	329	<div> <div>41%</div> <div>26%</div> <div>•</div> <div>31%</div> </div>
1	H	329	<div> <div>4%</div> <div>36%</div> <div>27%</div> <div>•</div> <div>34%</div> </div>
2	C	1342	<div> <div>64%</div> <div>31%</div> <div>•</div> </div>
2	I	1342	<div> <div>2%</div> <div>65%</div> <div>30%</div> <div>•</div> </div>

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Mol	Chain	Length	Quality of chain
3	D	1407	<div><div>%</div><div><div></div><div>49%</div><div>28%</div><div>5%</div><div>17%</div></div></div>
3	J	1407	<div><div>2%</div><div><div></div><div>49%</div><div>28%</div><div>5%</div><div>18%</div></div></div>
4	E	91	<div><div></div><div><div>78%</div><div>15%</div><div></div><div></div></div></div>
4	K	91	<div><div>23%</div><div><div></div><div>53%</div><div>31%</div><div></div><div>13%</div></div></div>
5	F	613	<div><div>4%</div><div><div></div><div>51%</div><div>23%</div><div></div><div>24%</div></div></div>
5	L	613	<div><div>4%</div><div><div></div><div>53%</div><div>20%</div><div></div><div>23%</div></div></div>

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 55638 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 DNA-directed RNA polymerase subunit alpha.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	235	Total	C	N	O	S	0	0	0
			1820	1132	323	358	7			
1	B	289	Total	C	N	O	S	0	0	0
			2234	1400	393	433	8			
1	G	227	Total	C	N	O	S	0	0	0
			1755	1093	311	345	6			
1	H	216	Total	C	N	O	S	0	0	0
			1662	1038	292	326	6			

- Molecule 2 is a protein called DNA-directed RNA polymerase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	1340	Total	C	N	O	S	0	0	0
			10570	6631	1841	2055	43			
2	I	1340	Total	C	N	O	S	0	0	0
			10560	6626	1837	2054	43			

- Molecule 3 is a protein called DNA-directed RNA polymerase subunit beta'.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1163	Total	C	N	O	S	0	0	0
			9029	5678	1613	1692	46			
3	J	1152	Total	C	N	O	S	0	0	0
			8980	5648	1605	1681	46			

- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	E	89	Total	C	N	O	S	0	0	0
			691	421	129	140	1			
4	K	79	Total	C	N	O	S	0	0	0
			627	382	118	126	1			

- Molecule 5 is a protein called RNA polymerase sigma factor RpoD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	F	468	Total	C	N	O	S	0	0	0
			3813	2389	678	723	23			
5	L	469	Total	C	N	O	S	0	0	0
			3821	2393	679	726	23			

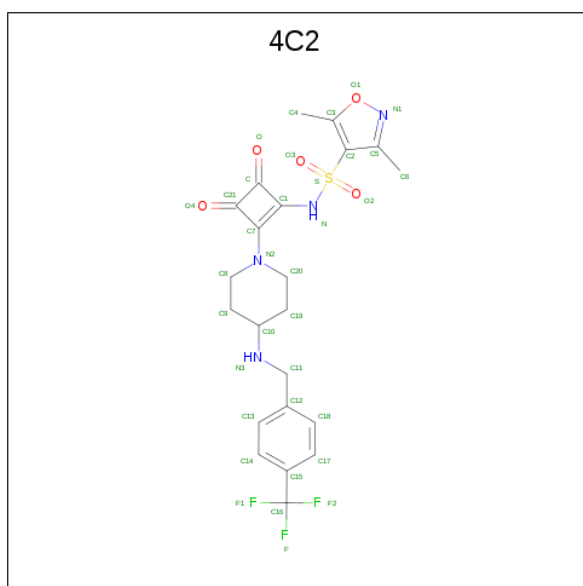
- Molecule 6 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	J	1	Total	Mg	0	0
			1	1		
6	D	1	Total	Mg	0	0
			1	1		

- Molecule 7 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	J	2	Total	Zn	0	0
			2	2		
7	D	2	Total	Zn	0	0
			2	2		

- Molecule 8 is N-[3,4-dioxo-2-(4-{[4-(trifluoromethyl)benzyl]amino}piperidin-1-yl)cyclobut-1-en-1-yl]-3,5-dimethyl-1,2-oxazole-4-sulfonamide (three-letter code: 4C2) (formula: C₂₂H₂₃F₃N₄O₅S).

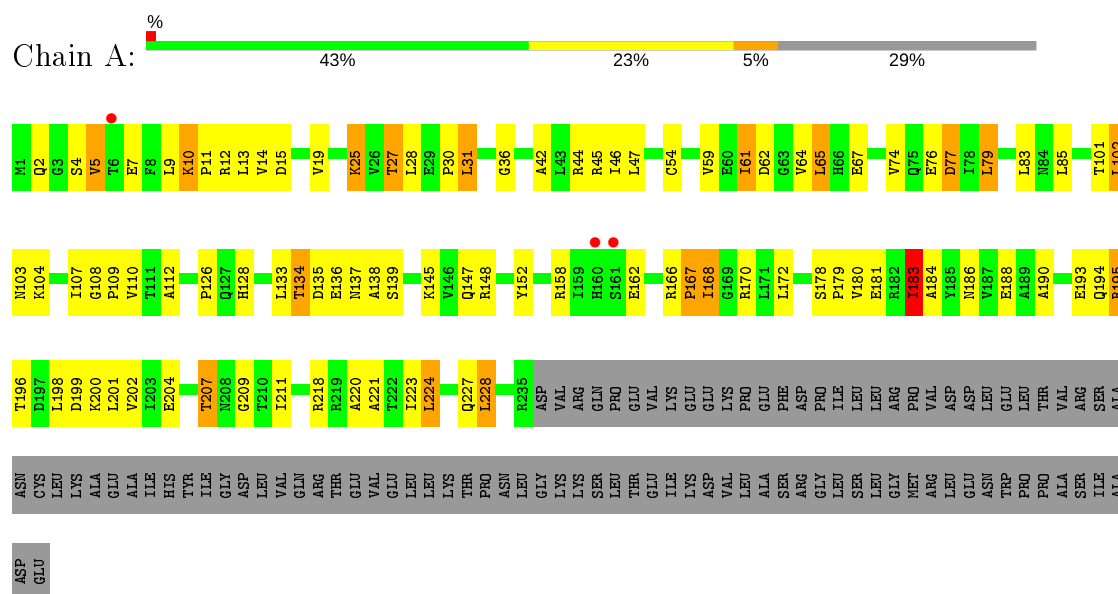


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	D	1	Total	C	F	N	O	S	0	0
			35	22	3	4	5	1		
8	J	1	Total	C	F	N	O	S	0	0
			35	22	3	4	5	1		

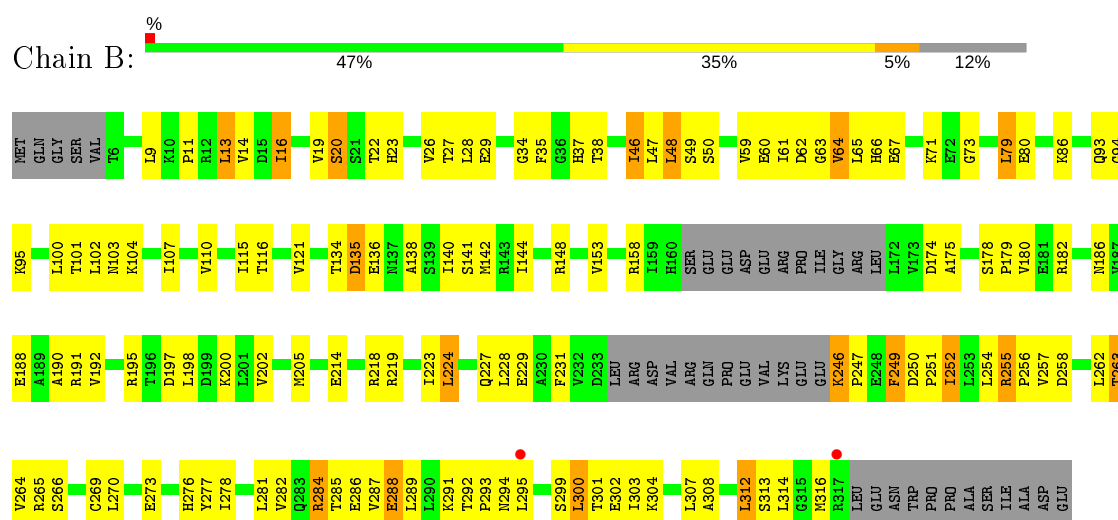
3 Residue-property plots

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: DNA-directed RNA polymerase subunit alpha

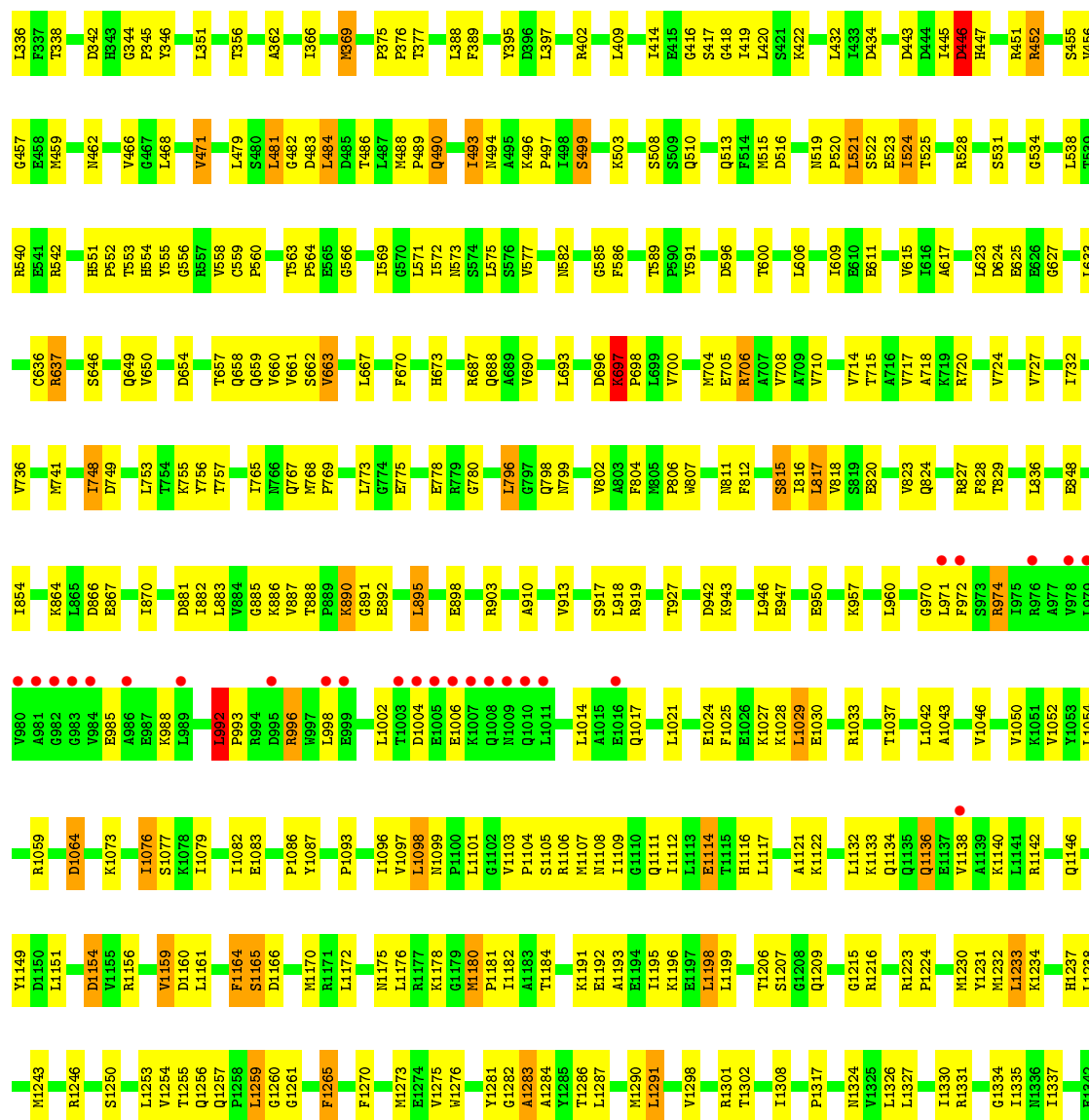


• Molecule 1: DNA-directed RNA polymerase subunit alpha

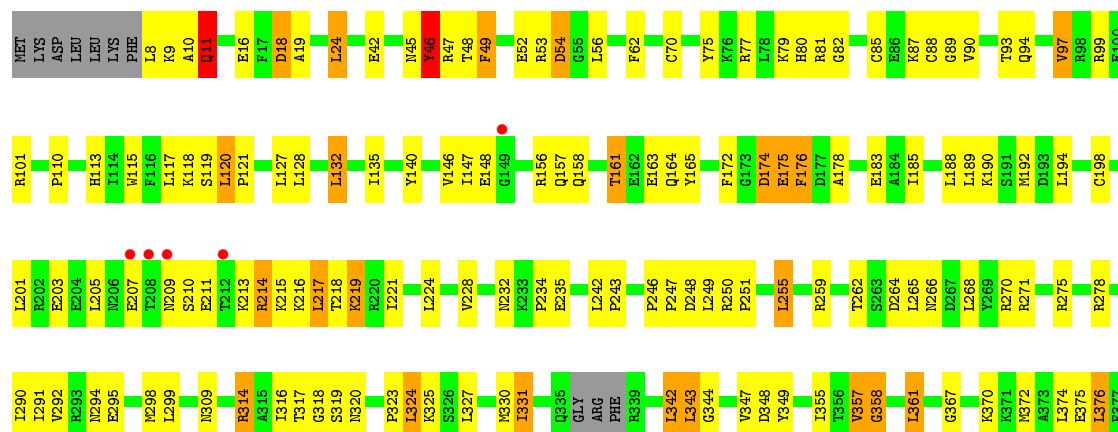


• Molecule 1: DNA-directed RNA polymerase subunit alpha





• Molecule 3: DNA-directed RNA polymerase subunit beta'

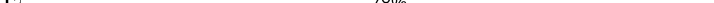


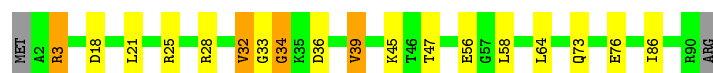


E91	E92	T93	Q94		V97	R98		R101		W115	F116	L117	K118	S119	L120	R123	I124	L132	R133	D134	L135	E136	V137	V138	V146	I147	E148	L154	E155	R156	L160	E162	E163	Q164	Y165		L169	F172	G173	D174	E175	F176	Q186	L188	L189		D193	Q196	E197										
MET	LYS	ASP	LEU	LEU	LYS	PHE	LEU	LYS	ALA	GLN	THR	LYS	THR	GLU	E16	F17	D18		L24	A25	S26		E42	T43	T44	N45	Y46	R47	T48	F49		E52	R53	D54	G55	L56	F57		F62		K66		B69	C70	L71		R77	L78	K79	H80	R81	G82		C85	E86	K87	C88	G89	T90

VAL	S1303	V1226	L1138	LEU	ALA	ILE	Y886	A804	T703	Y880	I394	P288	C198
THR	R1304	I1233	P1139	LYS	ASN	LYS	S887	Q805	E704	M881	K399	D289	L201
ALA	D1305	I1233	R1140	ILE	TRP	LEU	C888	D806	G496	G496	M400	E291	L202
GLU	L1306	I1233	V1141	VAL	ASP	SER	D889	T810	V706	K385	E497	E291	E203
ASP	L1307	E1237	A1142	ASP	PRO	ASN	F892	E811	I707	G586	E405	E295	E204
ALA	G1308	V1236	B1149	GLN	HIS	VAL	C893	E811	R709	Y889	E406	E295	L205
SER	L1309	Q1238	P1150	GLY	THR	LYS	C894	E811	D710	V592	V407	E207	E207
ALA	T1310	R1242	F1151	ASN	PRO	VAL	C895	E811	Q712	V502	V408	E207	E207
SER	K1311	R1242	P1151	ASP	MET	VAL	C895	E811	Q712	V502	V408	E207	E207
LEU	L1314	I1248	E1152	VAL	ILE	ASN	Y899	H817	Q716	D505	L411	E207	E207
ALA	A1315	I1248	P1153	THR	THR	SER	G900	G819	Q716	D505	L411	E207	E207
LEU	T1316	H1251	A1154	GLU	ILE	SER	R901	G819	Q716	D505	L411	E207	E207
LEU	E1317	H1252	I1155	VAL	GLU	SER	D902	G819	Q716	D505	L411	E207	E207
ASN	S1318	I1253	V1163	PRO	VAL	GLY	L903	G819	Q716	D505	L411	E207	E207
ASN	S1324	E1255	K1167	ASP	PHE	GLY	R905	G819	Q716	D505	L411	E207	E207
GLY	F1325	V1255	E1168	THR	VAL	ILE	I908	G819	Q716	D505	L411	E207	E207
GLY	Q1326	V1257	T1169	MET	ARG	THR	I909	G819	Q716	D505	L411	E207	E207
GLY	E1327	R1258	K1170	PRO	ARG	THR	I909	G819	Q716	D505	L411	E207	E207
ASP	T1329	Q1259	R1173	ALA	PHE	SER	I909	G819	Q716	D505	L411	E207	E207
ASN	T1329	M1260	R1174	GLN	THR	ARG	I909	G819	Q716	D505	L411	E207	E207
GLU	L1332	L1261	R1175	LEU	THR	ARG	I909	G819	Q716	D505	L411	E207	E207
	T1333	K1262	L1175	LEU	THR	ARG	I909	G819	Q716	D505	L411	E207	E207
	E1334	A1264	V1176	PRO	ASP	GLY	I909	G819	Q716	D505	L411	E207	E207
	V1337	I1265	T1177	LYS	GLY	GLN	I909	G819	Q716	D505	L411	E207	E207
	E1343	I1266	D1181	ILE	THR	ILE	I909	G819	Q716	D505	L411	E207	E207
	L1344	V1267	D1184	VAL	THR	GLU	I909	G819	Q716	D505	L411	E207	E207
	K1348	N1268	P1185	GLN	ARG	PHE	I909	G819	Q716	D505	L411	E207	E207
	E1349	G1270	P1186	LEU	GLN	GLY	I909	G819	Q716	D505	L411	E207	E207
	N1350	D1273	E1187	ASP	ASP	THR	I909	G819	Q716	D505	L411	E207	E207
	V1351	F1274	E1188	GLY	GLY	LYS	I909	G819	Q716	D505	L411	E207	E207
	I1352	L1275	E1188	VAL	VAL	GLU	I909	G819	Q716	D505	L411	E207	E207
	I1357	E1277	K1192	GLN	THR	THR	I909	G819	Q716	D505	L411	E207	E207
	P1358	V1280	V1193	ILE	GLY	THR	I909	G819	Q716	D505	L411	E207	E207
	A1359	E1281	R1194	SER	SER	LYS	I909	G819	Q716	D505	L411	E207	E207
	G1360	Y1282	H1197	GLY	SER	VAL	I909	G819	Q716	D505	L411	E207	E207
	T1361	S1283	V1198	THR	LEU	THR	I909	G819	Q716	D505	L411	E207	E207
	Y1365	R1284	F1199	LEU	VAL	GLY	I909	G819	Q716	D505	L411	E207	E207
	H1366	V1285	E1200	ALA	VAL	ALA	I909	G819	Q716	D505	L411	E207	E207
	R1369	K1286	G1202	ALA	LEU	VAL	I909	G819	Q716	D505	L411	E207	E207
		N1289	E1203	ARG	ASP	THR	I909	G819	Q716	D505	L411	E207	E207
		R1290	V1204	PRO	GLU	GLY	I909	G819	Q716	D505	L411	E207	E207
		E1291	D1208	GLN	GLU	GLY	I909	G819	Q716	D505	L411	E207	E207
		L1292	V1209	SER	THR	THR	I909	G819	Q716	D505	L411	E207	E207
		A1294	I1210	GLY	ALA	GLY	I909	G819	Q716	D505	L411	E207	E207
		K1297	E1215	THR	GLY	VAL	I909	G819	Q716	D505	L411	E207	E207
		G1298	A1216	LYS	LYS	ALA	I909	G819	Q716	D505	L411	E207	E207
		H1299	D1219	ASP	ASP	GLY	I909	G819	Q716	D505	L411	E207	E207
		A1300	I1221	ILE	LEU	GLY	I909	G819	Q716	D505	L411	E207	E207
		T1301	L1221	THR	ARG	THR	I909	G819	Q716	D505	L411	E207	E207
		Y1302		ALA	ALA	VAL	I909	G819	Q716	D505	L411	E207	E207

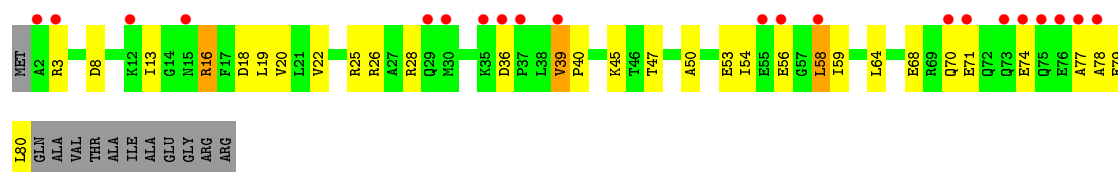
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E:  78% 15% . .



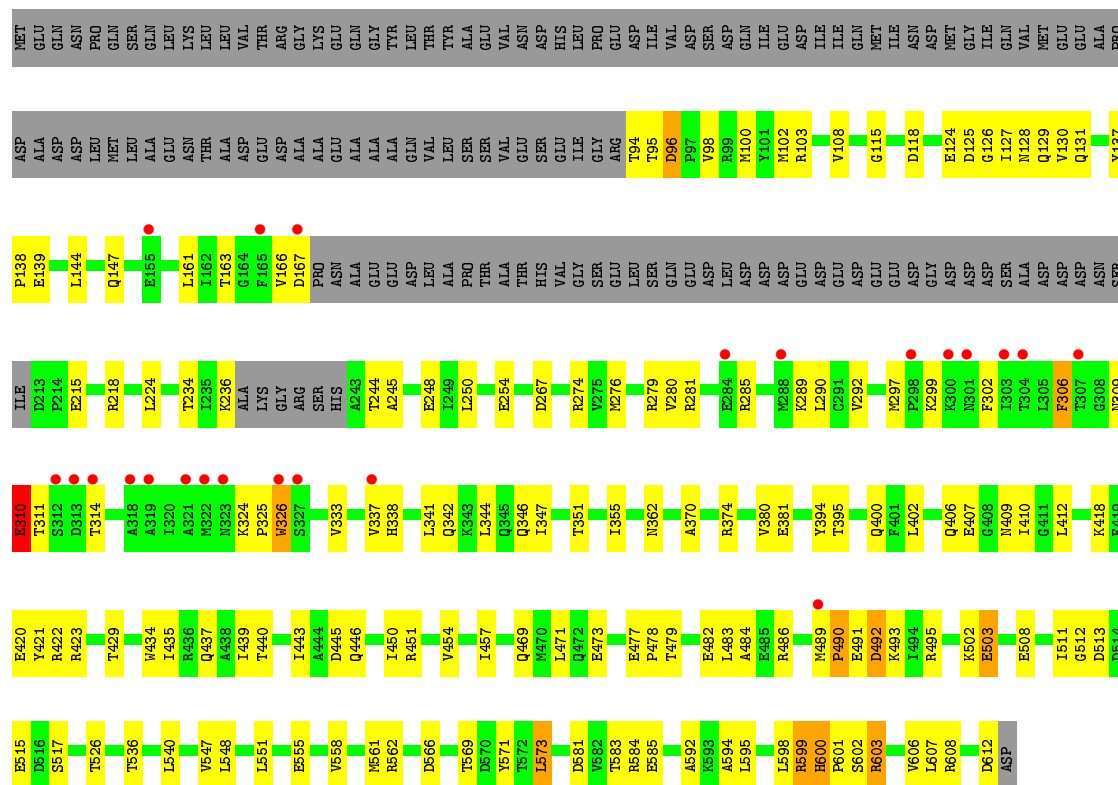
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain K: 



- Molecule 5: RNA polymerase sigma factor RpoD

Chain F: 



- Molecule 5: RNA polymerase sigma factor RpoD

Chain L: 





4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	191.25Å 206.57Å 312.15Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.96 – 3.82 30.16 – 3.82	Depositor EDS
% Data completeness (in resolution range)	88.9 (29.96-3.82) 77.9 (30.16-3.82)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.43 (at 3.86Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.222 , 0.270 0.226 , 0.275	Depositor DCC
R_{free} test set	2003 reflections (1.87%)	wwPDB-VP
Wilson B-factor (Å ²)	136.8	Xtriage
Anisotropy	0.348	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 114.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	55638	wwPDB-VP
Average B, all atoms (Å ²)	188.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.83% 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: ZN, 4C2, MG

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	0.77	0/1842	0.98	5/2495 (0.2%)
1	B	0.82	2/2260 (0.1%)	0.87	0/3059
1	G	0.82	0/1777	0.89	1/2408 (0.0%)
1	H	1.03	1/1681 (0.1%)	0.97	2/2278 (0.1%)
2	C	0.83	5/10739 (0.0%)	0.90	3/14489 (0.0%)
2	I	0.76	1/10729 (0.0%)	0.86	10/14477 (0.1%)
3	D	0.86	1/9167 (0.0%)	0.92	10/12380 (0.1%)
3	J	0.79	0/9118	0.89	9/12312 (0.1%)
4	E	0.76	0/693	0.78	0/935
4	K	1.14	0/629	0.96	3/847 (0.4%)
5	F	0.90	2/3864 (0.1%)	0.86	0/5194
5	L	0.89	3/3872 (0.1%)	0.84	0/5205
All	All	0.83	15/56371 (0.0%)	0.89	43/76079 (0.1%)

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	291	CYS	CB-SG	10.11	1.99	1.82
3	D	454	CYS	CB-SG	-7.01	1.70	1.82
5	L	315	TRP	CB-CG	6.64	1.62	1.50
5	F	326	TRP	CB-CG	6.03	1.61	1.50
5	F	337	VAL	CA-CB	6.00	1.67	1.54
1	B	67	GLU	CG-CD	5.95	1.60	1.51
2	C	90	VAL	CA-CB	-5.95	1.42	1.54
1	H	111	THR	CA-CB	5.66	1.68	1.53
2	C	700	VAL	CA-CB	-5.47	1.43	1.54
2	C	663	VAL	CA-CB	-5.12	1.44	1.54
5	L	326	TRP	CB-CG	5.11	1.59	1.50
1	B	67	GLU	CB-CG	5.08	1.61	1.52
2	I	1064	ASP	CB-CG	5.07	1.62	1.51
2	C	764	CYS	CB-SG	-5.03	1.73	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	745	GLU	CB-CG	5.02	1.61	1.52

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	849	LEU	CA-CB-CG	9.21	136.48	115.30
3	D	426	ALA	C-N-CD	7.92	145.02	128.40
2	I	521	LEU	CA-CB-CG	7.53	132.62	115.30
1	H	54	CYS	CA-CB-SG	7.17	126.91	114.00
3	D	376	LEU	CA-CB-CG	-6.83	99.59	115.30
2	I	1259	LEU	CB-CG-CD2	-6.47	100.00	111.00
3	J	1332	LEU	CB-CG-CD1	-6.24	100.39	111.00
3	D	361	LEU	CB-CG-CD2	-6.10	100.63	111.00
3	D	449	LEU	CB-CG-CD2	-6.04	100.73	111.00
2	C	482	GLY	N-CA-C	5.97	128.02	113.10
2	I	1064	ASP	CB-CG-OD1	5.97	123.67	118.30
1	H	131	CYS	CA-CB-SG	5.96	124.73	114.00
2	I	397	LEU	CB-CG-CD1	-5.83	101.10	111.00
2	I	1291	LEU	CA-CB-CG	5.78	128.59	115.30
2	I	817	LEU	CA-CB-CG	5.77	128.58	115.30
1	A	183	ILE	CG1-CB-CG2	-5.70	98.87	111.40
3	D	1332	LEU	CB-CG-CD1	-5.66	101.38	111.00
1	A	65	LEU	CA-CB-CG	5.58	128.13	115.30
2	C	680	LEU	CB-CG-CD1	-5.57	101.53	111.00
4	K	58	LEU	CA-CB-CG	5.53	128.01	115.30
1	A	102	LEU	CA-CB-CG	5.43	127.78	115.30
3	J	745	GLY	N-CA-C	5.36	126.50	113.10
3	J	814	CYS	CA-CB-SG	5.35	123.62	114.00
2	I	992	LEU	CA-CB-CG	5.33	127.56	115.30
3	J	426	ALA	C-N-CD	5.30	139.52	128.40
3	D	888	CYS	CA-CB-SG	-5.25	104.55	114.00
2	I	481	LEU	CA-CB-CG	5.23	127.33	115.30
3	J	306	LEU	CA-CB-CG	5.22	127.31	115.30
1	A	54	CYS	CA-CB-SG	-5.21	104.62	114.00
3	J	888	CYS	CA-CB-SG	-5.19	104.66	114.00
3	J	579	LEU	CA-CB-CG	5.18	127.22	115.30
4	K	16	ARG	NE-CZ-NH1	5.15	122.87	120.30
3	J	120	LEU	C-N-CD	5.13	139.17	128.40
2	I	484	LEU	CA-CB-CG	5.11	127.05	115.30
4	K	80	LEU	CA-CB-CG	5.10	127.03	115.30
3	D	903	LEU	N-CA-C	-5.10	97.23	111.00
2	I	996	ARG	NE-CZ-NH1	5.08	122.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	746	LEU	CB-CG-CD1	-5.07	102.39	111.00
1	G	65	LEU	CB-CG-CD2	5.06	119.60	111.00
2	C	794	LEU	CB-CG-CD2	-5.05	102.42	111.00
1	A	228	LEU	CB-CG-CD2	-5.00	102.49	111.00
3	D	217	LEU	CA-CB-CG	5.00	126.80	115.30
3	D	327	LEU	CB-CG-CD2	-5.00	102.50	111.00

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	1820	0	1850	62	0
1	B	2234	0	2291	90	0
1	G	1755	0	1773	63	0
1	H	1662	0	1687	81	0
2	C	10570	0	10582	318	0
2	I	10560	0	10565	296	0
3	D	9029	0	9175	334	0
3	J	8980	0	9148	338	0
4	E	691	0	695	7	0
4	K	627	0	634	20	0
5	F	3813	0	3880	101	0
5	L	3821	0	3884	92	0
6	D	1	0	0	0	0
6	J	1	0	0	0	0
7	D	2	0	0	0	0
7	J	2	0	0	0	0
8	D	35	0	23	1	0
8	J	35	0	23	2	0
All	All	55638	0	56210	1683	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 15.

All (1683) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:ARG:HG3	1:B:255:ARG:HH11	1.24	1.03
3:J:1215:GLU:HG3	3:J:1220:ILE:HD11	1.39	1.01
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.46	0.94
2:C:1160:ASP:HB2	2:C:1161:LEU:HA	1.48	0.93
1:G:195:ARG:HG2	1:G:198:LEU:HG	1.53	0.91
2:I:1160:ASP:HB2	2:I:1161:LEU:HA	1.52	0.91
1:A:11:PRO:HA	1:A:30:PRO:HG2	1.53	0.91
1:G:45:ARG:HG2	1:H:38:THR:HB	1.50	0.91
3:D:1176:VAL:HG22	3:D:1187:GLU:HB3	1.50	0.90
1:H:48:LEU:HD21	3:J:535:ARG:HG3	1.53	0.90
3:D:849:LEU:HG	3:D:853:THR:HG23	1.51	0.90
3:J:479:GLU:OE1	3:J:1361:THR:OG1	1.91	0.89
2:C:796:LEU:H	2:C:796:LEU:HD12	1.37	0.89
1:B:301:THR:HA	1:B:304:LYS:HE2	1.53	0.88
3:D:1227:HIS:HB2	3:J:1293:GLU:HG2	1.55	0.87
3:J:514:THR:HG21	3:J:596:LEU:HD23	1.57	0.87
2:C:255:ILE:HG23	2:C:285:ILE:HD13	1.56	0.86
3:J:450:HIS:HE1	3:J:452:LEU:HD12	1.41	0.85
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.41	0.85
3:D:515:ARG:NH2	3:D:717:VAL:O	2.10	0.85
5:L:551:LEU:HD11	5:L:598:LEU:HD21	1.58	0.84
3:D:77:ARG:HG3	3:D:79:LYS:H	1.40	0.84
2:C:292:ILE:HG23	2:C:295:LYS:HB2	1.60	0.84
2:C:1073:LYS:HE3	3:D:462:ASP:HB2	1.60	0.83
2:C:757:THR:HG23	2:C:765:ILE:HG23	1.60	0.83
3:J:513:MET:HE1	3:J:579:LEU:HD13	1.59	0.83
1:H:195:ARG:HB3	1:H:198:LEU:HD21	1.60	0.83
4:E:39:VAL:HG21	4:E:56:GLU:HG3	1.61	0.82
3:J:1280:VAL:HG11	3:J:1304:ARG:HE	1.44	0.82
3:J:814:CYS:SG	3:J:889:ASP:HB3	2.19	0.82
3:J:857:LEU:HD13	3:J:872:LEU:HD21	1.62	0.81
1:B:255:ARG:HH11	1:B:255:ARG:CG	1.94	0.80
3:D:425:ARG:NH1	3:D:464:ASP:OD1	2.15	0.80
3:D:552:ILE:HD11	3:D:570:LYS:HG3	1.63	0.80
1:B:86:LYS:HD3	1:B:174:ASP:HB2	1.62	0.80
3:D:147:ILE:HG22	3:D:188:LEU:HG	1.63	0.80
2:C:582:ASN:HB3	2:C:586:PHE:H	1.47	0.80
2:I:806:PRO:HB3	3:J:505:ASP:OD1	1.82	0.80
2:I:1142:ARG:HH22	2:I:1165:SER:HB2	1.46	0.80
2:I:957:LYS:HG3	2:I:1029:LEU:HD11	1.61	0.79
3:D:1282:TYR:HD2	3:D:1286:LYS:HZ2	1.29	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1344:LEU:HB3	3:J:1350:ASN:HD21	1.48	0.79
2:C:1160:ASP:CB	2:C:1161:LEU:HA	2.12	0.79
2:C:818:VAL:HG22	2:C:1096:ILE:HG12	1.65	0.79
2:C:839:VAL:HG12	2:C:1049:ILE:HG12	1.64	0.79
2:C:1283:ALA:HB1	2:C:1286:THR:HB	1.65	0.79
2:C:976:ARG:HD2	2:C:989:LEU:HD23	1.64	0.78
2:I:700:VAL:HG11	2:I:1114:GLU:HG2	1.65	0.78
1:G:228:LEU:HD21	1:H:224:LEU:HB3	1.66	0.78
2:C:696:ASP:O	2:C:697:LYS:HB3	1.84	0.78
1:H:185:TYR:HB2	1:H:201:LEU:HD11	1.66	0.78
3:J:1167:LYS:HD3	3:J:1174:ARG:HD2	1.65	0.78
5:L:98:VAL:HB	5:L:402:LEU:HD11	1.66	0.77
3:D:797:THR:HG23	3:D:924:GLY:HA3	1.67	0.77
1:B:27:THR:HG22	1:B:202:VAL:HG22	1.65	0.77
3:D:189:LEU:HB3	3:D:234:PRO:HB2	1.66	0.77
2:C:703:GLY:N	2:C:705:GLU:OE2	2.17	0.76
2:I:732:ILE:HD11	2:I:769:PRO:HB3	1.68	0.76
2:I:815:SER:HG	3:J:461:PHE:HD1	1.31	0.76
2:I:1142:ARG:HH12	2:I:1165:SER:HA	1.50	0.76
2:C:1297:ASP:OD1	2:C:1300:GLY:N	2.17	0.76
3:D:93:THR:HG22	3:D:94:GLN:H	1.51	0.76
2:I:1103:VAL:HG11	2:I:1112:ILE:HD11	1.68	0.76
5:L:454:VAL:HA	5:L:457:ILE:HD12	1.68	0.76
3:J:826:ILE:HA	3:J:831:VAL:HA	1.68	0.75
2:C:132:ASP:OD1	2:C:132:ASP:N	2.20	0.75
3:D:514:THR:O	3:D:514:THR:OG1	2.02	0.74
5:L:484:ALA:HB1	5:L:491:GLU:HB2	1.68	0.74
2:C:1142:ARG:HH22	2:C:1165:SER:HB2	1.51	0.74
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.20	0.74
1:G:12:ARG:HG3	1:H:230:ALA:HB1	1.70	0.74
3:J:491:LEU:HB2	3:J:904:ALA:HA	1.68	0.74
2:C:1275:VAL:HG13	2:C:1287:LEU:HD11	1.69	0.73
3:J:697:MET:SD	3:J:741:ALA:HB3	2.28	0.73
1:A:135:ASP:HB3	1:A:138:ALA:HB2	1.70	0.73
5:F:297:MET:HG3	5:F:326:TRP:HB2	1.70	0.73
1:H:220:ALA:HA	1:H:223:ILE:HD12	1.69	0.73
2:I:971:LEU:HD21	2:I:1014:LEU:O	1.89	0.73
1:H:99:ILE:HG12	1:H:143:ARG:HG2	1.70	0.73
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.70	0.72
5:F:483:LEU:H	5:F:483:LEU:HD12	1.54	0.72
3:J:47:ARG:NH1	5:L:500:ILE:HD11	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:898:GLU:HB3	5:F:540:LEU:HD22	1.70	0.72
5:F:469:GLN:NE2	5:F:473:GLU:OE2	2.18	0.72
1:B:35:PHE:HA	1:B:38:THR:HG22	1.70	0.72
2:I:1151:LEU:HG	2:I:1198:LEU:HD23	1.71	0.72
3:J:450:HIS:CE1	3:J:452:LEU:HD12	2.24	0.72
3:J:1238:GLN:NE2	3:J:1248:ILE:O	2.23	0.72
3:D:1280:VAL:HG11	3:D:1304:ARG:NE	2.04	0.71
2:I:1160:ASP:CB	2:I:1161:LEU:HA	2.19	0.71
2:C:1255:THR:O	2:C:1257:GLN:N	2.22	0.71
1:G:12:ARG:H	1:G:30:PRO:HD2	1.55	0.71
2:I:528:ARG:NH2	2:I:575:LEU:HD23	2.05	0.71
2:C:14:ASP:N	2:C:1157:GLN:OE1	2.22	0.71
3:D:275:ARG:HD3	3:D:298:MET:HB3	1.72	0.71
1:H:118:ASP:HB2	1:H:121:VAL:HB	1.71	0.71
5:L:137:TYR:CE2	5:L:139:GLU:HB2	2.25	0.71
2:C:802:VAL:HG12	2:C:1228:GLY:O	1.91	0.71
3:J:843:VAL:HG13	3:J:883:ARG:HD3	1.73	0.71
2:C:591:TYR:OH	2:C:637:ARG:NH2	2.22	0.70
3:J:93:THR:HG22	3:J:94:GLN:H	1.54	0.70
5:L:229:VAL:HA	5:L:232:ARG:HH12	1.56	0.70
1:A:152:TYR:CD1	2:C:824:GLN:HG2	2.26	0.70
2:C:1099:ASN:HD21	2:C:1101:LEU:HB2	1.55	0.70
1:A:218:ARG:HG3	1:B:231:PHE:O	1.91	0.70
2:C:1276:TRP:CZ2	3:D:801:VAL:HG11	2.27	0.70
2:C:1246:ARG:NH2	3:D:348:ASP:OD1	2.19	0.70
2:I:208:ILE:HG23	2:I:366:ILE:HD11	1.74	0.70
3:J:770:LEU:HD22	3:J:770:LEU:H	1.55	0.70
5:F:128:ASN:HA	5:F:131:GLN:HE21	1.57	0.69
3:D:770:LEU:H	3:D:770:LEU:HD22	1.55	0.69
2:I:94:ALA:HB2	2:I:129:LEU:HD11	1.74	0.69
3:J:490:ILE:HD12	3:J:500:ILE:HG13	1.73	0.69
3:D:343:LEU:HB3	3:D:344:GLY:HA3	1.74	0.69
3:J:746:LEU:HG	3:J:758:PRO:HB3	1.74	0.69
3:D:1179:PRO:HD3	3:D:1184:ASP:HB3	1.74	0.69
2:I:1122:LYS:NZ	2:I:1178:LYS:O	2.21	0.69
2:C:453:ILE:HD11	2:C:530:ILE:HD12	1.74	0.69
2:C:1330:ILE:HG23	3:D:331:ILE:HD11	1.74	0.69
3:J:858:VAL:HG11	3:J:872:LEU:HD11	1.72	0.69
1:A:190:ALA:HB2	1:A:200:LYS:HB2	1.75	0.69
3:J:824:PRO:HD3	3:J:835:LEU:HB2	1.75	0.69
3:D:201:LEU:HB2	3:D:221:ILE:HD13	1.73	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:918:ILE:HG13	3:D:919:ALA:N	2.08	0.69
3:J:279:LEU:HD12	3:J:295:GLU:HB3	1.73	0.69
5:L:547:VAL:HG22	5:L:603:ARG:HD3	1.74	0.68
3:J:515:ARG:NH2	3:J:717:VAL:O	2.26	0.68
3:J:733:SER:O	3:J:737:ILE:HG12	1.93	0.68
2:C:1106:ARG:O	2:C:1108:ASN:N	2.24	0.68
2:I:250:THR:HA	2:I:268:ARG:HA	1.74	0.68
2:I:319:LEU:HA	2:I:322:LEU:HD12	1.76	0.68
2:I:796:LEU:H	2:I:796:LEU:HD12	1.58	0.68
2:C:1269:ARG:CZ	3:D:343:LEU:HD13	2.24	0.68
3:D:190:LYS:HD3	3:D:235:GLU:HG2	1.74	0.68
3:J:88:CYS:O	3:J:90:VAL:N	2.27	0.68
2:C:1142:ARG:HH12	2:C:1165:SER:HA	1.58	0.67
3:D:1167:LYS:HD3	3:D:1174:ARG:HD2	1.76	0.67
3:J:846:GLU:HA	3:J:860:ARG:HE	1.59	0.67
1:A:59:VAL:HG21	1:A:85:LEU:HD13	1.76	0.67
2:I:213:LEU:HD22	2:I:422:LYS:HG2	1.76	0.67
2:C:848:GLU:HG2	2:C:888:THR:HG22	1.74	0.67
2:C:269:ILE:HG23	2:C:273:HIS:HB2	1.76	0.67
3:D:210:SER:HB2	3:D:213:LYS:HB2	1.77	0.67
3:D:1203:ARG:HH22	3:D:1205:GLU:HG2	1.58	0.67
3:D:847:ASP:N	3:D:847:ASP:OD1	2.28	0.67
1:H:54:CYS:SG	1:H:92:VAL:HG23	2.34	0.67
5:L:470:MET:CE	5:L:483:LEU:HG	2.25	0.67
3:D:1178:THR:HG23	3:D:1184:ASP:OD1	1.95	0.67
1:G:154:PRO:HD2	1:G:157:THR:OG1	1.95	0.67
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.77	0.67
2:C:551:HIS:CG	2:C:552:PRO:HD2	2.31	0.66
5:F:139:GLU:HG2	5:F:351:THR:HA	1.78	0.66
3:J:47:ARG:HH12	5:L:500:ILE:HD11	1.60	0.66
3:J:290:ILE:HD12	3:J:290:ILE:H	1.59	0.66
2:C:704:MET:O	2:C:706:ARG:N	2.28	0.66
1:H:62:ASP:HB3	1:H:141:SER:O	1.96	0.66
2:I:162:GLY:H	2:I:170:VAL:HG12	1.59	0.66
2:I:798:GLN:HB2	2:I:828:PHE:HE1	1.60	0.66
3:D:596:LEU:HD12	3:D:601:ILE:HG13	1.75	0.66
5:F:479:THR:HG22	5:F:482:GLU:HB2	1.77	0.66
2:C:319:LEU:HA	2:C:322:LEU:HD12	1.77	0.66
3:J:488:ASN:HB3	4:K:16:ARG:NH2	2.11	0.66
1:B:46:ILE:HD12	1:B:224:LEU:HD22	1.77	0.66
2:I:1087:TYR:HE1	2:I:1215:GLY:HA2	1.60	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.10	0.66
5:F:124:GLU:HA	5:F:127:ILE:HG12	1.77	0.66
1:G:191:ARG:HH22	1:G:197:ASP:HA	1.61	0.66
5:L:292:VAL:HG11	5:L:299:LYS:HE3	1.78	0.66
1:A:112:ALA:HB3	1:A:126:PRO:HA	1.78	0.66
1:H:59:VAL:HG23	1:H:173:VAL:HG21	1.77	0.66
5:L:492:ASP:HB2	5:L:495:ARG:HH12	1.61	0.66
3:D:536:LEU:HD12	3:D:542:ALA:HB2	1.77	0.66
2:I:972:PHE:CE2	2:I:998:LEU:HD11	2.31	0.66
5:F:215:GLU:HG2	5:F:218:ARG:HH21	1.61	0.65
3:J:885:VAL:O	3:J:1258:ARG:NH1	2.28	0.65
2:I:519:ASN:HB3	2:I:522:SER:HB2	1.77	0.65
3:J:647:PRO:HD3	3:J:697:MET:HB3	1.79	0.65
3:D:1266:ILE:HD13	3:D:1272:SER:HB3	1.78	0.65
1:A:45:ARG:HG2	1:B:38:THR:HB	1.77	0.65
3:D:275:ARG:HG2	3:D:278:ARG:HH12	1.60	0.65
2:I:1273:MET:HA	2:I:1276:TRP:CE3	2.32	0.65
3:J:767:LEU:HD23	3:J:771:GLN:HB3	1.79	0.65
5:F:380:VAL:HG13	5:F:412:LEU:HD23	1.79	0.65
3:J:1252:HIS:O	3:J:1255:VAL:HG13	1.95	0.65
2:I:1077:SER:HA	3:J:356:THR:OG1	1.97	0.65
2:C:748:ILE:HD11	2:C:967:LEU:HA	1.79	0.64
3:D:357:VAL:HG22	3:D:461:PHE:CD1	2.32	0.64
3:J:489:ASN:HA	3:J:904:ALA:HB1	1.78	0.64
2:I:338:THR:HG22	2:I:345:PRO:HB3	1.79	0.64
3:J:1264:ALA:O	3:J:1277:GLY:HA2	1.97	0.64
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.29	0.64
2:C:124:MET:HB2	2:C:498:ILE:HD13	1.78	0.64
2:C:95:PRO:HA	2:C:126:GLU:HG2	1.79	0.64
1:H:182:ARG:HB3	1:H:206:GLU:HG3	1.78	0.64
2:I:807:TRP:HH2	2:I:1216:ARG:HD3	1.62	0.64
2:I:95:PRO:HA	2:I:126:GLU:HG2	1.80	0.64
5:F:370:ALA:HB1	5:F:374:ARG:HH22	1.63	0.64
3:J:700:ASN:O	3:J:704:GLU:HB2	1.98	0.64
2:C:1254:VAL:HG13	2:C:1255:THR:H	1.63	0.64
3:J:1311:LYS:O	3:J:1314:LEU:HB3	1.98	0.64
4:K:70:GLN:O	4:K:74:GLU:HG2	1.97	0.64
5:L:485:GLU:HB2	5:L:486:ARG:NH2	2.12	0.64
1:B:214:GLU:HG2	1:B:218:ARG:NH2	2.13	0.64
2:C:88:ARG:HB2	2:C:88:ARG:HH11	1.62	0.64
2:I:344:GLY:HA3	2:I:346:TYR:CZ	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:255:ARG:HD3	1:B:256:PRO:HD2	1.80	0.63
2:C:1017:GLN:O	2:C:1021:LEU:HG	1.99	0.63
2:C:1305:TYR:CE1	3:D:379:PRO:HG3	2.33	0.63
2:I:296:VAL:HB	2:I:336:LEU:HD12	1.80	0.63
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.46	0.63
3:J:367:GLY:HA3	3:J:448:GLN:HB2	1.79	0.63
3:D:650:LYS:NZ	3:D:765:GLU:OE2	2.30	0.63
3:D:1227:HIS:CB	3:J:1293:GLU:HG2	2.29	0.63
2:I:1073:LYS:HE3	3:J:462:ASP:HB2	1.79	0.63
3:J:147:ILE:HG22	3:J:188:LEU:HG	1.80	0.63
2:I:221:LEU:HD11	2:I:314:ASN:HB2	1.81	0.63
3:J:425:ARG:NH1	3:J:464:ASP:OD1	2.31	0.63
2:C:389:PHE:HB3	2:C:420:LEU:HD12	1.81	0.63
2:C:1313:HIS:HD2	3:D:477:GLN:HE22	1.47	0.63
3:J:549:LYS:HB3	3:J:569:LEU:HD23	1.79	0.63
2:C:36:GLN:HE21	2:C:40:GLU:HG3	1.64	0.63
2:I:389:PHE:HB3	2:I:420:LEU:HD12	1.80	0.63
2:I:61:SER:HB3	2:I:479:LEU:HB3	1.81	0.63
3:J:502:PRO:HB3	3:J:506:VAL:HG21	1.80	0.63
1:H:102:LEU:O	1:H:141:SER:HA	1.97	0.63
2:C:519:ASN:HB3	2:C:522:SER:HB2	1.81	0.62
2:I:488:MET:O	2:I:490:GLN:N	2.31	0.62
1:B:59:VAL:HG22	1:B:144:ILE:HG13	1.82	0.62
1:G:134:THR:HG21	2:I:727:VAL:O	2.00	0.62
4:K:39:VAL:HG21	4:K:56:GLU:HG3	1.81	0.62
3:D:844:THR:HG23	3:D:864:LEU:HD11	1.81	0.62
5:F:547:VAL:HG13	5:F:598:LEU:HD22	1.81	0.62
1:H:59:VAL:HG13	1:H:144:ILE:HG22	1.81	0.62
2:I:551:HIS:ND1	2:I:553:THR:OG1	2.29	0.62
3:J:814:CYS:HG	3:J:888:CYS:HG	1.41	0.62
3:D:1299:GLY:H	3:J:1301:THR:HG21	1.64	0.62
3:J:615:LYS:HE2	3:J:616:PRO:HD3	1.80	0.62
1:B:219:ARG:O	1:B:223:ILE:HG13	2.00	0.62
3:D:205:LEU:HD23	3:D:217:LEU:HB3	1.81	0.62
3:D:615:LYS:HE2	3:D:616:PRO:HD3	1.81	0.62
3:J:203:GLU:O	3:J:207:GLU:HG2	1.98	0.62
2:C:13:LYS:HD3	2:C:1149:TYR:HA	1.82	0.62
2:I:748:ILE:HD12	2:I:970:GLY:HA3	1.81	0.62
3:J:642:ASP:HA	3:J:764:ARG:NH2	2.14	0.62
3:J:903:LEU:HB3	3:J:905:ARG:H	1.64	0.62
5:L:121:LYS:NZ	5:L:124:GLU:OE1	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:596:LEU:HD12	3:J:601:ILE:HG13	1.80	0.62
1:B:192:VAL:HB	1:B:195:ARG:HB2	1.81	0.62
2:C:94:ALA:HB2	2:C:129:LEU:HD11	1.82	0.62
3:D:450:HIS:HE1	3:D:452:LEU:HD12	1.65	0.62
3:J:857:LEU:HD13	3:J:872:LEU:CD2	2.30	0.62
3:J:275:ARG:HD3	3:J:298:MET:HB3	1.82	0.62
2:C:221:LEU:HD11	2:C:314:ASN:HB2	1.82	0.61
3:D:1316:THR:HG22	3:D:1318:SER:H	1.65	0.61
5:L:561:MET:HG3	5:L:567:MET:HE3	1.82	0.61
1:A:221:ALA:HB1	1:B:228:LEU:HD22	1.82	0.61
2:C:483:ASP:HB3	2:C:486:THR:CG2	2.30	0.61
2:I:886:LYS:H	2:I:917:SER:HB3	1.65	0.61
3:J:97:VAL:HG11	3:J:101:ARG:NH2	2.15	0.61
5:L:234:THR:O	5:L:245:ALA:HB2	2.01	0.61
1:A:11:PRO:HD2	1:B:227:GLN:O	2.00	0.61
5:F:484:ALA:HB1	5:F:491:GLU:HB2	1.82	0.61
2:I:231:GLU:HG2	2:I:332:ARG:HD3	1.83	0.61
2:C:344:GLY:HA3	2:C:346:TYR:CZ	2.36	0.61
3:D:316:ILE:HA	3:D:323:PRO:HA	1.82	0.61
2:I:97:ARG:HB3	2:I:121:GLU:HB2	1.83	0.61
2:I:183:TRP:HB2	2:I:199:ASP:HA	1.81	0.61
2:I:452:ARG:HH12	2:I:585:GLY:HA3	1.66	0.61
1:B:252:ILE:HG22	1:B:278:ILE:HD11	1.82	0.61
3:D:1193:TRP:HB2	3:D:1194:ARG:NH1	2.15	0.61
1:H:84:ASN:O	1:H:128:HIS:HE1	1.83	0.61
1:B:255:ARG:HG3	1:B:255:ARG:NH1	2.03	0.61
2:C:1330:ILE:CG2	3:D:331:ILE:HD11	2.31	0.61
1:H:51:MET:HB3	1:H:178:SER:CB	2.31	0.61
1:H:23:HIS:CE1	1:H:204:GLU:HG2	2.35	0.61
2:C:241:LEU:HD21	2:C:246:LEU:HD11	1.83	0.61
2:I:251:ALA:HB2	2:I:269:ILE:HD11	1.82	0.60
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.82	0.60
2:C:1142:ARG:HH22	2:C:1165:SER:CB	2.13	0.60
2:I:1250:SER:HB3	2:I:1259:LEU:O	2.01	0.60
1:A:13:LEU:H	1:A:13:LEU:HD23	1.66	0.60
2:C:241:LEU:HD11	2:C:246:LEU:HD11	1.83	0.60
3:J:1173:ARG:HB2	3:J:1192:LYS:HD2	1.82	0.60
3:D:278:ARG:HD2	3:D:295:GLU:OE1	2.01	0.60
3:D:810:THR:HG22	3:D:893:GLY:HA3	1.83	0.60
3:J:800:LEU:HD23	3:J:920:ALA:HA	1.82	0.60
3:D:1215:GLU:HG3	3:D:1220:ILE:HD11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:190:ALA:HB2	1:B:200:LYS:HB2	1.83	0.60
2:C:1024:GLU:HG3	2:C:1027:LYS:HE2	1.84	0.60
5:F:600:HIS:CD2	5:F:601:PRO:HD2	2.37	0.60
2:C:1117:LEU:HD12	2:C:1195:ILE:HG12	1.82	0.60
2:C:202:ARG:NH2	2:C:368:ARG:HH12	2.00	0.60
1:G:152:TYR:CD1	2:I:824:GLN:HG2	2.35	0.60
2:C:1120:ALA:HB1	2:C:1198:LEU:HD12	1.83	0.60
2:C:32:LEU:HD23	2:C:130:MET:SD	2.42	0.60
3:J:118:LYS:O	3:J:311:ARG:NH1	2.35	0.60
1:B:100:LEU:HD11	1:B:121:VAL:HG21	1.83	0.60
2:C:726:TYR:CE2	2:C:728:ASP:HB2	2.37	0.60
3:D:697:MET:SD	3:D:741:ALA:HB3	2.41	0.60
5:L:311:THR:HG21	5:L:348:GLU:OE1	2.02	0.60
2:C:495:ALA:HA	2:C:498:ILE:HD12	1.84	0.59
1:B:285:THR:HG23	1:B:287:VAL:HB	1.84	0.59
3:D:491:LEU:HB2	3:D:904:ALA:HA	1.84	0.59
1:H:82:LEU:O	1:H:86:LYS:HG3	2.03	0.59
2:I:75:LEU:HD11	2:I:127:ILE:HD11	1.84	0.59
1:A:45:ARG:HH21	2:C:1216:ARG:HA	1.66	0.59
3:D:884:SER:OG	3:D:886:VAL:HG12	2.01	0.59
3:D:901:ARG:HB2	3:D:907:HIS:O	2.02	0.59
3:D:392:THR:HG21	5:F:606:VAL:HA	1.85	0.59
3:D:706:VAL:HG12	3:D:715:LYS:HB3	1.85	0.59
3:J:85:CYS:SG	3:J:87:LYS:HB2	2.43	0.59
3:J:44:ILE:HG13	5:L:450:ILE:HG22	1.84	0.59
2:C:22:LEU:HD22	2:C:23:ASP:N	2.18	0.59
2:I:525:THR:HG21	2:I:687:ARG:HD2	1.85	0.59
3:J:1255:VAL:O	3:J:1259:GLN:HG2	2.03	0.59
3:J:833:GLU:HB2	3:J:1242:ARG:HD3	1.85	0.59
2:I:1108:ASN:OD1	2:I:1111:GLN:NE2	2.36	0.59
2:I:1287:LEU:HD13	3:J:1357:ILE:HD11	1.84	0.59
3:J:418:GLU:HG3	4:K:45:LYS:H	1.67	0.59
5:L:412:LEU:HD13	5:L:435:ILE:HD11	1.85	0.59
2:C:1158:LYS:O	2:C:1159:VAL:HG13	2.02	0.59
1:H:23:HIS:HE1	1:H:204:GLU:HG2	1.68	0.59
2:I:1282:GLY:O	2:I:1284:ALA:N	2.34	0.59
1:A:14:VAL:HG13	1:A:15:ASP:H	1.67	0.59
3:D:358:GLY:O	3:D:361:LEU:HD12	2.03	0.59
3:J:1280:VAL:HG11	3:J:1304:ARG:NE	2.16	0.59
3:D:661:VAL:HG12	3:D:685:ILE:HD11	1.85	0.58
2:I:1099:ASN:HD21	2:I:1101:LEU:HB2	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1209:GLN:HB3	2:I:1224:PRO:HB2	1.84	0.58
3:J:210:SER:O	3:J:214:ARG:HG2	2.03	0.58
3:J:405:GLU:O	3:J:408:VAL:HG22	2.03	0.58
2:C:230:PHE:CD1	2:C:292:ILE:HD11	2.38	0.58
2:C:704:MET:O	2:C:707:ALA:N	2.36	0.58
3:D:824:PRO:HD3	3:D:835:LEU:HB2	1.86	0.58
3:J:132:LEU:HA	3:J:135:ILE:HD12	1.85	0.58
1:B:269:CYS:HB3	1:B:292:THR:HG21	1.84	0.58
3:D:156:ARG:NH1	3:D:157:GLN:HE21	2.01	0.58
5:F:547:VAL:HG22	5:F:603:ARG:HD3	1.85	0.58
2:I:1033:ARG:O	2:I:1037:THR:HG23	2.03	0.58
2:I:499:SER:O	2:I:503:LYS:HB2	2.03	0.58
2:I:807:TRP:CH2	2:I:1216:ARG:HD3	2.38	0.58
5:L:229:VAL:HA	5:L:232:ARG:NH1	2.17	0.58
2:I:757:THR:HG23	2:I:765:ILE:HG23	1.85	0.58
3:J:514:THR:HG23	3:J:576:ARG:HG2	1.85	0.58
5:L:485:GLU:HB2	5:L:486:ARG:HH22	1.67	0.58
2:C:883:LEU:HB2	2:C:918:LEU:HD23	1.84	0.58
2:I:660:VAL:HG13	2:I:661:VAL:HG13	1.85	0.58
3:J:189:LEU:HB3	3:J:234:PRO:HB2	1.84	0.58
3:J:479:GLU:HG3	4:K:20:VAL:HG11	1.85	0.58
3:D:825:VAL:HG22	3:D:833:GLU:H	1.69	0.58
2:C:119:GLU:HB2	2:C:489:PRO:HG2	1.86	0.58
2:C:138:ILE:HB	2:C:143:ARG:HD3	1.84	0.58
3:D:216:LYS:HA	3:D:219:LYS:HE3	1.85	0.58
2:C:1106:ARG:HE	3:D:731:ARG:HH21	1.52	0.58
3:D:528:THR:O	3:D:551:ARG:HB3	2.04	0.58
4:K:26:ARG:HG2	4:K:59:ILE:HG21	1.86	0.58
3:J:124:ILE:HG12	3:J:237:MET:SD	2.44	0.58
3:J:77:ARG:HG3	3:J:79:LYS:H	1.69	0.58
1:H:190:ALA:HB2	1:H:200:LYS:HB2	1.86	0.58
2:I:1017:GLN:O	2:I:1021:LEU:HG	2.03	0.58
2:I:848:GLU:HG2	2:I:888:THR:HG22	1.85	0.58
5:L:445:ASP:OD2	5:L:451:ARG:NH1	2.37	0.58
3:J:857:LEU:HD22	3:J:872:LEU:HD23	1.86	0.57
2:C:799:ASN:ND2	2:C:799:ASN:H	2.02	0.57
3:D:423:LEU:HB3	3:D:466:MET:CE	2.33	0.57
3:D:45:ASN:O	3:D:46:TYR:HB3	2.04	0.57
3:D:701:LEU:HD12	3:D:723:TYR:HB2	1.85	0.57
5:F:606:VAL:HG13	5:F:607:LEU:HD12	1.86	0.57
3:J:885:VAL:HG12	3:J:894:VAL:HG11	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:399:LYS:NZ	5:L:612:ASP:HB3	2.18	0.57
1:A:11:PRO:HA	1:A:30:PRO:CG	2.33	0.57
2:I:13:LYS:HD3	2:I:1149:TYR:HA	1.85	0.57
5:F:592:ALA:HA	5:F:595:LEU:HD12	1.86	0.57
2:I:250:THR:OG1	2:I:268:ARG:HB3	2.03	0.57
5:L:503:GLU:CD	5:L:504:PRO:HD2	2.25	0.57
2:C:69:GLN:HE21	2:C:101:ARG:HD2	1.69	0.57
2:C:985:GLU:O	2:C:989:LEU:N	2.37	0.57
5:F:94:THR:HG21	5:F:103:ARG:HH22	1.70	0.57
3:J:210:SER:HB2	3:J:213:LYS:HB2	1.85	0.57
2:C:1282:GLY:O	2:C:1284:ALA:N	2.37	0.57
2:C:964:LEU:HD13	2:C:1025:PHE:HB2	1.87	0.57
2:I:1196:LYS:HA	2:I:1199:LEU:HD12	1.85	0.57
5:L:145:LEU:HD21	5:L:224:LEU:HD23	1.86	0.57
1:B:16:ILE:HG22	1:B:26:VAL:HG22	1.85	0.57
2:C:1103:VAL:HG11	2:C:1112:ILE:HD11	1.87	0.57
3:J:502:PRO:HB3	3:J:506:VAL:CG2	2.35	0.57
3:D:232:ASN:ND2	3:D:1337:VAL:O	2.36	0.57
1:G:169:GLY:O	1:G:171:LEU:HD22	2.04	0.57
3:J:1344:LEU:HB3	3:J:1350:ASN:ND2	2.18	0.57
3:J:205:LEU:HD23	3:J:217:LEU:HB3	1.87	0.57
1:B:273:GLU:OE2	1:B:293:PRO:HD2	2.05	0.57
5:F:492:ASP:HB2	5:F:495:ARG:HH12	1.68	0.57
2:I:720:ARG:HD3	2:I:749:ASP:OD1	2.05	0.57
2:I:807:TRP:HE1	2:I:1086:PRO:CG	2.18	0.57
2:C:37:LYS:NZ	2:C:40:GLU:OE2	2.30	0.57
3:D:242:LEU:HD23	3:D:243:PRO:O	2.05	0.57
2:I:1281:TYR:HE1	3:J:489:ASN:HD21	1.52	0.57
1:A:31:LEU:HD22	1:A:36:GLY:HA2	1.86	0.56
1:A:4:SER:OG	1:A:5:VAL:N	2.37	0.56
2:C:251:ALA:HB2	2:C:269:ILE:HD11	1.87	0.56
3:D:113:HIS:CE1	3:D:115:TRP:HB2	2.40	0.56
3:D:161:THR:HG23	3:D:163:GLU:H	1.70	0.56
2:I:798:GLN:HB2	2:I:828:PHE:CE1	2.39	0.56
3:J:679:TYR:CZ	3:J:683:ILE:HD11	2.40	0.56
3:D:209:ASN:HA	3:D:214:ARG:HE	1.70	0.56
3:D:9:LYS:HZ3	3:D:11:GLN:HA	1.69	0.56
2:I:231:GLU:OE2	2:I:233:ARG:NH1	2.38	0.56
2:C:1327:LEU:HD23	2:C:1337:ILE:HG23	1.87	0.56
2:C:202:ARG:HH22	2:C:368:ARG:HH22	1.51	0.56
3:D:549:LYS:HD3	3:D:569:LEU:HD23	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:K:19:LEU:CD1	4:K:54:ILE:HG21	2.35	0.56
1:B:263:THR:HG22	1:B:302:GLU:HG2	1.86	0.56
2:I:1256:GLN:HB3	2:I:1301:ARG:HH22	1.70	0.56
3:J:1357:ILE:HG22	3:J:1359:ALA:H	1.70	0.56
3:J:538:ARG:HH11	3:J:538:ARG:HA	1.70	0.56
2:C:175:ARG:HH11	2:C:183:TRP:HZ3	1.53	0.56
3:D:93:THR:HG22	3:D:94:GLN:N	2.20	0.56
4:K:19:LEU:HD13	4:K:54:ILE:HG21	1.87	0.56
2:C:1103:VAL:H	2:C:1104:PRO:HD2	1.71	0.56
3:J:899:TYR:O	3:J:1251:LYS:HD3	2.06	0.56
5:L:511:ILE:HG13	5:L:512:GLY:H	1.71	0.56
2:C:1281:TYR:CE1	3:D:484:MET:HA	2.41	0.56
3:D:161:THR:HG22	3:D:164:GLN:H	1.70	0.56
2:I:1024:GLU:HG3	2:I:1027:LYS:HE2	1.87	0.56
1:B:104:LYS:HG2	1:B:110:VAL:HG22	1.86	0.56
2:C:1099:ASN:ND2	2:C:1101:LEU:HB2	2.21	0.56
1:H:51:MET:HB3	1:H:178:SER:HB2	1.87	0.56
3:J:817:HIS:O	3:J:845:ALA:HB1	2.05	0.56
2:C:741:MET:HG2	2:C:974:ARG:HH21	1.71	0.56
2:C:798:GLN:OE1	2:C:827:ARG:HB2	2.05	0.56
1:H:27:THR:HG22	1:H:202:VAL:HG13	1.87	0.56
3:J:515:ARG:HG2	3:J:719:PHE:CZ	2.41	0.56
3:J:71:LEU:HB3	3:J:88:CYS:SG	2.46	0.56
3:D:318:GLY:O	3:D:320:ASN:N	2.34	0.55
3:D:343:LEU:HB3	3:D:344:GLY:CA	2.36	0.55
5:F:370:ALA:O	5:F:374:ARG:HB2	2.06	0.55
5:F:584:ARG:NH1	5:F:584:ARG:HA	2.21	0.55
5:F:600:HIS:CG	5:F:601:PRO:HD2	2.40	0.55
2:I:496:LYS:HB3	2:I:497:PRO:HD3	1.88	0.55
2:C:1272:GLU:O	2:C:1275:VAL:N	2.39	0.55
5:F:370:ALA:HB1	5:F:374:ARG:NH2	2.21	0.55
2:I:1283:ALA:HB1	2:I:1286:THR:HB	1.88	0.55
3:J:220:ARG:O	3:J:224:LEU:N	2.38	0.55
3:J:343:LEU:HD12	3:J:343:LEU:H	1.71	0.55
5:L:484:ALA:HB1	5:L:491:GLU:CB	2.37	0.55
3:D:9:LYS:CE	3:D:11:GLN:HA	2.37	0.55
4:E:25:ARG:HD3	4:E:64:LEU:HD13	1.87	0.55
5:F:454:VAL:HA	5:F:457:ILE:HD12	1.88	0.55
2:I:1324:ASN:HA	2:I:1327:LEU:HD12	1.87	0.55
2:I:985:GLU:HG2	2:I:988:LYS:HD2	1.87	0.55
3:J:1178:THR:HA	3:J:1184:ASP:HB3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1311:LYS:O	3:D:1314:LEU:HB3	2.07	0.55
1:H:118:ASP:HB2	1:H:121:VAL:CB	2.36	0.55
5:L:324:LYS:HB3	5:L:325:PRO:HD2	1.88	0.55
2:C:22:LEU:HD22	2:C:23:ASP:H	1.72	0.55
3:D:357:VAL:HG12	3:D:358:GLY:H	1.71	0.55
3:D:77:ARG:HB3	3:D:80:HIS:CE1	2.42	0.55
3:D:842:ARG:HB3	3:D:882:VAL:HG11	1.89	0.55
2:I:138:ILE:HB	2:I:143:ARG:HD3	1.87	0.55
3:J:1289:ASN:O	3:J:1290:ARG:NH1	2.40	0.55
2:C:19:PRO:HA	2:C:1156:ARG:HH11	1.72	0.55
3:D:9:LYS:NZ	3:D:11:GLN:HG3	2.22	0.55
1:G:104:LYS:HG2	1:G:110:VAL:HG22	1.89	0.55
1:H:109:PRO:HA	1:H:132:HIS:HA	1.88	0.55
2:I:1166:ASP:O	2:I:1170:MET:HG2	2.07	0.55
1:G:45:ARG:HH21	2:I:1216:ARG:HA	1.71	0.55
2:I:237:LEU:HD11	2:I:292:ILE:HD11	1.89	0.55
2:I:820:GLU:HA	2:I:1079:ILE:HD11	1.88	0.55
3:J:288:PRO:HG2	3:J:291:ILE:HD12	1.88	0.55
3:D:1257:VAL:O	3:D:1260:MET:N	2.40	0.55
3:J:1253:ILE:O	3:J:1257:VAL:HG23	2.07	0.55
3:D:88:CYS:O	3:D:90:VAL:N	2.38	0.55
2:I:571:LEU:O	2:I:572:ILE:HD13	2.07	0.55
4:K:50:ALA:O	4:K:54:ILE:HG12	2.07	0.55
2:C:528:ARG:NH2	2:C:575:LEU:HD23	2.22	0.55
2:C:582:ASN:HB3	2:C:586:PHE:N	2.20	0.55
3:D:1178:THR:HA	3:D:1184:ASP:HB3	1.89	0.55
3:D:1191:PRO:HB2	3:D:1194:ARG:HH11	1.72	0.55
3:D:1140:ARG:HH21	3:D:1236:GLU:HG2	1.72	0.55
3:J:57:PHE:HB3	3:J:98:ARG:HH22	1.71	0.55
1:B:140:ILE:HG13	1:B:141:SER:N	2.22	0.54
2:C:175:ARG:CZ	2:C:200:ARG:HH12	2.20	0.54
1:B:182:ARG:NH1	3:D:534:GLU:OE2	2.40	0.54
1:G:150:ARG:HH11	1:H:6:THR:HG23	1.73	0.54
1:B:107:ILE:HG12	1:B:135:ASP:HA	1.89	0.54
3:D:248:ASP:O	3:D:251:PRO:HG3	2.06	0.54
1:G:218:ARG:HG3	1:H:231:PHE:O	2.06	0.54
1:G:45:ARG:HH22	1:H:37:HIS:HB3	1.73	0.54
5:L:392:LYS:O	5:L:395:THR:HG23	2.07	0.54
3:D:658:GLU:O	3:D:661:VAL:HG22	2.07	0.54
3:D:644:MET:HG2	3:D:722:ILE:HD13	1.90	0.54
3:J:1269:ALA:HB2	3:J:1274:PHE:CD1	2.42	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:612:GLY:O	2:C:639:LYS:HG2	2.07	0.54
2:I:158:ASP:OD1	2:I:159:SER:N	2.37	0.54
2:I:60:GLN:HB3	2:I:67:GLU:HG3	1.90	0.54
2:I:670:PHE:HB3	2:I:673:HIS:HD2	1.72	0.54
3:J:1280:VAL:HG21	3:J:1304:ARG:NE	2.23	0.54
3:J:399:LYS:HZ1	5:L:612:ASP:HB3	1.73	0.54
3:D:527:LEU:HB2	3:D:550:VAL:HG12	1.88	0.54
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.08	0.54
3:D:262:THR:HG1	3:D:266:ASN:ND2	2.04	0.54
3:D:357:VAL:HG22	3:D:461:PHE:CE1	2.43	0.54
1:H:54:CYS:HB2	1:H:90:VAL:O	2.08	0.54
2:I:71:VAL:HB	2:I:99:LYS:HB2	1.90	0.54
3:J:1178:THR:HG23	3:J:1184:ASP:OD1	2.07	0.54
2:C:1151:LEU:HD21	2:C:1197:GLU:HB3	1.89	0.54
2:I:510:GLN:CD	2:I:534:GLY:HA2	2.28	0.54
3:J:742:GLY:O	3:J:762:ASN:HB3	2.07	0.54
3:J:418:GLU:H	4:K:45:LYS:HZ2	1.55	0.54
5:L:316:PHE:HZ	5:L:334:SER:HA	1.72	0.54
1:B:16:ILE:HG22	1:B:26:VAL:HG13	1.90	0.54
3:D:1341:ARG:NH1	3:D:1343:GLU:OE2	2.41	0.54
3:D:901:ARG:HG3	3:D:902:ASP:N	2.23	0.54
1:H:84:ASN:HB3	1:H:130:ILE:HA	1.90	0.54
2:I:1308:ILE:HG21	3:J:379:PRO:HB2	1.90	0.54
2:C:98:VAL:O	2:C:121:GLU:HA	2.08	0.54
2:C:120:GLN:HG3	2:C:121:GLU:HG2	1.89	0.54
2:C:589:THR:OG1	2:C:659:GLN:NE2	2.41	0.54
3:D:458:ASN:O	3:D:458:ASN:ND2	2.40	0.54
3:D:741:ALA:O	3:D:762:ASN:ND2	2.41	0.54
3:J:853:THR:HG22	3:J:854:ALA:H	1.72	0.54
3:D:630:ALA:O	3:D:633:ALA:HB3	2.07	0.53
3:D:746:LEU:HA	3:D:758:PRO:HB3	1.90	0.53
1:H:125:LYS:HD3	1:H:128:HIS:HB2	1.88	0.53
1:H:67:GLU:OE1	1:H:171:LEU:HD13	2.07	0.53
3:J:278:ARG:HD2	3:J:295:GLU:OE1	2.08	0.53
2:C:796:LEU:H	2:C:796:LEU:CD1	2.04	0.53
3:D:744:ARG:HG3	3:D:744:ARG:O	2.09	0.53
2:I:1327:LEU:HD23	2:I:1337:ILE:HG23	1.91	0.53
2:I:520:PRO:HB3	2:I:714:VAL:HG21	1.91	0.53
3:J:901:ARG:HG3	3:J:902:ASP:N	2.24	0.53
5:L:295:CYS:SG	5:L:333:VAL:HB	2.48	0.53
1:B:140:ILE:HD11	1:B:142:MET:HE3	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:146:VAL:HB	3:D:156:ARG:O	2.08	0.53
3:D:209:ASN:HA	3:D:214:ARG:NE	2.24	0.53
5:F:492:ASP:HB2	5:F:495:ARG:HH22	1.73	0.53
1:H:61:ILE:HB	1:H:64:VAL:O	2.07	0.53
1:B:47:LEU:HB3	1:B:180:VAL:HG11	1.90	0.53
2:C:1132:LEU:HD22	2:C:1177:ARG:CZ	2.37	0.53
3:D:140:TYR:HB3	5:F:100:MET:SD	2.49	0.53
3:D:870:ASP:O	3:D:874:GLU:HG3	2.08	0.53
5:F:280:VAL:HG11	5:F:355:ILE:HD12	1.91	0.53
2:I:103:VAL:HG12	2:I:116:ASP:HB3	1.90	0.53
5:L:506:SER:O	5:L:509:THR:OG1	2.15	0.53
2:C:306:THR:HG23	2:C:308:GLU:H	1.74	0.53
1:H:29:GLU:HB3	1:H:200:LYS:HG3	1.89	0.53
1:H:181:GLU:HB3	1:H:206:GLU:HB2	1.90	0.53
3:J:189:LEU:HD13	3:J:234:PRO:O	2.07	0.53
3:J:343:LEU:CB	3:J:344:GLY:HA3	2.39	0.53
2:C:820:GLU:O	2:C:823:VAL:HG12	2.08	0.53
5:F:492:ASP:HB2	5:F:495:ARG:NH1	2.23	0.53
2:I:12:ARG:HG3	2:I:1181:PRO:C	2.29	0.53
3:J:46:TYR:CD1	5:L:452:ILE:HG22	2.43	0.53
3:J:845:ALA:O	3:J:860:ARG:NH2	2.42	0.53
3:D:174:ASP:O	3:D:176:PHE:N	2.42	0.53
3:D:216:LYS:HA	3:D:219:LYS:CE	2.39	0.53
2:I:1103:VAL:H	2:I:1104:PRO:HD2	1.74	0.53
2:I:1298:VAL:HG23	2:I:1301:ARG:HH12	1.74	0.53
2:I:591:TYR:OH	2:I:611:GLU:OE1	2.23	0.53
3:J:154:LEU:HD22	3:J:160:LEU:HD11	1.90	0.53
2:C:1327:LEU:HD23	2:C:1337:ILE:CG2	2.38	0.53
2:I:698:PRO:HG3	2:I:1231:TYR:CE2	2.44	0.53
3:J:517:CYS:HA	3:J:716:GLN:HE22	1.74	0.53
3:J:810:THR:HG23	3:J:811:GLU:H	1.74	0.53
3:D:423:LEU:HB3	3:D:466:MET:HE2	1.90	0.53
1:H:118:ASP:HB2	1:H:121:VAL:CG2	2.39	0.53
3:J:1151:LYS:O	3:J:1153:PRO:HD3	2.08	0.53
5:L:315:TRP:CZ2	5:L:341:LEU:HD11	2.44	0.53
2:C:837:ALA:HB2	2:C:1051:LYS:HG2	1.91	0.52
5:F:290:LEU:HB3	5:F:333:VAL:HG21	1.91	0.52
2:I:26:TYR:CE2	2:I:28:LEU:HB2	2.44	0.52
2:I:974:ARG:HD2	2:I:1014:LEU:HD21	1.91	0.52
3:J:557:LYS:HA	3:J:562:GLU:O	2.09	0.52
2:I:898:GLU:HB3	5:L:540:LEU:HD22	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1005:GLU:HB3	2:C:1007:LYS:H	1.74	0.52
2:C:563:THR:OG1	2:C:564:PRO:HD2	2.09	0.52
5:F:511:ILE:HG13	5:F:512:GLY:H	1.74	0.52
2:I:1254:VAL:HG13	2:I:1255:THR:H	1.73	0.52
1:B:287:VAL:O	1:B:291:LYS:HG2	2.10	0.52
3:D:1323:ALA:HB1	3:D:1328:THR:HG23	1.91	0.52
4:E:73:GLN:HA	4:E:76:GLU:HB2	1.90	0.52
5:F:292:VAL:HG11	5:F:299:LYS:HE3	1.90	0.52
2:C:382:GLU:O	2:C:386:GLU:HG2	2.10	0.52
3:D:1238:GLN:O	3:D:1242:ARG:HB2	2.10	0.52
3:D:367:GLY:HA3	3:D:448:GLN:HB2	1.92	0.52
3:D:796:LEU:HG	3:D:800:LEU:HD13	1.92	0.52
1:G:14:VAL:HG13	1:G:15:ASP:H	1.75	0.52
3:J:93:THR:HG22	3:J:94:GLN:N	2.24	0.52
3:D:9:LYS:NZ	3:D:11:GLN:HA	2.25	0.52
2:C:1314:GLN:HG2	4:E:28:ARG:CZ	2.40	0.52
2:I:1243:MET:HA	3:J:353:SER:HB3	1.90	0.52
2:C:42:ASP:OD2	2:C:44:GLU:HG3	2.10	0.52
1:A:158:ARG:NH1	1:A:172:LEU:HD23	2.25	0.52
2:C:130:MET:SD	2:C:134:GLY:HA2	2.49	0.52
3:D:127:LEU:HG	3:D:127:LEU:O	2.10	0.52
1:G:45:ARG:NH2	2:I:1216:ARG:HA	2.24	0.52
1:H:67:GLU:OE2	1:H:171:LEU:HB3	2.10	0.52
1:H:79:LEU:HA	1:H:82:LEU:HD12	1.92	0.52
1:H:83:LEU:HD12	1:H:86:LYS:HE2	1.90	0.52
5:L:490:PRO:HG2	5:L:493:LYS:HE3	1.91	0.52
1:A:102:LEU:O	1:A:103:ASN:ND2	2.43	0.52
1:A:207:THR:HG21	1:A:211:ILE:HG22	1.91	0.52
2:C:69:GLN:HG3	2:C:101:ARG:HB3	1.91	0.52
2:I:818:VAL:HG22	2:I:1096:ILE:HG12	1.91	0.52
1:A:83:LEU:HD23	2:C:694:ARG:HE	1.75	0.52
2:C:202:ARG:HH22	2:C:368:ARG:HH12	1.57	0.52
2:C:417:SER:OG	2:C:418:GLY:N	2.42	0.52
2:C:516:ASP:O	2:C:522:SER:HB3	2.10	0.52
3:D:343:LEU:CB	3:D:344:GLY:HA3	2.37	0.52
3:J:613:GLY:HA3	3:J:615:LYS:HZ1	1.75	0.52
3:J:821:MET:CE	3:J:879:ALA:HB1	2.39	0.52
2:C:925:SER:O	2:C:1056:VAL:HG13	2.09	0.52
5:F:311:THR:HG22	5:F:344:LEU:HD23	1.92	0.52
5:F:489:MET:O	5:F:491:GLU:N	2.43	0.52
1:G:190:ALA:HB2	1:G:200:LYS:CB	2.31	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:577:VAL:HG23	2:I:661:VAL:O	2.10	0.52
3:J:825:VAL:C	3:J:826:ILE:HG13	2.29	0.52
4:K:39:VAL:HG22	4:K:40:PRO:HD2	1.92	0.52
1:A:195:ARG:HG2	1:A:198:LEU:HD11	1.91	0.51
1:B:29:GLU:OE2	1:B:200:LYS:HE3	2.10	0.51
2:C:16:GLY:O	2:C:1156:ARG:HG2	2.10	0.51
2:C:378:ARG:NH1	2:C:382:GLU:OE1	2.43	0.51
1:G:133:LEU:HD12	1:G:138:ALA:HB1	1.92	0.51
2:I:1024:GLU:OE2	2:I:1028:LYS:HD2	2.11	0.51
1:B:94:GLY:HA2	1:B:277:TYR:CE2	2.45	0.51
1:B:282:VAL:HG21	1:B:312:LEU:HD23	1.91	0.51
2:C:202:ARG:HH12	2:C:368:ARG:NH2	2.08	0.51
3:D:859:PRO:HD2	3:D:862:THR:HG21	1.91	0.51
2:I:235:ASN:OD1	2:I:236:LYS:HG2	2.10	0.51
1:A:76:GLU:OE1	1:A:76:GLU:N	2.43	0.51
3:D:1280:VAL:HG11	3:D:1304:ARG:HE	1.74	0.51
3:D:203:GLU:O	3:D:207:GLU:HG2	2.09	0.51
5:F:281:ARG:HD3	5:F:285:ARG:NH1	2.25	0.51
1:G:18:GLN:NE2	1:G:24:ALA:HB2	2.25	0.51
2:I:344:GLY:HA3	2:I:346:TYR:CE1	2.45	0.51
3:J:148:GLU:H	3:J:156:ARG:HG3	1.75	0.51
3:J:525:MET:O	3:J:548:VAL:HG13	2.10	0.51
3:J:908:ILE:HD13	3:J:909:ILE:O	2.11	0.51
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.91	0.51
2:I:1121:ALA:HB2	2:I:1182:ILE:HD12	1.90	0.51
2:I:306:THR:HG23	2:I:308:GLU:H	1.75	0.51
3:J:1233:ILE:O	3:J:1237:VAL:HG13	2.10	0.51
2:C:818:VAL:O	2:C:1079:ILE:HD12	2.11	0.51
3:D:1176:VAL:HG22	3:D:1187:GLU:CB	2.33	0.51
3:D:490:ILE:HD12	3:D:500:ILE:HG13	1.93	0.51
3:D:903:LEU:HB3	3:D:905:ARG:H	1.75	0.51
5:F:276:MET:O	5:F:280:VAL:HG23	2.11	0.51
5:F:280:VAL:CG1	5:F:355:ILE:HD12	2.41	0.51
3:J:1264:ALA:HB2	3:J:1280:VAL:HG22	1.91	0.51
3:J:532:GLU:HA	3:J:535:ARG:HB3	1.93	0.51
3:J:863:LEU:HD11	3:J:901:ARG:HB3	1.93	0.51
2:C:1043:ALA:O	2:C:1046:VAL:HG12	2.10	0.51
2:C:1176:LEU:HD22	2:C:1180:MET:HG2	1.93	0.51
3:D:1184:ASP:C	3:D:1186:TYR:H	2.14	0.51
2:I:1134:GLN:HE21	2:I:1136:GLN:NE2	2.09	0.51
3:J:495:ASN:O	3:J:497:GLU:N	2.43	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:130:VAL:O	5:L:134:VAL:HG23	2.11	0.51
2:C:820:GLU:HA	2:C:1079:ILE:HD11	1.93	0.51
3:D:491:LEU:HA	3:D:498:PRO:HA	1.92	0.51
5:F:420:GLU:OE1	5:F:423:ARG:NH2	2.44	0.51
1:G:48:LEU:HA	1:G:180:VAL:HG21	1.91	0.51
1:H:14:VAL:HG13	1:H:15:ASP:H	1.75	0.51
1:H:47:LEU:HD13	1:H:183:ILE:HG12	1.91	0.51
2:I:736:VAL:HG23	2:I:748:ILE:HA	1.93	0.51
3:J:930:LEU:HD12	3:J:1138:LEU:HD13	1.93	0.51
3:J:1155:ILE:O	3:J:1210:ILE:HB	2.10	0.51
3:J:146:VAL:HB	3:J:156:ARG:O	2.11	0.51
1:B:62:ASP:OD2	1:B:140:ILE:HD12	2.11	0.51
2:C:232:ILE:HG23	2:C:237:LEU:H	1.76	0.51
3:D:1343:GLU:HG3	3:D:1373:ARG:CZ	2.40	0.51
3:D:347:VAL:HG12	3:D:348:ASP:O	2.11	0.51
3:D:609:TYR:HE2	3:D:614:LEU:HD12	1.75	0.51
3:D:819:GLY:O	3:D:1227:HIS:HE1	1.94	0.51
1:G:229:GLU:HA	1:G:231:PHE:CE2	2.46	0.51
3:J:385:LEU:CD2	3:J:411:ILE:HG13	2.40	0.51
3:J:66:LYS:HD3	3:J:69:GLU:OE2	2.10	0.51
5:L:165:PHE:O	5:L:260:ARG:HD3	2.09	0.51
1:A:61:ILE:HG13	1:A:64:VAL:HB	1.92	0.51
2:C:1142:ARG:HD3	2:C:1161:LEU:HD22	1.92	0.51
2:C:1313:HIS:CD2	3:D:477:GLN:HE22	2.28	0.51
2:C:618:GLN:CD	3:D:770:LEU:HD21	2.31	0.51
5:F:562:ARG:NH1	5:F:571:TYR:O	2.44	0.51
2:I:122:VAL:HG11	2:I:493:ILE:HG21	1.93	0.51
3:J:814:CYS:HB2	3:J:889:ASP:OD1	2.10	0.51
1:A:188:GLU:HG3	1:A:200:LYS:HB3	1.93	0.51
3:D:613:GLY:C	3:D:616:PRO:HD2	2.31	0.51
3:D:860:ARG:HB3	3:D:860:ARG:CZ	2.41	0.51
5:F:147:GLN:HB3	5:F:161:LEU:HD13	1.93	0.51
1:H:124:VAL:HG21	1:H:209:GLY:O	2.11	0.51
2:I:1234:LYS:HE2	2:I:1238:LEU:HD21	1.93	0.51
3:J:24:LEU:HB2	3:J:232:ASN:OD1	2.10	0.51
3:J:693:VAL:HG11	3:J:743:MET:HG2	1.91	0.51
1:B:292:THR:HB	1:B:295:LEU:HB2	1.93	0.50
3:D:357:VAL:HG12	3:D:358:GLY:N	2.26	0.50
2:I:854:ILE:HD11	2:I:885:GLY:HA3	1.93	0.50
1:B:303:ILE:O	1:B:307:LEU:HB2	2.10	0.50
2:C:1209:GLN:HB3	2:C:1224:PRO:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:468:LEU:O	2:C:471:VAL:HG12	2.10	0.50
3:D:1203:ARG:NH2	3:D:1205:GLU:HG2	2.25	0.50
3:D:701:LEU:CD1	3:D:723:TYR:HB2	2.41	0.50
1:G:150:ARG:NH1	1:H:6:THR:HG23	2.27	0.50
2:I:1259:LEU:HD12	2:I:1260:GLY:H	1.76	0.50
2:I:798:GLN:OE1	2:I:827:ARG:HB2	2.10	0.50
2:C:615:VAL:HG12	2:C:651:ASP:OD2	2.10	0.50
3:D:647:PRO:HD3	3:D:697:MET:HB3	1.94	0.50
3:D:700:ASN:O	3:D:704:GLU:HB2	2.11	0.50
5:F:108:VAL:HG11	5:F:381:GLU:HB3	1.92	0.50
2:I:1331:ARG:HA	2:I:1335:ILE:O	2.11	0.50
2:C:1112:ILE:O	2:C:1115:THR:N	2.44	0.50
3:D:290:ILE:HD12	3:D:290:ILE:H	1.77	0.50
3:D:348:ASP:HB3	3:D:349:TYR:CD1	2.45	0.50
3:D:495:ASN:O	3:D:497:GLU:N	2.44	0.50
2:I:696:ASP:O	2:I:697:LYS:HB3	2.12	0.50
3:J:366:CYS:HB3	3:J:437:PHE:CD1	2.46	0.50
5:L:108:VAL:HG11	5:L:381:GLU:HB3	1.93	0.50
2:C:514:PHE:HB3	2:C:760:ASN:HD22	1.76	0.50
2:I:10:ARG:CD	2:I:1181:PRO:HG2	2.42	0.50
2:I:19:PRO:HA	2:I:1156:ARG:HH11	1.77	0.50
3:J:385:LEU:HD21	3:J:411:ILE:HG13	1.93	0.50
3:J:823:THR:HA	3:J:835:LEU:HD13	1.93	0.50
5:L:143:TYR:CD2	5:L:269:LEU:HD21	2.46	0.50
3:D:1284:ARG:HE	3:D:1304:ARG:NH2	2.09	0.50
3:D:549:LYS:HG3	3:D:571:ASP:OD1	2.11	0.50
2:I:169:LYS:O	2:I:170:VAL:HG22	2.12	0.50
2:I:22:LEU:HD22	2:I:23:ASP:N	2.26	0.50
2:I:88:ARG:HH11	2:I:88:ARG:HB2	1.77	0.50
3:J:660:GLU:O	3:J:664:ILE:HG12	2.11	0.50
3:J:325:LYS:HD3	5:L:508:GLU:HG2	1.92	0.50
2:C:688:GLN:OE1	2:C:1237:HIS:HE1	1.95	0.50
3:D:1284:ARG:HA	3:D:1287:ILE:HG12	1.94	0.50
3:D:518:VAL:HG11	3:D:707:ILE:HB	1.94	0.50
3:J:156:ARG:NH2	3:J:188:LEU:HD23	2.27	0.50
5:L:380:VAL:HG13	5:L:412:LEU:HD23	1.94	0.50
3:D:117:LEU:HD23	3:D:118:LYS:HG2	1.92	0.50
5:F:94:THR:CG2	5:F:103:ARG:HH22	2.25	0.50
2:I:943:LYS:HG2	2:I:947:GLU:OE1	2.12	0.50
3:J:97:VAL:HG11	3:J:101:ARG:CZ	2.42	0.50
5:L:385:ARG:HA	5:L:388:ILE:HD12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:47:LEU:O	1:A:180:VAL:HG21	2.11	0.50
2:C:1214:ASP:HB2	2:C:1221:PHE:CZ	2.47	0.50
2:C:71:VAL:HB	2:C:99:LYS:HB2	1.93	0.50
3:D:9:LYS:HZ2	3:D:11:GLN:HG3	1.77	0.50
2:I:274:ILE:HG22	2:I:278:GLU:OE1	2.12	0.50
3:J:621:ALA:HA	3:J:624:ILE:HD12	1.93	0.50
1:A:107:ILE:HD11	1:A:136:GLU:HG2	1.93	0.49
3:D:1351:VAL:HG12	8:D:2004:4C2:O2	2.12	0.49
3:D:520:ALA:HB1	3:D:543:SER:HB3	1.94	0.49
5:F:302:PHE:O	5:F:306:PHE:HB2	2.12	0.49
5:F:445:ASP:OD2	5:F:451:ARG:NH1	2.45	0.49
2:I:1172:LEU:O	2:I:1172:LEU:HD22	2.12	0.49
3:J:248:ASP:O	3:J:251:PRO:HG3	2.12	0.49
3:J:317:THR:HG23	3:J:320:ASN:HB3	1.94	0.49
5:L:306:PHE:CE2	5:L:310:GLU:HG2	2.47	0.49
5:L:297:MET:HG3	5:L:326:TRP:HB2	1.94	0.49
1:B:300:LEU:O	1:B:300:LEU:HD13	2.12	0.49
3:D:161:THR:H	3:D:164:GLN:HB2	1.76	0.49
5:F:324:LYS:HB3	5:F:325:PRO:HD2	1.93	0.49
5:F:548:LEU:HA	5:F:551:LEU:HD12	1.94	0.49
5:F:584:ARG:HH11	5:F:584:ARG:HA	1.76	0.49
2:I:992:LEU:HB2	2:I:993:PRO:HD2	1.95	0.49
3:J:1149:ARG:HG3	3:J:1216:ALA:HB2	1.94	0.49
3:J:1280:VAL:HG11	3:J:1304:ARG:HH21	1.76	0.49
5:L:536:THR:O	5:L:539:SER:HB3	2.13	0.49
5:L:555:GLU:HA	5:L:558:VAL:HG12	1.94	0.49
1:A:102:LEU:HD22	1:A:103:ASN:H	1.77	0.49
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.93	0.49
3:D:1230:THR:O	3:D:1234:VAL:HG13	2.11	0.49
3:D:211:GLU:O	3:D:215:LYS:HB2	2.13	0.49
3:J:349:TYR:HE2	3:J:379:PRO:HG2	1.77	0.49
1:B:263:THR:HG23	1:B:266:SER:OG	2.13	0.49
1:B:29:GLU:HB3	1:B:200:LYS:HG3	1.94	0.49
3:D:81:ARG:HG3	3:D:82:GLY:H	1.77	0.49
3:D:85:CYS:SG	3:D:87:LYS:HB2	2.52	0.49
5:F:115:GLY:HA2	5:F:118:ASP:OD1	2.13	0.49
2:I:151:ARG:HH21	2:I:156:PHE:HE2	1.54	0.49
2:C:886:LYS:HE3	2:C:916:SER:O	2.13	0.49
3:D:425:ARG:O	3:D:426:ALA:O	2.30	0.49
5:F:234:THR:O	5:F:245:ALA:HB2	2.12	0.49
3:J:507:VAL:HG11	3:J:598:LYS:HG3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:735:ALA:HA	3:J:738:ARG:NH1	2.28	0.49
3:J:91:GLU:OE1	3:J:93:THR:OG1	2.31	0.49
2:C:1271:GLY:CA	3:D:343:LEU:HD23	2.43	0.49
2:C:466:VAL:HA	2:C:469:VAL:HG22	1.94	0.49
3:D:606:ASN:HD21	3:D:610:ARG:HE	1.61	0.49
2:I:250:THR:HG23	2:I:268:ARG:N	2.26	0.49
2:I:389:PHE:HA	2:I:395:TYR:CD1	2.47	0.49
3:J:800:LEU:O	3:J:803:VAL:HG12	2.13	0.49
5:L:270:VAL:HG13	5:L:274:ARG:HH21	1.78	0.49
2:C:1103:VAL:N	2:C:1104:PRO:HD2	2.28	0.49
3:D:1298:VAL:H	3:D:1299:GLY:HA3	1.78	0.49
3:D:679:TYR:CZ	3:D:683:ILE:HD11	2.47	0.49
1:H:99:ILE:HD12	1:H:145:LYS:HB2	1.93	0.49
2:I:615:VAL:HG13	2:I:650:VAL:HA	1.95	0.49
2:I:724:VAL:HG23	2:I:775:GLU:O	2.13	0.49
2:I:848:GLU:CG	2:I:888:THR:HG22	2.43	0.49
3:J:201:LEU:HB2	3:J:221:ILE:HD13	1.95	0.49
3:J:26:SER:HB2	3:J:236:TRP:CZ2	2.48	0.49
1:B:308:ALA:HA	1:B:312:LEU:O	2.12	0.49
1:A:45:ARG:HH12	1:B:37:HIS:HB2	1.77	0.49
3:D:10:ALA:O	3:D:11:GLN:HB2	2.13	0.49
3:D:853:THR:HG22	3:D:854:ALA:H	1.78	0.49
1:H:58:GLU:HG3	1:H:145:LYS:HD3	1.94	0.49
2:C:1319:MET:HG3	2:C:1320:PRO:HD2	1.95	0.49
2:C:569:ILE:H	2:C:569:ILE:HD12	1.78	0.49
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.95	0.49
5:F:573:LEU:H	5:F:573:LEU:HD23	1.77	0.49
1:H:182:ARG:NH1	3:J:581:MET:SD	2.86	0.49
3:J:232:ASN:ND2	3:J:1337:VAL:O	2.46	0.49
2:C:314:ASN:ND2	2:C:314:ASN:O	2.46	0.49
2:C:519:ASN:OD1	2:C:796:LEU:HD23	2.12	0.49
3:D:811:GLU:OE1	3:D:890:THR:HG23	2.13	0.49
1:H:67:GLU:HA	1:H:78:ILE:HG21	1.94	0.49
2:I:1276:TRP:CZ2	3:J:801:VAL:HG11	2.48	0.49
2:C:262:TYR:HE1	2:C:280:ASP:OD2	1.96	0.48
2:C:903:ARG:O	2:C:907:GLY:HA2	2.12	0.48
3:D:75:TYR:CE1	3:D:85:CYS:HA	2.47	0.48
5:F:511:ILE:HG22	5:F:517:SER:O	2.12	0.48
2:I:417:SER:OG	2:I:418:GLY:N	2.46	0.48
2:I:446:ASP:N	2:I:446:ASP:OD1	2.43	0.48
5:L:476:ARG:HD2	5:L:477:GLU:HG2	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:ARG:O	1:A:168:ILE:N	2.46	0.48
3:D:435:GLN:HB2	3:D:457:TYR:OH	2.12	0.48
5:F:280:VAL:CG2	5:F:347:ILE:HG21	2.43	0.48
1:G:179:PRO:HA	1:G:208:ASN:HD21	1.78	0.48
1:H:196:THR:HG23	3:J:443:GLU:HG3	1.95	0.48
3:J:559:ALA:O	3:J:561:GLY:N	2.45	0.48
1:B:265:ARG:NH2	1:B:294:ASN:HB3	2.28	0.48
1:B:270:LEU:HD22	1:B:281:LEU:HD13	1.96	0.48
2:C:1013:GLN:O	2:C:1017:GLN:HG2	2.13	0.48
2:C:250:THR:HA	2:C:268:ARG:HA	1.94	0.48
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.95	0.48
2:C:994:ARG:HD2	2:C:997:TRP:CZ2	2.48	0.48
3:D:427:PRO:O	3:D:429:LEU:HD22	2.13	0.48
5:F:250:LEU:O	5:F:254:GLU:HG2	2.14	0.48
1:H:91:ARG:HG3	1:H:122:GLU:HB3	1.94	0.48
2:I:468:LEU:O	2:I:471:VAL:HG12	2.13	0.48
2:I:824:GLN:HE22	2:I:1082:ILE:HD11	1.78	0.48
3:J:1327:GLU:OE1	3:J:1329:THR:HB	2.13	0.48
3:J:1352:ILE:HA	8:J:2004:4C2:O2	2.13	0.48
3:J:915:ILE:HA	3:J:918:ILE:HG12	1.95	0.48
2:C:175:ARG:HD3	2:C:183:TRP:CZ3	2.49	0.48
2:C:10:ARG:NH2	2:C:791:LEU:HD12	2.28	0.48
3:D:97:VAL:HG12	3:D:101:ARG:HG3	1.94	0.48
5:F:125:ASP:O	5:F:129:GLN:HB2	2.14	0.48
3:J:1198:VAL:HG23	3:J:1204:VAL:HG11	1.94	0.48
3:J:45:ASN:O	3:J:46:TYR:HB3	2.11	0.48
3:J:818:GLU:CG	3:J:887:SER:HB2	2.43	0.48
2:C:26:TYR:HE2	2:C:32:LEU:HD12	1.79	0.48
1:H:51:MET:HB3	1:H:178:SER:HB3	1.95	0.48
3:J:1316:THR:HG22	3:J:1318:SER:H	1.79	0.48
3:J:343:LEU:HB3	3:J:344:GLY:HA3	1.95	0.48
3:J:515:ARG:HG3	3:J:516:ASP:N	2.29	0.48
3:J:94:GLN:O	3:J:97:VAL:HG23	2.14	0.48
5:L:561:MET:HG3	5:L:567:MET:CE	2.43	0.48
1:B:79:LEU:H	1:B:79:LEU:HD23	1.78	0.48
5:F:555:GLU:O	5:F:558:VAL:HG12	2.14	0.48
2:I:715:THR:HG23	2:I:717:VAL:HG23	1.95	0.48
2:I:1291:LEU:HD22	8:J:2004:4C2:H16	1.94	0.48
3:J:642:ASP:HA	3:J:764:ARG:HH21	1.76	0.48
1:A:134:THR:OG1	1:A:134:THR:O	2.32	0.48
1:A:178:SER:HA	1:A:179:PRO:HD3	1.68	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:176:ILE:HD11	2:C:428:VAL:HG11	1.95	0.48
3:D:1157:ALA:HB2	3:D:1210:ILE:HD11	1.96	0.48
2:C:1269:ARG:NE	3:D:343:LEU:HD22	2.29	0.48
2:I:816:ILE:O	2:I:1076:ILE:HD12	2.13	0.48
2:I:197:ARG:HH22	2:I:203:LYS:HE3	1.78	0.48
2:I:563:THR:OG1	2:I:564:PRO:HD2	2.13	0.48
2:I:882:ILE:HD11	2:I:919:ARG:HH12	1.79	0.48
3:J:133:ARG:O	3:J:137:ARG:HB2	2.14	0.48
3:J:363:LEU:HD23	3:J:487:THR:HG22	1.95	0.48
1:B:246:LYS:HB3	1:B:246:LYS:HE3	1.66	0.48
1:B:73:GLY:HA2	1:B:134:THR:HB	1.96	0.48
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.95	0.48
3:D:1298:VAL:N	3:D:1299:GLY:HA3	2.29	0.48
3:D:268:LEU:HD21	3:D:324:LEU:HD13	1.96	0.48
5:F:139:GLU:CG	5:F:351:THR:HA	2.42	0.48
5:F:492:ASP:HB2	5:F:495:ARG:NH2	2.27	0.48
1:G:195:ARG:HG2	1:G:198:LEU:CG	2.35	0.48
2:I:1255:THR:O	2:I:1257:GLN:N	2.47	0.48
2:I:582:ASN:HB3	2:I:586:PHE:H	1.77	0.48
3:J:193:ASP:CG	3:J:196:GLN:HG2	2.34	0.48
5:L:561:MET:HA	5:L:567:MET:HE1	1.96	0.48
2:C:17:LYS:HG2	2:C:1154:ASP:O	2.13	0.48
2:C:1235:LEU:O	2:C:1237:HIS:N	2.45	0.48
3:D:1309:ILE:HG13	3:D:1310:THR:N	2.29	0.48
2:I:1117:LEU:HD12	2:I:1195:ILE:HG12	1.95	0.48
3:J:218:THR:HA	3:J:221:ILE:HG22	1.96	0.48
3:J:857:LEU:HD12	3:J:858:VAL:H	1.79	0.48
5:L:147:GLN:O	5:L:151:VAL:HG23	2.13	0.48
2:C:435:ILE:HG12	2:C:440:GLY:HA3	1.95	0.48
2:C:600:THR:HB	2:C:602:GLU:HG2	1.96	0.48
3:D:161:THR:HG22	3:D:164:GLN:HG3	1.95	0.48
3:D:688:ALA:O	3:D:692:ARG:HG3	2.14	0.48
5:F:484:ALA:HB1	5:F:491:GLU:CB	2.44	0.48
3:J:770:LEU:HD22	3:J:770:LEU:N	2.27	0.48
2:C:10:ARG:NH2	2:C:790:ASP:OD2	2.42	0.47
3:J:1238:GLN:O	3:J:1242:ARG:HB2	2.14	0.47
4:K:77:ALA:C	4:K:79:GLU:H	2.17	0.47
2:C:131:THR:HG22	2:C:132:ASP:N	2.29	0.47
2:C:274:ILE:O	2:C:278:GLU:HG3	2.14	0.47
2:C:886:LYS:H	2:C:917:SER:HB3	1.79	0.47
2:C:848:GLU:CG	2:C:888:THR:HG22	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:214:GLU:HA	1:G:217:ILE:HG22	1.96	0.47
2:I:253:PHE:CZ	2:I:287:VAL:HG12	2.49	0.47
2:I:375:PRO:HA	2:I:376:PRO:HD3	1.77	0.47
3:J:407:VAL:O	3:J:411:ILE:HG12	2.13	0.47
1:B:252:ILE:O	1:B:255:ARG:HB2	2.15	0.47
1:B:313:SER:OG	1:B:314:LEU:N	2.45	0.47
3:D:1282:TYR:HD2	3:D:1286:LYS:NZ	2.07	0.47
3:D:372:MET:O	3:D:376:LEU:HD12	2.14	0.47
3:D:557:LYS:HA	3:D:562:GLU:O	2.14	0.47
3:D:854:ALA:HB2	3:J:1372:ARG:HG3	1.95	0.47
5:F:166:VAL:HG12	5:F:167:ASP:OD1	2.14	0.47
2:I:27:LEU:O	2:I:528:ARG:NH1	2.40	0.47
2:C:147:SER:OG	2:C:455:SER:HB3	2.14	0.47
2:C:263:VAL:HG22	2:C:273:HIS:CD2	2.49	0.47
2:C:117:ILE:HD11	2:C:485:ASP:OD1	2.14	0.47
3:D:800:LEU:O	3:D:803:VAL:HG12	2.15	0.47
1:G:81:ILE:HG12	1:G:131:CYS:HB3	1.96	0.47
3:J:165:TYR:CZ	3:J:169:LEU:HD11	2.49	0.47
3:J:325:LYS:HE3	3:J:330:MET:HB3	1.96	0.47
3:J:846:GLU:HA	3:J:860:ARG:NE	2.28	0.47
1:H:109:PRO:HB3	1:H:132:HIS:HD2	1.78	0.47
2:I:807:TRP:O	2:I:807:TRP:HE3	1.97	0.47
2:I:5:TYR:O	2:I:8:LYS:HG2	2.15	0.47
3:J:265:LEU:HG	3:J:330:MET:HE1	1.97	0.47
2:C:101:ARG:HH21	2:C:118:LYS:HE2	1.79	0.47
3:D:110:PRO:HG2	3:D:183:GLU:HG3	1.96	0.47
2:I:510:GLN:NE2	2:I:534:GLY:HA2	2.29	0.47
2:C:1192:GLU:HA	2:C:1195:ILE:HD12	1.97	0.47
2:C:865:LEU:HD22	2:C:869:GLY:O	2.15	0.47
3:D:342:LEU:O	3:D:343:LEU:O	2.33	0.47
3:D:698:MET:O	3:D:702:GLN:HB2	2.15	0.47
1:G:161:SER:O	1:G:163:GLU:HG3	2.15	0.47
1:G:218:ARG:HD3	1:H:233:ASP:CB	2.44	0.47
2:I:1103:VAL:N	2:I:1104:PRO:HD2	2.29	0.47
1:A:104:LYS:HG2	1:A:110:VAL:HG22	1.97	0.47
5:F:594:ALA:O	5:F:598:LEU:HG	2.15	0.47
1:G:68:TYR:HE2	2:I:927:THR:HB	1.79	0.47
1:H:154:PRO:HD2	1:H:157:THR:OG1	2.15	0.47
3:J:1266:ILE:HD12	3:J:1274:PHE:C	2.35	0.47
3:J:555:TYR:CE1	3:J:565:ALA:HB2	2.49	0.47
3:J:847:ASP:OD2	3:J:860:ARG:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:145:LEU:CD2	5:L:224:LEU:HD23	2.45	0.47
3:D:128:LEU:HD23	3:D:192:MET:HE3	1.96	0.47
3:D:825:VAL:C	3:D:826:ILE:HG13	2.35	0.47
1:G:102:LEU:O	1:G:141:SER:HA	2.15	0.47
2:I:1042:LEU:HB3	2:I:1046:VAL:HG13	1.96	0.47
2:I:720:ARG:HB2	2:I:749:ASP:OD1	2.15	0.47
2:I:864:LYS:NZ	2:I:881:ASP:OD2	2.42	0.47
3:J:209:ASN:C	3:J:214:ARG:HH21	2.19	0.47
3:J:479:GLU:CG	4:K:20:VAL:HG11	2.45	0.47
5:L:468:ARG:HA	5:L:471:LEU:HD12	1.96	0.47
2:C:69:GLN:NE2	2:C:101:ARG:HD2	2.29	0.47
3:D:210:SER:O	3:D:214:ARG:HG2	2.15	0.47
3:D:382:TYR:HE1	3:D:401:VAL:HG21	1.79	0.47
5:F:137:TYR:CZ	5:F:139:GLU:HB2	2.50	0.47
2:C:906:PHE:HE2	5:F:608:ARG:HH11	1.60	0.47
3:J:211:GLU:O	3:J:215:LYS:HB2	2.15	0.47
3:J:343:LEU:HB3	3:J:344:GLY:CA	2.45	0.47
5:L:248:GLU:HG3	5:L:251:LYS:HZ1	1.79	0.47
3:D:201:LEU:O	3:D:217:LEU:HD12	2.15	0.47
3:D:194:LEU:HD13	3:D:228:VAL:HG22	1.97	0.47
1:H:107:ILE:HG23	1:H:134:THR:O	2.15	0.47
1:H:27:THR:HG22	1:H:202:VAL:HG22	1.97	0.47
1:H:79:LEU:HD23	1:H:79:LEU:H	1.79	0.47
2:I:138:ILE:HD12	2:I:138:ILE:HA	1.75	0.47
3:J:342:LEU:O	3:J:343:LEU:O	2.33	0.47
3:J:430:HIS:ND1	3:J:925:GLU:HG3	2.30	0.47
1:A:67:GLU:HG3	1:A:79:LEU:HD23	1.95	0.46
2:C:169:LYS:O	2:C:170:VAL:HG22	2.14	0.46
2:C:494:ASN:O	2:C:497:PRO:HD2	2.15	0.46
3:D:1198:VAL:HG23	3:D:1204:VAL:HG11	1.96	0.46
3:D:812:ASP:O	3:D:896:ALA:HB3	2.14	0.46
5:F:412:LEU:HD13	5:F:435:ILE:HD11	1.96	0.46
1:G:126:PRO:HD2	1:G:127:GLN:NE2	2.31	0.46
2:I:1106:ARG:CZ	3:J:731:ARG:HH21	2.28	0.46
2:I:131:THR:HG22	2:I:132:ASP:N	2.29	0.46
2:I:462:ASN:O	2:I:466:VAL:HG23	2.15	0.46
3:J:1357:ILE:HG22	3:J:1359:ALA:N	2.30	0.46
1:H:83:LEU:HD21	3:J:526:VAL:HB	1.96	0.46
5:L:114:GLU:HA	5:L:117:ILE:HD12	1.95	0.46
2:C:1120:ALA:HB2	2:C:1199:LEU:HG	1.97	0.46
1:H:73:GLY:HA3	1:H:138:ALA:HB1	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:224:LEU:O	1:H:228:LEU:HD12	2.14	0.46
2:I:174:ALA:HB2	2:I:432:LEU:HD13	1.96	0.46
1:G:70:THR:CG2	2:I:755:LYS:HE2	2.46	0.46
3:J:698:MET:O	3:J:702:GLN:HB2	2.16	0.46
3:J:810:THR:HG23	3:J:811:GLU:N	2.29	0.46
3:J:847:ASP:N	3:J:860:ARG:HA	2.30	0.46
3:J:849:LEU:HG	3:J:853:THR:HG23	1.98	0.46
4:K:22:VAL:HG13	4:K:64:LEU:HD12	1.96	0.46
1:B:255:ARG:NH1	1:B:255:ARG:CG	2.61	0.46
2:C:555:TYR:CE1	2:C:637:ARG:CZ	2.99	0.46
2:C:700:VAL:HG11	2:C:1114:GLU:HG2	1.97	0.46
3:D:1250:ASP:O	3:D:1251:LYS:C	2.53	0.46
3:D:165:TYR:CE2	3:D:178:ALA:HB3	2.50	0.46
5:F:407:GLU:HA	5:F:410:ILE:HD12	1.97	0.46
1:G:187:VAL:HG22	1:G:201:LEU:HD13	1.97	0.46
1:H:187:VAL:HG22	1:H:201:LEU:HD13	1.98	0.46
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.98	0.46
2:I:718:ALA:HB3	2:I:780:GLY:H	1.80	0.46
3:J:902:ASP:O	3:J:903:LEU:HD13	2.15	0.46
5:L:490:PRO:HD2	5:L:493:LYS:HD2	1.97	0.46
3:J:46:TYR:HD1	5:L:500:ILE:HG21	1.79	0.46
3:D:405:GLU:O	3:D:408:VAL:HG22	2.14	0.46
5:F:285:ARG:O	5:F:289:LYS:HG3	2.15	0.46
1:G:188:GLU:OE2	1:G:200:LYS:HD3	2.15	0.46
3:J:814:CYS:HB2	3:J:889:ASP:HB3	1.98	0.46
2:C:617:ALA:HA	2:C:636:CYS:SG	2.56	0.46
2:C:985:GLU:HB3	2:C:988:LYS:HB2	1.98	0.46
3:D:615:LYS:HG3	3:D:615:LYS:H	1.49	0.46
3:D:826:ILE:HA	3:D:831:VAL:HA	1.98	0.46
3:D:1227:HIS:CG	3:J:1293:GLU:HG2	2.51	0.46
3:J:824:PRO:CD	3:J:835:LEU:HB2	2.45	0.46
1:B:19:VAL:O	1:B:23:HIS:HB3	2.16	0.46
2:C:1259:LEU:HD12	2:C:1260:GLY:H	1.80	0.46
2:C:1289:GLU:OE2	3:D:473:THR:HG22	2.14	0.46
2:C:158:ASP:HB3	2:C:173:ASN:OD1	2.15	0.46
3:D:412:LEU:O	3:D:416:ILE:HG12	2.16	0.46
3:D:495:ASN:ND2	3:D:497:GLU:HB2	2.31	0.46
1:G:75:GLN:HG3	1:G:76:GLU:OE1	2.14	0.46
2:I:883:LEU:HD22	2:I:1052:VAL:HG11	1.98	0.46
2:I:836:LEU:HB3	2:I:918:LEU:HD21	1.97	0.46
1:B:188:GLU:HG3	1:B:200:LYS:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:455:SER:O	2:C:457:GLY:N	2.49	0.46
2:I:1142:ARG:HH22	2:I:1165:SER:CB	2.22	0.46
2:I:693:LEU:HB2	2:I:829:THR:O	2.14	0.46
3:J:615:LYS:HG3	3:J:615:LYS:H	1.37	0.46
5:L:600:HIS:CG	5:L:601:PRO:HD2	2.50	0.46
3:D:1169:THR:OG1	3:D:1192:LYS:HD3	2.16	0.46
3:D:75:TYR:HE1	3:D:85:CYS:HA	1.81	0.46
2:I:30:ILE:HD12	2:I:30:ILE:H	1.81	0.46
3:J:400:MET:HG2	3:J:405:GLU:OE2	2.16	0.46
3:J:526:VAL:HG12	3:J:569:LEU:HD21	1.98	0.46
1:A:44:ARG:HG3	1:A:183:ILE:HG22	1.98	0.46
1:B:286:GLU:OE2	1:B:300:LEU:HD11	2.16	0.46
1:B:299:SER:O	1:B:303:ILE:HG12	2.16	0.46
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.97	0.46
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.97	0.46
2:C:1256:GLN:HB3	2:C:1301:ARG:HH22	1.80	0.46
2:C:992:LEU:HB2	2:C:993:PRO:HD2	1.98	0.46
3:D:1357:ILE:HG22	3:D:1359:ALA:H	1.80	0.46
3:D:268:LEU:HD23	3:D:271:ARG:NH1	2.31	0.46
3:J:101:ARG:O	3:J:246:PRO:HG3	2.16	0.46
3:J:797:THR:HG23	3:J:924:GLY:HA3	1.98	0.46
2:C:50:GLU:HG2	2:C:73:TYR:HE1	1.81	0.45
2:C:820:GLU:O	2:C:823:VAL:N	2.49	0.45
2:C:930:ASP:OD2	2:C:931:VAL:N	2.49	0.45
5:F:98:VAL:HB	5:F:402:LEU:HD11	1.97	0.45
1:H:125:LYS:CD	1:H:128:HIS:HB2	2.47	0.45
3:J:514:THR:HG23	3:J:576:ARG:CG	2.46	0.45
3:J:612:LEU:HB3	3:J:616:PRO:HG2	1.98	0.45
3:J:62:PHE:CD1	3:J:247:PRO:HD3	2.51	0.45
5:L:137:TYR:HA	5:L:138:PRO:HD3	1.71	0.45
1:B:191:ARG:HA	1:B:198:LEU:HD23	1.98	0.45
2:C:798:GLN:HB2	2:C:828:PHE:HE1	1.81	0.45
3:D:1164:SER:O	3:D:1175:LEU:HD12	2.16	0.45
3:D:148:GLU:H	3:D:156:ARG:HG3	1.80	0.45
3:D:370:LYS:N	3:D:442:ILE:O	2.49	0.45
5:F:279:ARG:NH2	5:F:346:GLN:OE1	2.50	0.45
2:I:802:VAL:HG21	2:I:1098:LEU:HD22	1.98	0.45
2:I:646:SER:HB3	2:I:649:GLN:CD	2.37	0.45
3:J:1358:PRO:HB3	3:J:1366:HIS:CD2	2.51	0.45
5:L:479:THR:HG22	5:L:482:GLU:HB2	1.98	0.45
2:C:1070:HIS:CD2	2:C:1111:GLN:HA	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:67:GLU:O	1:H:78:ILE:HB	2.17	0.45
2:I:1030:GLU:OE1	2:I:1033:ARG:NH2	2.50	0.45
3:J:418:GLU:HB2	4:K:45:LYS:HB2	1.97	0.45
2:C:119:GLU:CB	2:C:489:PRO:HG2	2.45	0.45
3:D:19:ALA:HB2	3:D:1373:ARG:NH2	2.31	0.45
3:D:378:LYS:HB2	3:D:379:PRO:HD3	1.97	0.45
3:D:842:ARG:HB3	3:D:882:VAL:CG1	2.46	0.45
5:F:346:GLN:O	5:F:346:GLN:HG2	2.16	0.45
2:I:804:PHE:CE1	2:I:1098:LEU:HD23	2.52	0.45
2:I:1106:ARG:O	2:I:1108:ASN:N	2.44	0.45
2:I:807:TRP:HE1	2:I:1086:PRO:HG3	1.81	0.45
3:J:491:LEU:HD22	3:J:496:GLY:O	2.16	0.45
2:C:106:GLU:OE1	2:C:114:VAL:HG22	2.16	0.45
2:C:481:LEU:H	2:C:481:LEU:HD22	1.81	0.45
3:D:770:LEU:N	3:D:770:LEU:HD22	2.28	0.45
1:G:112:ALA:HB3	1:G:126:PRO:HA	1.98	0.45
1:G:191:ARG:NH2	1:G:197:ASP:HA	2.28	0.45
2:I:1334:GLY:O	3:J:25:ALA:HB3	2.17	0.45
2:I:402:ARG:HG2	2:I:416:GLY:H	1.82	0.45
2:I:62:TYR:C	2:I:64:GLY:H	2.18	0.45
2:I:753:LEU:HD23	2:I:767:GLN:HB3	1.97	0.45
3:J:117:LEU:HD23	3:J:118:LYS:HG2	1.99	0.45
5:L:483:LEU:H	5:L:483:LEU:HD12	1.80	0.45
1:A:13:LEU:O	1:A:13:LEU:HG	2.17	0.45
2:C:551:HIS:CE1	2:C:553:THR:HG1	2.33	0.45
3:D:16:GLU:HG3	3:D:1369:ARG:NH1	2.31	0.45
3:D:423:LEU:HB3	3:D:466:MET:HE1	1.99	0.45
2:C:1276:TRP:CE2	3:D:801:VAL:HG11	2.51	0.45
1:G:178:SER:HA	1:G:179:PRO:HD3	1.82	0.45
1:G:45:ARG:HH12	1:H:37:HIS:HB2	1.80	0.45
1:H:83:LEU:HD11	3:J:526:VAL:HG23	1.99	0.45
3:J:694:SER:O	3:J:698:MET:HB2	2.17	0.45
3:J:81:ARG:HG3	3:J:82:GLY:H	1.81	0.45
1:B:251:PRO:HA	1:B:254:LEU:HD12	1.97	0.45
2:C:483:ASP:HB3	2:C:486:THR:HG21	1.98	0.45
3:D:537:TYR:CE1	3:D:544:LEU:HB2	2.52	0.45
3:D:712:GLN:HB2	3:D:713:GLU:H	1.51	0.45
3:D:880:VAL:HG12	3:D:882:VAL:HG23	1.99	0.45
3:D:325:LYS:HD3	5:F:508:GLU:HG2	1.99	0.45
1:G:12:ARG:H	1:G:30:PRO:CD	2.25	0.45
3:J:268:LEU:HD13	3:J:306:LEU:HA	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:488:ASN:HB3	4:K:16:ARG:HH21	1.82	0.45
5:L:277:MET:HG3	5:L:362:ASN:ND2	2.31	0.45
5:L:547:VAL:HG13	5:L:598:LEU:HD22	1.98	0.45
2:C:1042:LEU:HB3	2:C:1046:VAL:HG13	1.98	0.45
2:C:17:LYS:HE3	2:C:1154:ASP:HB3	1.98	0.45
2:C:185:ASP:O	2:C:196:VAL:HA	2.16	0.45
3:D:355:ILE:HG22	3:D:447:ILE:HB	1.99	0.45
1:G:76:GLU:OE1	1:G:76:GLU:N	2.49	0.45
1:H:51:MET:HA	1:H:52:PRO:HD3	1.85	0.45
5:L:573:LEU:H	5:L:573:LEU:HD23	1.82	0.45
5:L:600:HIS:CD2	5:L:601:PRO:HD2	2.51	0.45
1:B:269:CYS:O	1:B:273:GLU:HB2	2.16	0.45
1:B:288:GLU:H	1:B:288:GLU:HG2	1.49	0.45
2:C:268:ARG:HH21	2:C:270:THR:HG21	1.81	0.45
1:H:10:LYS:HA	1:H:11:PRO:HD3	1.62	0.45
2:I:617:ALA:HA	2:I:636:CYS:SG	2.56	0.45
2:I:741:MET:HG2	2:I:974:ARG:HH21	1.82	0.45
2:I:890:LYS:NZ	2:I:891:GLY:O	2.28	0.45
3:J:789:LYS:HD3	3:J:1138:LEU:HD23	1.99	0.45
3:J:811:GLU:O	3:J:895:CYS:HA	2.16	0.45
3:J:858:VAL:HA	3:J:859:PRO:HD3	1.81	0.45
2:C:453:ILE:HG23	2:C:453:ILE:O	2.16	0.45
2:C:660:VAL:HG22	2:C:660:VAL:O	2.16	0.45
3:D:1179:PRO:CD	3:D:1184:ASP:HB3	2.44	0.45
3:D:1194:ARG:O	3:D:1196:LEU:HD22	2.17	0.45
3:D:1266:ILE:H	3:D:1266:ILE:HG13	1.55	0.45
3:D:654:ILE:O	3:D:658:GLU:HG3	2.17	0.45
3:D:865:HIS:HB2	3:D:866:GLU:H	1.60	0.45
3:J:1280:VAL:HA	3:J:1283:SER:HB3	1.99	0.45
3:J:362:ARG:HB2	3:J:365:GLN:HG2	1.99	0.45
3:J:610:ARG:HG2	3:J:866:GLU:CD	2.38	0.45
3:J:826:ILE:HD12	3:J:826:ILE:O	2.17	0.45
5:L:594:ALA:O	5:L:598:LEU:HG	2.17	0.45
1:B:289:LEU:HB3	1:B:300:LEU:CD2	2.46	0.44
3:D:622:ASP:O	3:D:625:MET:N	2.50	0.44
3:D:9:LYS:HG2	3:D:11:GLN:H	1.83	0.44
5:F:515:GLU:HB3	5:F:517:SER:OG	2.17	0.44
1:G:207:THR:HG22	1:G:208:ASN:N	2.32	0.44
1:G:91:ARG:HB3	1:G:122:GLU:HB3	1.98	0.44
2:I:1232:MET:C	2:I:1233:LEU:HD13	2.38	0.44
2:I:34:SER:OG	2:I:455:SER:O	2.25	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:201:LEU:O	3:J:217:LEU:HD11	2.17	0.44
5:L:230:VAL:HG13	5:L:248:GLU:HG2	1.99	0.44
2:C:1196:LYS:HD2	2:C:1206:THR:OG1	2.17	0.44
2:C:37:LYS:HA	2:C:37:LYS:HD3	1.79	0.44
3:D:451:PRO:HD2	3:D:625:MET:SD	2.58	0.44
2:I:198:ILE:HG22	2:I:199:ASP:OD2	2.17	0.44
2:I:867:GLU:HG3	2:I:867:GLU:H	1.60	0.44
2:I:885:GLY:HA2	2:I:917:SER:CB	2.48	0.44
3:J:53:ARG:HA	3:J:54:ASP:HA	1.59	0.44
3:J:858:VAL:CG1	3:J:872:LEU:HD11	2.42	0.44
2:C:1271:GLY:HA3	3:D:343:LEU:HD23	1.99	0.44
2:C:671:LEU:O	2:C:673:HIS:N	2.51	0.44
2:C:722:GLY:HA2	2:C:737:ASN:OD1	2.17	0.44
3:D:900:GLY:O	3:D:908:ILE:HG12	2.16	0.44
2:I:551:HIS:CG	2:I:552:PRO:HD2	2.53	0.44
3:J:1263:LYS:HD2	3:J:1277:GLY:O	2.18	0.44
3:J:527:LEU:HB2	3:J:550:VAL:HG12	1.99	0.44
5:L:137:TYR:CZ	5:L:139:GLU:HB2	2.53	0.44
5:L:387:VAL:HG22	5:L:435:ILE:HD13	2.00	0.44
2:C:1272:GLU:O	2:C:1275:VAL:HB	2.18	0.44
3:D:250:ARG:HB3	3:D:265:LEU:HD12	1.99	0.44
3:D:740:LEU:HD12	3:D:740:LEU:HA	1.84	0.44
3:D:825:VAL:O	3:D:826:ILE:HG13	2.18	0.44
3:D:899:TYR:O	3:D:1251:LYS:HD3	2.18	0.44
2:I:870:ILE:HG12	2:I:1050:VAL:HG11	1.98	0.44
2:I:213:LEU:HB3	2:I:422:LYS:HD3	1.99	0.44
2:I:972:PHE:HE2	2:I:998:LEU:HD11	1.82	0.44
3:J:24:LEU:HA	3:J:24:LEU:HD13	1.81	0.44
5:L:483:LEU:HA	5:L:486:ARG:NH1	2.32	0.44
5:L:540:LEU:HD23	5:L:540:LEU:O	2.17	0.44
2:C:138:ILE:HA	2:C:138:ILE:HD12	1.59	0.44
2:C:297:VAL:HG12	2:C:315:MET:O	2.17	0.44
2:C:496:LYS:HE3	2:C:496:LYS:HB3	1.77	0.44
3:D:400:MET:HG2	3:D:405:GLU:OE2	2.16	0.44
5:F:95:THR:HA	5:F:100:MET:HE3	2.00	0.44
1:H:153:VAL:HA	1:H:154:PRO:HD3	1.61	0.44
2:I:388:LEU:HB3	2:I:389:PHE:CE2	2.52	0.44
3:J:342:LEU:HB3	3:J:343:LEU:H	1.61	0.44
3:J:821:MET:HE1	3:J:879:ALA:HB1	1.99	0.44
1:B:102:LEU:HD23	1:B:103:ASN:N	2.32	0.44
2:C:496:LYS:HB3	2:C:497:PRO:HD3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:210:SER:HB2	3:D:213:LYS:CB	2.46	0.44
3:D:255:LEU:HA	3:D:255:LEU:HD13	1.63	0.44
5:F:137:TYR:HA	5:F:138:PRO:HD3	1.76	0.44
5:F:394:TYR:CD2	5:F:439:ILE:HG21	2.53	0.44
1:G:100:LEU:HD21	1:G:121:VAL:HG21	1.98	0.44
2:I:811:ASN:HD21	2:I:1097:VAL:HG12	1.83	0.44
3:D:1302:TYR:OH	3:J:1291:GLU:HG2	2.16	0.44
3:D:218:THR:HA	3:D:221:ILE:HG22	2.00	0.44
3:D:397:ALA:O	3:D:401:VAL:HG13	2.18	0.44
5:F:583:THR:HG22	5:F:584:ARG:N	2.33	0.44
2:I:1164:PHE:HD1	2:I:1164:PHE:HA	1.71	0.44
2:I:748:ILE:HG12	2:I:748:ILE:O	2.18	0.44
1:B:287:VAL:O	1:B:291:LYS:HE2	2.18	0.44
2:C:145:ILE:HG22	2:C:456:VAL:HG22	1.99	0.44
2:C:484:LEU:HB2	2:C:485:ASP:H	1.62	0.44
2:C:646:SER:HB3	2:C:649:GLN:HB2	1.99	0.44
3:D:317:THR:CG2	3:D:320:ASN:HB3	2.47	0.44
3:D:442:ILE:HA	3:D:442:ILE:HD13	1.63	0.44
3:D:858:VAL:HA	3:D:859:PRO:HD3	1.71	0.44
1:H:84:ASN:O	1:H:128:HIS:CE1	2.66	0.44
2:I:103:VAL:HG12	2:I:116:ASP:CB	2.47	0.44
2:I:556:GLY:HA2	2:I:659:GLN:O	2.18	0.44
2:I:811:ASN:O	2:I:1099:ASN:HB2	2.17	0.44
3:J:707:ILE:HD11	3:J:716:GLN:HG2	1.99	0.44
5:L:584:ARG:NH1	5:L:584:ARG:HA	2.33	0.44
1:A:207:THR:HB	1:A:209:GLY:H	1.82	0.44
2:C:528:ARG:CZ	2:C:575:LEU:HD23	2.48	0.44
3:D:854:ALA:CB	3:J:1372:ARG:HG3	2.48	0.44
2:I:176:ILE:HB	2:I:184:LEU:HB3	2.00	0.44
2:I:197:ARG:HH12	2:I:203:LYS:HB2	1.83	0.44
2:I:388:LEU:HB3	2:I:389:PHE:CD2	2.52	0.44
2:I:494:ASN:O	2:I:497:PRO:HD2	2.17	0.44
3:J:1140:ARG:NH2	3:J:1236:GLU:HG2	2.32	0.44
3:J:1269:ALA:HB2	3:J:1274:PHE:HD1	1.83	0.44
3:J:115:TRP:HZ3	3:J:1332:LEU:HD22	1.83	0.44
3:J:614:LEU:O	3:J:618:VAL:HG23	2.18	0.44
2:I:1276:TRP:CE2	3:J:801:VAL:HG11	2.53	0.44
3:J:801:VAL:O	3:J:805:GLN:HB2	2.18	0.44
1:A:10:LYS:HE3	1:B:229:GLU:OE1	2.17	0.43
2:C:61:SER:HB3	2:C:479:LEU:HB3	2.00	0.43
3:D:515:ARG:HG3	3:D:516:ASP:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:280:VAL:HG22	5:F:347:ILE:HG21	2.00	0.43
1:H:100:LEU:HD21	1:H:121:VAL:HG11	1.99	0.43
2:I:1176:LEU:HD22	2:I:1180:MET:HG2	2.00	0.43
2:I:281:ASP:OD1	2:I:283:LYS:HE3	2.18	0.43
2:I:704:MET:O	2:I:706:ARG:N	2.51	0.43
3:J:1264:ALA:CB	3:J:1280:VAL:HG22	2.48	0.43
3:J:843:VAL:HG13	3:J:883:ARG:HB2	2.00	0.43
1:A:31:LEU:HD13	1:A:201:LEU:HB2	2.00	0.43
1:B:73:GLY:CA	1:B:134:THR:HB	2.48	0.43
1:B:289:LEU:O	1:B:295:LEU:HD22	2.18	0.43
1:B:61:ILE:HB	1:B:64:VAL:O	2.17	0.43
2:C:56:VAL:HG11	2:C:468:LEU:HB3	1.99	0.43
2:C:757:THR:OG1	2:C:758:ARG:N	2.51	0.43
3:D:1319:PHE:O	3:D:1322:ALA:HB3	2.18	0.43
3:D:660:GLU:HB3	3:D:685:ILE:HD12	2.01	0.43
3:D:298:MET:SD	5:F:406:GLN:HG3	2.58	0.43
5:F:418:LYS:HD2	5:F:434:TRP:CH2	2.52	0.43
1:G:107:ILE:HD11	1:G:136:GLU:HG2	2.00	0.43
2:I:1142:ARG:HD3	2:I:1161:LEU:HD13	2.00	0.43
2:I:1276:TRP:CD1	3:J:801:VAL:HG21	2.53	0.43
3:J:1184:ASP:N	3:J:1185:PRO:HD3	2.33	0.43
3:J:242:LEU:HD23	3:J:243:PRO:O	2.18	0.43
3:J:265:LEU:HD23	3:J:265:LEU:HA	1.84	0.43
5:L:496:LYS:O	5:L:500:ILE:HG12	2.18	0.43
1:A:167:PRO:O	1:A:170:ARG:HB2	2.18	0.43
1:A:4:SER:O	1:A:5:VAL:HG13	2.18	0.43
1:B:153:VAL:HB	1:B:175:ALA:HB3	1.99	0.43
2:C:189:ASP:HB3	2:C:195:PHE:CE2	2.52	0.43
3:D:510:LEU:HA	3:D:513:MET:HE2	2.00	0.43
3:D:674:THR:OG1	3:D:677:GLU:HB2	2.17	0.43
5:F:502:LYS:O	5:F:503:GLU:HB2	2.19	0.43
1:G:179:PRO:HA	1:G:208:ASN:ND2	2.33	0.43
2:I:1087:TYR:CE1	2:I:1215:GLY:HA2	2.47	0.43
2:I:452:ARG:NH1	2:I:585:GLY:HA3	2.30	0.43
3:J:592:VAL:HA	3:J:596:LEU:HD21	2.00	0.43
3:J:819:GLY:HA3	3:J:882:VAL:O	2.19	0.43
2:C:1073:LYS:HE3	3:D:462:ASP:CB	2.39	0.43
2:C:1067:ALA:O	2:C:1233:LEU:HD22	2.19	0.43
2:C:202:ARG:HD3	2:C:369:MET:HG2	2.00	0.43
3:D:930:LEU:HD11	3:D:1241:TYR:CE2	2.53	0.43
2:C:676:ALA:HA	3:D:772:TYR:OH	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:91:ARG:HD3	1:G:210:THR:O	2.18	0.43
1:H:178:SER:HA	1:H:179:PRO:HD3	1.66	0.43
2:I:1087:TYR:HA	2:I:1093:PRO:HA	2.00	0.43
2:I:207:THR:HG21	2:I:351:LEU:HG	2.00	0.43
3:J:641:ILE:HD13	3:J:644:MET:CE	2.49	0.43
2:C:1166:ASP:O	2:C:1168:GLU:N	2.52	0.43
2:C:285:ILE:HG13	2:C:285:ILE:O	2.19	0.43
2:C:717:VAL:HG12	2:C:718:ALA:N	2.33	0.43
2:C:881:ASP:OD1	2:C:881:ASP:N	2.51	0.43
3:D:1299:GLY:HA2	3:D:1300:ALA:HA	1.72	0.43
3:D:801:VAL:O	3:D:801:VAL:HG22	2.19	0.43
5:F:144:LEU:HD23	5:F:224:LEU:HD21	2.01	0.43
3:J:784:ALA:O	3:J:787:ALA:HB3	2.19	0.43
5:L:448:ARG:HH21	5:L:450:ILE:HG13	1.83	0.43
1:A:108:GLY:HA2	1:A:109:PRO:HD3	1.77	0.43
1:B:293:PRO:O	1:B:294:ASN:HB2	2.17	0.43
2:C:842:ASP:N	2:C:1045:GLY:O	2.49	0.43
2:C:1114:GLU:OE2	2:C:1230:MET:HA	2.19	0.43
2:C:1286:THR:O	2:C:1290:MET:HB2	2.18	0.43
5:F:469:GLN:O	5:F:473:GLU:HB2	2.18	0.43
2:I:17:LYS:HE3	2:I:1154:ASP:HB3	2.01	0.43
2:I:1259:LEU:HD12	2:I:1260:GLY:N	2.33	0.43
3:J:1139:PRO:O	3:J:1142:ALA:HB3	2.18	0.43
2:C:1127:LYS:HE2	2:C:1203:ASP:OD2	2.18	0.43
2:C:673:HIS:HB3	2:C:1109:ILE:HG22	2.00	0.43
2:C:718:ALA:HB3	2:C:780:GLY:H	1.84	0.43
3:D:599:LYS:HD3	3:D:599:LYS:HA	1.76	0.43
5:F:490:PRO:O	5:F:491:GLU:HG2	2.18	0.43
1:G:166:ARG:O	1:G:167:PRO:C	2.57	0.43
3:J:497:GLU:HA	3:J:498:PRO:HD3	1.77	0.43
3:J:66:LYS:HD3	3:J:69:GLU:CD	2.39	0.43
3:J:741:ALA:O	3:J:762:ASN:ND2	2.52	0.43
3:J:892:PHE:H	3:J:1281:GLU:HG2	1.82	0.43
4:K:25:ARG:NH2	4:K:68:GLU:OE1	2.52	0.43
1:A:194:GLN:O	1:A:195:ARG:HB2	2.18	0.43
1:B:62:ASP:OD2	1:B:71:LYS:NZ	2.51	0.43
2:C:310:ILE:HD13	2:C:325:LEU:HA	1.99	0.43
2:C:213:LEU:HD22	2:C:422:LYS:HG2	2.00	0.43
2:C:840:SER:O	2:C:1047:LEU:N	2.51	0.43
3:D:259:ARG:HD3	5:F:502:LYS:HD2	2.00	0.43
3:D:532:GLU:HA	3:D:535:ARG:HB3	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:865:HIS:HE1	3:D:867:GLN:HB2	1.84	0.43
5:F:512:GLY:O	5:F:513:ASP:HB3	2.19	0.43
2:I:1101:LEU:HB3	3:J:731:ARG:HD3	2.01	0.43
2:I:292:ILE:HG23	2:I:295:LYS:HB2	2.00	0.43
2:I:417:SER:OG	2:I:419:ILE:HG13	2.18	0.43
3:J:161:THR:HG23	3:J:163:GLU:H	1.84	0.43
5:L:280:VAL:O	5:L:284:GLU:HB2	2.18	0.43
5:L:379:MET:O	5:L:383:ASN:ND2	2.52	0.43
1:A:42:ALA:O	1:A:46:ILE:HG12	2.19	0.43
1:B:11:PRO:HB2	1:B:28:LEU:HD11	2.00	0.43
1:B:252:ILE:CG2	1:B:278:ILE:HD11	2.48	0.43
1:B:313:SER:HB3	1:B:316:MET:SD	2.59	0.43
2:C:1099:ASN:OD1	2:C:1100:PRO:HD2	2.19	0.43
2:C:178:PRO:HG3	2:C:395:TYR:CE1	2.52	0.43
2:C:175:ARG:NH1	2:C:183:TRP:HZ3	2.15	0.43
3:D:650:LYS:HE2	3:D:654:ILE:HD11	2.01	0.43
4:E:3:ARG:HA	4:E:3:ARG:NE	2.33	0.43
5:F:477:GLU:HB2	5:F:478:PRO:HD2	2.00	0.43
1:H:158:ARG:HB3	1:H:172:LEU:HD23	2.00	0.43
2:I:1223:ARG:HB3	2:I:1223:ARG:NH1	2.33	0.43
3:J:1216:ALA:HB3	3:J:1219:ASP:OD2	2.19	0.43
1:A:133:LEU:HA	1:A:133:LEU:HD13	1.78	0.43
1:A:25:LYS:HG3	1:A:204:GLU:HG3	2.01	0.43
1:A:77:ASP:N	1:A:77:ASP:OD1	2.52	0.43
1:B:180:VAL:O	1:B:180:VAL:HG23	2.19	0.43
1:A:2:GLN:HE22	1:B:249:PHE:HZ	1.67	0.43
2:C:80:PHE:HB3	2:C:84:GLU:HB2	2.00	0.43
2:C:854:ILE:HD11	2:C:885:GLY:HA3	2.01	0.43
3:D:572:THR:HG23	3:D:573:THR:N	2.34	0.43
2:I:820:GLU:O	2:I:823:VAL:HG12	2.19	0.43
3:J:357:VAL:HB	3:J:358:GLY:H	1.53	0.43
2:C:1191:LYS:HD3	2:C:1193:ALA:N	2.22	0.42
2:C:1234:LYS:HZ3	2:C:1238:LEU:HD21	1.84	0.42
2:C:1330:ILE:HA	2:C:1333:LEU:HD12	2.01	0.42
2:C:551:HIS:CE1	2:C:552:PRO:HG2	2.53	0.42
3:D:132:LEU:HA	3:D:135:ILE:HD12	2.01	0.42
5:F:489:MET:HE2	5:F:493:LYS:HD2	2.01	0.42
1:G:46:ILE:HD11	1:H:38:THR:HG21	2.01	0.42
2:I:1099:ASN:ND2	2:I:1101:LEU:HB2	2.33	0.42
2:I:1142:ARG:HH12	2:I:1165:SER:CA	2.27	0.42
2:I:670:PHE:CD1	2:I:1184:THR:HG21	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1273:MET:HG2	2:I:1276:TRP:CZ3	2.53	0.42
2:I:1301:ARG:HG3	2:I:1302:THR:N	2.33	0.42
2:I:455:SER:O	2:I:457:GLY:N	2.51	0.42
2:I:510:GLN:OE1	2:I:534:GLY:HA2	2.19	0.42
3:J:416:ILE:HG21	3:J:441:LEU:HD23	2.01	0.42
3:J:825:VAL:HG22	3:J:833:GLU:H	1.83	0.42
5:L:577:GLY:HA3	5:L:583:THR:HG23	2.01	0.42
1:A:137:ASN:OD1	1:A:137:ASN:N	2.51	0.42
1:A:218:ARG:NH1	1:B:231:PHE:O	2.52	0.42
1:B:94:GLY:HA2	1:B:277:TYR:CZ	2.54	0.42
2:C:93:SER:OG	2:C:126:GLU:OE1	2.24	0.42
3:D:48:THR:O	3:D:49:PHE:C	2.56	0.42
1:H:92:VAL:HA	1:H:120:ASP:O	2.19	0.42
2:I:10:ARG:HG3	2:I:1175:ASN:HB3	2.01	0.42
3:J:123:ARG:NH2	3:J:1334:GLU:HG3	2.34	0.42
3:J:255:LEU:HD13	3:J:255:LEU:HA	1.65	0.42
1:B:47:LEU:O	1:B:180:VAL:HG21	2.19	0.42
3:D:1343:GLU:HG3	3:D:1373:ARG:NH2	2.35	0.42
3:D:53:ARG:HA	3:D:54:ASP:HA	1.64	0.42
1:G:124:VAL:O	1:G:126:PRO:HD3	2.19	0.42
1:G:56:VAL:HG13	1:G:173:VAL:HG21	2.01	0.42
3:J:1306:LEU:HD23	3:J:1307:LEU:N	2.34	0.42
3:J:420:PRO:HA	3:J:439:PRO:HD3	2.01	0.42
3:J:528:THR:O	3:J:551:ARG:HB3	2.20	0.42
3:J:596:LEU:HD11	3:J:604:MET:CE	2.50	0.42
5:L:348:GLU:HA	5:L:353:LEU:O	2.19	0.42
1:B:246:LYS:HA	1:B:247:PRO:HD3	1.93	0.42
3:D:1140:ARG:HH21	3:D:1236:GLU:CG	2.32	0.42
3:D:378:LYS:CB	3:D:379:PRO:HD3	2.50	0.42
3:D:810:THR:HG23	3:D:811:GLU:N	2.33	0.42
5:F:127:ILE:HG13	5:F:128:ASN:N	2.34	0.42
5:F:126:GLY:O	5:F:130:VAL:HG22	2.19	0.42
1:G:108:GLY:HA2	1:G:109:PRO:HD3	1.76	0.42
2:I:1298:VAL:HG23	2:I:1301:ARG:NH1	2.33	0.42
2:I:18:ARG:HA	2:I:19:PRO:HD3	1.83	0.42
2:I:895:LEU:HG	2:I:895:LEU:H	1.71	0.42
3:J:1297:LYS:HD2	3:J:1297:LYS:HA	1.64	0.42
1:B:101:THR:HG22	1:B:116:THR:HG21	2.01	0.42
2:C:1198:LEU:HD22	2:C:1198:LEU:HA	1.88	0.42
2:C:274:ILE:HG22	2:C:278:GLU:OE1	2.20	0.42
2:C:635:THR:HG22	2:C:644:LEU:HD22	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:24:LEU:HA	3:D:24:LEU:HD13	1.65	0.42
3:D:385:LEU:HD23	3:D:411:ILE:HG13	2.00	0.42
3:D:505:ASP:HB2	3:D:629:PHE:HE1	1.85	0.42
3:D:62:PHE:CD1	3:D:247:PRO:HD3	2.55	0.42
1:G:165:GLU:OE2	1:G:172:LEU:HD11	2.18	0.42
2:I:667:LEU:HD11	2:I:708:VAL:HG21	2.01	0.42
3:J:1221:LEU:CD2	3:J:1226:VAL:HG22	2.49	0.42
1:A:77:ASP:OD2	2:C:755:LYS:NZ	2.42	0.42
3:D:491:LEU:HD22	3:D:496:GLY:O	2.20	0.42
5:F:540:LEU:HD23	5:F:540:LEU:O	2.19	0.42
2:I:1326:LEU:O	2:I:1330:ILE:HG22	2.18	0.42
2:I:1330:ILE:HG12	2:I:1335:ILE:HB	2.01	0.42
2:I:274:ILE:O	2:I:278:GLU:HG3	2.19	0.42
2:I:445:ILE:O	2:I:447:HIS:N	2.53	0.42
3:J:242:LEU:HG	3:J:243:PRO:HD2	2.02	0.42
3:J:482:ALA:HB3	4:K:20:VAL:HG22	2.02	0.42
5:L:343:LYS:H	5:L:343:LYS:HD2	1.84	0.42
1:A:220:ALA:HA	1:A:223:ILE:HD12	2.02	0.42
1:A:31:LEU:HB2	1:A:199:ASP:O	2.19	0.42
2:C:338:THR:HG22	2:C:345:PRO:HB3	2.01	0.42
2:C:518:ASN:OD1	2:C:518:ASN:N	2.52	0.42
2:C:582:ASN:HD21	2:C:584:TYR:HB2	1.84	0.42
2:C:618:GLN:CG	3:D:770:LEU:HD21	2.50	0.42
3:D:1297:LYS:HA	3:D:1298:VAL:HA	1.65	0.42
3:D:613:GLY:O	3:D:616:PRO:HD2	2.20	0.42
5:F:421:TYR:CE2	5:F:422:ARG:HG3	2.54	0.42
5:F:583:THR:HG22	5:F:584:ARG:H	1.84	0.42
2:I:1103:VAL:CG1	2:I:1112:ILE:HD11	2.46	0.42
2:I:1122:LYS:HZ3	2:I:1178:LYS:C	2.14	0.42
2:I:1230:MET:HG2	2:I:1232:MET:HG3	2.02	0.42
3:J:1261:LEU:H	3:J:1261:LEU:HG	1.57	0.42
3:J:1266:ILE:HG13	3:J:1266:ILE:H	1.51	0.42
3:J:609:TYR:HE2	3:J:614:LEU:HD12	1.85	0.42
3:J:888:CYS:SG	3:J:889:ASP:N	2.92	0.42
4:K:71:GLU:HA	4:K:74:GLU:HB2	2.02	0.42
5:L:113:ARG:O	5:L:117:ILE:HD12	2.20	0.42
1:B:20:SER:OG	1:B:22:THR:HG22	2.20	0.42
2:C:1294:LYS:HB3	3:D:347:VAL:HG13	2.02	0.42
2:C:587:LEU:HD23	2:C:587:LEU:HA	1.84	0.42
3:D:909:ILE:HG13	3:D:910:ASN:N	2.33	0.42
1:H:144:ILE:HG13	1:H:144:ILE:O	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:53:GLY:HA3	1:H:177:TYR:O	2.20	0.42
2:I:132:ASP:N	2:I:132:ASP:OD1	2.53	0.42
2:I:356:THR:HG21	2:I:362:ALA:HA	2.02	0.42
2:I:591:TYR:HD2	2:I:606:LEU:HD13	1.83	0.42
2:I:673:HIS:HB3	2:I:1109:ILE:HG22	2.00	0.42
3:J:1208:ASP:O	3:J:1210:ILE:HG12	2.20	0.42
3:J:1258:ARG:HA	3:J:1261:LEU:HD11	2.02	0.42
3:J:294:ASN:HD22	5:L:406:GLN:NE2	2.15	0.42
2:C:268:ARG:NH2	2:C:270:THR:HG21	2.34	0.42
2:C:530:ILE:HG23	2:C:530:ILE:HD12	1.67	0.42
3:D:247:PRO:O	3:D:249:LEU:N	2.53	0.42
3:D:490:ILE:HG23	3:D:491:LEU:HG	2.02	0.42
3:D:99:ARG:HA	3:D:248:ASP:HB2	2.02	0.42
2:I:1191:LYS:HD3	2:I:1193:ALA:H	1.85	0.42
2:I:147:SER:OG	2:I:455:SER:HB3	2.20	0.42
2:I:22:LEU:HD22	2:I:23:ASP:H	1.84	0.42
2:I:237:LEU:HD13	2:I:237:LEU:HA	1.76	0.42
2:I:942:ASP:O	2:I:946:LEU:HD12	2.20	0.42
3:J:1137:GLY:O	3:J:1140:ARG:HB3	2.20	0.42
3:J:1343:GLU:O	3:J:1344:LEU:HB2	2.20	0.42
3:J:442:ILE:HA	3:J:442:ILE:HD13	1.70	0.42
3:J:518:VAL:HG11	3:J:707:ILE:HB	2.02	0.42
5:L:601:PRO:HA	5:L:604:SER:HB3	2.01	0.42
1:B:48:LEU:CD2	3:D:539:SER:HB3	2.50	0.42
2:C:478:ARG:HH11	2:C:481:LEU:HD23	1.85	0.42
2:C:596:ASP:O	2:C:648:ASP:OD1	2.38	0.42
1:H:95:LYS:HD3	1:H:120:ASP:OD2	2.19	0.42
2:I:253:PHE:HA	2:I:265:LYS:HG3	2.02	0.42
2:I:572:ILE:O	2:I:573:ASN:HB2	2.19	0.42
3:J:1280:VAL:CG1	3:J:1304:ARG:HH21	2.32	0.42
3:J:700:ASN:HA	3:J:704:GLU:OE1	2.20	0.42
3:J:814:CYS:CB	3:J:889:ASP:HB3	2.49	0.42
1:A:45:ARG:NH1	1:B:34:GLY:O	2.53	0.41
2:C:1053:TYR:CD1	2:C:1053:TYR:N	2.87	0.41
2:C:30:ILE:HG13	2:C:30:ILE:H	1.56	0.41
2:C:732:ILE:HD11	2:C:769:PRO:HB3	2.02	0.41
3:D:1314:LEU:HD12	3:D:1326:GLN:OE1	2.20	0.41
3:D:146:VAL:HG23	3:D:158:GLN:O	2.19	0.41
3:D:294:ASN:HD22	5:F:406:GLN:NE2	2.17	0.41
3:D:507:VAL:HG11	3:D:598:LYS:HG3	2.01	0.41
3:D:825:VAL:CG2	3:D:833:GLU:H	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:E:32:VAL:O	4:E:34:GLY:N	2.42	0.41
2:I:1024:GLU:HA	2:I:1027:LYS:HG2	2.02	0.41
3:J:419:HIS:HA	3:J:420:PRO:HD3	1.96	0.41
5:L:453:PRO:HB2	5:L:455:HIS:CE1	2.55	0.41
5:L:468:ARG:O	5:L:471:LEU:HB2	2.20	0.41
5:L:512:GLY:O	5:L:513:ASP:HB3	2.20	0.41
1:A:27:THR:HG23	1:A:202:VAL:HG22	2.01	0.41
2:C:1043:ALA:HB1	2:C:1044:PRO:HD2	2.02	0.41
2:C:1148:ALA:HB1	2:C:1180:MET:CE	2.50	0.41
2:C:253:PHE:CE1	2:C:255:ILE:HG12	2.56	0.41
2:C:866:ASP:HA	2:C:872:TYR:OH	2.19	0.41
3:D:264:ASP:N	3:D:264:ASP:OD2	2.52	0.41
5:F:421:TYR:CZ	5:F:422:ARG:HG3	2.55	0.41
1:G:118:ASP:HB3	1:G:121:VAL:CG2	2.50	0.41
2:I:107:ARG:HA	2:I:108:GLU:HA	1.64	0.41
2:I:1324:ASN:O	2:I:1327:LEU:HB2	2.21	0.41
2:I:141:THR:O	2:I:143:ARG:HG3	2.20	0.41
2:I:663:VAL:H	2:I:663:VAL:HG22	1.58	0.41
2:I:768:MET:HA	2:I:769:PRO:HD3	1.90	0.41
2:I:903:ARG:HE	2:I:910:ALA:HB2	1.85	0.41
3:J:930:LEU:HB2	3:J:1138:LEU:HB2	2.02	0.41
3:J:770:LEU:H	3:J:770:LEU:CD2	2.27	0.41
3:J:872:LEU:HD22	3:J:877:VAL:HG11	2.01	0.41
1:A:12:ARG:H	1:A:30:PRO:CD	2.34	0.41
2:C:107:ARG:HA	2:C:108:GLU:HA	1.43	0.41
2:C:421:SER:O	2:C:425:ILE:HD12	2.20	0.41
2:C:549:ASP:OD1	3:D:777:HIS:CE1	2.73	0.41
5:F:124:GLU:HA	5:F:127:ILE:CG1	2.46	0.41
5:F:139:GLU:HG3	5:F:351:THR:HG22	2.02	0.41
1:H:60:GLU:HG3	1:H:143:ARG:O	2.20	0.41
2:I:30:ILE:HD12	2:I:30:ILE:N	2.36	0.41
2:I:971:LEU:HG	2:I:1014:LEU:HD23	2.02	0.41
3:J:1252:HIS:HA	3:J:1255:VAL:HG13	2.02	0.41
3:J:1289:ASN:ND2	3:J:1290:ARG:HH12	2.18	0.41
1:B:307:LEU:HD23	1:B:313:SER:O	2.19	0.41
2:C:1296:ASP:HB3	2:C:1321:GLU:H	1.86	0.41
2:C:162:GLY:H	2:C:170:VAL:HG12	1.86	0.41
2:C:214:ASN:OD1	2:C:359:ARG:HD2	2.20	0.41
2:C:657:THR:OG1	2:C:1187:PHE:HB2	2.19	0.41
2:C:722:GLY:HA3	2:C:735:LYS:O	2.20	0.41
3:D:1372:ARG:NH2	3:J:854:ALA:HB2	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:174:ASP:C	3:D:176:PHE:H	2.24	0.41
3:D:291:ILE:HD11	5:F:409:ASN:HB3	2.02	0.41
3:D:375:GLU:OE1	3:D:378:LYS:HE3	2.21	0.41
3:D:492:SER:HA	3:D:493:PRO:HD3	1.76	0.41
3:D:810:THR:CG2	3:D:893:GLY:HA3	2.49	0.41
2:I:1064:ASP:OD2	2:I:1238:LEU:HD23	2.20	0.41
2:I:528:ARG:CZ	2:I:575:LEU:HD23	2.49	0.41
3:J:225:GLU:HA	3:J:228:VAL:HG23	2.03	0.41
3:J:304:ASP:OD2	3:J:312:ARG:NH2	2.40	0.41
3:J:749:LYS:HB3	3:J:755:ILE:HD11	2.03	0.41
1:B:257:VAL:HG12	1:B:278:ILE:HG22	2.02	0.41
2:C:374:GLU:HA	2:C:375:PRO:HD3	1.87	0.41
2:C:471:VAL:HG21	2:C:493:ILE:HD12	2.02	0.41
3:D:156:ARG:NH1	3:D:157:GLN:NE2	2.67	0.41
3:D:18:ASP:O	3:D:19:ALA:HB3	2.20	0.41
3:D:554:GLU:OE2	3:D:570:LYS:NZ	2.36	0.41
3:D:720:ASN:OD1	3:D:722:ILE:HG22	2.20	0.41
1:G:87:GLY:O	1:G:128:HIS:CE1	2.73	0.41
2:I:1043:ALA:O	2:I:1046:VAL:HG12	2.20	0.41
2:I:1275:VAL:HG13	2:I:1287:LEU:HD11	2.01	0.41
2:I:960:LEU:HB3	2:I:1025:PHE:HE2	1.85	0.41
3:J:1221:LEU:HD21	3:J:1226:VAL:HG22	2.01	0.41
3:J:518:VAL:HA	3:J:547:ARG:HH12	1.85	0.41
3:J:804:ALA:O	3:J:806:ASP:N	2.53	0.41
3:J:888:CYS:HG	3:J:889:ASP:N	2.18	0.41
2:C:559:CYS:HA	2:C:560:PRO:HD3	1.92	0.41
2:C:691:PRO:HB3	2:C:788:SER:OG	2.20	0.41
2:C:864:LYS:NZ	2:C:881:ASP:OD2	2.52	0.41
3:D:1327:GLU:OE1	3:D:1329:THR:HB	2.20	0.41
3:D:850:LYS:HB3	3:D:851:PRO:HD2	2.01	0.41
3:D:430:HIS:ND1	3:D:925:GLU:HG3	2.35	0.41
3:D:418:GLU:HG3	4:E:45:LYS:H	1.85	0.41
3:D:394:ILE:HG12	5:F:536:THR:HG22	2.01	0.41
1:G:179:PRO:HG2	1:G:211:ILE:HG13	2.03	0.41
1:H:69:SER:H	1:H:78:ILE:CD1	2.33	0.41
2:I:1246:ARG:HD2	2:I:1265:PHE:O	2.21	0.41
2:I:148:GLN:HG2	2:I:531:SER:O	2.21	0.41
2:I:551:HIS:HB3	2:I:554:HIS:CE1	2.55	0.41
1:H:84:ASN:ND2	3:J:551:ARG:HH12	2.18	0.41
3:J:866:GLU:N	3:J:866:GLU:OE1	2.51	0.41
3:J:818:GLU:HG3	3:J:887:SER:HB2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:748:ILE:HD13	2:C:748:ILE:N	2.36	0.41
3:D:1151:LYS:O	3:D:1153:PRO:HD3	2.20	0.41
3:D:1159:ILE:HG13	3:D:1160:SER:N	2.36	0.41
3:D:309:ASN:OD1	3:D:314:ARG:HA	2.20	0.41
2:I:202:ARG:HD3	2:I:369:MET:HG2	2.03	0.41
2:I:409:LEU:HD23	2:I:409:LEU:HA	1.91	0.41
2:I:688:GLN:OE1	2:I:1237:HIS:HE1	2.04	0.41
2:I:748:ILE:HD13	2:I:748:ILE:N	2.36	0.41
3:J:746:LEU:HG	3:J:758:PRO:CB	2.49	0.41
2:C:268:ARG:HH21	2:C:270:THR:CG2	2.33	0.41
2:C:1279:GLU:HG2	3:D:1357:ILE:CD1	2.51	0.41
3:D:347:VAL:CG1	3:D:348:ASP:N	2.83	0.41
5:F:137:TYR:CE2	5:F:139:GLU:HB2	2.56	0.41
5:F:440:THR:HA	5:F:443:ILE:HD12	2.03	0.41
1:G:192:VAL:O	1:G:194:GLN:N	2.54	0.41
2:I:1138:VAL:O	2:I:1142:ARG:HB2	2.21	0.41
2:I:521:LEU:HA	2:I:524:ILE:HG22	2.02	0.41
3:J:1265:THR:N	3:J:1303:SER:O	2.51	0.41
3:J:474:LEU:HD12	3:J:477:GLN:NE2	2.36	0.41
3:J:557:LYS:HA	3:J:563:LEU:HA	2.02	0.41
1:A:152:TYR:CE1	2:C:824:GLN:HA	2.56	0.41
2:C:86:GLN:HA	2:C:140:GLY:HA2	2.03	0.41
3:D:1216:ALA:O	3:D:1220:ILE:HG12	2.21	0.41
3:D:1343:GLU:O	3:D:1344:LEU:HB2	2.20	0.41
1:H:74:VAL:HG11	1:H:81:ILE:HD11	2.02	0.41
2:I:62:TYR:C	2:I:64:GLY:N	2.74	0.41
2:I:1105:SER:HA	3:J:736:GLN:OE1	2.20	0.41
4:K:53:GLU:HB3	4:K:59:ILE:HB	2.02	0.41
1:B:14:VAL:HB	1:B:28:LEU:HD13	2.03	0.41
2:C:157:PHE:CE2	2:C:431:LYS:HG2	2.55	0.41
2:C:748:ILE:O	2:C:748:ILE:HG12	2.20	0.41
2:C:818:VAL:HG22	2:C:1096:ILE:CG1	2.44	0.41
2:C:987:GLU:HG2	2:C:991:LYS:HE3	2.03	0.41
3:D:1280:VAL:HB	3:D:1304:ARG:HH21	1.86	0.41
1:H:44:ARG:O	1:H:48:LEU:HB2	2.21	0.41
2:I:1270:PHE:CZ	2:I:1290:MET:HG2	2.56	0.41
2:I:471:VAL:HG21	2:I:493:ILE:HD12	2.02	0.41
5:L:139:GLU:HG3	5:L:351:THR:HG22	2.03	0.41
5:L:567:MET:CE	5:L:571:TYR:HE2	2.34	0.41
1:A:158:ARG:HH12	1:A:172:LEU:HD23	1.86	0.41
1:A:67:GLU:HG3	1:A:79:LEU:CD2	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:GLY:C	1:B:134:THR:HB	2.41	0.41
2:C:1098:LEU:HD12	2:C:1098:LEU:HA	1.85	0.41
2:C:145:ILE:HA	2:C:511:LEU:O	2.21	0.41
2:C:269:ILE:HA	2:C:273:HIS:ND1	2.35	0.41
2:C:995:ASP:O	2:C:998:LEU:HD12	2.21	0.41
3:D:1138:LEU:N	3:D:1139:PRO:CD	2.84	0.41
3:D:246:PRO:HA	3:D:247:PRO:HD3	1.91	0.41
3:D:848:VAL:HG12	3:D:858:VAL:CG2	2.51	0.41
1:G:124:VAL:HG11	1:G:208:ASN:O	2.21	0.41
2:I:1327:LEU:HD23	2:I:1337:ILE:CG2	2.50	0.41
2:I:993:PRO:HG2	2:I:996:ARG:HB2	2.03	0.41
3:J:1309:ILE:HG13	3:J:1310:THR:N	2.36	0.41
3:J:596:LEU:HD11	3:J:604:MET:HE1	2.02	0.41
2:C:1161:LEU:HA	2:C:1161:LEU:HD12	1.92	0.40
2:C:1174:GLU:OE2	2:C:1177:ARG:NH1	2.54	0.40
2:C:325:LEU:O	2:C:330:HIS:HB2	2.20	0.40
2:C:61:SER:O	2:C:63:SER:N	2.54	0.40
3:D:234:PRO:HD2	3:D:235:GLU:OE2	2.21	0.40
3:D:527:LEU:HD23	3:D:532:GLU:HG3	2.03	0.40
3:D:559:ALA:O	3:D:561:GLY:N	2.52	0.40
1:G:89:ALA:HB3	1:G:125:LYS:HD3	2.04	0.40
2:I:515:MET:SD	2:I:523:GLU:HG2	2.62	0.40
2:I:522:SER:O	2:I:525:THR:HG22	2.21	0.40
2:I:589:THR:OG1	2:I:659:GLN:NE2	2.54	0.40
3:J:1286:LYS:HA	3:J:1289:ASN:OD1	2.21	0.40
3:J:1325:PHE:CD2	3:J:1326:GLN:HG3	2.57	0.40
3:J:425:ARG:NH2	3:J:426:ALA:HB3	2.36	0.40
3:J:678:ARG:HG3	3:J:679:TYR:N	2.36	0.40
3:J:853:THR:O	3:J:854:ALA:HB3	2.21	0.40
2:C:1082:ILE:HD12	2:C:1082:ILE:H	1.87	0.40
2:C:1225:VAL:HA	3:D:638:SER:HB2	2.04	0.40
2:C:312:ALA:H	2:C:315:MET:HE1	1.85	0.40
2:C:383:SER:O	2:C:387:ASN:ND2	2.54	0.40
2:C:745:GLU:O	2:C:746:ALA:C	2.60	0.40
2:C:798:GLN:HB2	2:C:828:PHE:CE1	2.56	0.40
5:F:595:LEU:HB3	5:F:599:ARG:CZ	2.51	0.40
2:I:559:CYS:HA	2:I:560:PRO:HD3	1.85	0.40
2:I:710:VAL:HA	2:I:715:THR:HG21	2.03	0.40
3:D:1299:GLY:N	3:J:1301:THR:HG21	2.35	0.40
3:J:1324:SER:HB3	3:J:1348:LYS:NZ	2.36	0.40
5:L:139:GLU:HG2	5:L:351:THR:HA	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:145:ILE:O	2:C:145:ILE:HG22	2.21	0.40
3:D:1160:SER:HB2	3:D:1206:ARG:HG2	2.03	0.40
3:D:147:ILE:O	3:D:148:GLU:HB2	2.21	0.40
3:D:357:VAL:CG1	3:D:358:GLY:H	2.29	0.40
3:D:600:ALA:O	3:D:603:LYS:HG2	2.22	0.40
3:D:518:VAL:CG1	3:D:707:ILE:HB	2.51	0.40
1:G:105:SER:HA	1:G:138:ALA:O	2.21	0.40
2:I:624:ASP:OD1	2:I:625:GLU:N	2.48	0.40
3:J:363:LEU:O	3:J:363:LEU:HG	2.21	0.40
3:J:580:TRP:HB2	3:J:589:TYR:HE1	1.86	0.40
5:L:387:VAL:HG22	5:L:435:ILE:CD1	2.51	0.40
1:A:27:THR:C	1:A:28:LEU:HD12	2.42	0.40
1:B:178:SER:HA	1:B:179:PRO:HD3	1.81	0.40
1:B:197:ASP:O	1:B:198:LEU:HD13	2.21	0.40
1:B:284:ARG:HA	1:B:284:ARG:HD2	1.90	0.40
2:C:414:ILE:HG13	2:C:414:ILE:H	1.80	0.40
3:D:495:ASN:HD21	3:D:497:GLU:HB2	1.86	0.40
5:F:309:ASN:HB3	5:F:310:GLU:H	1.72	0.40
2:I:455:SER:HA	2:I:459:MET:HE2	2.03	0.40
2:I:119:GLU:HG3	2:I:489:PRO:HD2	2.03	0.40
2:I:555:TYR:CE1	2:I:637:ARG:CZ	3.05	0.40
2:I:670:PHE:CE1	2:I:1184:THR:HG21	2.57	0.40
3:J:1140:ARG:HH21	3:J:1236:GLU:HG2	1.86	0.40
3:J:186:GLN:HA	3:J:189:LEU:HD12	2.02	0.40
3:J:425:ARG:HD3	3:J:459:ALA:HB2	2.04	0.40
3:J:474:LEU:HD12	3:J:474:LEU:HA	1.85	0.40
3:J:821:MET:HE3	3:J:879:ALA:HB1	2.02	0.40
5:L:608:ARG:HD2	5:L:608:ARG:HH11	1.77	0.40
1:A:224:LEU:HD23	1:A:228:LEU:HD11	2.02	0.40
2:C:1046:VAL:O	2:C:1046:VAL:HG13	2.22	0.40
2:C:1077:SER:OG	2:C:1078:LYS:N	2.54	0.40
2:C:746:ALA:HA	2:C:974:ARG:HE	1.87	0.40
3:D:1337:VAL:HG23	3:D:1338:ALA:N	2.36	0.40
3:D:135:ILE:HG23	3:D:185:ILE:HD12	2.04	0.40
3:D:266:ASN:O	3:D:270:ARG:HB2	2.21	0.40
3:D:515:ARG:HG2	3:D:719:PHE:CZ	2.56	0.40
3:D:817:HIS:O	3:D:845:ALA:HB1	2.21	0.40
5:F:128:ASN:HA	5:F:131:GLN:NE2	2.32	0.40
1:G:188:GLU:HG3	1:G:200:LYS:HB3	2.03	0.40
2:I:1330:ILE:HG21	2:I:1330:ILE:HD13	1.67	0.40
2:I:5:TYR:HD2	2:I:778:GLU:HB2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:134:ASP:O	3:J:138:VAL:HG23	2.21	0.40
3:J:425:ARG:HH21	3:J:426:ALA:HB3	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	233/329 (71%)	211 (91%)	16 (7%)	6 (3%)	5	35
1	B	283/329 (86%)	247 (87%)	28 (10%)	8 (3%)	5	34
1	G	225/329 (68%)	205 (91%)	15 (7%)	5 (2%)	6	38
1	H	212/329 (64%)	196 (92%)	14 (7%)	2 (1%)	17	54
2	C	1338/1342 (100%)	1194 (89%)	112 (8%)	32 (2%)	6	37
2	I	1338/1342 (100%)	1185 (89%)	122 (9%)	31 (2%)	6	38
3	D	1157/1407 (82%)	1036 (90%)	91 (8%)	30 (3%)	5	35
3	J	1146/1407 (81%)	1030 (90%)	85 (7%)	31 (3%)	5	35
4	E	87/91 (96%)	77 (88%)	6 (7%)	4 (5%)	2	24
4	K	77/91 (85%)	69 (90%)	7 (9%)	1 (1%)	12	48
5	F	462/613 (75%)	419 (91%)	34 (7%)	9 (2%)	8	41
5	L	463/613 (76%)	425 (92%)	30 (6%)	8 (2%)	9	43
All	All	7021/8222 (85%)	6294 (90%)	560 (8%)	167 (2%)	6	37

All (167) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	196	THR

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Mol	Chain	Res	Type
1	B	13	LEU
1	B	50	SER
1	B	135	ASP
2	C	456	VAL
2	C	705	GLU
2	C	1136	GLN
2	C	1159	VAL
2	C	1317	PRO
3	D	49	PHE
3	D	89	GLY
3	D	175	GLU
3	D	343	LEU
3	D	357	VAL
3	D	426	ALA
3	D	585	LYS
3	D	826	ILE
3	D	860	ARG
3	D	1169	THR
3	D	1274	PHE
3	D	1294	ALA
5	F	96	ASP
5	F	395	THR
5	F	602	SER
1	G	193	GLU
1	H	138	ALA
2	I	237	LEU
2	I	456	VAL
2	I	756	TYR
2	I	1283	ALA
3	J	49	PHE
3	J	89	GLY
3	J	175	GLU
3	J	343	LEU
3	J	357	VAL
3	J	426	ALA
3	J	585	LYS
3	J	745	GLY
3	J	826	ILE
3	J	860	ARG
3	J	1169	THR
3	J	1297	LYS
5	L	96	ASP

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Mol	Chain	Res	Type
5	L	395	THR
5	L	602	SER
1	A	167	PRO
1	A	193	GLU
1	A	195	ARG
1	B	49	SER
2	C	62	TYR
2	C	482	GLY
2	C	490	GLN
2	C	756	TYR
2	C	1059	ARG
2	C	1107	MET
2	C	1261	GLY
3	D	46	TYR
3	D	174	ASP
3	D	496	GLY
3	D	745	GLY
3	D	805	GLN
3	D	1344	LEU
4	E	34	GLY
1	G	162	GLU
2	I	47	TYR
2	I	162	GLY
2	I	169	LYS
2	I	446	ASP
2	I	482	GLY
2	I	490	GLN
2	I	705	GLU
2	I	1059	ARG
2	I	1107	MET
2	I	1136	GLN
2	I	1317	PRO
3	J	46	TYR
3	J	174	ASP
3	J	342	LEU
3	J	417	ARG
3	J	710	ASP
3	J	805	GLN
3	J	1294	ALA
4	K	78	ALA
2	C	26	TYR
2	C	162	GLY

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Mol	Chain	Res	Type
2	C	170	VAL
2	C	596	ASP
2	C	627	GLY
2	C	697	LYS
2	C	1283	ALA
3	D	11	GLN
3	D	417	ARG
3	D	559	ALA
5	F	569	THR
5	F	585	GLU
1	G	229	GLU
2	I	62	TYR
2	I	170	VAL
2	I	596	ASP
2	I	627	GLY
2	I	1004	ASP
2	I	1261	GLY
3	J	496	GLY
3	J	854	ALA
3	J	1344	LEU
5	L	360	ASP
5	L	569	THR
1	A	162	GLU
1	B	63	GLY
1	B	93	GLN
1	B	138	ALA
2	C	114	VAL
2	C	121	GLU
2	C	236	LYS
2	C	484	LEU
2	C	566	GLY
2	C	746	ALA
2	C	1153	ALA
2	C	1167	GLU
3	D	1167	LYS
3	D	1276	GLU
4	E	86	ILE
5	F	503	GLU
1	G	167	PRO
1	H	193	GLU
2	I	121	GLU
2	I	160	ASP

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Mol	Chain	Res	Type
2	I	236	LYS
2	I	697	LYS
3	J	559	ALA
3	J	902	ASP
3	J	1270	GLY
3	J	1326	GLN
1	B	136	GLU
2	C	237	LEU
2	C	812	PHE
2	C	1165	SER
2	C	1341	ASP
3	D	314	ARG
3	D	710	ASP
3	D	1297	LYS
3	D	1326	GLN
5	F	310	GLU
5	F	581	ASP
2	I	484	LEU
2	I	812	PHE
3	J	560	ASN
3	J	712	GLN
3	J	1276	GLU
2	I	1165	SER
3	J	1209	VAL
5	L	296	LYS
5	L	581	ASP
4	E	33	GLY
3	J	586	GLY
2	C	905	ILE
3	D	358	GLY
3	D	1270	GLY
4	E	32	VAL
5	F	490	PRO
2	I	1159	VAL
1	G	232	VAL
2	I	114	VAL
5	L	490	PRO
3	D	1209	VAL
2	I	566	GLY

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	202/286 (71%)	175 (87%)	27 (13%)	4	22
1	B	248/286 (87%)	215 (87%)	33 (13%)	4	22
1	G	193/286 (68%)	181 (94%)	12 (6%)	18	49
1	H	183/286 (64%)	169 (92%)	14 (8%)	13	43
2	C	1155/1157 (100%)	1053 (91%)	102 (9%)	10	38
2	I	1153/1157 (100%)	1058 (92%)	95 (8%)	11	40
3	D	959/1168 (82%)	849 (88%)	110 (12%)	5	27
3	J	959/1168 (82%)	861 (90%)	98 (10%)	7	31
4	E	72/75 (96%)	65 (90%)	7 (10%)	8	33
4	K	67/75 (89%)	58 (87%)	9 (13%)	4	22
5	F	417/540 (77%)	386 (93%)	31 (7%)	13	44
5	L	418/540 (77%)	385 (92%)	33 (8%)	12	42
All	All	6026/7024 (86%)	5455 (90%)	571 (10%)	8	34

All (571) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	7	GLU
1	A	10	LYS
1	A	19	VAL
1	A	25	LYS
1	A	27	THR
1	A	31	LEU
1	A	61	ILE
1	A	62	ASP
1	A	65	LEU
1	A	74	VAL
1	A	77	ASP
1	A	79	LEU
1	A	101	THR

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Mol	Chain	Res	Type
1	A	128	HIS
1	A	134	THR
1	A	139	SER
1	A	145	LYS
1	A	147	GLN
1	A	148	ARG
1	A	168	ILE
1	A	181	GLU
1	A	183	ILE
1	A	186	ASN
1	A	207	THR
1	A	224	LEU
1	A	227	GLN
1	B	9	LEU
1	B	13	LEU
1	B	16	ILE
1	B	20	SER
1	B	46	ILE
1	B	48	LEU
1	B	60	GLU
1	B	64	VAL
1	B	65	LEU
1	B	66	HIS
1	B	79	LEU
1	B	80	GLU
1	B	95	LYS
1	B	115	ILE
1	B	148	ARG
1	B	158	ARG
1	B	186	ASN
1	B	205	MET
1	B	224	LEU
1	B	246	LYS
1	B	249	PHE
1	B	250	ASP
1	B	252	ILE
1	B	255	ARG
1	B	258	ASP
1	B	262	LEU
1	B	263	THR
1	B	264	VAL
1	B	276	HIS

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Mol	Chain	Res	Type
1	B	284	ARG
1	B	288	GLU
1	B	300	LEU
1	B	312	LEU
2	C	10	ARG
2	C	22	LEU
2	C	29	SER
2	C	30	ILE
2	C	56	VAL
2	C	88	ARG
2	C	90	VAL
2	C	115	LYS
2	C	116	ASP
2	C	132	ASP
2	C	135	THR
2	C	138	ILE
2	C	145	ILE
2	C	148	GLN
2	C	156	PHE
2	C	185	ASP
2	C	189	ASP
2	C	202	ARG
2	C	208	ILE
2	C	209	ILE
2	C	237	LEU
2	C	238	GLN
2	C	285	ILE
2	C	319	LEU
2	C	321	LEU
2	C	369	MET
2	C	374	GLU
2	C	377	THR
2	C	414	ILE
2	C	419	ILE
2	C	434	ASP
2	C	443	ASP
2	C	451	ARG
2	C	452	ARG
2	C	456	VAL
2	C	481	LEU
2	C	483	ASP
2	C	484	LEU

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Mol	Chain	Res	Type
2	C	486	THR
2	C	493	ILE
2	C	499	SER
2	C	516	ASP
2	C	522	SER
2	C	524	ILE
2	C	525	THR
2	C	538	LEU
2	C	540	ARG
2	C	542	ARG
2	C	554	HIS
2	C	558	VAL
2	C	568	ASN
2	C	600	THR
2	C	623	LEU
2	C	633	LEU
2	C	637	ARG
2	C	657	THR
2	C	658	GLN
2	C	663	VAL
2	C	690	VAL
2	C	697	LYS
2	C	706	ARG
2	C	741	MET
2	C	748	ILE
2	C	773	LEU
2	C	796	LEU
2	C	799	ASN
2	C	815	SER
2	C	817	LEU
2	C	842	ASP
2	C	866	ASP
2	C	890	LYS
2	C	892	GLU
2	C	913	VAL
2	C	950	GLU
2	C	971	LEU
2	C	974	ARG
2	C	992	LEU
2	C	1002	LEU
2	C	1006	GLU
2	C	1029	LEU

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Mol	Chain	Res	Type
2	C	1054	LEU
2	C	1073	LYS
2	C	1076	ILE
2	C	1083	GLU
2	C	1098	LEU
2	C	1109	ILE
2	C	1114	GLU
2	C	1132	LEU
2	C	1140	LYS
2	C	1146	GLN
2	C	1154	ASP
2	C	1159	VAL
2	C	1164	PHE
2	C	1180	MET
2	C	1186	VAL
2	C	1206	THR
2	C	1207	SER
2	C	1233	LEU
2	C	1253	LEU
2	C	1265	PHE
2	C	1287	LEU
2	C	1330	ILE
3	D	8	LEU
3	D	11	GLN
3	D	18	ASP
3	D	24	LEU
3	D	42	GLU
3	D	46	TYR
3	D	47	ARG
3	D	52	GLU
3	D	54	ASP
3	D	56	LEU
3	D	70	CYS
3	D	97	VAL
3	D	119	SER
3	D	120	LEU
3	D	132	LEU
3	D	161	THR
3	D	172	PHE
3	D	175	GLU
3	D	176	PHE
3	D	198	CYS

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Mol	Chain	Res	Type
3	D	214	ARG
3	D	219	LYS
3	D	224	LEU
3	D	255	LEU
3	D	292	VAL
3	D	299	LEU
3	D	319	SER
3	D	324	LEU
3	D	330	MET
3	D	331	ILE
3	D	342	LEU
3	D	374	LEU
3	D	392	THR
3	D	394	ILE
3	D	412	LEU
3	D	415	VAL
3	D	442	ILE
3	D	460	ASP
3	D	514	THR
3	D	526	VAL
3	D	528	THR
3	D	536	LEU
3	D	545	HIS
3	D	569	LEU
3	D	571	ASP
3	D	614	LEU
3	D	635	SER
3	D	641	ILE
3	D	643	ASP
3	D	660	GLU
3	D	663	GLU
3	D	674	THR
3	D	698	MET
3	D	701	LEU
3	D	707	ILE
3	D	708	ASN
3	D	710	ASP
3	D	712	GLN
3	D	716	GLN
3	D	717	VAL
3	D	720	ASN
3	D	721	SER

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Mol	Chain	Res	Type
3	D	727	ASP
3	D	731	ARG
3	D	740	LEU
3	D	751	ASP
3	D	764	ARG
3	D	770	LEU
3	D	788	LEU
3	D	797	THR
3	D	844	THR
3	D	847	ASP
3	D	849	LEU
3	D	853	THR
3	D	855	ASP
3	D	857	LEU
3	D	860	ARG
3	D	867	GLN
3	D	878	ASP
3	D	895	CYS
3	D	903	LEU
3	D	908	ILE
3	D	918	ILE
3	D	928	THR
3	D	1135	THR
3	D	1140	ARG
3	D	1163	VAL
3	D	1169	THR
3	D	1170	LYS
3	D	1172	LYS
3	D	1177	ILE
3	D	1181	ASP
3	D	1184	ASP
3	D	1186	TYR
3	D	1194	ARG
3	D	1195	GLN
3	D	1208	ASP
3	D	1209	VAL
3	D	1266	ILE
3	D	1273	ASP
3	D	1275	LEU
3	D	1276	GLU
3	D	1305	ASP
3	D	1306	LEU

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Mol	Chain	Res	Type
3	D	1310	THR
3	D	1314	LEU
3	D	1327	GLU
3	D	1328	THR
3	D	1343	GLU
3	D	1365	TYR
4	E	3	ARG
4	E	18	ASP
4	E	21	LEU
4	E	36	ASP
4	E	39	VAL
4	E	47	THR
4	E	58	LEU
5	F	96	ASP
5	F	102	MET
5	F	163	THR
5	F	236	LYS
5	F	244	THR
5	F	248	GLU
5	F	267	ASP
5	F	274	ARG
5	F	306	PHE
5	F	310	GLU
5	F	314	THR
5	F	338	HIS
5	F	341	LEU
5	F	342	GLN
5	F	362	ASN
5	F	400	GLN
5	F	429	THR
5	F	437	GLN
5	F	446	GLN
5	F	450	ILE
5	F	471	LEU
5	F	486	ARG
5	F	492	ASP
5	F	526	THR
5	F	561	MET
5	F	566	ASP
5	F	573	LEU
5	F	599	ARG
5	F	600	HIS

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Mol	Chain	Res	Type
5	F	603	ARG
5	F	612	ASP
1	G	27	THR
1	G	51	MET
1	G	65	LEU
1	G	79	LEU
1	G	96	ASP
1	G	140	ILE
1	G	145	LYS
1	G	148	ARG
1	G	168	ILE
1	G	178	SER
1	G	217	ILE
1	G	224	LEU
1	H	45	ARG
1	H	48	LEU
1	H	49	SER
1	H	50	SER
1	H	60	GLU
1	H	62	ASP
1	H	79	LEU
1	H	95	LYS
1	H	96	ASP
1	H	102	LEU
1	H	127	GLN
1	H	135	ASP
1	H	143	ARG
1	H	206	GLU
2	I	22	LEU
2	I	29	SER
2	I	30	ILE
2	I	39	ILE
2	I	44	GLU
2	I	90	VAL
2	I	115	LYS
2	I	119	GLU
2	I	132	ASP
2	I	135	THR
2	I	138	ILE
2	I	148	GLN
2	I	156	PHE
2	I	185	ASP

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Mol	Chain	Res	Type
2	I	189	ASP
2	I	202	ARG
2	I	208	ILE
2	I	237	LEU
2	I	238	GLN
2	I	285	ILE
2	I	319	LEU
2	I	321	LEU
2	I	342	ASP
2	I	369	MET
2	I	377	THR
2	I	414	ILE
2	I	434	ASP
2	I	443	ASP
2	I	446	ASP
2	I	451	ARG
2	I	452	ARG
2	I	471	VAL
2	I	481	LEU
2	I	483	ASP
2	I	486	THR
2	I	493	ILE
2	I	499	SER
2	I	508	SER
2	I	513	GLN
2	I	516	ASP
2	I	524	ILE
2	I	538	LEU
2	I	540	ARG
2	I	542	ARG
2	I	558	VAL
2	I	569	ILE
2	I	600	THR
2	I	609	ILE
2	I	623	LEU
2	I	633	LEU
2	I	637	ARG
2	I	654	ASP
2	I	657	THR
2	I	658	GLN
2	I	663	VAL
2	I	690	VAL

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Mol	Chain	Res	Type
2	I	697	LYS
2	I	706	ARG
2	I	748	ILE
2	I	773	LEU
2	I	796	LEU
2	I	799	ASN
2	I	815	SER
2	I	817	LEU
2	I	866	ASP
2	I	887	VAL
2	I	890	LYS
2	I	892	GLU
2	I	895	LEU
2	I	913	VAL
2	I	950	GLU
2	I	974	ARG
2	I	992	LEU
2	I	1002	LEU
2	I	1006	GLU
2	I	1029	LEU
2	I	1054	LEU
2	I	1076	ILE
2	I	1083	GLU
2	I	1098	LEU
2	I	1114	GLU
2	I	1132	LEU
2	I	1133	LYS
2	I	1140	LYS
2	I	1146	GLN
2	I	1154	ASP
2	I	1159	VAL
2	I	1164	PHE
2	I	1180	MET
2	I	1198	LEU
2	I	1206	THR
2	I	1207	SER
2	I	1233	LEU
2	I	1253	LEU
2	I	1265	PHE
3	J	18	ASP
3	J	42	GLU
3	J	44	ILE

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Mol	Chain	Res	Type
3	J	46	TYR
3	J	52	GLU
3	J	54	ASP
3	J	56	LEU
3	J	70	CYS
3	J	97	VAL
3	J	119	SER
3	J	120	LEU
3	J	132	LEU
3	J	161	THR
3	J	172	PHE
3	J	175	GLU
3	J	176	PHE
3	J	198	CYS
3	J	214	ARG
3	J	217	LEU
3	J	219	LYS
3	J	244	VAL
3	J	252	LEU
3	J	255	LEU
3	J	259	ARG
3	J	299	LEU
3	J	319	SER
3	J	324	LEU
3	J	330	MET
3	J	331	ILE
3	J	342	LEU
3	J	392	THR
3	J	394	ILE
3	J	412	LEU
3	J	415	VAL
3	J	416	ILE
3	J	417	ARG
3	J	425	ARG
3	J	442	ILE
3	J	460	ASP
3	J	475	GLU
3	J	505	ASP
3	J	518	VAL
3	J	526	VAL
3	J	545	HIS
3	J	569	LEU

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Mol	Chain	Res	Type
3	J	571	ASP
3	J	641	ILE
3	J	643	ASP
3	J	660	GLU
3	J	674	THR
3	J	678	ARG
3	J	698	MET
3	J	701	LEU
3	J	706	VAL
3	J	707	ILE
3	J	708	ASN
3	J	712	GLN
3	J	717	VAL
3	J	731	ARG
3	J	740	LEU
3	J	764	ARG
3	J	770	LEU
3	J	788	LEU
3	J	797	THR
3	J	844	THR
3	J	847	ASP
3	J	849	LEU
3	J	857	LEU
3	J	860	ARG
3	J	878	ASP
3	J	903	LEU
3	J	908	ILE
3	J	928	THR
3	J	1140	ARG
3	J	1163	VAL
3	J	1169	THR
3	J	1170	LYS
3	J	1177	ILE
3	J	1181	ASP
3	J	1186	TYR
3	J	1194	ARG
3	J	1208	ASP
3	J	1209	VAL
3	J	1261	LEU
3	J	1266	ILE
3	J	1268	ASN
3	J	1273	ASP

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Mol	Chain	Res	Type
3	J	1275	LEU
3	J	1284	ARG
3	J	1290	ARG
3	J	1293	GLU
3	J	1306	LEU
3	J	1310	THR
3	J	1314	LEU
3	J	1327	GLU
3	J	1343	GLU
3	J	1365	TYR
3	J	1369	ARG
4	K	3	ARG
4	K	8	ASP
4	K	13	ILE
4	K	18	ASP
4	K	28	ARG
4	K	36	ASP
4	K	39	VAL
4	K	47	THR
4	K	58	LEU
5	L	102	MET
5	L	114	GLU
5	L	236	LYS
5	L	244	THR
5	L	248	GLU
5	L	267	ASP
5	L	274	ARG
5	L	277	MET
5	L	306	PHE
5	L	310	GLU
5	L	314	THR
5	L	333	VAL
5	L	338	HIS
5	L	341	LEU
5	L	342	GLN
5	L	360	ASP
5	L	362	ASN
5	L	400	GLN
5	L	402	LEU
5	L	437	GLN
5	L	471	LEU
5	L	476	ARG

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Mol	Chain	Res	Type
5	L	481	GLU
5	L	486	ARG
5	L	526	THR
5	L	561	MET
5	L	566	ASP
5	L	573	LEU
5	L	587	ILE
5	L	599	ARG
5	L	600	HIS
5	L	603	ARG
5	L	613	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	227	GLN
1	B	132	HIS
1	B	268	ASN
2	C	31	GLN
2	C	36	GLN
2	C	69	GLN
2	C	120	GLN
2	C	139	ASN
2	C	330	HIS
2	C	387	ASN
2	C	582	ASN
2	C	659	GLN
2	C	760	ASN
2	C	799	ASN
2	C	1134	GLN
2	C	1136	GLN
2	C	1146	GLN
2	C	1220	GLN
2	C	1237	HIS
2	C	1268	GLN
3	D	157	GLN
3	D	232	ASN
3	D	364	HIS
3	D	365	GLN
3	D	435	GLN
3	D	450	HIS
3	D	458	ASN

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Mol	Chain	Res	Type
3	D	477	GLN
3	D	680	ASN
3	D	716	GLN
3	D	817	HIS
3	D	1227	HIS
3	D	1366	HIS
5	F	131	GLN
5	F	227	GLN
5	F	258	GLN
5	F	362	ASN
5	F	406	GLN
5	F	472	GLN
5	F	600	HIS
1	G	18	GLN
1	G	41	ASN
1	H	23	HIS
1	H	128	HIS
2	I	31	GLN
2	I	582	ASN
2	I	673	HIS
2	I	760	ASN
2	I	808	ASN
2	I	824	GLN
2	I	834	GLN
2	I	955	GLN
2	I	1116	HIS
2	I	1134	GLN
2	I	1136	GLN
2	I	1146	GLN
2	I	1237	HIS
2	I	1256	GLN
2	I	1314	GLN
3	J	294	ASN
3	J	364	HIS
3	J	365	GLN
3	J	424	ASN
3	J	450	HIS
3	J	458	ASN
3	J	477	GLN
3	J	489	ASN
3	J	716	GLN
3	J	762	ASN

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Mol	Chain	Res	Type
3	J	771	GLN
3	J	1197	ASN
3	J	1279	GLN
3	J	1366	HIS
5	L	129	GLN
5	L	131	GLN
5	L	227	GLN
5	L	406	GLN
5	L	600	HIS

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 8 ligands modelled in this entry, 6 are monoatomic - leaving 2 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
8	4C2	D	2004	-	36,38,38	1.23	4 (11%)	48,58,58	2.02	12 (25%)
8	4C2	J	2004	-	36,38,38	0.97	2 (5%)	48,58,58	1.79	7 (14%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
8	4C2	D	2004	-	-	2/14/52/52	0/4/4/4
8	4C2	J	2004	-	-	1/14/52/52	0/4/4/4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	2004	4C2	C2-C3	4.51	1.42	1.38
8	D	2004	4C2	C1-N	4.04	1.46	1.42
8	D	2004	4C2	C7-N2	-3.04	1.25	1.36
8	D	2004	4C2	O-C	-2.60	1.17	1.23
8	D	2004	4C2	C1-C7	-2.55	1.37	1.41
8	J	2004	4C2	C2-S	-2.22	1.75	1.79

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	2004	4C2	C11-N3-C10	-7.49	103.43	114.14
8	J	2004	4C2	C19-C10-N3	-5.75	85.95	110.57
8	D	2004	4C2	C19-C10-N3	-5.69	86.20	110.57
8	D	2004	4C2	C4-C3-C2	5.00	134.67	129.47
8	D	2004	4C2	C1-C-C21	-4.96	84.47	88.37
8	D	2004	4C2	O2-S-C2	-4.54	102.00	108.74
8	D	2004	4C2	C7-C1-C	4.18	95.75	91.68
8	J	2004	4C2	C4-C3-C2	4.12	133.76	129.47
8	D	2004	4C2	C11-N3-C10	-4.02	108.40	114.14
8	J	2004	4C2	C3-C2-C5	-3.23	103.79	106.15
8	J	2004	4C2	C1-N-S	3.23	128.86	121.34
8	D	2004	4C2	O3-S-C2	3.13	113.39	108.74
8	J	2004	4C2	O2-S-C2	-2.99	104.31	108.74
8	D	2004	4C2	C-C1-N	-2.95	128.33	137.83
8	D	2004	4C2	C1-N-S	2.68	127.57	121.34
8	D	2004	4C2	C7-C1-N	2.61	135.91	129.93
8	D	2004	4C2	C3-C2-C5	-2.54	104.29	106.15
8	J	2004	4C2	O3-S-C2	2.37	112.27	108.74
8	D	2004	4C2	O-C-C1	2.04	139.78	136.36

There are no chirality outliers.

All (3) torsion outliers are listed below:

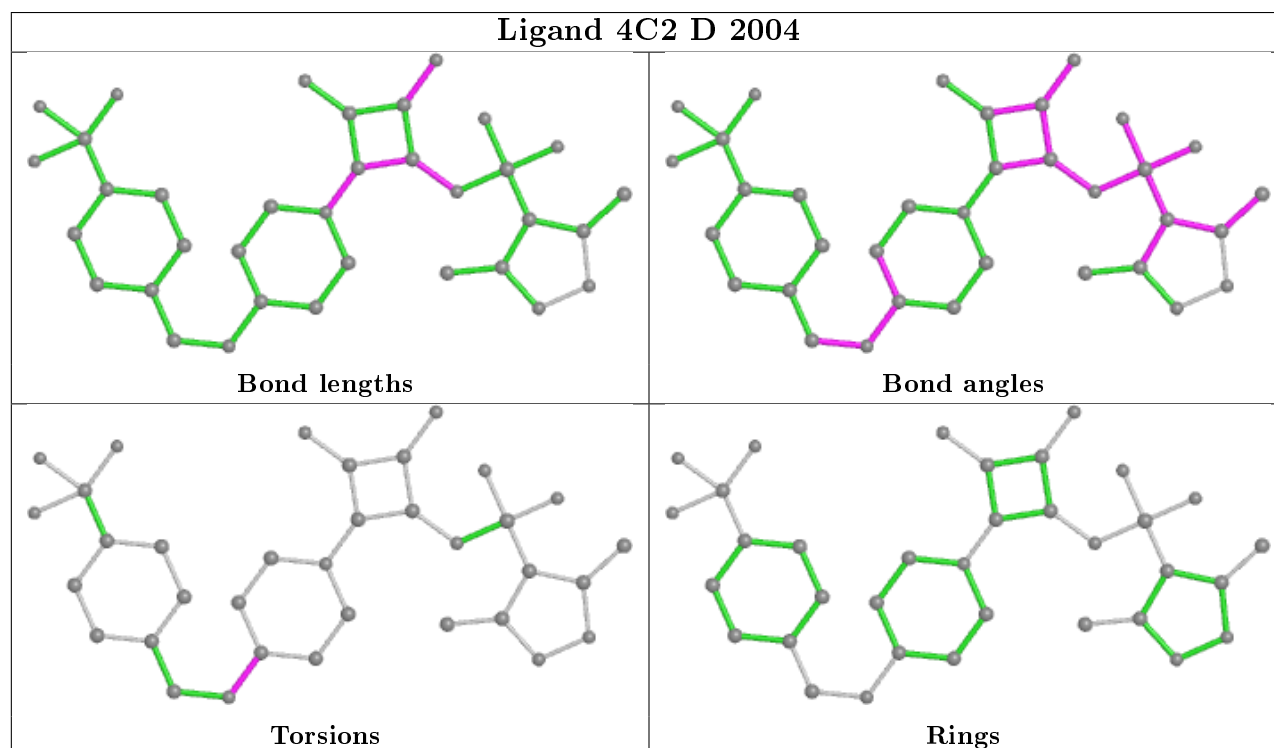
Mol	Chain	Res	Type	Atoms
8	D	2004	4C2	C9-C10-N3-C11
8	J	2004	4C2	C9-C10-N3-C11
8	D	2004	4C2	C19-C10-N3-C11

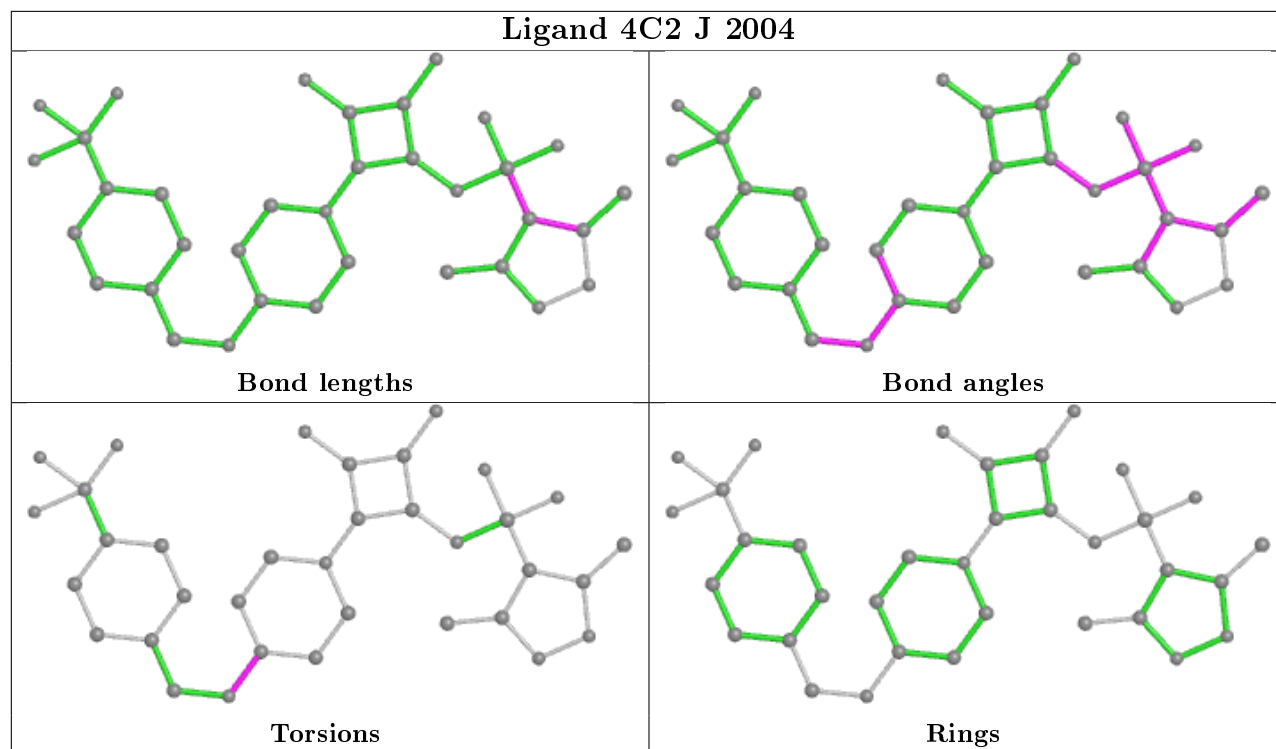
There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
8	D	2004	4C2	1	0
8	J	2004	4C2	2	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 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	235/329 (71%)	-0.34	3 (1%) 77 70	140, 166, 193, 222	0
1	B	289/329 (87%)	-0.13	2 (0%) 87 83	146, 203, 247, 259	0
1	G	227/329 (68%)	-0.22	2 (0%) 84 78	189, 214, 238, 246	0
1	H	216/329 (65%)	0.18	12 (5%) 24 20	201, 246, 255, 259	0
2	C	1340/1342 (99%)	-0.34	8 (0%) 89 85	115, 159, 222, 268	0
2	I	1340/1342 (99%)	-0.15	29 (2%) 62 53	153, 185, 240, 340	0
3	D	1163/1407 (82%)	-0.22	12 (1%) 82 76	121, 156, 213, 257	0
3	J	1152/1407 (81%)	-0.08	33 (2%) 51 41	151, 192, 247, 273	0
4	E	89/91 (97%)	-0.08	0 100 100	174, 192, 209, 216	0
4	K	79/91 (86%)	1.28	21 (26%) 0 0	262, 289, 297, 302	0
5	F	468/613 (76%)	-0.00	23 (4%) 29 25	150, 211, 305, 326	0
5	L	469/613 (76%)	0.01	25 (5%) 26 22	163, 215, 294, 309	0
All	All	7067/8222 (85%)	-0.15	170 (2%) 59 50	115, 183, 255, 340	0

All (170) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
5	L	318	ALA	6.8
2	I	1004	ASP	6.7
5	L	321	ALA	6.4
5	F	323	ASN	6.1
5	F	301	ASN	5.5
2	I	976	ARG	5.4
5	F	319	ALA	5.2
5	L	319	ALA	5.1
5	L	327	SER	5.0
4	K	37	PRO	5.0
5	L	314	THR	5.0

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Mol	Chain	Res	Type	RSRZ
4	K	35	LYS	5.0
2	I	979	LEU	4.9
5	F	337	VAL	4.8
5	L	312	SER	4.7
5	L	322	MET	4.4
3	J	586	GLY	4.3
2	I	972	PHE	4.3
2	C	231	GLU	4.1
5	F	314	THR	4.1
3	J	1188	GLU	4.0
2	I	982	GLY	4.0
5	F	167	ASP	4.0
5	L	317	ASN	4.0
4	K	75	GLN	4.0
3	J	856	ILE	3.8
3	J	857	LEU	3.8
5	L	315	TRP	3.8
2	I	998	LEU	3.8
2	I	1005	GLU	3.8
4	K	55	GLU	3.8
5	L	323	ASN	3.7
3	J	1299	GLY	3.7
3	D	209	ASN	3.7
2	I	981	ALA	3.7
5	L	489	MET	3.7
4	K	36	ASP	3.6
5	F	288	MET	3.6
5	L	316	PHE	3.6
5	L	338	HIS	3.6
5	F	322	MET	3.6
2	I	983	GLY	3.5
5	F	298	PRO	3.5
3	J	1168	GLU	3.5
2	I	1007	LYS	3.5
2	I	1138	VAL	3.5
5	F	300	LYS	3.4
2	I	999	GLU	3.4
5	L	313	ASP	3.4
1	H	145	LYS	3.3
1	G	95	LYS	3.3
4	K	15	ASN	3.3
3	D	1203	ARG	3.2

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Mol	Chain	Res	Type	RSRZ
5	L	490	PRO	3.2
5	F	313	ASP	3.2
4	K	77	ALA	3.2
4	K	56	GLU	3.2
5	F	318	ALA	3.2
3	J	1175	LEU	3.2
1	H	182	ARG	3.2
2	C	332	ARG	3.2
5	F	304	THR	3.2
5	L	167	ASP	3.1
3	J	477	GLN	3.1
4	K	12	LYS	3.1
2	I	980	VAL	3.1
3	J	1197	ASN	3.1
3	J	1201	GLY	3.1
1	H	205	MET	3.0
5	L	304	THR	3.0
3	J	208	THR	3.0
4	K	71	GLU	3.0
3	J	1169	THR	3.0
5	F	327	SER	2.9
5	F	303	ILE	2.9
1	H	112	ALA	2.9
2	I	978	VAL	2.9
1	H	113	ALA	2.9
3	J	707	ILE	2.9
2	I	1010	GLN	2.8
5	F	307	THR	2.8
4	K	70	GLN	2.8
3	J	1187	GLU	2.8
5	F	326	TRP	2.8
2	I	989	LEU	2.7
1	A	160	HIS	2.7
1	B	295	LEU	2.7
5	F	312	SER	2.7
3	D	1300	ALA	2.6
4	K	3	ARG	2.6
2	I	971	LEU	2.6
1	H	108	GLY	2.6
2	I	1006	GLU	2.6
1	H	96	ASP	2.6
4	K	78	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
2	C	266	GLY	2.6
3	J	1300	ALA	2.6
1	H	12	ARG	2.6
3	J	829	GLY	2.6
4	K	74	GLU	2.6
5	L	320	ILE	2.5
5	L	305	LEU	2.5
3	D	1198	VAL	2.5
1	B	317	ARG	2.5
2	I	1011	LEU	2.5
2	I	1003	THR	2.5
5	L	488	LEU	2.5
2	I	105	TYR	2.4
2	C	252	SER	2.4
3	D	1202	GLU	2.4
5	F	155	GLU	2.4
2	I	995	ASP	2.4
3	J	212	THR	2.4
3	J	1198	VAL	2.4
4	K	73	GLN	2.4
1	A	161	SER	2.4
3	D	930	LEU	2.4
3	J	811	GLU	2.4
5	F	321	ALA	2.3
1	A	6	THR	2.3
3	J	878	ASP	2.3
3	D	1201	GLY	2.3
4	K	39	VAL	2.3
3	D	208	THR	2.3
5	L	292	VAL	2.3
2	I	165	HIS	2.3
2	I	1016	GLU	2.3
4	K	30	MET	2.3
1	G	164	ASP	2.3
1	H	211	ILE	2.3
1	H	24	ALA	2.3
3	J	1152	GLU	2.2
3	D	149	GLY	2.2
5	L	514	ASP	2.2
3	J	876	SER	2.2
3	J	830	ASP	2.2
3	D	207	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
5	L	337	VAL	2.2
4	K	2	ALA	2.2
5	F	284	GLU	2.2
2	I	231	GLU	2.2
2	I	1008	GLN	2.2
3	D	212	THR	2.2
2	C	317	LEU	2.2
2	C	745	GLU	2.2
2	C	1000	LEU	2.1
3	J	849	LEU	2.1
4	K	29	GLN	2.1
3	J	554	GLU	2.1
1	H	98	VAL	2.1
2	I	986	ALA	2.1
2	I	1009	ASN	2.1
3	J	1200	GLU	2.1
3	J	1186	TYR	2.1
3	J	1372	ARG	2.1
5	F	165	PHE	2.1
3	D	1299	GLY	2.1
4	K	76	GLU	2.1
1	H	97	GLU	2.1
2	I	984	VAL	2.1
2	C	331	LYS	2.1
3	J	209	ASN	2.1
3	J	1203	ARG	2.0
3	J	1151	LYS	2.0
3	J	555	TYR	2.0
3	J	89	GLY	2.0
4	K	58	LEU	2.0
5	F	489	MET	2.0
5	L	425	TYR	2.0
5	L	293	GLU	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 ⓘ

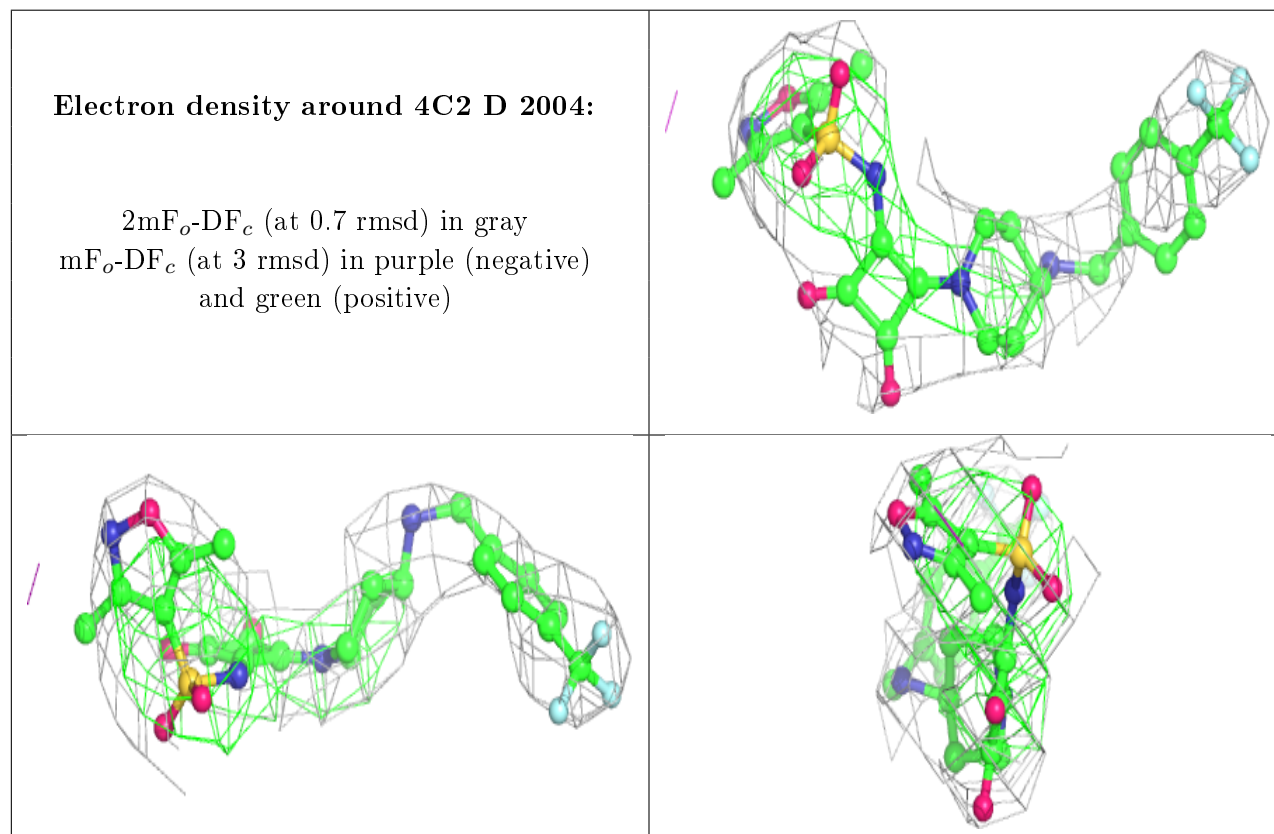
There are no carbohydrates in this entry.

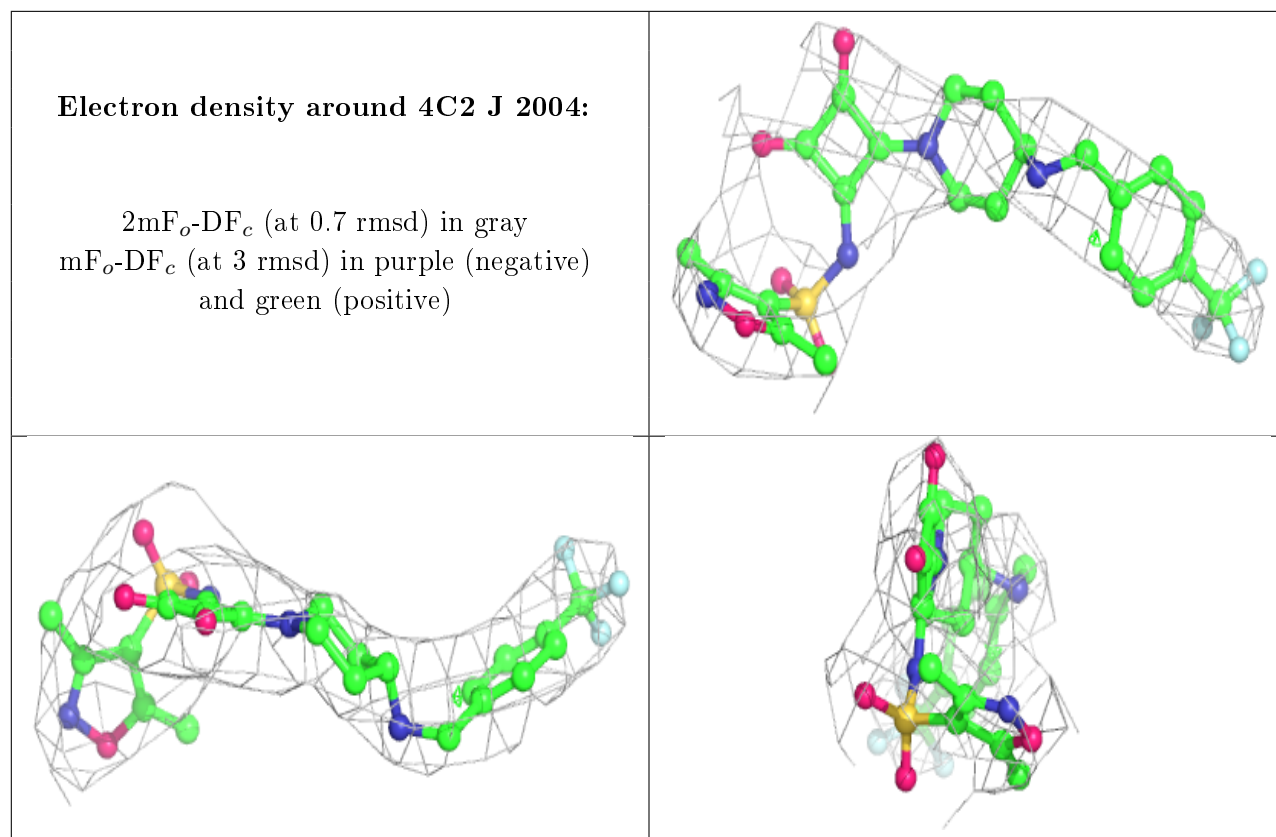
6.4 Ligands ⓘ

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. 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	B-factors(Å ²)	Q<0.9
8	4C2	D	2004	35/35	0.92	0.39	166,166,166,175	0
6	MG	J	2001	1/1	0.94	0.29	166,166,166,166	0
7	ZN	J	2002	1/1	0.94	0.08	201,201,201,201	0
8	4C2	J	2004	35/35	0.94	0.29	166,166,171,175	0
6	MG	D	2001	1/1	0.95	0.16	166,166,166,166	0
7	ZN	D	2002	1/1	0.98	0.13	166,166,166,166	0
7	ZN	J	2003	1/1	0.99	0.13	217,217,217,217	0
7	ZN	D	2003	1/1	1.00	0.24	166,166,166,166	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.





6.5 Other polymers [i](#)

There are no such residues in this entry.