



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:47 PM UTC

PDB ID : 4YFN / pdb_00004yfn
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 types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references](#) ①) were used in the production of this report:

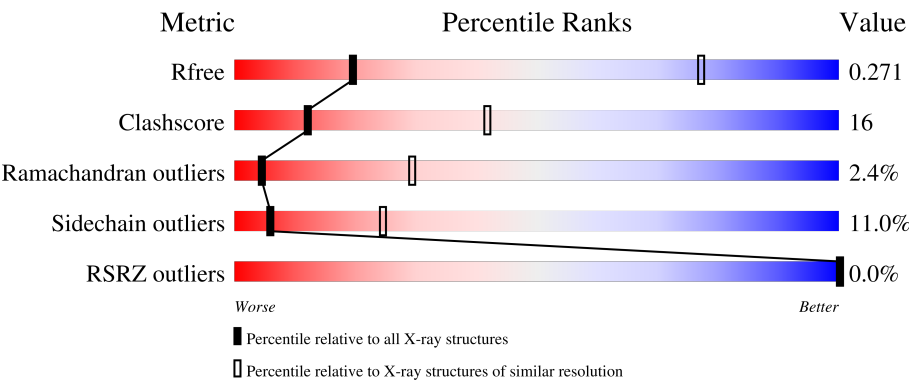
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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}	180053	1043 (3.98-3.66)
Clashscore	190562	1075 (3.98-3.66)
Ramachandran outliers	187476	1029 (3.98-3.66)
Sidechain outliers	187428	1024 (3.98-3.66)
RSRZ outliers	180081	1042 (3.98-3.66)

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 of 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	41%24%6%•29%
1	B	329	45%35%7%12%
1	G	329	38%27%•31%
1	H	329	32%27%6%•34%
2	C	1342	59%34%6%•

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Mol	Chain	Length	Quality of chain
2	I	1342	
3	D	1407	
3	J	1407	
4	E	91	
4	K	91	
5	F	613	
5	L	613	

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			

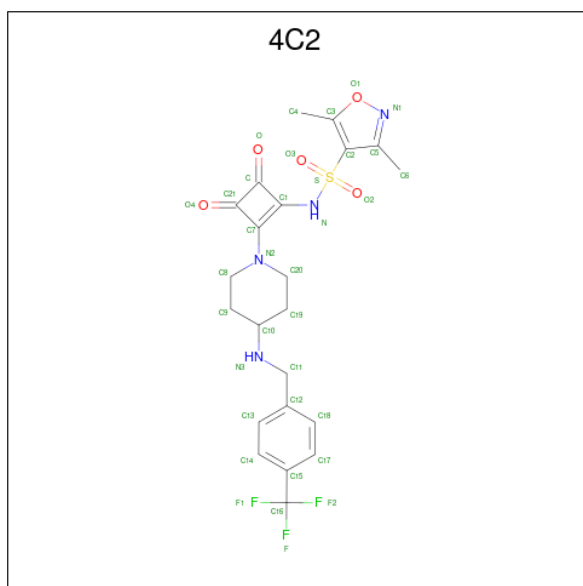
- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

- Molecule 7 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	D	2	Total	Zn	0	0
			2	2		
7	J	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 (CCD ID: 4C2) (formula: C₂₂H₂₃F₃N₄O₅S).

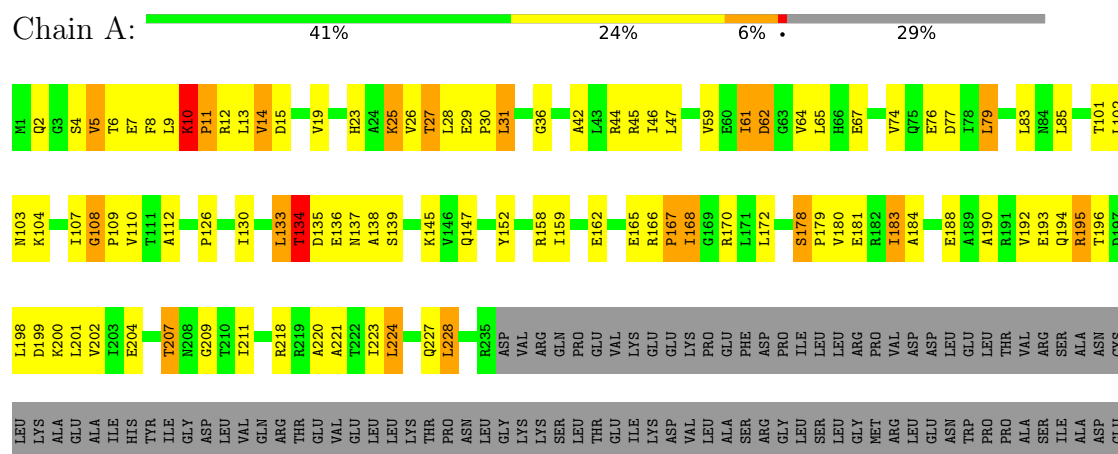


Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
8	D	1	Total	C	F	N	O	S	0	0
			35	22	3	4	5	1		
8	J	1	Total	C	F	N	O	S	0	0
			35	22	3	4	5	1		

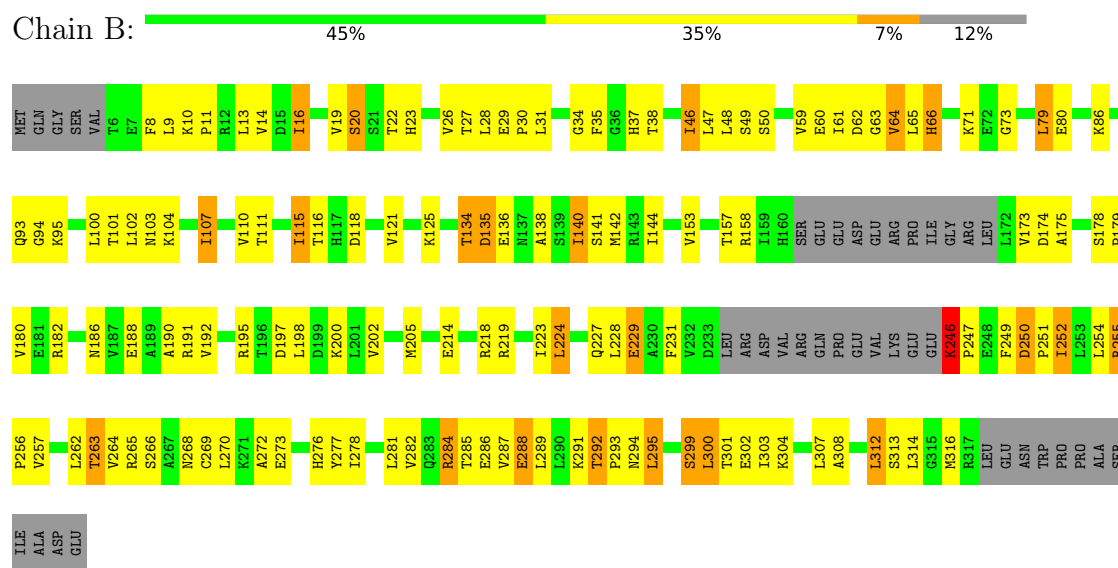
3 Residue-property plots

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

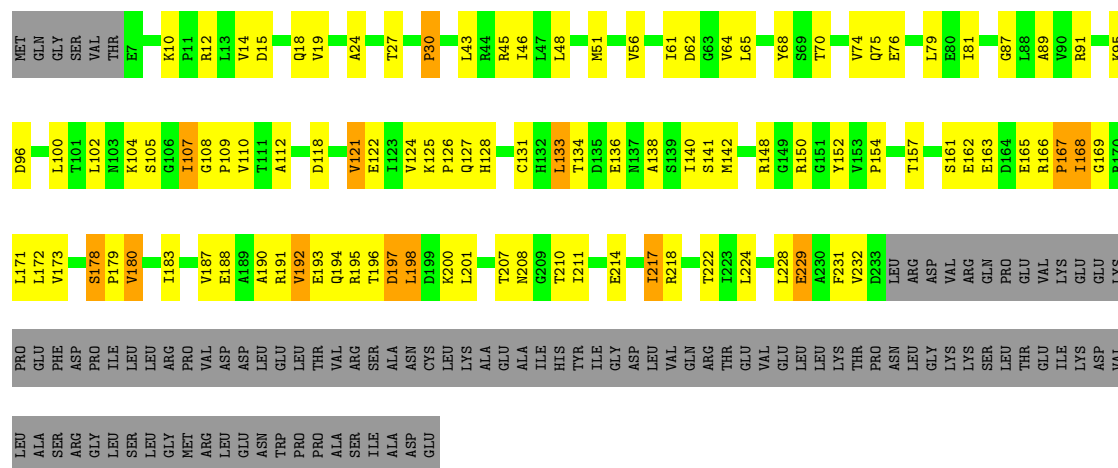


• Molecule 1: DNA-directed RNA polymerase subunit alpha

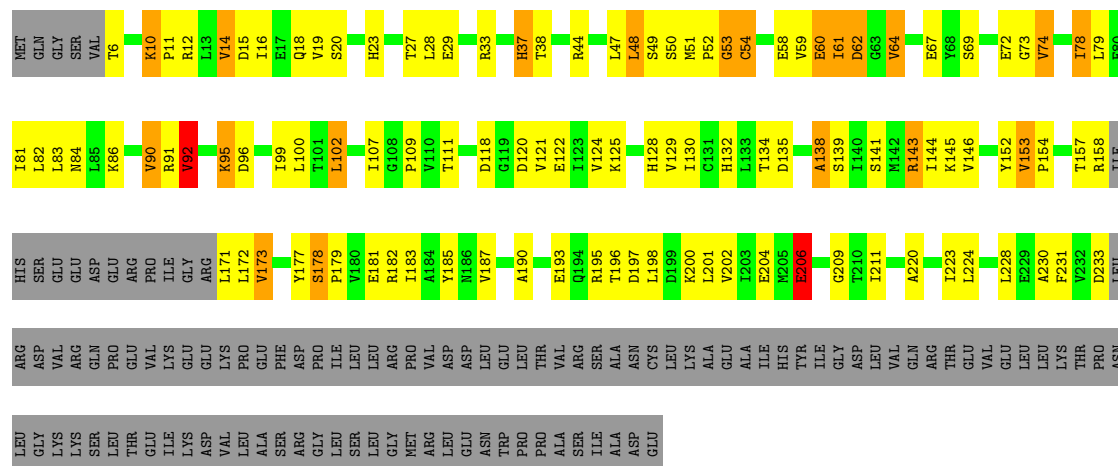


• Molecule 1: DNA-directed RNA polymerase subunit alpha

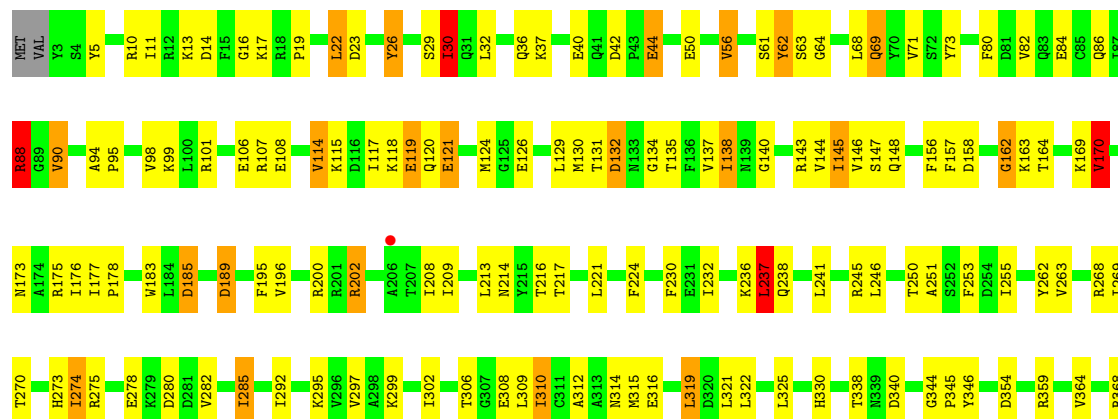


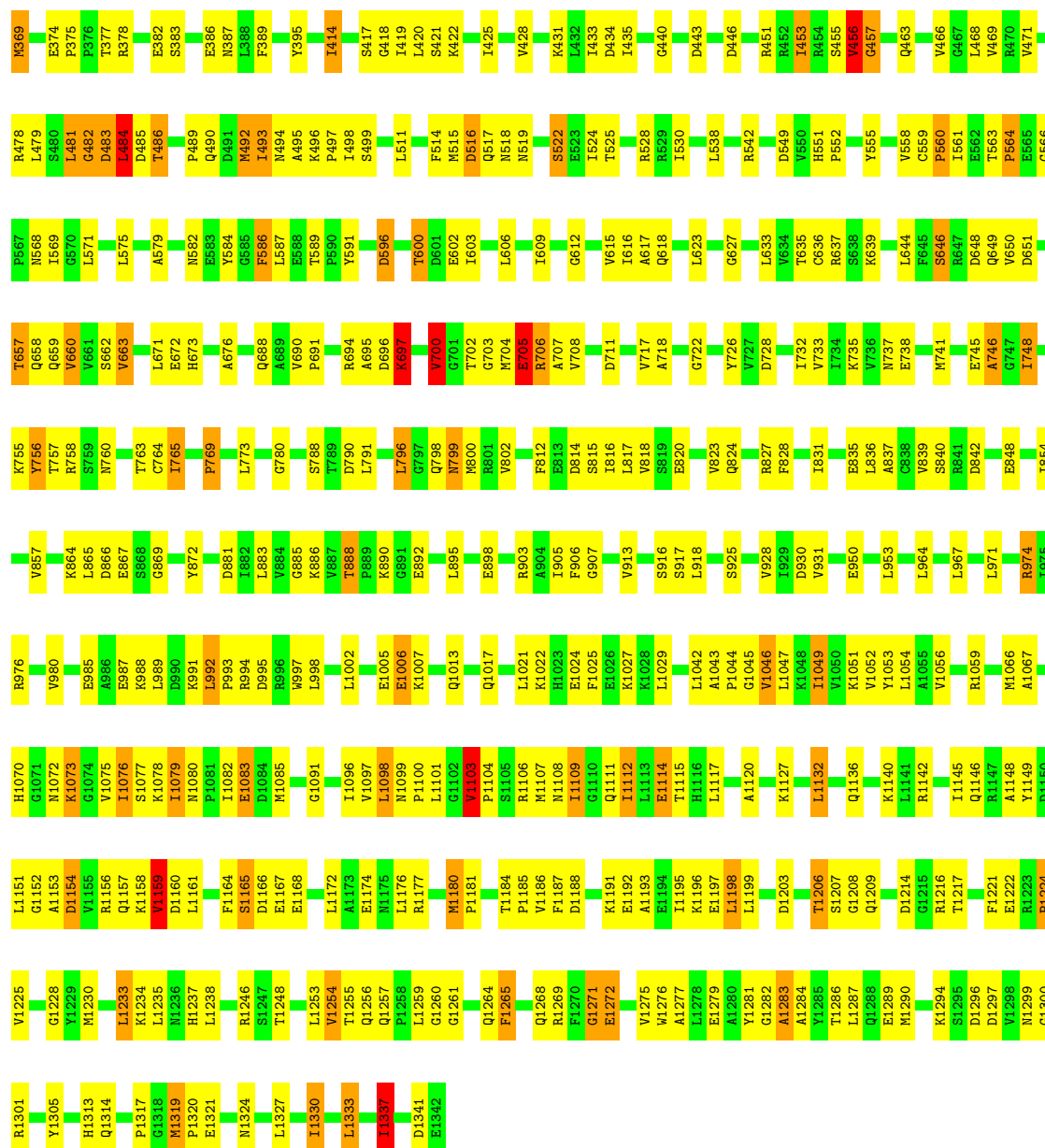


• Molecule 1: DNA-directed RNA polymerase subunit alpha



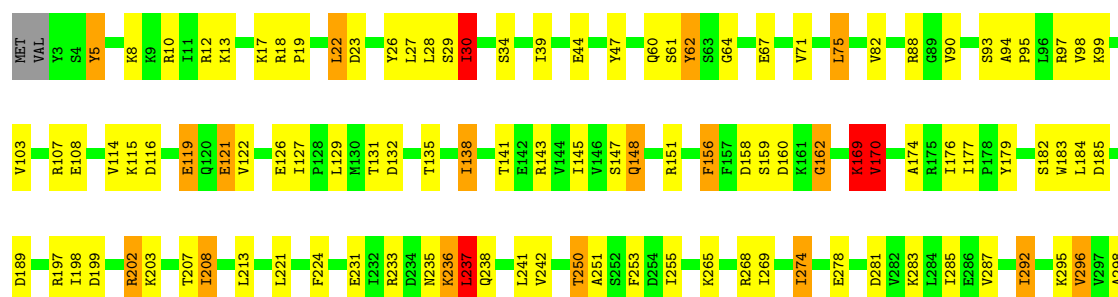
• Molecule 2: DNA-directed RNA polymerase subunit beta

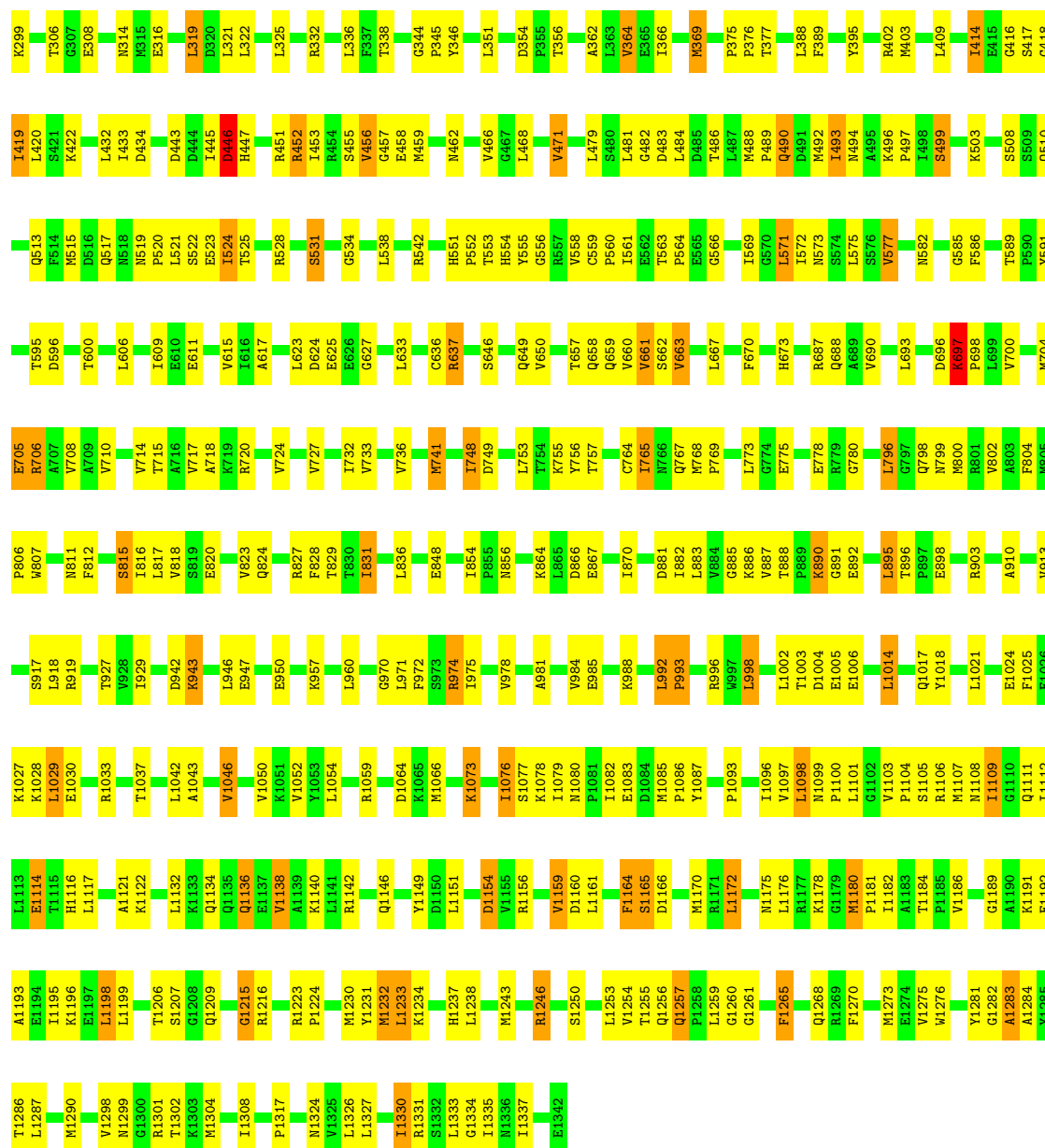




• Molecule 2: DNA-directed RNA polymerase subunit beta

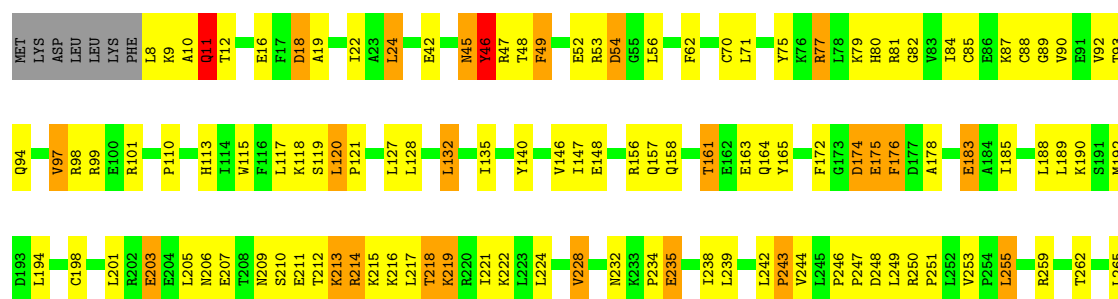
Chain I: 62% 32% 6%

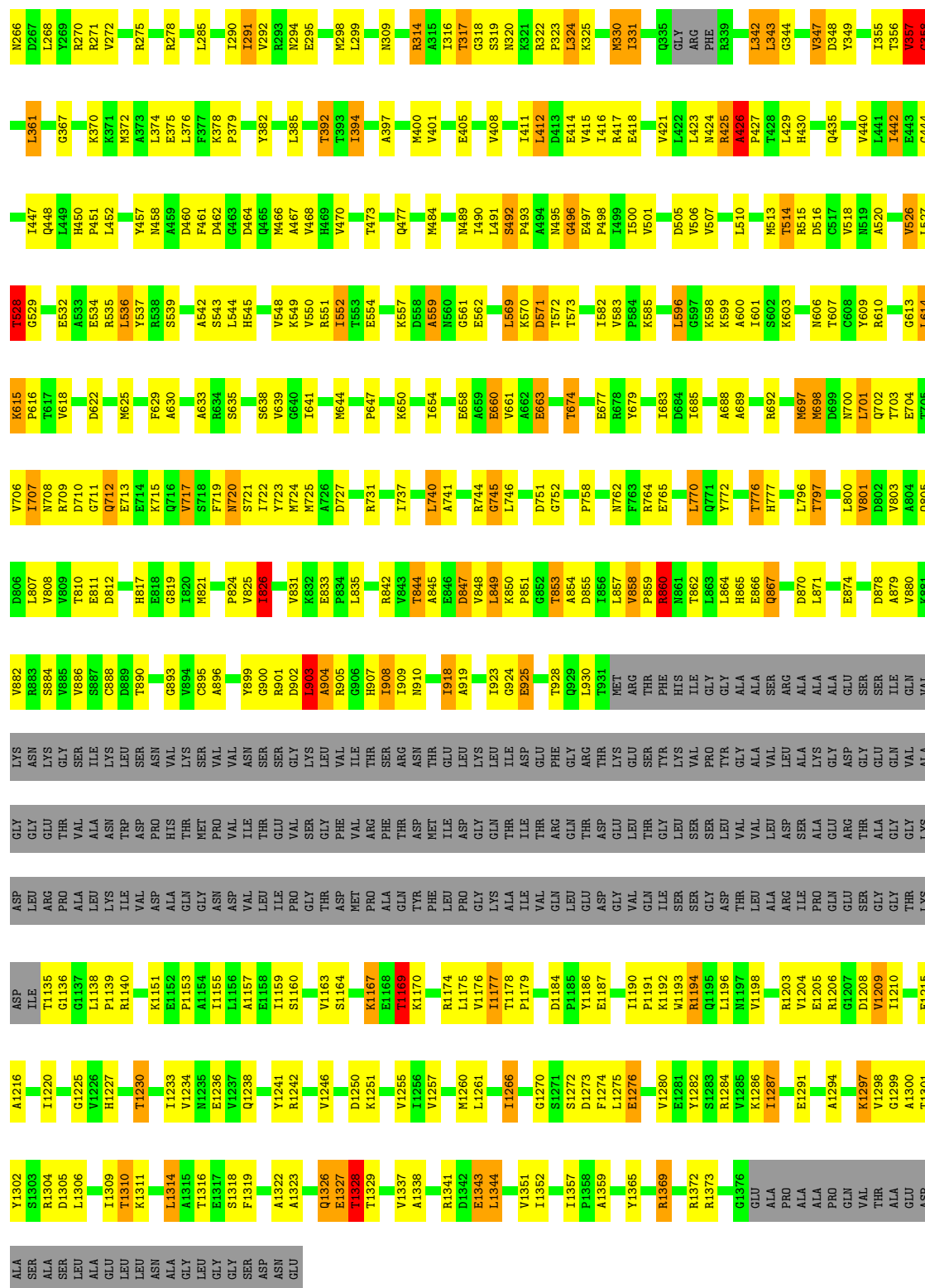




• Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain D: 45% 30% 7% 17%

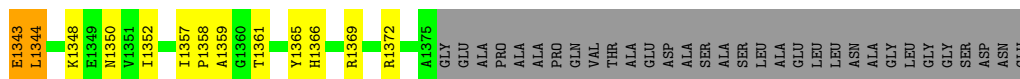




- Molecule 3: DNA-directed RNA polymerase subunit beta'

Chain J: 47% 28% 6% 18%

MET	LYS	ASP	LEU	LEU	LEU	PHE	LEU	LYS	GLN	THR	THR	GLU	E16	F17	A23	A25	S26	I30	K40	P41	E42	T43	I44	N45	Y46	R47	T48	F49	E52	R53	D54	G55	L56	F57	F62	K66	E69	C70	L71	R77	L78	K79	H80	R81	G82	C85	E86									
K87	C88	G89	V90	E91	V92	T93	Q94	V97	R98	R101	W115	F116	L117	K118	S119	L120	R123	I124	L128	L132	R133	D134	I135	E136	R137	V138	L139	V146	I147	E148	L154	G55	L56	F57	F62	K66	E69	C70	L71	R77	L78	K79	H80	R81	G82	C85	E86									
L188	L189	R259	L265	L362	L268	Q196	E197	C198	L201	R202	E203	E204	N205	N206	E207	T208	N209	S210	E211	K212	R214	K215	K216	L217	K218	R219	R220	I221	K222	L223	L224	E225	V228	N232	K233	P234	E235	M236	M237	I238	T239	T240	V241	L242	P243	V244	L245	P246	P247	D248	P251	L252	L255			
F461	D462	G463	R362	L363	Q465	M466	L474	C366	R275	G367	L285	L385	T392	T393	I394	I291	K399	M400	E295	E405	A406	V407	V408	I411	L412	L306	R311	I416	R417	E418	G318	H419	S319	P420	N320	L423	M424	R425	A426	M330	I331	Q335	GLY	ARG	PHE	R339	L342	L343	G344	V347	D348	Y349	V453	S353	A459	D460
K549	V550	R551	Y555	E556	K557	D558	A559	N560	G561	E562	L563	Y564	A565	L569	K570	D571	R576	L579	V580	M581	I582	P584	K585	V501	P502	D505	V506	S507	M513	T514	R515	D516	C517	Y518	M525	V526	L527	T528	G529	E532	R535	L536	Y537	R538	H545	A546	R547	V548								
D643	M644	P647	Y655	E656	K657	D658	A659	G661	E662	L663	Y664	A665	L669	K670	D671	R676	L679	V680	M681	I682	P684	K685	V601	P602	D605	V606	S607	M613	T614	R615	D616	C617	Y618	M625	V626	L627	T628	G629	E632	R635	L636	Y637	R638	H645	A646	R647	V648									
G745	L746	K749	P750	D751	Y755	P758	N762	F763	R764	E765	L767	N769	G770	L771	A784	Y877	L788	K789	T797	L800	V801	P802	K803	V804	D805	S806	T810	E811	C814	H817	E818	G819	T820	M821	H822	T823	P824	Y825	T826	Y831	H832	Y833	Y834	E835	L836	R837										
V843	T844	A845	E846	D847	Y848	L849	T853	A854	D855	L856	L857	H858	R859	L863	E866	L872	V877	D878	A879	V882	S884	V885	P886	S887	K888	L889	F892	G893	H894	C895	Y899	G900	R901	D902	L903	A904	R905	I908	P909	T915	Y918	A919	A920	G924												
E925	T928	Q929	L930	T931	MET	ARG	THR	PHE	THR	ILE	GLY	GLY	ALA	ALA	ALA	ALA	ALA	GLN	VAL	LYS	ASN	GLY	THR	VAL	VAL	ASN	THR	LYS	SER	PRO	ASN	SER	GLY	VAL	GLY	THR	VAL	GLY	THR	ARG	THR	ILE	GLY	LEU	LYS	ILE										
ASP	GLU	PHE	GLN	ASP	THR	LYS	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR								
ILE	VAL	GLN	LEU	ASP	THR	GLY	VAL	GLY	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR	THR							
G1182	S1183	T1184	P1185	I1180	P1191	K1192	W1193	R1194	V1198	F1199	T1204	D1208	I1209	L1210	E1215	A1216	D1219	I1220	L1221	ASP	V1226	I1233	E1236	V1237	Q1238	R1242	V1246	K1247	I1248	M1249	D1250	K1251	H1252	I1253	E1254	V1255	I1256	T1257	R1258	K1259	G1171	K1172	R1173	K1263	A1264	T1265	V1266	L1267								
N1268	A1269	G1270	D1273	F1274	L1275	G1277	V1280	E1281	L1282	S1283	K1284	V1285	K1286	N1289	L1290	E1291	S1293	A1294	I1297	L1298	G1299	A1300	T1301	F1302	S1303	R1304	D1305	L1306	L1307	G1308	I1309	T1310	K1311	L1314	A1315	T1316	E1317	S1318	S1324	F1325	Q1326	E1327	T1328	T1329	L1332	K1333	A1334	V1337								

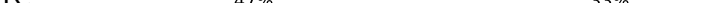


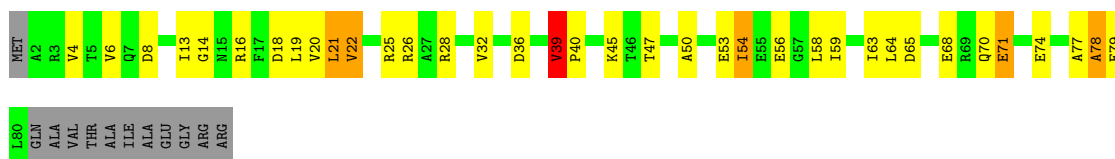
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 73% 22% .



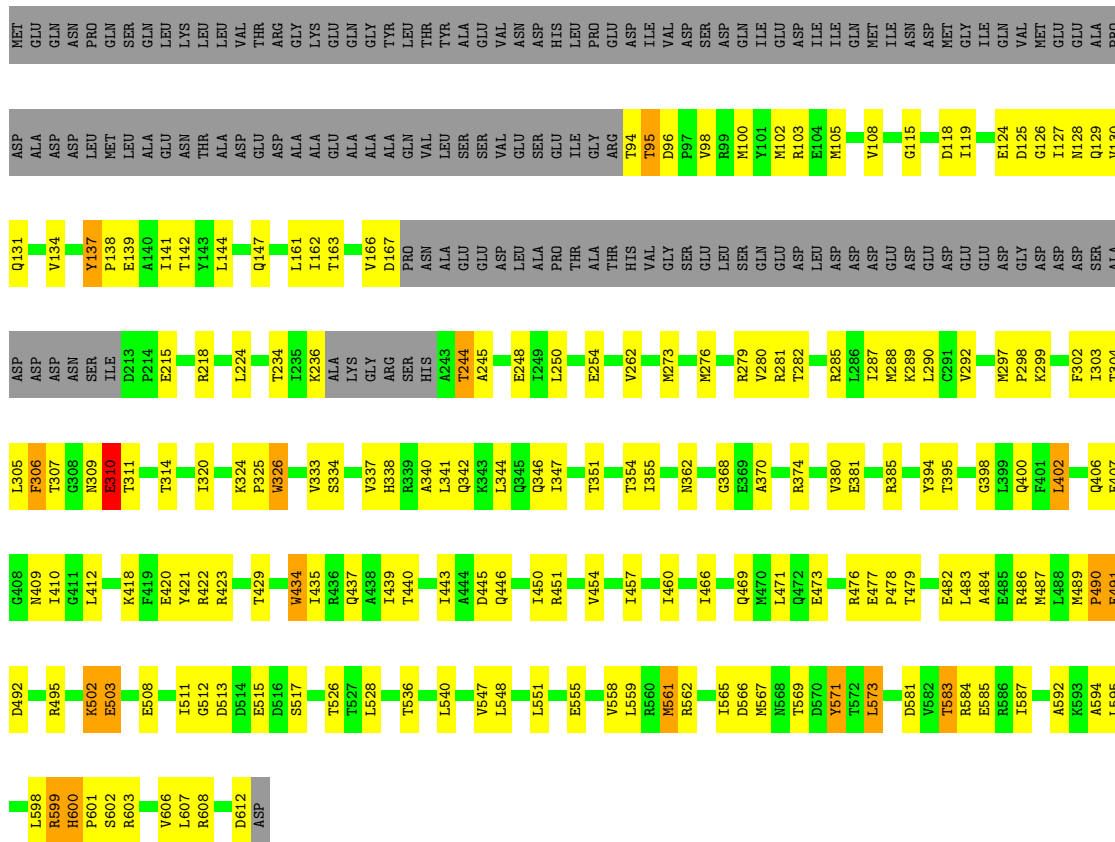
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain K:  47% 33% 5% • 13%



- Molecule 5: RNA polymerase sigma factor RpoD

Chain F: 46% 27% . 24%



- Molecule 5: RNA polymerase sigma factor RpoD



MET	GLU	GLN	ASN	PRO	GLN	SER	GLN	LEU	LYS	LEU	VAL	THR	ARG	GLY	LYS	GLU	GLN	GLY	TYR	LEU	THR	THR	ALA	GLU	VAL	ASN	ASP	HIS	LEU	PRO	GLU	ASP	ILE	VAL	ASP	SER	ASP	GLN	ILE	GLU	ASP	ILE	GLN	MET	ILE	GLN	VAL	MET	GLU	GLU	ALA	PRO		
ASP	ALA	ASP	ASP	LEU	MET	LEU	ALA	GLU	ASN	THR	ALA	ASP	GLU	ASP	ALA	ALA	ALA	ALA	ALA	GLN	VAL	LEU	TYR	LEU	SER	SER	GLU	GLU	HIS	ILE	GLY	ARG	T94	T95	D96	P97	V98	M102	M105	V108	E109	L110	R113	E114	R117	K121	E124	V130	V134					
Y137	P138	E139		T142	Y143	L144	L145	E146	Q147	V151	F165	V166	D167	PRO	ASN	GLY	ALA	ALA	GLU	ASP	GLU	VAL	THR	THR	ALA	THR	HIS	VAL	GLY	SER	GLY	LEU	SER	GLU	SER	GLU	GLN	ASP	ASP	GLU	ASP	GLU	ASP	GLY	ASP	ASP	ASP	ASP	ASP	ASP	SER			
ILE	D213	E219	L224	V229	V230	T231	R232	D233	T234	I235	K236	ALA	LYS	GLY	ARG	SER	HIS	A243	T244	A245	E248	K251	V255	R260	L269	V270	M273	R274	V275	M276	M277	V280	E284	K289	L290	C291	V292	C295	K296	M297	P298	K299	T304	L305	F306									
E310	T311	T314	W315	F316	K324	P325	W326	V333	S334	V337	L341	Q342	K343	E348	T351	G352	L353	D360	I361	N362	M365	S366	I367	M379	V380	E381	A382	N383	L384	R385	L386	V387	I388	K392	T395	Q400	F401	L402	Q406	L412	I435	R436												
Q437	D445	R448	T449	I450	R451	I452	P453	V454	H455	H456	I457	I466	S467	R468	Q469	M470	L471	M474	G475	R476	E477	P478	T479	P480	E481	E482	L483	A484	E485	R486	M487	L488	M489	P490	E491	D492	K493	I494	R495	K496	V497	L498	K499	I500	E503	P504	I505	S506	M507	E508	T509	P510	I511	G512
D513	T526	L530	T536	S539	L540	V547	L551	E555	V558	L559	R560	M561	D566	M567	R568	T569	D570	Y571	T572	L573	G577	D581	V582	T583	R584	I587	R588	A594	L598	R599	H600	P601	S602	R603	S604	R608	D612	D613																

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 29.96 – 3.82	Depositor EDS
% Data completeness (in resolution range)	88.9 (29.96-3.82) 77.7 (29.96-3.82)	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 0.229 , 0.271	Depositor DCC
R_{free} test set	2003 reflections (1.66%)	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)	0.28 , 123.9	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: MG, 4C2, ZN

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.05	5/1842 (0.3%)	1.34	12/2495 (0.5%)
1	B	1.08	6/2260 (0.3%)	1.28	14/3059 (0.5%)
1	G	1.16	6/1777 (0.3%)	1.27	9/2408 (0.4%)
1	H	1.46	20/1681 (1.2%)	1.45	16/2278 (0.7%)
2	C	1.11	22/10739 (0.2%)	1.26	59/14489 (0.4%)
2	I	1.01	14/10729 (0.1%)	1.23	44/14477 (0.3%)
3	D	1.16	27/9167 (0.3%)	1.29	53/12380 (0.4%)
3	J	1.08	18/9118 (0.2%)	1.28	48/12312 (0.4%)
4	E	0.93	0/693	1.13	0/935
4	K	1.66	6/629 (1.0%)	1.57	8/847 (0.9%)
5	F	1.23	22/3864 (0.6%)	1.32	13/5194 (0.3%)
5	L	1.19	16/3872 (0.4%)	1.32	16/5205 (0.3%)
All	All	1.13	162/56371 (0.3%)	1.28	292/76079 (0.4%)

All (162) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	307	THR	CA-CB	10.09	1.65	1.53
1	H	111	THR	CA-CB	9.80	1.68	1.53
5	F	337	VAL	CA-CB	9.47	1.67	1.54
3	J	1190	ILE	CA-CB	9.01	1.61	1.54
2	C	90	VAL	CA-CB	-8.97	1.42	1.54
3	J	703	THR	CA-CB	8.88	1.66	1.53
2	C	663	VAL	CA-CB	-8.71	1.44	1.54
1	H	129	VAL	CA-CB	8.40	1.64	1.54
3	J	856	ILE	CA-CB	8.08	1.63	1.53
3	D	1246	VAL	CA-CB	-7.99	1.44	1.54
1	G	192	VAL	CA-CB	7.84	1.63	1.53
5	L	275	VAL	CA-CB	7.71	1.64	1.54
3	D	1287	ILE	CA-CB	7.67	1.65	1.54
2	I	975	ILE	CA-CB	7.67	1.64	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	292	VAL	CA-CB	7.64	1.63	1.54
2	I	984	VAL	CA-CB	7.49	1.62	1.54
2	C	660	VAL	CA-CB	-7.47	1.44	1.54
3	D	1177	ILE	CA-CB	7.46	1.62	1.54
2	C	700	VAL	CA-CB	-7.45	1.43	1.53
5	L	234	THR	CA-CB	7.41	1.64	1.53
5	L	304	THR	CA-CB	7.38	1.64	1.53
3	D	468	VAL	CA-CB	-7.37	1.44	1.54
5	F	304	THR	CA-CB	7.34	1.64	1.53
3	J	877	VAL	CA-CB	7.27	1.62	1.53
5	F	583	THR	CA-CB	7.13	1.64	1.53
2	C	1079	ILE	CA-CB	-7.12	1.45	1.54
2	C	137	VAL	CA-CB	-7.04	1.45	1.54
2	C	816	ILE	CA-CB	-7.03	1.45	1.54
3	J	858	VAL	CA-C	6.95	1.57	1.52
5	F	320	ILE	CA-CB	6.94	1.63	1.54
3	D	801	VAL	CA-CB	-6.86	1.44	1.54
3	J	858	VAL	CA-CB	6.82	1.59	1.54
5	F	326	TRP	CA-C	6.78	1.61	1.53
3	D	467	ALA	CA-CB	-6.76	1.42	1.53
3	J	317	THR	CA-CB	6.74	1.63	1.53
3	D	470	VAL	CA-CB	-6.73	1.46	1.54
3	D	253	VAL	CA-CB	-6.72	1.45	1.54
3	J	1190	ILE	CA-C	6.70	1.57	1.52
5	L	337	VAL	CA-CB	6.68	1.61	1.54
3	D	22	ILE	CA-CB	-6.64	1.45	1.55
5	F	142	THR	CA-CB	6.64	1.63	1.53
3	J	518	VAL	CA-CB	6.60	1.62	1.54
5	L	314	THR	CA-CB	6.60	1.64	1.53
1	A	192	VAL	CA-CB	6.55	1.61	1.53
2	C	274	ILE	CA-CB	6.50	1.62	1.54
2	I	595	THR	CA-CB	6.37	1.62	1.53
2	I	274	ILE	CA-CB	6.36	1.61	1.54
1	H	64	VAL	CA-C	6.28	1.60	1.52
2	C	1097	VAL	CA-CB	-6.28	1.46	1.54
1	H	173	VAL	CA-C	6.27	1.60	1.52
2	I	250	THR	CA-CB	6.25	1.62	1.53
2	C	30	ILE	CA-CB	-6.23	1.47	1.54
3	D	218	THR	CA-CB	6.23	1.63	1.53
3	D	272	VAL	CA-CB	-6.23	1.47	1.54
2	I	1003	THR	CA-CB	6.20	1.62	1.53
3	D	1190	ILE	CA-C	6.16	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	J	221	ILE	CA-CB	6.10	1.61	1.54
3	D	506	VAL	CA-CB	-6.10	1.46	1.54
2	I	453	ILE	CA-C	6.09	1.59	1.52
4	K	22	VAL	CA-CB	6.09	1.61	1.54
5	F	298	PRO	CA-C	6.09	1.60	1.52
1	H	146	VAL	CA-CB	6.02	1.62	1.54
1	G	121	VAL	CA-CB	5.97	1.61	1.54
5	L	291	CYS	CA-C	5.95	1.60	1.53
2	I	896	THR	CA-CB	5.93	1.62	1.53
2	C	144	VAL	CA-CB	-5.92	1.47	1.54
1	H	16	ILE	CA-CB	5.92	1.62	1.54
1	H	14	VAL	CA-CB	5.88	1.62	1.54
5	F	303	ILE	CA-CB	5.85	1.62	1.54
2	I	981	ALA	CA-C	5.84	1.60	1.52
2	C	310	ILE	CA-CB	5.84	1.61	1.54
1	B	115	ILE	CA-CB	5.84	1.60	1.54
3	D	1190	ILE	CA-CB	5.84	1.61	1.54
5	L	230	VAL	CA-CB	5.83	1.62	1.54
1	A	14	VAL	CA-CB	5.82	1.62	1.54
3	D	238	ILE	CA-CB	-5.81	1.47	1.54
1	H	211	ILE	CA-CB	5.81	1.63	1.54
3	J	705	THR	CA-CB	5.81	1.63	1.53
2	C	708	VAL	CA-CB	-5.79	1.47	1.54
5	L	142	THR	CA-CB	5.79	1.62	1.53
3	D	470	VAL	CA-C	-5.78	1.48	1.53
3	D	317	THR	CA-CB	5.77	1.62	1.53
2	C	1277	ALA	CA-CB	-5.75	1.44	1.53
5	L	304	THR	CA-C	5.75	1.60	1.52
3	D	703	THR	CA-CB	5.74	1.64	1.53
2	C	1112	ILE	CA-CB	-5.73	1.47	1.54
5	L	280	VAL	CA-CB	5.73	1.62	1.54
4	K	6	VAL	CA-CB	5.71	1.62	1.54
1	H	74	VAL	CA-C	5.70	1.59	1.52
3	D	1352	ILE	CA-CB	-5.70	1.47	1.54
4	K	39	VAL	CA-CB	5.68	1.61	1.54
1	G	196	THR	CA-CB	5.66	1.62	1.53
1	H	61	ILE	CA-CB	5.66	1.61	1.54
3	D	356	THR	CA-CB	-5.65	1.45	1.53
5	F	287	ILE	CA-CB	5.65	1.60	1.54
3	J	853	THR	CA-C	5.63	1.60	1.53
1	H	28	LEU	CA-C	5.62	1.59	1.52
5	F	262	VAL	CA-C	5.62	1.58	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	460	ILE	CA-CB	5.59	1.60	1.54
3	J	882	VAL	CA-CB	5.58	1.62	1.54
1	A	134	THR	CA-CB	-5.55	1.46	1.54
2	C	888	THR	CA-CB	5.54	1.61	1.53
2	C	702	THR	CA-CB	-5.53	1.46	1.54
1	H	72	GLU	CA-C	5.53	1.60	1.52
1	B	107	ILE	CA-CB	5.52	1.62	1.54
5	L	291	CYS	CB-SG	5.51	1.99	1.81
1	H	129	VAL	CA-C	5.51	1.59	1.52
1	H	152	TYR	CA-C	5.50	1.58	1.52
4	K	32	VAL	CA-C	5.47	1.59	1.52
5	F	334	SER	CA-C	5.46	1.60	1.52
1	G	222	THR	CA-CB	5.45	1.61	1.53
3	D	421	VAL	CA-CB	-5.44	1.46	1.54
5	F	141	ILE	CA-CB	5.44	1.60	1.54
1	B	66	HIS	CA-C	5.43	1.59	1.52
1	G	30	PRO	CA-C	5.42	1.57	1.53
3	J	1155	ILE	CA-C	5.41	1.59	1.52
3	D	212	THR	CA-CB	5.40	1.61	1.53
3	J	1199	PHE	CA-C	5.39	1.59	1.52
1	B	125	LYS	CA-C	5.38	1.58	1.52
5	F	162	ILE	CA-C	5.34	1.59	1.52
1	H	173	VAL	CA-CB	5.34	1.64	1.55
5	F	288	MET	CA-C	5.34	1.59	1.52
3	D	489	ASN	CA-C	-5.33	1.47	1.53
2	C	1217	THR	CA-CB	-5.31	1.44	1.53
5	F	354	THR	CA-CB	5.31	1.61	1.53
5	F	307	THR	N-CA	5.29	1.53	1.46
3	D	206	ASN	CA-C	5.28	1.59	1.52
1	A	6	THR	CA-CB	5.28	1.62	1.53
2	I	1005	GLU	CA-C	5.28	1.58	1.52
1	B	111	THR	CA-CB	5.27	1.61	1.53
5	F	320	ILE	CA-C	5.25	1.61	1.52
3	J	1176	VAL	CA-C	5.25	1.59	1.52
1	B	299	SER	CA-C	5.25	1.59	1.52
2	C	282	VAL	CA-CB	5.25	1.59	1.53
1	A	11	PRO	CA-C	-5.23	1.47	1.52
1	H	173	VAL	N-CA	5.21	1.52	1.46
5	L	315	TRP	CA-C	5.20	1.59	1.52
2	C	1103	VAL	CA-CB	-5.20	1.47	1.54
2	C	650	VAL	CA-CB	-5.19	1.48	1.54
1	H	92	VAL	CA-CB	5.19	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	903	LEU	CA-C	-5.18	1.46	1.52
5	F	282	THR	CA-CB	5.15	1.61	1.53
3	D	440	VAL	CA-CB	-5.15	1.48	1.54
3	D	1233	ILE	CA-CB	-5.14	1.48	1.54
4	K	54	ILE	CA-CB	5.14	1.60	1.54
2	I	1018	TYR	CA-C	5.13	1.59	1.52
1	H	206	GLU	CA-C	5.13	1.59	1.52
1	H	19	VAL	CA-C	5.11	1.59	1.52
1	H	20	SER	CA-C	5.09	1.59	1.52
3	J	849	LEU	CA-C	5.09	1.58	1.52
1	G	107	ILE	CA-CB	5.08	1.59	1.53
2	I	978	VAL	CA-CB	5.08	1.61	1.54
2	I	1138	VAL	CA-CB	5.07	1.60	1.54
3	J	215	LYS	CA-C	5.06	1.59	1.52
5	F	244	THR	CA-CB	5.05	1.62	1.53
4	K	71	GLU	CA-C	5.05	1.59	1.52
5	L	219	GLU	CA-C	5.02	1.59	1.52
5	F	340	ALA	CA-C	5.02	1.59	1.52
2	I	998	LEU	CA-C	5.01	1.59	1.52
2	C	763	THR	CA-CB	-5.01	1.45	1.53
5	L	255	VAL	CA-CB	5.01	1.61	1.54
5	L	229	VAL	CA-CB	5.00	1.60	1.54

All (292) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	426	ALA	CA-C-N	-14.60	103.63	120.13
3	D	426	ALA	C-N-CA	-14.60	103.63	120.13
3	J	17	PHE	N-CA-C	9.82	123.01	110.24
2	C	561	ILE	N-CA-C	9.75	119.80	111.90
1	B	250	ASP	CA-C-N	9.54	129.25	118.85
1	B	250	ASP	C-N-CA	9.54	129.25	118.85
1	H	10	LYS	CA-C-N	9.43	131.03	120.85
1	H	10	LYS	C-N-CA	9.43	131.03	120.85
1	A	62	ASP	N-CA-C	9.36	122.43	111.02
3	D	925	GLU	CA-C-N	-9.23	110.29	121.00
3	D	925	GLU	C-N-CA	-9.23	110.29	121.00
3	J	426	ALA	CA-C-N	-9.14	109.80	120.13
3	J	426	ALA	C-N-CA	-9.14	109.80	120.13
1	A	10	LYS	CA-C-N	-8.88	110.98	120.66
1	A	10	LYS	C-N-CA	-8.88	110.98	120.66
3	J	120	LEU	CA-C-N	-8.30	109.47	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	120	LEU	C-N-CA	-8.30	109.47	119.84
2	C	561	ILE	CB-CA-C	-8.27	103.36	111.30
3	D	903	LEU	N-CA-C	-8.26	97.23	108.38
3	J	40	LYS	CA-C-N	8.19	129.18	120.83
3	J	40	LYS	C-N-CA	8.19	129.18	120.83
1	B	246	LYS	CA-C-N	8.15	130.03	119.84
1	B	246	LYS	C-N-CA	8.15	130.03	119.84
1	H	153	VAL	CA-C-N	8.09	128.24	120.31
1	H	153	VAL	C-N-CA	8.09	128.24	120.31
3	D	752	GLY	N-CA-C	-8.05	103.78	114.25
3	D	529	GLY	CA-C-N	-8.02	110.69	119.19
3	D	529	GLY	C-N-CA	-8.02	110.69	119.19
3	D	501	VAL	N-CA-C	7.98	116.59	107.89
3	D	45	ASN	N-CA-C	7.87	119.49	111.07
2	C	1333	LEU	N-CA-C	-7.83	98.34	110.17
5	L	96	ASP	CA-C-N	7.83	129.63	119.84
5	L	96	ASP	C-N-CA	7.83	129.63	119.84
3	D	12	THR	N-CA-C	-7.67	105.08	114.75
2	C	1046	VAL	N-CA-C	7.52	119.34	107.98
2	C	224	PHE	N-CA-C	7.41	119.44	111.36
3	J	233	LYS	CA-C-N	7.41	127.12	119.56
3	J	233	LYS	C-N-CA	7.41	127.12	119.56
1	H	53	GLY	N-CA-C	7.36	121.88	110.91
3	J	529	GLY	CA-C-N	-7.15	112.34	119.56
3	J	529	GLY	C-N-CA	-7.15	112.34	119.56
2	I	414	ILE	N-CA-C	-7.14	106.93	113.71
2	C	1319	MET	N-CA-C	7.09	119.01	110.07
3	J	1171	GLY	N-CA-C	-7.09	105.03	114.25
3	J	365	GLN	N-CA-C	7.08	121.03	109.85
5	F	368	GLY	N-CA-C	-7.04	104.01	113.24
2	I	1333	LEU	N-CA-C	-7.03	99.56	110.17
2	C	1337	ILE	CA-C-N	-6.97	111.65	122.59
2	C	1337	ILE	C-N-CA	-6.97	111.65	122.59
3	D	528	THR	N-CA-C	6.95	119.73	111.33
3	D	1136	GLY	N-CA-C	6.88	120.80	110.75
3	J	930	LEU	N-CA-C	6.85	119.57	110.53
3	D	1225	GLY	N-CA-C	6.76	119.40	111.63
5	L	137	TYR	CA-C-N	6.74	126.37	119.56
5	L	137	TYR	C-N-CA	6.74	126.37	119.56
2	I	561	ILE	N-CA-C	6.73	117.59	111.81
3	J	347	VAL	N-CA-C	6.73	119.21	108.85
2	C	1208	GLY	N-CA-C	-6.68	106.01	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	62	ASP	N-CA-C	6.67	122.31	111.37
1	B	10	LYS	CA-C-N	6.67	128.17	119.84
1	B	10	LYS	C-N-CA	6.67	128.17	119.84
3	D	470	VAL	N-CA-C	6.67	115.23	107.77
1	H	18	GLN	N-CA-C	6.61	119.68	108.90
3	J	888	CYS	N-CA-C	6.61	119.87	109.96
3	D	414	GLU	N-CA-C	6.60	118.27	111.14
1	A	8	PHE	N-CA-C	6.60	119.92	109.50
2	I	453	ILE	N-CA-C	6.57	117.37	108.17
5	L	487	MET	CA-C-N	6.54	129.93	120.38
5	L	487	MET	C-N-CA	6.54	129.93	120.38
3	J	1182	GLY	N-CA-C	6.52	123.25	112.30
3	D	444	GLY	N-CA-C	-6.51	101.98	110.45
2	C	275	ARG	CA-C-N	6.51	129.32	120.54
2	C	275	ARG	C-N-CA	6.51	129.32	120.54
3	D	358	GLY	CA-C-N	6.47	126.10	119.56
3	D	358	GLY	C-N-CA	6.47	126.10	119.56
1	H	72	GLU	N-CA-C	6.47	119.67	109.96
2	I	237	LEU	N-CA-C	6.43	124.50	110.80
5	F	95	THR	CB-CA-C	-6.41	109.16	116.54
5	F	338	HIS	N-CA-C	6.40	119.95	111.75
2	C	928	VAL	CA-C-N	-6.38	114.05	121.71
2	C	928	VAL	C-N-CA	-6.38	114.05	121.71
5	F	119	ILE	N-CA-C	6.38	116.41	110.42
1	H	139	SER	N-CA-C	6.37	118.90	108.52
5	F	502	LYS	N-CA-C	6.35	118.28	111.36
3	D	807	LEU	N-CA-C	6.34	118.78	108.63
1	G	43	LEU	N-CA-C	6.32	117.96	111.14
3	D	1246	VAL	N-CA-C	6.28	117.15	107.99
1	H	178	SER	CA-C-N	6.27	127.08	120.12
1	H	178	SER	C-N-CA	6.27	127.08	120.12
3	J	765	GLU	N-CA-C	-6.27	102.44	110.53
2	C	482	GLY	N-CA-C	6.26	128.02	113.18
3	J	769	VAL	N-CA-C	6.26	116.93	110.36
3	J	803	VAL	N-CA-C	6.18	116.97	110.72
2	C	1083	GLU	N-CA-C	6.18	118.10	111.36
5	F	137	TYR	CA-C-N	6.18	125.80	119.56
5	F	137	TYR	C-N-CA	6.18	125.80	119.56
2	I	98	VAL	N-CA-C	6.17	117.37	108.48
2	C	579	ALA	N-CA-C	6.15	119.14	110.23
3	J	139	LEU	N-CA-C	6.10	118.72	111.71
1	G	168	ILE	N-CA-C	6.09	116.83	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	811	GLU	N-CA-C	6.04	118.70	110.55
2	I	943	LYS	N-CA-C	6.03	117.52	111.07
2	C	340	ASP	N-CA-C	6.00	118.60	111.33
2	I	354	ASP	CA-C-N	6.00	127.34	119.84
2	I	354	ASP	C-N-CA	6.00	127.34	119.84
1	B	272	ALA	N-CA-C	5.99	118.77	111.82
2	C	560	PRO	CA-C-N	-5.98	116.86	122.66
2	C	560	PRO	C-N-CA	-5.98	116.86	122.66
3	J	1286	LYS	N-CA-C	5.96	119.02	111.69
3	D	347	VAL	N-CA-C	5.92	117.97	108.85
3	D	1328	THR	N-CA-C	5.92	117.81	111.36
3	J	23	ALA	N-CA-C	5.91	115.90	108.45
3	J	583	VAL	CA-C-N	5.91	126.11	119.90
3	J	583	VAL	C-N-CA	5.91	126.11	119.90
2	I	1138	VAL	N-CA-C	5.89	116.08	110.42
2	C	457	GLY	N-CA-C	5.89	119.77	112.64
3	J	492	SER	CA-C-N	5.86	126.74	120.47
3	J	492	SER	C-N-CA	5.86	126.74	120.47
2	I	1257	GLN	CA-C-N	5.83	127.13	119.84
2	I	1257	GLN	C-N-CA	5.83	127.13	119.84
2	I	741	MET	N-CA-C	5.83	118.07	110.43
2	I	298	ALA	N-CA-C	5.83	118.86	111.69
1	H	37	HIS	N-CA-C	5.83	117.71	111.36
2	I	831	ILE	N-CA-C	5.81	116.67	108.36
2	I	182	SER	N-CA-C	5.80	118.67	110.50
2	I	571	LEU	N-CA-C	-5.80	106.18	113.72
1	A	108	GLY	CA-C-N	5.78	125.71	119.76
1	A	108	GLY	C-N-CA	5.78	125.71	119.76
2	I	177	ILE	N-CA-C	5.77	112.81	107.56
1	B	292	THR	N-CA-C	5.77	117.26	109.24
3	J	849	LEU	CA-CB-CG	5.77	136.48	116.30
4	K	78	ALA	CA-C-N	5.76	128.47	120.29
4	K	78	ALA	C-N-CA	5.76	128.47	120.29
2	C	1152	GLY	N-CA-C	5.76	121.73	114.25
1	H	78	ILE	N-CA-C	5.75	115.94	110.42
1	B	268	ASN	N-CA-C	5.75	118.49	111.82
5	F	565	ILE	N-CA-C	5.74	116.68	108.93
2	C	1224	PRO	CA-C-O	-5.74	114.92	121.98
3	J	817	HIS	N-CA-C	-5.74	106.26	113.72
5	L	530	LEU	CA-C-N	-5.73	113.11	119.19
5	L	530	LEU	C-N-CA	-5.73	113.11	119.19
1	A	10	LYS	N-CA-C	-5.72	100.72	109.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	1299	GLY	N-CA-C	5.72	120.38	112.37
2	I	1246	ARG	N-CA-C	5.71	117.68	108.32
2	I	255	ILE	N-CA-C	5.70	112.31	106.21
3	D	904	ALA	N-CA-C	-5.70	106.28	113.18
2	I	531	SER	N-CA-C	5.69	118.72	108.48
2	I	1232	MET	N-CA-C	5.68	118.82	109.72
2	C	1184	THR	CB-CA-C	-5.68	104.74	110.65
3	D	203	GLU	CA-C-N	5.68	128.94	120.31
3	D	203	GLU	C-N-CA	5.68	128.94	120.31
3	D	635	SER	N-CA-C	5.67	119.01	111.75
2	I	364	VAL	N-CA-C	5.67	115.86	110.42
1	B	8	PHE	N-CA-C	5.64	118.88	110.14
1	B	140	ILE	N-CA-C	5.64	115.80	108.35
2	C	163	LYS	N-CA-C	5.64	118.97	111.75
2	C	146	VAL	N-CA-C	5.64	116.98	109.37
2	C	453	ILE	N-CA-C	5.63	115.98	107.75
2	C	1265	PHE	N-CA-C	5.63	117.80	110.43
3	J	1268	ASN	N-CA-C	5.63	118.67	110.17
2	C	606	LEU	N-CA-C	5.62	118.26	108.76
3	J	745	GLY	N-CA-C	5.62	126.50	113.18
2	I	30	ILE	CB-CA-C	-5.61	104.70	111.88
2	I	661	VAL	N-CA-C	5.60	120.99	109.34
1	H	90	VAL	CB-CA-C	-5.60	102.86	110.42
3	D	776	THR	N-CA-C	5.59	117.05	111.07
5	F	434	TRP	N-CA-C	5.59	117.37	111.28
1	B	66	HIS	N-CA-C	5.58	118.65	109.72
2	C	492	MET	N-CA-C	5.56	120.33	113.50
2	I	224	PHE	N-CA-C	5.56	119.23	112.23
3	J	925	GLU	CA-C-N	-5.55	114.56	121.00
3	J	925	GLU	C-N-CA	-5.55	114.56	121.00
2	I	1189	GLY	N-CA-C	5.55	121.62	112.30
1	H	135	ASP	N-CA-C	5.54	118.03	110.55
3	J	836	ARG	N-CA-C	5.54	117.76	111.11
3	J	343	LEU	N-CA-C	5.50	122.52	110.80
2	C	646	SER	N-CA-C	5.49	117.81	110.35
5	L	487	MET	N-CA-C	5.49	117.91	109.07
2	C	1052	VAL	CA-C-N	-5.49	115.47	122.77
2	C	1052	VAL	C-N-CA	-5.49	115.47	122.77
2	C	354	ASP	N-CA-C	5.48	117.49	109.71
2	C	764	CYS	N-CA-C	5.47	118.69	107.69
2	I	492	MET	N-CA-C	5.47	120.02	113.23
1	G	64	VAL	N-CA-C	5.47	115.77	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1271	GLY	N-CA-C	5.47	121.01	112.31
5	L	289	LYS	N-CA-C	5.46	117.32	111.36
4	K	65	ASP	CA-C-N	5.46	127.94	120.46
4	K	65	ASP	C-N-CA	5.46	127.94	120.46
5	L	343	LYS	CA-C-N	5.45	128.13	120.28
5	L	343	LYS	C-N-CA	5.45	128.13	120.28
3	J	1293	GLU	CB-CA-C	-5.45	109.30	115.79
3	D	1369	ARG	N-CA-C	5.45	117.30	111.36
5	F	398	GLY	N-CA-C	-5.45	107.69	115.64
3	J	1174	ARG	N-CA-C	5.44	117.56	110.43
1	H	54	CYS	CA-CB-SG	5.44	126.91	114.40
2	C	146	VAL	CB-CA-C	-5.43	102.73	111.59
3	D	808	VAL	N-CA-C	5.43	116.31	108.48
3	J	30	ILE	N-CA-C	-5.43	105.24	110.72
5	F	571	TYR	N-CA-C	5.42	118.30	109.24
2	C	1264	GLN	N-CA-C	5.42	117.31	108.63
2	I	242	VAL	CA-C-N	5.41	125.08	119.56
2	I	242	VAL	C-N-CA	5.41	125.08	119.56
2	C	237	LEU	N-CA-C	5.41	122.32	110.80
3	D	424	ASN	N-CA-C	5.41	118.21	109.40
3	D	583	VAL	CA-C-N	5.40	125.57	119.90
3	D	583	VAL	C-N-CA	5.40	125.57	119.90
2	C	814	ASP	N-CA-C	-5.38	105.75	114.09
3	D	663	GLU	N-CA-C	5.38	117.22	111.36
5	L	483	LEU	CA-C-N	5.38	128.24	120.38
5	L	483	LEU	C-N-CA	5.38	128.24	120.38
1	A	192	VAL	CB-CA-C	5.38	118.52	111.53
2	I	856	ASN	N-CA-C	5.37	119.00	111.74
2	C	1049	ILE	N-CA-C	5.37	115.85	108.12
2	C	831	ILE	N-CA-C	5.35	116.01	108.36
2	I	296	VAL	N-CA-C	5.35	115.95	108.89
2	I	241	LEU	N-CA-C	5.34	118.10	109.40
2	C	695	ALA	CA-C-N	-5.33	114.30	121.71
2	C	695	ALA	C-N-CA	-5.33	114.30	121.71
3	D	888	CYS	N-CA-C	5.33	117.95	109.96
3	D	492	SER	CA-C-N	5.31	125.78	120.04
3	D	492	SER	C-N-CA	5.31	125.78	120.04
3	D	239	LEU	N-CA-C	5.29	118.31	110.48
2	I	169	LYS	N-CA-C	5.28	122.06	110.80
2	C	245	ARG	N-CA-C	5.28	118.51	111.75
1	A	29	GLU	N-CA-C	5.27	121.46	109.81
3	J	240	THR	N-CA-C	-5.27	106.80	113.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	I	764	CYS	CA-C-N	-5.26	115.80	122.43
2	I	764	CYS	C-N-CA	-5.26	115.80	122.43
1	A	178	SER	CA-C-N	5.26	124.95	119.64
1	A	178	SER	C-N-CA	5.26	124.95	119.64
3	J	501	VAL	N-CA-C	5.25	113.62	107.89
2	C	177	ILE	N-CA-C	5.25	112.33	107.56
1	G	107	ILE	N-CA-C	5.24	115.89	107.98
3	D	689	ALA	N-CA-C	-5.23	105.66	111.36
3	D	322	ARG	CA-C-N	5.22	125.12	119.85
3	D	322	ARG	C-N-CA	5.22	125.12	119.85
3	D	361	LEU	N-CA-C	5.22	117.45	110.35
1	G	180	VAL	CB-CA-C	-5.22	105.85	111.59
2	I	974	ARG	CA-C-N	5.21	127.83	120.42
2	I	974	ARG	C-N-CA	5.21	127.83	120.42
3	D	526	VAL	N-CA-C	5.21	115.81	108.36
2	I	1215	GLY	N-CA-C	-5.20	108.21	114.66
2	C	616	ILE	N-CA-C	5.20	115.44	108.17
2	C	711	ASP	CA-C-N	-5.20	114.07	121.50
2	C	711	ASP	C-N-CA	-5.20	114.07	121.50
3	J	317	THR	N-CA-C	5.18	116.78	110.41
3	D	923	ILE	N-CA-C	5.17	115.84	110.82
3	J	1246	VAL	N-CA-C	5.17	115.54	107.99
5	F	528	LEU	N-CA-C	5.17	117.20	110.43
3	D	77	ARG	N-CA-C	5.16	117.92	110.28
5	F	282	THR	N-CA-C	-5.16	105.28	112.45
1	A	228	LEU	N-CA-C	-5.16	106.98	113.28
2	C	586	PHE	CA-C-N	-5.15	114.92	122.19
2	C	586	PHE	C-N-CA	-5.15	114.92	122.19
4	K	22	VAL	CA-C-N	5.15	127.18	120.28
4	K	22	VAL	C-N-CA	5.15	127.18	120.28
1	H	74	VAL	N-CA-C	5.13	115.51	108.12
1	G	10	LYS	N-CA-C	5.13	117.89	110.14
2	C	463	GLN	N-CA-C	5.13	117.77	111.82
2	C	564	PRO	N-CA-C	5.12	119.23	111.19
1	G	197	ASP	N-CA-C	5.12	117.42	108.76
2	C	857	VAL	N-CA-C	5.12	115.49	108.12
2	C	1272	GLU	N-CA-C	-5.11	105.60	111.07
3	D	727	ASP	N-CA-C	-5.11	105.71	111.28
2	I	1046	VAL	N-CA-C	5.11	115.69	107.98
3	D	1291	GLU	N-CA-C	5.10	116.92	111.36
5	L	588	ARG	N-CA-C	5.10	116.92	111.36
2	C	1006	GLU	N-CA-C	-5.09	107.02	113.18

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	K	21	LEU	CA-C-N	5.09	127.07	120.56
4	K	21	LEU	C-N-CA	5.09	127.07	120.56
5	L	95	THR	CB-CA-C	-5.08	109.76	117.07
3	D	1230	THR	N-CA-C	-5.07	105.83	111.36
3	J	438	GLU	CA-C-N	-5.07	114.40	120.13
3	J	438	GLU	C-N-CA	-5.07	114.40	120.13
3	D	858	VAL	CA-C-N	5.07	125.08	120.21
3	D	858	VAL	C-N-CA	5.07	125.08	120.21
2	C	571	LEU	N-CA-C	-5.07	107.15	113.38
3	J	1266	ILE	CB-CA-C	-5.07	105.78	111.45
2	C	5	TYR	N-CA-C	5.05	118.22	111.75
2	I	993	PRO	CA-C-N	5.05	127.75	120.38
2	I	993	PRO	C-N-CA	5.05	127.75	120.38
1	B	125	LYS	CA-C-N	5.05	126.05	120.45
1	B	125	LYS	C-N-CA	5.05	126.05	120.45
3	J	831	VAL	N-CA-C	5.05	115.91	109.30
3	D	243	PRO	CA-C-O	-5.05	115.86	122.12
2	C	769	PRO	CA-C-O	-5.04	115.02	120.92
3	D	213	LYS	N-CA-C	5.04	117.55	111.40
1	G	95	LYS	N-CA-C	5.04	117.73	110.28
2	I	577	VAL	N-CA-C	5.03	115.46	110.23
2	I	5	TYR	N-CA-C	5.02	117.48	111.71
2	C	88	ARG	N-CA-C	-5.00	105.72	111.07
3	D	745	GLY	N-CA-C	5.00	125.03	113.18

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1820	0	1850	63	0
1	B	2234	0	2291	91	0
1	G	1755	0	1773	64	0
1	H	1662	0	1687	83	0
2	C	10570	0	10582	337	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	10560	0	10565	308	0
3	D	9029	0	9175	340	0
3	J	8980	0	9148	345	0
4	E	691	0	695	8	0
4	K	627	0	634	20	0
5	F	3813	0	3880	107	0
5	L	3821	0	3884	102	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	1	0
All	All	55638	0	56210	1746	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 16.

All (1746) 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:HH11	1:B:255:ARG:HG3	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
5:L:561:MET:HG3	5:L:567:MET:HE1	1.52	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
3:J:821:MET:HE3	3:J:879:ALA:HB1	1.54	0.86
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:738:GLU:HA	2:C:741:MET:HE2	1.61	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:814:CYS:HG	3:J:888:CYS:HG	1.22	0.81
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
2:I:815:SER:HG	3:J:461:PHE:HD1	1.29	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:J:1344:LEU:HB3	3:J:1350:ASN:HD21	1.48	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:1160:ASP:CB	2:C:1161:LEU:HA	2.12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:F:105:MET:HE1	5:F:385:ARG:HG2	1.70	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:513:MET:HE3	3:J:579:LEU:HD22	1.69	0.73
5:L:474:MET:HE2	5:L:478:PRO:HA	1.70	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
5:L:274:ARG:NH2	5:L:365:MET:HE3	2.04	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
5:F:561:MET:HG3	5:F:567:MET:HE1	1.71	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:H	3:J:770:LEU:HD22	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
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
2:C:515:MET:HE3	2:C:517:GLN:HG3	1.76	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1167:LYS:HD3	3:D:1174:ARG:HD2	1.76	0.67
3:J:525:MET:HE2	3:J:527:LEU:HD11	1.75	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:847:ASP:N	3:D:847:ASP:OD1	2.28	0.67
3:D:1203:ARG:HH22	3:D:1205:GLU:HG2	1.58	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
5:L:105:MET:HE1	5:L:385:ARG:HG2	1.75	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:D:821:MET:HE3	3:D:879:ALA:HB1	1.76	0.66
3:J:290:ILE:H	3:J:290:ILE:HD12	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:128:LEU:HA	3:D:192:MET:HE1	1.77	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:95:PRO:HA	2:C:126:GLU:HG2	1.79	0.64
2:C:124:MET:HB2	2:C:498:ILE:HD13	1.78	0.64
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.29	0.64
1:H:182:ARG:HB3	1:H:206:GLU:HG3	1.78	0.64
2:I:95:PRO:HA	2:I:126:GLU:HG2	1.80	0.64
2:I:807:TRP:HH2	2:I:1216:ARG:HD3	1.62	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:D:918:ILE:HG13	3:D:919:ALA:N	2.08	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
1:B:255:ARG:HD3	1:B:256:PRO:HD2	1.80	0.63
2:C:37:LYS:NZ	2:C:40:GLU:OE2	2.30	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:515:MET:HE3	2:I:517:GLN:HG3	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:61:SER:HB3	2:I:479:LEU:HB3	1.81	0.63
2:I:389:PHE:HB3	2:I:420:LEU:HD12	1.80	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: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:D:697:MET:HE1	3:D:737:ILE:HG22	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
3:J:596:LEU:HD12	3:J:601:ILE:HG13	1.80	0.62
5:L:503:GLU:CD	5:L:504:PRO:HD2	2.25	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
5:F:95:THR:HA	5:F:100:MET:HE3	1.82	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:1080:ASN:HB3	2:C:1085:MET:HE3	1.82	0.61
2:C:1330:ILE:CG2	3:D:331:ILE:HD11	2.31	0.61
1:H:23:HIS:CE1	1:H:204:GLU:HG2	2.35	0.61
1:H:51:MET:HB3	1:H:178:SER:CB	2.31	0.61
2:C:241:LEU:HD21	2:C:246:LEU:HD11	1.83	0.61
3:J:325:LYS:HE2	3:J:330:MET:HE2	1.81	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:202:ARG:NH2	2:C:368:ARG:HH12	2.00	0.60
2:C:1117:LEU:HD12	2:C:1195:ILE:HG12	1.82	0.60
1:G:152:TYR:CD1	2:I:824:GLN:HG2	2.35	0.60
2:C:32:LEU:HD23	2:C:130:MET:SD	2.42	0.60
2:C:1120:ALA:HB1	2:C:1198:LEU:HD12	1.83	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
2:C:68:LEU:HD22	2:C:492:MET:HE3	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:392:THR:HG21	5:F:606:VAL:HA	1.85	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:706:VAL:HG12	3:D:715:LYS:HB3	1.85	0.59
3:J:44:ILE:HG13	5:L:450:ILE:HG22	1.84	0.59
3:J:85:CYS:SG	3:J:87:LYS:HB2	2.43	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:833:GLU:HB2	3:J:1242:ARG:HD3	1.85	0.59
3:J:1255:VAL:O	3:J:1259:GLN:HG2	2.03	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:499:SER:O	2:I:503:LYS:HB2	2.03	0.58
2:I:510:GLN:CD	2:I:534:GLY:HA2	2.28	0.58
2:I:807:TRP:CH2	2:I:1216:ARG:HD3	2.38	0.58
2:I:1033:ARG:O	2:I:1037:THR:HG23	2.03	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
2:C:1106:ARG:HE	3:D:731:ARG:HH21	1.52	0.58
3:D:216:LYS:HA	3:D:219:LYS:HE3	1.85	0.58
3:D:528:THR:O	3:D:551:ARG:HB3	2.04	0.58
4:E:30:MET:HE3	4:E:46:THR:HG22	1.85	0.58
4:K:26:ARG:HG2	4:K:59:ILE:HG21	1.86	0.58
3:D:719:PHE:O	3:D:724:MET:HE2	2.03	0.58
3:J:77:ARG:HG3	3:J:79:LYS:H	1.69	0.58
3:J:124:ILE:HG12	3:J:237:MET:SD	2.44	0.58
1:H:190:ALA:HB2	1:H:200:LYS:HB2	1.86	0.58
2:I:848:GLU:HG2	2:I:888:THR:HG22	1.85	0.58
2:I:1017:GLN:O	2:I:1021:LEU:HG	2.03	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:45:ASN:O	3:D:46:TYR:HB3	2.04	0.57
3:D:423:LEU:HB3	3:D:466:MET:CE	2.33	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

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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
3:J:885:VAL:HG12	3:J:894:VAL:HG11	1.86	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
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
3:J:825:VAL:C	3:J:826:ILE:HG13	2.29	0.57
2:C:964:LEU:HD13	2:C:1025:PHE:HB2	1.87	0.57
2:C:1282:GLY:O	2:C:1284:ALA:N	2.37	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:205:LEU:HD23	3:J:217:LEU:HB3	1.87	0.57
3:J:1344:LEU:HB3	3:J:1350:ASN:ND2	2.18	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
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
3:J:513:MET:HE1	3:J:579:LEU:HD13	1.85	0.57
1:A:31:LEU:HD22	1:A:36:GLY:HA2	1.86	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
2:C:1066:MET:HE2	2:C:1076:ILE:HG22	1.85	0.56
3:D:9:LYS:HZ3	3:D:11:GLN:HA	1.69	0.56
3:D:209:ASN:HA	3:D:214:ARG:HE	1.70	0.56
2:I:231:GLU:OE2	2:I:233:ARG:NH1	2.38	0.56
2:C:202:ARG:HH22	2:C:368:ARG:HH22	1.51	0.56
2:C:312:ALA:HB3	2:C:315:MET:HE3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1327:LEU:HD23	2:C:1337:ILE:HG23	1.87	0.56
3:D:549:LYS:HD3	3:D:569:LEU:HD23	1.86	0.56
2:I:12:ARG:HG3	2:I:1181:PRO:C	2.29	0.56
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:538:ARG:HH11	3:J:538:ARG:HA	1.70	0.56
3:J:1357:ILE:HG22	3:J:1359:ALA:H	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
1:A:4:SER:OG	1:A:5:VAL:N	2.37	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:D:1184:ASP:C	3:D:1186:TYR:H	2.14	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:71:LEU:HB3	3:J:88:CYS:SG	2.46	0.56
3:J:515:ARG:HG2	3:J:719:PHE:CZ	2.41	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:HA	5:F:584:ARG:NH1	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:618:GLN:CD	3:D:770:LEU:HD21	2.31	0.55
2:C:1272:GLU:O	2:C:1275:VAL:N	2.39	0.55
5:F:137:TYR:CD2	5:F:273:MET:HE2	2.41	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:H	3:J:343:LEU:HD12	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:985:GLU:HG2	2:I:988:LYS:HD2	1.87	0.55
2:I:1324:ASN:HA	2:I:1327:LEU:HD12	1.87	0.55
3:J:1178:THR:HA	3:J:1184:ASP:HB3	1.87	0.55
3:D:613:GLY:C	3:D:616:PRO:HD2	2.31	0.55
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
2:C:1066:MET:HE2	2:C:1076:ILE:CG2	2.36	0.55
3:D:77:ARG:HB3	3:D:80:HIS:CE1	2.42	0.55
3:D:357:VAL:HG12	3:D:358:GLY:H	1.71	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
5:L:134:VAL:HG13	5:L:273:MET:HE1	1.89	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:45:ARG:HH21	2:I:1216:ARG:HA	1.71	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: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
2:I:1166:ASP:O	2:I:1170:MET:HG2	2.07	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
5:L:506:SER:O	5:L:509:THR:OG1	2.15	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:1140:ARG:HH21	3:D:1236:GLU:HG2	1.72	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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:ARG:NH1	3:D:534:GLU:OE2	2.40	0.54
2:C:175:ARG:CZ	2:C:200:ARG:HH12	2.20	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:45:ARG:HH22	1:H:37:HIS:HB3	1.73	0.54
1:G:218:ARG:HG3	1:H:231:PHE:O	2.06	0.54
5:L:392:LYS:O	5:L:395:THR:HG23	2.07	0.54
3:D:644:MET:HG2	3:D:722:ILE:HD13	1.90	0.54
3:D:658:GLU:O	3:D:661:VAL:HG22	2.07	0.54
3:J:1269:ALA:HB2	3:J:1274:PHE:CD1	2.42	0.54
2:C:612:GLY:O	2:C:639:LYS:HG2	2.07	0.54
2:I:60:GLN:HB3	2:I:67:GLU:HG3	1.90	0.54
2:I:158:ASP:OD1	2:I:159:SER:N	2.37	0.54
2:I:670:PHE:HB3	2:I:673:HIS:HD2	1.72	0.54
3:J:399:LYS:HZ1	5:L:612:ASP:HB3	1.73	0.54
3:J:1280:VAL:HG21	3:J:1304:ARG:NE	2.23	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: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
3:J:742:GLY:O	3:J:762:ASN:HB3	2.07	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:901:ARG:HG3	3:D:902:ASP:N	2.23	0.54
3:D:1341:ARG:NH1	3:D:1343:GLU:OE2	2.41	0.54
1:H:84:ASN:HB3	1:H:130:ILE:HA	1.90	0.54
2:I:1304:MET:HE3	2:I:1308:ILE:HD11	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:262:THR:HG1	3:D:266:ASN:ND2	2.03	0.54
3:D:458:ASN:ND2	3:D:458:ASN:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:67:GLU:OE1	1:H:171:LEU:HD13	2.07	0.53
1:H:125:LYS:HD3	1:H:128:HIS:HB2	1.88	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:520:PRO:HB3	2:I:714:VAL:HG21	1.91	0.53
2:I:1327:LEU:HD23	2:I:1337:ILE:HG23	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
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
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
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:591:TYR:OH	2:I:611:GLU:OE1	2.23	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
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
1:H:118:ASP:HB2	1:H:121:VAL:CG2	2.39	0.53
3:J:193:ASP:CG	3:J:196:GLN:HG2	2.34	0.53
3:J:1151:LYS:O	3:J:1153:PRO:HD3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:864:LYS:NZ	2:I:881:ASP:OD2	2.42	0.52
2:I:898:GLU:HB3	5:L:540:LEU:HD22	1.91	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:C:563:THR:OG1	2:C:564:PRO:HD2	2.09	0.52
2:C:1005:GLU:HB3	2:C:1007:LYS:H	1.74	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
4:K:77:ALA:C	4:K:79:GLU:H	2.17	0.52
2:C:382:GLU:O	2:C:386:GLU:HG2	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
3:D:1238:GLN:O	3:D:1242:ARG:HB2	2.10	0.52
1:G:14:VAL:HG13	1:G:15:ASP:H	1.75	0.52
2:I:34:SER:OG	2:I:455:SER:O	2.25	0.52
3:J:93:THR:HG22	3:J:94:GLN:N	2.24	0.52
2:C:1314:GLN:HG2	4:E:28:ARG:CZ	2.40	0.52
3:D:9:LYS:NZ	3:D:11:GLN:HA	2.25	0.52
3:D:1282:TYR:HD2	3:D:1286:LYS:NZ	2.07	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:613:GLY:HA3	3:J:615:LYS:HZ1	1.75	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:140:TYR:CD2	5:F:100:MET:HE1	2.44	0.52
3:D:343:LEU:CB	3:D:344:GLY:HA3	2.37	0.52
3:J:1266:ILE:HD12	3:J:1274:PHE:C	2.35	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:61:ILE:HG23	1:G:142:MET:HE2	1.91	0.52
1:G:190:ALA:HB2	1:G:200:LYS:CB	2.31	0.52
2:I:577:VAL:HG23	2:I:661:VAL:O	2.10	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
3:D:825:VAL:C	3:D:826:ILE:HG13	2.35	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
3:J:209:ASN:C	3:J:214:ARG:HH21	2.19	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:N	1:A:76:GLU:OE1	2.43	0.51
3:D:203:GLU:O	3:D:207:GLU:HG2	2.09	0.51
3:D:1280:VAL:HG11	3:D:1304:ARG:HE	1.74	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:306:THR:HG23	2:I:308:GLU:H	1.75	0.51
2:I:1121:ALA:HB2	2:I:1182:ILE:HD12	1.90	0.51
3:J:1233:ILE:O	3:J:1237:VAL:HG13	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:818:VAL:O	2:C:1079:ILE:HD12	2.11	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
3:D:1176:VAL:HG22	3:D:1187:GLU:CB	2.33	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: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
3:J:1264:ALA:HB2	3:J:1280:VAL:HG22	1.91	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:423:LEU:HB3	3:D:466:MET:HE2	1.92	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
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:146:VAL:HB	3:J:156:ARG:O	2.11	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
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: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
3:D:1343:GLU:HG3	3:D:1373:ARG:CZ	2.40	0.51
1:G:229:GLU:HA	1:G:231:PHE:CE2	2.46	0.51
3:J:66:LYS:HD3	3:J:69:GLU:OE2	2.10	0.51
3:J:385:LEU:CD2	3:J:411:ILE:HG13	2.40	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
3:D:1250:ASP:O	3:D:1251:LYS:C	2.53	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:860:ARG:CZ	3:D:860:ARG:HB3	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:468:LEU:O	2:C:471:VAL:HG12	2.10	0.50
2:C:1209:GLN:HB3	2:C:1224:PRO:HB2	1.93	0.50
3:D:701:LEU:CD1	3:D:723:TYR:HB2	2.41	0.50
3:D:1203:ARG:NH2	3:D:1205:GLU:HG2	2.25	0.50
1:G:150:ARG:NH1	1:H:6:THR:HG23	2.27	0.50
2:I:798:GLN:OE1	2:I:827:ARG:HB2	2.10	0.50
2:I:1259:LEU:HD12	2:I:1260:GLY:H	1.76	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
3:J:697:MET:HE1	3:J:737:ILE:HG22	1.92	0.50
2:C:1112:ILE:O	2:C:1115:THR:N	2.44	0.50
3:D:290:ILE:H	3:D:290:ILE:HD12	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
2:I:646:SER:HB3	2:I:649:GLN:CD	2.37	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:549:LYS:HG3	3:D:571:ASP:OD1	2.11	0.50
3:D:1284:ARG:HE	3:D:1304:ARG:NH2	2.09	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:I:169:LYS:O	2:I:170:VAL:HG22	2.12	0.50
3:J:325:LYS:HD3	5:L:508:GLU:HG2	1.92	0.50
3:J:660:GLU:O	3:J:664:ILE:HG12	2.11	0.50
2:C:688:GLN:OE1	2:C:1237:HIS:HE1	1.95	0.50
3:D:518:VAL:HG11	3:D:707:ILE:HB	1.94	0.50
3:D:1284:ARG:HA	3:D:1287:ILE:HG12	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:62:TYR:C	2:I:64:GLY:H	2.18	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
1:A:47:LEU:O	1:A:180:VAL:HG21	2.11	0.50
2:C:71:VAL:HB	2:C:99:LYS:HB2	1.93	0.50
2:C:1214:ASP:HB2	2:C:1221:PHE:CZ	2.47	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:520:ALA:HB1	3:D:543:SER:HB3	1.94	0.49
3:D:1351:VAL:HG12	8:D:2004:4C2:O2	2.12	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:297:MET:HG3	5:L:326:TRP:HB2	1.94	0.49
5:L:306:PHE:CE2	5:L:310:GLU:HG2	2.47	0.49
1:B:300:LEU:HD13	1:B:300:LEU:O	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:HA	5:F:584:ARG:HH11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:211:GLU:O	3:D:215:LYS:HB2	2.13	0.49
3:D:1230:THR:O	3:D:1234:VAL:HG13	2.11	0.49
2:I:741:MET:HE3	2:I:974:ARG:CZ	2.42	0.49
3:J:349:TYR:HE2	3:J:379:PRO:HG2	1.77	0.49
3:J:423:LEU:HB3	3:J:466:MET:HE1	1.95	0.49
1:B:29:GLU:HB3	1:B:200:LYS:HG3	1.94	0.49
1:B:263:THR:HG23	1:B:266:SER:OG	2.13	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
3:J:610:ARG:HG2	3:J:866:GLU:CD	2.38	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
2:I:1232:MET:C	2:I:1233:LEU:HD13	2.38	0.49
3:J:91:GLU:OE1	3:J:93:THR:OG1	2.31	0.49
3:J:507:VAL:HG11	3:J:598:LYS:HG3	1.94	0.49
3:J:735:ALA:HA	3:J:738:ARG:NH1	2.28	0.49
5:L:466:ILE:HG22	5:L:470:MET:HE2	1.94	0.49
2:C:466:VAL:HA	2:C:469:VAL:HG22	1.94	0.49
2:C:1271:GLY:CA	3:D:343:LEU:HD23	2.43	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:679:TYR:CZ	3:D:683:ILE:HD11	2.47	0.49
3:D:1298:VAL:H	3:D:1299:GLY:HA3	1.78	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:26:SER:HB2	3:J:236:TRP:CZ2	2.48	0.49
3:J:201:LEU:HB2	3:J:221:ILE:HD13	1.95	0.49
1:A:45:ARG:HH12	1:B:37:HIS:HB2	1.77	0.49
1:B:308:ALA:HA	1:B:312:LEU:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:569:ILE:H	2:C:569:ILE:HD12	1.78	0.49
2:C:1319:MET:HG3	2:C:1320:PRO:HD2	1.95	0.49
3:D:120:LEU:HB3	3:D:121:PRO:HD3	1.95	0.49
5:F:573:LEU:HD23	5:F:573:LEU:H	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:O	2:C:314:ASN:ND2	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:OD1	2:I:446:ASP:N	2.43	0.48
5:L:476:ARG:HD2	5:L:477:GLU:HG2	1.95	0.48
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: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
2:C:1013:GLN:O	2:C:1017:GLN:HG2	2.13	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:915:ILE:HA	3:J:918:ILE:HG12	1.95	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:10:ARG:NH2	2:C:791:LEU:HD12	2.28	0.48
2:C:175:ARG:HD3	2:C:183:TRP:CZ3	2.49	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: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
3:J:1198:VAL:HG23	3:J:1204:VAL:HG11	1.94	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:94:GLN:O	3:J:97:VAL:HG23	2.14	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:1316:THR:HG22	3:J:1318:SER:H	1.79	0.48
1:B:79:LEU:HD23	1:B:79:LEU:H	1.78	0.48
3:D:554:GLU:OE2	3:D:570:LYS:NZ	2.36	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
3:J:642:ASP:HA	3:J:764:ARG:HH21	1.76	0.48
1:A:134:THR:O	1:A:134:THR:OG1	2.32	0.48
1:A:178:SER:HA	1:A:179:PRO:HD3	1.68	0.48
2:C:176:ILE:HD11	2:C:428:VAL:HG11	1.95	0.48
2:C:1269:ARG:NE	3:D:343:LEU:HD22	2.29	0.48
3:D:1157:ALA:HB2	3:D:1210:ILE:HD11	1.96	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:816:ILE:O	2:I:1076:ILE:HD12	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:73:GLY:HA2	1:B:134:THR:HB	1.96	0.48
1:B:246:LYS:HE3	1:B:246:LYS:HB3	1.66	0.48
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.95	0.48
3:D:268:LEU:HD21	3:D:324:LEU:HD13	1.96	0.48
3:D:1298:VAL:N	3:D:1299:GLY:HA3	2.29	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:582:ASN:HB3	2:I:586:PHE:H	1.77	0.48
2:I:1255:THR:O	2:I:1257:GLN:N	2.47	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:G:166:ARG:O	1:G:167:PRO:C	2.57	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
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:848:GLU:CG	2:C:888:THR:HG22	2.43	0.47
2:C:886:LYS:H	2:C:917:SER:HB3	1.79	0.47
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
5:L:134:VAL:HG22	5:L:273:MET:HE1	1.96	0.47
1:B:252:ILE:O	1:B:255:ARG:HB2	2.15	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
3:J:66:LYS:HD3	3:J:69:GLU:CD	2.39	0.47
1:B:140:ILE:HD11	1:B:142:MET:HE3	1.95	0.47
2:C:117:ILE:HD11	2:C:485:ASP:OD1	2.14	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
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
3:D:48:THR:O	3:D:49:PHE:C	2.56	0.47
1:H:109:PRO:HB3	1:H:132:HIS:HD2	1.78	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:5:TYR:O	2:I:8:LYS:HG2	2.15	0.47
2:I:807:TRP:HE3	2:I:807:TRP:O	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
5:L:489:MET:HE2	5:L:493:LYS:HB3	1.97	0.47
1:A:104:LYS:HG2	1:A:110:VAL:HG22	1.97	0.47
2:C:865:LEU:HD22	2:C:869:GLY:O	2.15	0.47
2:C:1192:GLU:HA	2:C:1195:ILE:HD12	1.97	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
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: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
1:H:154:PRO:HD2	1:H:157:THR:OG1	2.15	0.47
2:I:1103:VAL:N	2:I:1104:PRO:HD2	2.29	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
5:L:145:LEU:CD2	5:L:224:LEU:HD23	2.45	0.47
5:L:470:MET:HE1	5:L:483:LEU:HG	1.94	0.47
1:G:102:LEU:O	1:G:141:SER:HA	2.15	0.47
2:I:93:SER:OG	2:I:126:GLU:OE1	2.23	0.47
2:I:510:GLN:NE2	2:I:534:GLY:HA2	2.29	0.47
2:I:720:ARG:HB2	2:I:749:ASP:OD1	2.15	0.47
2:I:1042:LEU:HB3	2:I:1046:VAL:HG13	1.96	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
2:C:906:PHE:HE2	5:F:608:ARG:HH11	1.60	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:134:VAL:HG13	5:F:273:MET:HE1	1.96	0.47
5:F:137:TYR:CZ	5:F:139:GLU:HB2	2.50	0.47
2:I:1122:LYS:HZ3	2:I:1178:LYS:C	2.14	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:194:LEU:HD13	3:D:228:VAL:HG22	1.97	0.47
3:D:201:LEU:O	3:D:217:LEU:HD12	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:107:ILE:HG23	1:H:134:THR:O	2.15	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
1:B:313:SER:OG	1:B:314:LEU:N	2.45	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:812:ASP:O	3:D:896:ALA:HB3	2.14	0.46
3:D:1198:VAL:HG23	3:D:1204:VAL:HG11	1.96	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
1:H:83:LEU:HD21	3:J:526:VAL:HB	1.96	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
2:I:1106:ARG:CZ	3:J:731:ARG:HH21	2.28	0.46
3:J:1357:ILE:HG22	3:J:1359:ALA:N	2.30	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
3:D:423:LEU:HB3	3:D:466:MET:HE1	1.97	0.46
1:G:70:THR:CG2	2:I:755:LYS:HE2	2.46	0.46
1:H:73:GLY:HA3	1:H:138:ALA:HB1	1.98	0.46
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
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:CG	1:B:255:ARG:NH1	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: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:46:TYR:HD1	5:L:500:ILE:HG21	1.79	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:H	3:D:615:LYS:HG3	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
3:D:174:ASP:C	3:D:176:PHE:H	2.24	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:836:LEU:HB3	2:I:918:LEU:HD21	1.97	0.46
2:I:883:LEU:HD22	2:I:1052:VAL:HG11	1.98	0.46
1:B:188:GLU:HG3	1:B:200:LYS:HB3	1.97	0.46
2:C:455:SER:O	2:C:457:GLY:N	2.49	0.46
2:C:1100:PRO:HB2	3:D:725:MET:HE1	1.98	0.46
2:I:693:LEU:HB2	2:I:829:THR:O	2.14	0.46
2:I:1142:ARG:HH22	2:I:1165:SER:CB	2.22	0.46
3:J:615:LYS:H	3:J:615:LYS:HG3	1.37	0.46
5:L:600:HIS:CG	5:L:601:PRO:HD2	2.50	0.46
3:D:75:TYR:HE1	3:D:85:CYS:HA	1.81	0.46
3:D:1169:THR:OG1	3:D:1192:LYS:HD3	2.16	0.46
2:I:30:ILE:HD12	2:I:30:ILE:H	1.81	0.46
3:J:128:LEU:HA	3:J:192:MET:HE1	1.97	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:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.97	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
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.97	0.46
2:C:992:LEU:HB2	2:C:993:PRO:HD2	1.98	0.46
2:C:1256:GLN:HB3	2:C:1301:ARG:HH22	1.80	0.46
3:D:268:LEU:HD23	3:D:271:ARG:NH1	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1357:ILE:HG22	3:D:1359:ALA:H	1.80	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
2:I:1080:ASN:HB3	2:I:1085:MET:HE3	1.98	0.45
3:J:62:PHE:CD1	3:J:247:PRO:HD3	2.51	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
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: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
3:D:1164:SER:O	3:D:1175:LEU:HD12	2.16	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
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
1:H:67:GLU:O	1:H:78:ILE:HB	2.17	0.45
2:I:62:TYR:C	2:I:64:GLY:N	2.74	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:510:LEU:HA	3:D:513:MET:HE2	1.97	0.45
3:D:842:ARG:HB3	3:D:882:VAL:CG1	2.46	0.45
5:F:346:GLN:HG2	5:F:346:GLN:O	2.16	0.45
2:I:804:PHE:CE1	2:I:1098:LEU:HD23	2.52	0.45
2:I:807:TRP:HE1	2:I:1086:PRO:HG3	1.81	0.45
2:I:1106:ARG:O	2:I:1108:ASN:N	2.44	0.45
3:J:491:LEU:HD22	3:J:496:GLY:O	2.16	0.45
1:B:73:GLY:C	1:B:134:THR:HB	2.41	0.45
2:C:106:GLU:OE1	2:C:114:VAL:HG22	2.16	0.45
2:C:481:LEU:HD22	2:C:481:LEU:H	1.81	0.45
2:C:745:GLU:O	2:C:746:ALA:C	2.60	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:770:LEU:HD22	3:D:770:LEU:N	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:402:ARG:HG2	2:I:416:GLY:H	1.82	0.45
2:I:753:LEU:HD23	2:I:767:GLN:HB3	1.97	0.45
2:I:1334:GLY:O	3:J:25:ALA:HB3	2.17	0.45
3:J:117:LEU:HD23	3:J:118:LYS:HG2	1.99	0.45
5:L:483:LEU:HD12	5:L:483:LEU:H	1.80	0.45
1:A:13:LEU:HG	1:A:13:LEU:O	2.17	0.45
2:C:1276:TRP:CE2	3:D:801:VAL:HG11	2.51	0.45
3:D:16:GLU:HG3	3:D:1369:ARG:NH1	2.31	0.45
1:G:45:ARG:HH12	1:H:37:HIS:HB2	1.80	0.45
1:G:178:SER:HA	1:G:179:PRO:HD3	1.82	0.45
1:H:83:LEU:HD11	3:J:526:VAL:HG23	1.99	0.45
3:J:81:ARG:HG3	3:J:82:GLY:H	1.81	0.45
3:J:694:SER:O	3:J:698:MET:HB2	2.17	0.45
1:A:27:THR:C	1:A:28:LEU:HD12	2.42	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:325:LYS:HD3	5:F:508:GLU:HG2	1.99	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
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
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: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
2:C:1042:LEU:HB3	2:C:1046:VAL:HG13	1.98	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:HD23	5:L:573:LEU:H	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
2:C:671:LEU:O	2:C:672:GLU:C	2.60	0.45
1:H:10:LYS:HA	1:H:11:PRO:HD3	1.62	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	2:C:660:VAL:HG22	2.16	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: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:J:362:ARG:HB2	3:J:365:GLN:HG2	1.99	0.45
3:J:826:ILE:HD12	3:J:826:ILE:O	2.17	0.45
3:J:1280:VAL:HA	3:J:1283:SER:HB3	1.99	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:9:LYS:HG2	3:D:11:GLN:H	1.83	0.44
3:D:622:ASP:O	3:D:625:MET:N	2.50	0.44
5:F:515:GLU:HB3	5:F:517:SER:OG	2.17	0.44
1:G:91:ARG:HB3	1:G:122:GLU:HB3	1.98	0.44
1:G:207:THR:HG22	1:G:208:ASN:N	2.32	0.44
3:J:201:LEU:O	3:J:217:LEU:HD11	2.17	0.44
3:J:719:PHE:O	3:J:724:MET:HE2	2.17	0.44
5:L:230:VAL:HG13	5:L:248:GLU:HG2	1.99	0.44
2:C:37:LYS:HD3	2:C:37:LYS:HA	1.79	0.44
2:C:1196:LYS:HD2	2:C:1206:THR:OG1	2.17	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:H	2:I:867:GLU:HG3	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:671:LEU:O	2:C:673:HIS:N	2.51	0.44
2:C:705:GLU:H	2:C:705:GLU:CD	2.25	0.44
2:C:722:GLY:HA2	2:C:737:ASN:OD1	2.17	0.44
2:C:1271:GLY:HA3	3:D:343:LEU:HD23	1.99	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:527:LEU:HB2	3:J:550:VAL:HG12	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:1263:LYS:HD2	3:J:1277:GLY:O	2.18	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
2:C:1319:MET:HE3	2:C:1324:ASN:OD1	2.17	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:213:LEU:HB3	2:I:422:LYS:HD3	1.99	0.44
2:I:870:ILE:HG12	2:I:1050:VAL:HG11	1.98	0.44
2:I:972:PHE:HE2	2:I:998:LEU:HD11	1.82	0.44
3:J:24:LEU:HD13	3:J:24:LEU:HA	1.81	0.44
3:J:48:THR:O	3:J:49:PHE:C	2.60	0.44
5:L:483:LEU:HA	5:L:486:ARG:NH1	2.32	0.44
5:L:540:LEU:O	5:L:540:LEU:HD23	2.17	0.44
2:C:138:ILE:HD12	2:C:138:ILE:HA	1.59	0.44
2:C:297:VAL:HG12	2:C:315:MET:O	2.17	0.44
2:C:496:LYS:HB3	2:C:496:LYS:HE3	1.77	0.44
3:D:400:MET:HG2	3:D:405:GLU:OE2	2.16	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
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
2:C:1111:GLN:HB2	2:C:1230:MET:HE1	2.00	0.44
3:D:210:SER:HB2	3:D:213:LYS:CB	2.46	0.44
3:D:255:LEU:HD13	3:D:255:LEU:HA	1.63	0.44
3:D:1302:TYR:OH	3:J:1291:GLU:HG2	2.16	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: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
1:H:33:ARG:HH12	2:I:820:GLU:CD	2.25	0.44
2:I:179:TYR:OH	2:I:458:GLU:OE2	2.32	0.44
2:I:748:ILE:O	2:I:748:ILE:HG12	2.18	0.44
2:I:1164:PHE:HD1	2:I:1164:PHE:HA	1.71	0.44
1:B:287:VAL:O	1:B:291:LYS:HE2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:I:1276:TRP:CE2	3:J:801:VAL:HG11	2.53	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
3:J:801:VAL:O	3:J:805:GLN:HB2	2.18	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
4:K:14:GLY:C	4:K:16:ARG:H	2.26	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
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: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
2:I:1176:LEU:HD22	2:I:1180:MET:HG2	2.00	0.43
3:J:613:GLY:O	3:J:617:THR:OG1	2.33	0.43
3:J:843:VAL:HG13	3:J:883:ARG:HB2	2.00	0.43
3:J:1264:ALA:CB	3:J:1280:VAL:HG22	2.48	0.43
1:A:31:LEU:HD13	1:A:201:LEU:HB2	2.00	0.43
1:B:61:ILE:HB	1:B:64:VAL:O	2.17	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
2:C:56:VAL:HG11	2:C:468:LEU:HB3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:757:THR:OG1	2:C:758:ARG:N	2.51	0.43
2:C:865:LEU:HD22	2:C:869:GLY:C	2.43	0.43
3:D:298:MET:SD	5:F:406:GLN:HG3	2.58	0.43
3:D:660:GLU:HB3	3:D:685:ILE:HD12	2.01	0.43
3:D:1319:PHE:O	3:D:1322:ALA:HB3	2.18	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: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
3:J:1184:ASP:N	3:J:1185:PRO:HD3	2.33	0.43
5:L:496:LYS:O	5:L:500:ILE:HG12	2.18	0.43
1:A:4:SER:O	1:A:5:VAL:HG13	2.18	0.43
1:A:167:PRO:O	1:A:170:ARG:HB2	2.18	0.43
1:B:153:VAL:HB	1:B:175:ALA:HB3	1.99	0.43
2:C:62:TYR:C	2:C:64:GLY:H	2.26	0.43
2:C:189:ASP:HB3	2:C:195:PHE:CE2	2.52	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:452:ARG:NH1	2:I:585:GLY:HA3	2.30	0.43
2:I:1087:TYR:CE1	2:I:1215:GLY:HA2	2.47	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:202:ARG:HD3	2:C:369:MET:HG2	2.00	0.43
2:C:676:ALA:HA	3:D:772:TYR:OH	2.17	0.43
2:C:1067:ALA:O	2:C:1233:LEU:HD22	2.19	0.43
2:C:1073:LYS:HE3	3:D:462:ASP:CB	2.39	0.43
3:D:515:ARG:HG3	3:D:516:ASP:N	2.33	0.43
3:D:930:LEU:HD11	3:D:1241:TYR:CE2	2.53	0.43
5:F:137:TYR:HD2	5:F:273:MET:HE2	1.82	0.43
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:207:THR:HG21	2:I:351:LEU:HG	2.00	0.43
2:I:1087:TYR:HA	2:I:1093:PRO:HA	2.00	0.43
3:J:641:ILE:HD13	3:J:644:MET:CE	2.49	0.43
2:C:285:ILE:O	2:C:285:ILE:HG13	2.19	0.43
2:C:717:VAL:HG12	2:C:718:ALA:N	2.33	0.43
2:C:800:MET:HE3	2:C:800:MET:HB3	1.74	0.43
2:C:881:ASP:OD1	2:C:881:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1166:ASP:O	2:C:1168:GLU:N	2.52	0.43
3:D:801:VAL:O	3:D:801:VAL:HG22	2.19	0.43
3:D:1299:GLY:HA2	3:D:1300:ALA:HA	1.72	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: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
2:C:1127:LYS:HE2	2:C:1203:ASP:OD2	2.18	0.43
3:D:599:LYS:HA	3:D:599:LYS:HD3	1.76	0.43
5:F:490:PRO:O	5:F:491:GLU:HG2	2.18	0.43
3:J:497:GLU:HA	3:J:498:PRO:HD3	1.77	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:213:LEU:HD22	2:C:422:LYS:HG2	2.00	0.43
2:C:310:ILE:HD13	2:C:325:LEU:HA	1.99	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
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: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
2:I:1101:LEU:HB3	3:J:731:ARG:HD3	2.01	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:175:ARG:NH1	2:C:183:TRP:HZ3	2.15	0.43
2:C:178:PRO:HG3	2:C:395:TYR:CE1	2.52	0.43
2:C:1099:ASN:OD1	2:C:1100:PRO:HD2	2.19	0.43
3:D:650:LYS:HE2	3:D:654:ILE:HD11	2.01	0.43
4:E:3:ARG:NE	4:E:3:ARG:HA	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:NH1	2:I:1223:ARG:HB3	2.33	0.43
3:J:1216:ALA:HB3	3:J:1219:ASP:OD2	2.19	0.43
1:A:2:GLN:HE22	1:B:249:PHE:HZ	1.67	0.43
1:A:25:LYS:HG3	1:A:204:GLU:HG3	2.01	0.43
1:A:77:ASP:OD1	1:A:77:ASP:N	2.52	0.43
1:A:133:LEU:HA	1:A:133:LEU:HD13	1.78	0.43
1:B:180:VAL:O	1:B:180:VAL:HG23	2.19	0.43
2:C:80:PHE:HB3	2:C:84:GLU:HB2	2.00	0.43
2:C:835:GLU:C	2:C:836:LEU:HD12	2.44	0.43
2:C:854:ILE:HD11	2:C:885:GLY:HA3	2.01	0.43
2:C:864:LYS:NZ	2:C:881:ASP:OD2	2.52	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
3:J:1250:ASP:O	3:J:1251:LYS:C	2.62	0.43
5:L:490:PRO:C	5:L:492:ASP:H	2.26	0.43
2:C:551:HIS:CE1	2:C:552:PRO:HG2	2.53	0.42
2:C:1191:LYS:HD3	2:C:1193:ALA:N	2.22	0.42
2:C:1330:ILE:HA	2:C:1333:LEU:HD12	2.01	0.42
3:D:132:LEU:HA	3:D:135:ILE:HD12	2.01	0.42
1:G:46:ILE:HD11	1:H:38:THR:HG21	2.01	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
2:I:670:PHE:CD1	2:I:1184:THR:HG21	2.54	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: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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
3:J:693:VAL:HG21	3:J:743:MET:HE3	2.00	0.42
1:B:47:LEU:O	1:B:180:VAL:HG21	2.19	0.42
3:D:53:ARG:HA	3:D:54:ASP:HA	1.64	0.42
3:D:1343:GLU:HG3	3:D:1373:ARG:NH2	2.35	0.42
1:G:56:VAL:HG13	1:G:173:VAL:HG21	2.01	0.42
1:G:124:VAL:O	1:G:126:PRO:HD3	2.19	0.42
1:H:197:ASP:C	1:H:198:LEU:HD22	2.45	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
3:J:1306:LEU:HD23	3:J:1307:LEU:N	2.34	0.42
5:L:348:GLU:HA	5:L:353:LEU:O	2.19	0.42
1:B:30:PRO:C	1:B:31:LEU:HD22	2.44	0.42
1:B:246:LYS:HA	1:B:247:PRO:HD3	1.93	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
3:D:1140:ARG:HH21	3:D:1236:GLU:CG	2.32	0.42
5:F:126:GLY:O	5:F:130:VAL:HG22	2.19	0.42
5:F:127:ILE:HG13	5:F:128:ASN:N	2.34	0.42
1:G:108:GLY:HA2	1:G:109:PRO:HD3	1.76	0.42
2:I:18:ARG:HA	2:I:19:PRO:HD3	1.83	0.42
2:I:895:LEU:H	2:I:895:LEU:HG	1.71	0.42
2:I:1298:VAL:HG23	2:I:1301:ARG:NH1	2.33	0.42
3:J:1297:LYS:HA	3:J:1297:LYS:HD2	1.64	0.42
1:B:101:THR:HG22	1:B:116:THR:HG21	2.01	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
2:C:1198:LEU:HD22	2:C:1198:LEU:HA	1.88	0.42
3:D:24:LEU:HD13	3:D:24:LEU:HA	1.65	0.42
3:D:62:PHE:CD1	3:D:247:PRO:HD3	2.55	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
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
2:I:1100:PRO:HB2	3:J:725:MET:HE1	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:O	5:F:540:LEU:HD23	2.19	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
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
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
5:L:470:MET:HE3	5:L:478:PRO:HG3	2.02	0.42
1:A:31:LEU:HB2	1:A:199:ASP:O	2.19	0.42
1:A:220:ALA:HA	1:A:223:ILE:HD12	2.02	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:325:LYS:HE2	3:D:330:MET:HE2	2.00	0.42
3:D:1297:LYS:HA	3:D:1298:VAL:HA	1.65	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:455:SER:HA	2:I:459:MET:HE2	2.01	0.42
2:I:1103:VAL:CG1	2:I:1112:ILE:HD11	2.46	0.42
2:I:1230:MET:HG2	2:I:1232:MET:HG3	2.02	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
3:J:1261:LEU:H	3:J:1261:LEU:HG	1.57	0.42
3:J:1266:ILE:H	3:J:1266:ILE:HG13	1.51	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:587:LEU:HD23	2:C:587:LEU:HA	1.84	0.42
2:C:1294:LYS:HB3	3:D:347:VAL:HG13	2.02	0.42
3:D:909:ILE:HG13	3:D:910:ASN:N	2.33	0.42
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:294:ASN:HD22	5:L:406:GLN:NE2	2.15	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:A:159:ILE:HD12	1:A:165:GLU:CD	2.45	0.42
2:C:268:ARG:NH2	2:C:270:THR:HG21	2.34	0.42
2:C:530:ILE:HD12	2:C:530:ILE:HG23	1.67	0.42
3:D:99:ARG:HA	3:D:248:ASP:HB2	2.02	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
1:H:144:ILE:O	1:H:144:ILE:HG13	2.20	0.42
2:I:22:LEU:HD22	2:I:23:ASP:H	1.84	0.42
2:I:147:SER:OG	2:I:455:SER:HB3	2.20	0.42
2:I:237:LEU:HA	2:I:237:LEU:HD13	1.76	0.42
2:I:942:ASP:O	2:I:946:LEU:HD12	2.20	0.42
2:I:1191:LYS:HD3	2:I:1193:ALA:H	1.85	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
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
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
2:C:755:LYS:O	2:C:756:TYR:C	2.62	0.42
5:F:466:ILE:HD11	5:F:487:MET:HE3	2.02	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: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
3:J:1280:VAL:CG1	3:J:1304:ARG:HH21	2.32	0.42
1:A:45:ARG:NH1	1:B:34:GLY:O	2.53	0.41
2:C:30:ILE:H	2:C:30:ILE:HG13	1.56	0.41
2:C:732:ILE:HD11	2:C:769:PRO:HB3	2.02	0.41
2:C:1053:TYR:CD1	2:C:1053:TYR:N	2.87	0.41
2:C:1075:VAL:O	2:C:1076:ILE:C	2.63	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:613:GLY:O	3:D:616:PRO:HD2	2.20	0.41
3:D:825:VAL:CG2	3:D:833:GLU:H	2.33	0.41
3:D:1314:LEU:HD12	3:D:1326:GLN:OE1	2.20	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:848:GLU:CD	2:I:888:THR:HG22	2.44	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: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
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
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: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
2:I:1324:ASN:O	2:I:1327:LEU:HB2	2.21	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
3:J:930:LEU:HB2	3:J:1138:LEU:HB2	2.02	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: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
2:C:1296:ASP:HB3	2:C:1321:GLU:H	1.86	0.41
3:D:291:ILE:HD11	5:F:409:ASN:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:D:1372:ARG:NH2	3:J:854:ALA:HB2	2.35	0.41
2:I:528:ARG:CZ	2:I:575:LEU:HD23	2.49	0.41
2:I:1064:ASP:OD2	2:I:1238:LEU:HD23	2.20	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:18:ASP:O	3:D:19:ALA:HB3	2.20	0.41
3:D:156:ARG:NH1	3:D:157:GLN:NE2	2.67	0.41
3:D:720:ASN:OD1	3:D:722:ILE:HG22	2.20	0.41
3:D:1282:TYR:HD2	3:D:1286:LYS:HZ1	1.68	0.41
1:G:87:GLY:O	1:G:128:HIS:CE1	2.73	0.41
2:I:960:LEU:HB3	2:I:1025:PHE:HE2	1.85	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
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:1221:LEU:HD21	3:J:1226:VAL:HG22	2.01	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
3:D:394:ILE:HG12	5:F:536:THR:HG22	2.01	0.41
3:D:418:GLU:HG3	4:E:45:LYS:H	1.85	0.41
3:D:430:HIS:ND1	3:D:925:GLU:HG3	2.35	0.41
3:D:850:LYS:HB3	3:D:851:PRO:HD2	2.01	0.41
3:D:1327:GLU:OE1	3:D:1329:THR:HB	2.20	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
1:H:84:ASN:ND2	3:J:551:ARG:HH12	2.18	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
2:I:1246:ARG:HD2	2:I:1265:PHE:O	2.21	0.41
3:J:818:GLU:HG3	3:J:887:SER:HB2	2.02	0.41
3:J:866:GLU:OE1	3:J:866:GLU:N	2.51	0.41
5:L:489:MET:HE2	5:L:493:LYS:CB	2.50	0.41
2:C:496:LYS:HD2	2:C:496:LYS:C	2.46	0.41
2:C:704:MET:O	2:C:705:GLU:C	2.63	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:309:ASN:OD1	3:D:314:ARG:HA	2.20	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
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
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:521:LEU:HA	2:I:524:ILE:HG22	2.02	0.41
2:I:1138:VAL:O	2:I:1142:ARG:HB2	2.21	0.41
3:J:186:GLN:CD	3:J:238:ILE:HB	2.45	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
3:J:1265:THR:N	3:J:1303:SER:O	2.51	0.41
1:A:152:TYR:CE1	2:C:824:GLN:HA	2.56	0.41
1:B:14:VAL:HB	1:B:28:LEU:HD13	2.03	0.41
2:C:86:GLN:HA	2:C:140:GLY:HA2	2.03	0.41
2:C:157:PHE:CE2	2:C:431:LYS:HG2	2.55	0.41
2:C:748:ILE:HG12	2:C:748:ILE:O	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:709:ARG:C	3:D:711:GLY:H	2.28	0.41
3:D:1216:ALA:O	3:D:1220:ILE:HG12	2.21	0.41
3:D:1280:VAL:HB	3:D:1304:ARG:HH21	1.86	0.41
3:D:1343:GLU:O	3:D:1344:LEU:HB2	2.20	0.41
1:H:44:ARG:O	1:H:48:LEU:HB2	2.21	0.41
1:H:74:VAL:HG11	1:H:81:ILE:HD11	2.02	0.41
2:I:403:MET:HE3	2:I:403:MET:HB3	1.81	0.41
2:I:471:VAL:HG21	2:I:493:ILE:HD12	2.02	0.41
2:I:1105:SER:HA	3:J:736:GLN:OE1	2.20	0.41
2:I:1270:PHE:CZ	2:I:1290:MET:HG2	2.56	0.41
4:K:53:GLU:HB3	4:K:59:ILE:HB	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: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:A:158:ARG:HH12	1:A:172:LEU:HD23	1.86	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
2:C:1098:LEU:HA	2:C:1098:LEU:HD12	1.85	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
3:D:1138:LEU:N	3:D:1139:PRO:CD	2.84	0.41
1:G:124:VAL:HG11	1:G:208:ASN:O	2.21	0.41
2:I:993:PRO:HG2	2:I:996:ARG:HB2	2.03	0.41
2:I:1327:LEU:HD23	2:I:1337:ILE:CG2	2.50	0.41
3:J:1309:ILE:HG13	3:J:1310:THR:N	2.36	0.41
2:C:61:SER:O	2:C:63:SER:N	2.54	0.40
2:C:62:TYR:C	2:C:64:GLY:N	2.79	0.40
2:C:325:LEU:O	2:C:330:HIS:HB2	2.20	0.40
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
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
2:I:800:MET:HE3	2:I:800:MET:HB3	1.80	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
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
5:L:365:MET:C	5:L:367:ILE:H	2.29	0.40
2:C:383:SER:O	2:C:387:ASN:ND2	2.54	0.40
2:C:798:GLN:HB2	2:C:828:PHE:CE1	2.56	0.40
2:C:1082:ILE:H	2:C:1082:ILE:HD12	1.87	0.40
2:C:1225:VAL:HA	3:D:638:SER:HB2	2.04	0.40
2:C:1234:LYS:HZ3	2:C:1238:LEU:HD21	1.86	0.40
3:D:372:MET:HE2	3:D:372:MET:HB3	1.97	0.40
3:D:1299:GLY:N	3:J:1301:THR:HG21	2.35	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:145:ILE:HG22	2:C:145:ILE:O	2.21	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:518:VAL:CG1	3:D:707:ILE:HB	2.51	0.40
3:D:600:ALA:O	3:D:603:LYS:HG2	2.22	0.40
3:D:1160:SER:HB2	3:D:1206:ARG:HG2	2.03	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
2:I:848:GLU:CD	2:I:886:LYS:HZ3	2.28	0.40
2:I:1066:MET:HE3	2:I:1066:MET:HB2	1.87	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: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:H	2:C:414:ILE:HG13	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: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: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:1140:ARG:HH21	3:J:1236:GLU:HG2	1.86	0.40
5:L:608:ARG:HH11	5:L:608:ARG:HD2	1.77	0.40
1:A:224:LEU:HD23	1:A:228:LEU:HD11	2.02	0.40
2:C:216:THR:O	2:C:217:THR:C	2.64	0.40
2:C:746:ALA:HA	2:C:974:ARG:HE	1.87	0.40
2:C:1046:VAL:HG13	2:C:1046:VAL:O	2.22	0.40
2:C:1077:SER:OG	2:C:1078:LYS:N	2.54	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
3:D:1337:VAL:HG23	3:D:1338:ALA:N	2.36	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:5:TYR:HD2	2:I:778:GLU:HB2	1.86	0.40
2:I:1330:ILE:HD13	2:I:1330:ILE:HG21	1.67	0.40
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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	233/329 (71%)	211 (91%)	16 (7%)	6 (3%)	4	28
1	B	283/329 (86%)	247 (87%)	28 (10%)	8 (3%)	4	27
1	G	225/329 (68%)	205 (91%)	15 (7%)	5 (2%)	5	30
1	H	212/329 (64%)	196 (92%)	14 (7%)	2 (1%)	14	46
2	C	1338/1342 (100%)	1194 (89%)	112 (8%)	32 (2%)	4	29
2	I	1338/1342 (100%)	1185 (89%)	122 (9%)	31 (2%)	5	30
3	D	1157/1407 (82%)	1036 (90%)	91 (8%)	30 (3%)	4	28
3	J	1146/1407 (81%)	1030 (90%)	85 (7%)	31 (3%)	4	27
4	E	87/91 (96%)	77 (88%)	6 (7%)	4 (5%)	2	19
4	K	77/91 (85%)	69 (90%)	7 (9%)	1 (1%)	9	39
5	F	462/613 (75%)	419 (91%)	34 (7%)	9 (2%)	6	33
5	L	463/613 (76%)	425 (92%)	30 (6%)	8 (2%)	7	34
All	All	7021/8222 (85%)	6294 (90%)	560 (8%)	167 (2%)	4	29

All (167) Ramachandran outliers are listed below:

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

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Mol	Chain	Res	Type
5	L	96	ASP
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

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Mol	Chain	Res	Type
2	C	162	GLY
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

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Mol	Chain	Res	Type
2	I	160	ASP
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	19
1	B	248/286 (87%)	214 (86%)	34 (14%)	3	18
1	G	193/286 (68%)	177 (92%)	16 (8%)	10	34
1	H	183/286 (64%)	171 (93%)	12 (7%)	15	41
2	C	1155/1157 (100%)	1031 (89%)	124 (11%)	6	25
2	I	1153/1157 (100%)	1039 (90%)	114 (10%)	7	29
3	D	959/1168 (82%)	833 (87%)	126 (13%)	4	20
3	J	959/1168 (82%)	837 (87%)	122 (13%)	4	21
4	E	72/75 (96%)	63 (88%)	9 (12%)	4	21
4	K	67/75 (89%)	56 (84%)	11 (16%)	2	14
5	F	417/540 (77%)	386 (93%)	31 (7%)	13	38
5	L	418/540 (77%)	383 (92%)	35 (8%)	10	34
All	All	6026/7024 (86%)	5365 (89%)	661 (11%)	6	24

All (661) 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	23	HIS
1	A	25	LYS
1	A	26	VAL
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	79	LEU

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Mol	Chain	Res	Type
1	A	101	THR
1	A	130	ILE
1	A	133	LEU
1	A	134	THR
1	A	139	SER
1	A	145	LYS
1	A	147	GLN
1	A	168	ILE
1	A	181	GLU
1	A	183	ILE
1	A	207	THR
1	A	224	LEU
1	A	227	GLN
1	B	9	LEU
1	B	16	ILE
1	B	20	SER
1	B	46	ILE
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	118	ASP
1	B	134	THR
1	B	157	THR
1	B	158	ARG
1	B	173	VAL
1	B	186	ASN
1	B	205	MET
1	B	224	LEU
1	B	229	GLU
1	B	246	LYS
1	B	250	ASP
1	B	252	ILE
1	B	255	ARG
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	295	LEU
1	B	300	LEU
1	B	312	LEU
2	C	11	ILE
2	C	22	LEU
2	C	29	SER
2	C	30	ILE
2	C	44	GLU
2	C	56	VAL
2	C	69	GLN
2	C	82	VAL
2	C	88	ARG
2	C	90	VAL
2	C	115	LYS
2	C	119	GLU
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	164	THR
2	C	170	VAL
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	299	LYS
2	C	316	GLU
2	C	319	LEU
2	C	321	LEU
2	C	364	VAL
2	C	369	MET
2	C	377	THR
2	C	414	ILE
2	C	419	ILE

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Mol	Chain	Res	Type
2	C	433	ILE
2	C	434	ASP
2	C	443	ASP
2	C	446	ASP
2	C	451	ARG
2	C	456	VAL
2	C	481	LEU
2	C	483	ASP
2	C	484	LEU
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	542	ARG
2	C	558	VAL
2	C	568	ASN
2	C	600	THR
2	C	603	ILE
2	C	609	ILE
2	C	623	LEU
2	C	633	LEU
2	C	657	THR
2	C	658	GLN
2	C	663	VAL
2	C	690	VAL
2	C	697	LYS
2	C	700	VAL
2	C	705	GLU
2	C	706	ARG
2	C	733	VAL
2	C	748	ILE
2	C	765	ILE
2	C	773	LEU
2	C	796	LEU
2	C	799	ASN
2	C	815	SER
2	C	817	LEU
2	C	867	GLU

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Mol	Chain	Res	Type
2	C	890	LYS
2	C	892	GLU
2	C	895	LEU
2	C	913	VAL
2	C	950	GLU
2	C	953	LEU
2	C	971	LEU
2	C	974	ARG
2	C	980	VAL
2	C	992	LEU
2	C	1002	LEU
2	C	1006	GLU
2	C	1022	LYS
2	C	1029	LEU
2	C	1054	LEU
2	C	1073	LYS
2	C	1076	ILE
2	C	1083	GLU
2	C	1098	LEU
2	C	1103	VAL
2	C	1109	ILE
2	C	1114	GLU
2	C	1132	LEU
2	C	1140	LYS
2	C	1145	ILE
2	C	1146	GLN
2	C	1154	ASP
2	C	1159	VAL
2	C	1164	PHE
2	C	1172	LEU
2	C	1180	MET
2	C	1186	VAL
2	C	1198	LEU
2	C	1206	THR
2	C	1207	SER
2	C	1222	GLU
2	C	1233	LEU
2	C	1248	THR
2	C	1253	LEU
2	C	1254	VAL
2	C	1265	PHE
2	C	1268	GLN

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Mol	Chain	Res	Type
2	C	1299	ASN
2	C	1330	ILE
2	C	1337	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	71	LEU
3	D	84	ILE
3	D	92	VAL
3	D	97	VAL
3	D	98	ARG
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	183	GLU
3	D	198	CYS
3	D	214	ARG
3	D	219	LYS
3	D	222	LYS
3	D	224	LEU
3	D	228	VAL
3	D	235	GLU
3	D	244	VAL
3	D	255	LEU
3	D	285	LEU
3	D	291	ILE
3	D	292	VAL
3	D	299	LEU
3	D	319	SER
3	D	324	LEU

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Mol	Chain	Res	Type
3	D	330	MET
3	D	331	ILE
3	D	342	LEU
3	D	357	VAL
3	D	374	LEU
3	D	392	THR
3	D	394	ILE
3	D	412	LEU
3	D	415	VAL
3	D	425	ARG
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	548	VAL
3	D	552	ILE
3	D	569	LEU
3	D	571	ASP
3	D	582	ILE
3	D	596	LEU
3	D	607	THR
3	D	614	LEU
3	D	615	LYS
3	D	618	VAL
3	D	639	VAL
3	D	641	ILE
3	D	660	GLU
3	D	663	GLU
3	D	674	THR
3	D	697	MET
3	D	698	MET
3	D	701	LEU
3	D	707	ILE
3	D	708	ASN
3	D	712	GLN
3	D	717	VAL
3	D	720	ASN
3	D	721	SER
3	D	740	LEU

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Mol	Chain	Res	Type
3	D	751	ASP
3	D	764	ARG
3	D	770	LEU
3	D	776	THR
3	D	797	THR
3	D	826	ILE
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	871	LEU
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	1155	ILE
3	D	1163	VAL
3	D	1169	THR
3	D	1170	LYS
3	D	1177	ILE
3	D	1194	ARG
3	D	1208	ASP
3	D	1209	VAL
3	D	1255	VAL
3	D	1261	LEU
3	D	1266	ILE
3	D	1273	ASP
3	D	1275	LEU
3	D	1276	GLU
3	D	1301	THR
3	D	1305	ASP
3	D	1306	LEU
3	D	1310	THR
3	D	1314	LEU
3	D	1327	GLU

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Mol	Chain	Res	Type
3	D	1328	THR
3	D	1343	GLU
3	D	1365	TYR
4	E	13	ILE
4	E	18	ASP
4	E	21	LEU
4	E	36	ASP
4	E	39	VAL
4	E	47	THR
4	E	58	LEU
4	E	63	ILE
4	E	84	THR
5	F	102	MET
5	F	163	THR
5	F	236	LYS
5	F	244	THR
5	F	248	GLU
5	F	305	LEU
5	F	306	PHE
5	F	310	GLU
5	F	314	THR
5	F	341	LEU
5	F	342	GLN
5	F	362	ASN
5	F	400	GLN
5	F	402	LEU
5	F	429	THR
5	F	437	GLN
5	F	446	GLN
5	F	450	ILE
5	F	471	LEU
5	F	476	ARG
5	F	486	ARG
5	F	491	GLU
5	F	526	THR
5	F	559	LEU
5	F	561	MET
5	F	566	ASP
5	F	573	LEU
5	F	587	ILE
5	F	599	ARG
5	F	600	HIS

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Mol	Chain	Res	Type
5	F	612	ASP
1	G	19	VAL
1	G	27	THR
1	G	51	MET
1	G	65	LEU
1	G	74	VAL
1	G	79	LEU
1	G	96	ASP
1	G	133	LEU
1	G	140	ILE
1	G	148	ARG
1	G	168	ILE
1	G	178	SER
1	G	183	ILE
1	G	198	LEU
1	G	217	ILE
1	G	224	LEU
1	H	12	ARG
1	H	48	LEU
1	H	49	SER
1	H	50	SER
1	H	60	GLU
1	H	62	ASP
1	H	92	VAL
1	H	95	LYS
1	H	96	ASP
1	H	102	LEU
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	75	LEU
2	I	82	VAL
2	I	90	VAL
2	I	115	LYS
2	I	119	GLU
2	I	135	THR
2	I	138	ILE
2	I	145	ILE

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Mol	Chain	Res	Type
2	I	148	GLN
2	I	156	PHE
2	I	170	VAL
2	I	185	ASP
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	292	ILE
2	I	299	LYS
2	I	316	GLU
2	I	319	LEU
2	I	321	LEU
2	I	325	LEU
2	I	364	VAL
2	I	369	MET
2	I	377	THR
2	I	414	ILE
2	I	419	ILE
2	I	433	ILE
2	I	434	ASP
2	I	443	ASP
2	I	446	ASP
2	I	451	ARG
2	I	452	ARG
2	I	456	VAL
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	524	ILE
2	I	538	LEU
2	I	542	ARG
2	I	558	VAL
2	I	569	ILE
2	I	600	THR

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Mol	Chain	Res	Type
2	I	609	ILE
2	I	623	LEU
2	I	633	LEU
2	I	637	ARG
2	I	657	THR
2	I	658	GLN
2	I	663	VAL
2	I	690	VAL
2	I	697	LYS
2	I	705	GLU
2	I	706	ARG
2	I	733	VAL
2	I	748	ILE
2	I	765	ILE
2	I	773	LEU
2	I	796	LEU
2	I	799	ASN
2	I	815	SER
2	I	817	LEU
2	I	831	ILE
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	929	ILE
2	I	950	GLU
2	I	992	LEU
2	I	1002	LEU
2	I	1006	GLU
2	I	1014	LEU
2	I	1029	LEU
2	I	1054	LEU
2	I	1073	LYS
2	I	1076	ILE
2	I	1078	LYS
2	I	1083	GLU
2	I	1098	LEU
2	I	1109	ILE
2	I	1114	GLU
2	I	1132	LEU

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Mol	Chain	Res	Type
2	I	1140	LYS
2	I	1146	GLN
2	I	1154	ASP
2	I	1159	VAL
2	I	1164	PHE
2	I	1172	LEU
2	I	1180	MET
2	I	1186	VAL
2	I	1198	LEU
2	I	1206	THR
2	I	1207	SER
2	I	1233	LEU
2	I	1253	LEU
2	I	1265	PHE
2	I	1268	GLN
2	I	1299	ASN
2	I	1330	ILE
3	J	24	LEU
3	J	42	GLU
3	J	44	ILE
3	J	46	TYR
3	J	52	GLU
3	J	54	ASP
3	J	56	LEU
3	J	70	CYS
3	J	71	LEU
3	J	92	VAL
3	J	97	VAL
3	J	98	ARG
3	J	119	SER
3	J	120	LEU
3	J	132	LEU
3	J	154	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	222	LYS

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Mol	Chain	Res	Type
3	J	224	LEU
3	J	228	VAL
3	J	244	VAL
3	J	252	LEU
3	J	255	LEU
3	J	259	ARG
3	J	285	LEU
3	J	291	ILE
3	J	299	LEU
3	J	306	LEU
3	J	319	SER
3	J	324	LEU
3	J	330	MET
3	J	331	ILE
3	J	342	LEU
3	J	357	VAL
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	430	HIS
3	J	442	ILE
3	J	453	VAL
3	J	460	ASP
3	J	475	GLU
3	J	506	VAL
3	J	518	VAL
3	J	526	VAL
3	J	536	LEU
3	J	545	HIS
3	J	548	VAL
3	J	569	LEU
3	J	571	ASP
3	J	582	ILE
3	J	596	LEU
3	J	615	LYS
3	J	641	ILE
3	J	660	GLU
3	J	674	THR

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Mol	Chain	Res	Type
3	J	678	ARG
3	J	697	MET
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	721	SER
3	J	731	ARG
3	J	740	LEU
3	J	751	ASP
3	J	764	ARG
3	J	770	LEU
3	J	788	LEU
3	J	797	THR
3	J	826	ILE
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	918	ILE
3	J	928	THR
3	J	1155	ILE
3	J	1163	VAL
3	J	1167	LYS
3	J	1169	THR
3	J	1170	LYS
3	J	1177	ILE
3	J	1194	ARG
3	J	1208	ASP
3	J	1209	VAL
3	J	1219	ASP
3	J	1242	ARG
3	J	1255	VAL
3	J	1261	LEU
3	J	1266	ILE

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Mol	Chain	Res	Type
3	J	1268	ASN
3	J	1273	ASP
3	J	1275	LEU
3	J	1280	VAL
3	J	1284	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	4	VAL
4	K	8	ASP
4	K	13	ILE
4	K	18	ASP
4	K	21	LEU
4	K	28	ARG
4	K	36	ASP
4	K	39	VAL
4	K	47	THR
4	K	58	LEU
4	K	63	ILE
5	L	102	MET
5	L	110	LEU
5	L	114	GLU
5	L	236	LYS
5	L	244	THR
5	L	248	GLU
5	L	277	MET
5	L	305	LEU
5	L	310	GLU
5	L	314	THR
5	L	333	VAL
5	L	341	LEU
5	L	342	GLN
5	L	362	ASN
5	L	400	GLN
5	L	402	LEU
5	L	437	GLN
5	L	450	ILE

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Mol	Chain	Res	Type
5	L	469	GLN
5	L	471	LEU
5	L	476	ARG
5	L	481	GLU
5	L	486	ARG
5	L	491	GLU
5	L	498	LEU
5	L	526	THR
5	L	540	LEU
5	L	559	LEU
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	613	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (123) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	23	HIS
1	A	194	GLN
1	A	227	GLN
1	B	18	GLN
1	B	132	HIS
1	B	137	ASN
1	B	268	ASN
2	C	31	GLN
2	C	36	GLN
2	C	69	GLN
2	C	120	GLN
2	C	314	ASN
2	C	330	HIS
2	C	387	ASN
2	C	490	GLN
2	C	618	GLN
2	C	649	GLN
2	C	658	GLN
2	C	659	GLN
2	C	799	ASN
2	C	952	GLN

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Mol	Chain	Res	Type
2	C	1008	GLN
2	C	1038	GLN
2	C	1134	GLN
2	C	1146	GLN
2	C	1237	HIS
2	C	1268	GLN
2	C	1313	HIS
3	D	157	GLN
3	D	196	GLN
3	D	274	ASN
3	D	364	HIS
3	D	365	GLN
3	D	419	HIS
3	D	435	GLN
3	D	450	HIS
3	D	458	ASN
3	D	593	ASN
3	D	665	GLN
3	D	716	GLN
3	D	805	GLN
3	D	817	HIS
3	D	1227	HIS
3	D	1235	ASN
3	D	1259	GLN
3	D	1289	ASN
3	D	1366	HIS
3	D	1367	GLN
4	E	31	GLN
5	F	131	GLN
5	F	227	GLN
5	F	258	GLN
5	F	271	ASN
5	F	317	ASN
5	F	342	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	G	66	HIS
1	G	117	HIS

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Mol	Chain	Res	Type
1	H	23	HIS
1	H	37	HIS
1	H	103	ASN
1	H	128	HIS
1	H	137	ASN
1	H	186	ASN
2	I	36	GLN
2	I	276	GLN
2	I	494	ASN
2	I	618	GLN
2	I	673	HIS
2	I	760	ASN
2	I	762	ASN
2	I	799	ASN
2	I	824	GLN
2	I	832	HIS
2	I	834	GLN
2	I	952	GLN
2	I	955	GLN
2	I	1008	GLN
2	I	1070	HIS
2	I	1134	GLN
2	I	1146	GLN
2	I	1237	HIS
2	I	1256	GLN
2	I	1299	ASN
2	I	1314	GLN
3	J	94	GLN
3	J	200	GLN
3	J	266	ASN
3	J	274	ASN
3	J	364	HIS
3	J	365	GLN
3	J	450	HIS
3	J	458	ASN
3	J	465	GLN
3	J	489	ASN
3	J	665	GLN
3	J	680	ASN
3	J	700	ASN
3	J	739	GLN
3	J	762	ASN

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Mol	Chain	Res	Type
3	J	805	GLN
3	J	929	GLN
3	J	1197	ASN
3	J	1235	ASN
3	J	1268	ASN
3	J	1279	GLN
3	J	1289	ASN
3	J	1366	HIS
5	L	129	GLN
5	L	227	GLN
5	L	271	ASN
5	L	301	ASN
5	L	317	ASN
5	L	406	GLN
5	L	437	GLN
5	L	545	HIS
5	L	579	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 oligosaccharides 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	1.09	4 (11%)	49,58,58	1.59	8 (16%)
8	4C2	J	2004	-	36,38,38	0.43	0	49,58,58	1.72	4 (8%)

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	-	-	6/22/52/52	0/4/4/4
8	4C2	J	2004	-	-	3/22/52/52	0/4/4/4

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	D	2004	4C2	C1-N	3.87	1.46	1.42
8	D	2004	4C2	C7-N2	-2.92	1.25	1.36
8	D	2004	4C2	O-C	-2.53	1.17	1.23
8	D	2004	4C2	C1-C7	-2.45	1.37	1.41

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	J	2004	4C2	C5-C2-S	7.40	132.74	127.23
8	J	2004	4C2	C11-N3-C10	-6.28	103.43	113.84
8	J	2004	4C2	C19-C10-N3	-4.93	85.95	110.56
8	D	2004	4C2	C19-C10-N3	-4.88	86.20	110.56
8	D	2004	4C2	C1-C-C21	-4.71	84.47	88.30
8	D	2004	4C2	C7-C1-C	4.36	95.75	91.74
8	D	2004	4C2	C11-N3-C10	-3.28	108.40	113.84
8	D	2004	4C2	C-C1-N	-3.15	128.33	137.84
8	J	2004	4C2	C1-N-S	3.04	128.86	121.03
8	D	2004	4C2	C7-C1-N	2.85	135.91	129.88
8	D	2004	4C2	C1-N-S	2.54	127.57	121.03
8	D	2004	4C2	O-C-C1	2.00	139.78	136.49

There are no chirality outliers.

All (9) torsion outliers are listed below:

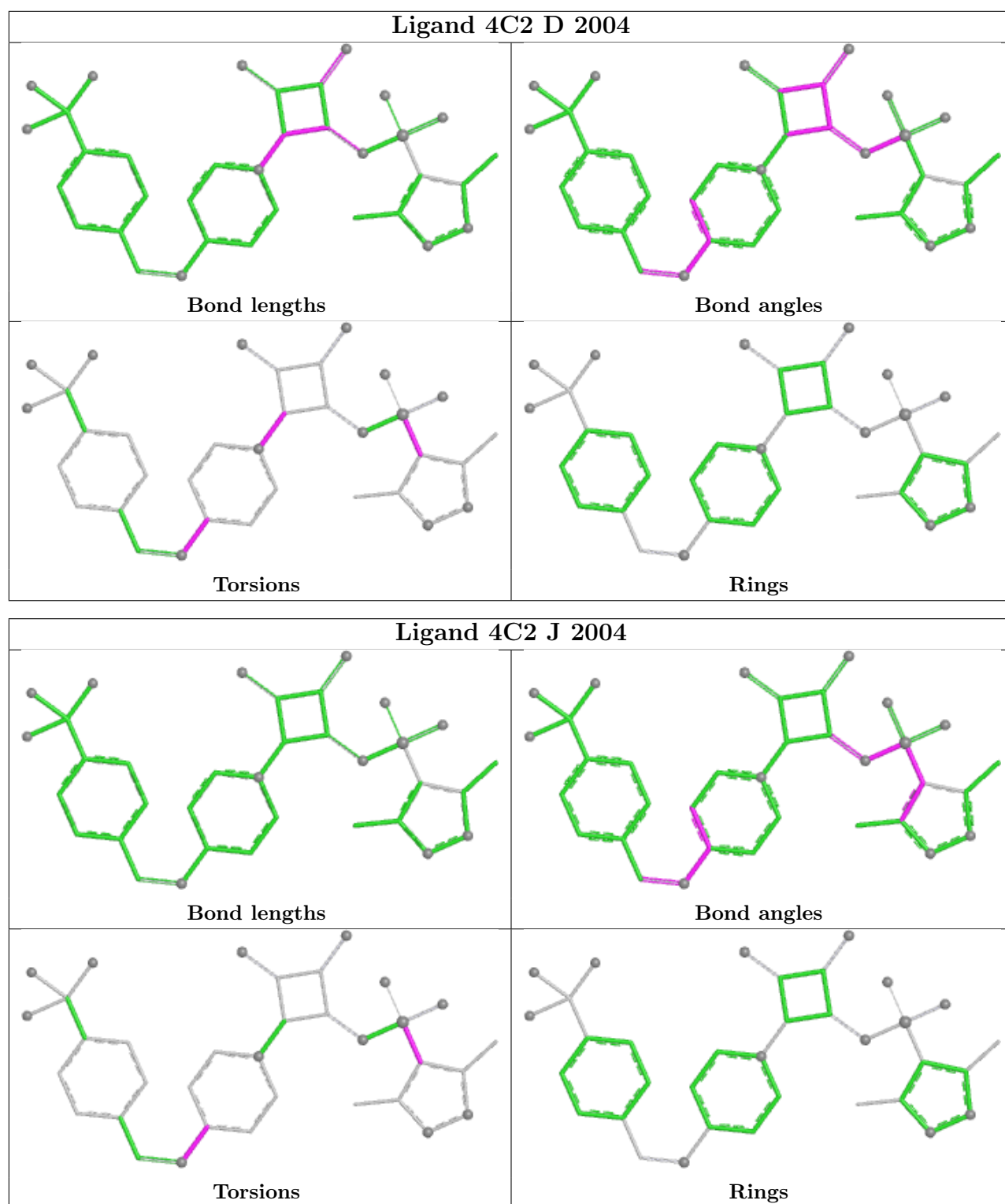
Mol	Chain	Res	Type	Atoms
8	D	2004	4C2	C3-C2-S-O2
8	D	2004	4C2	C3-C2-S-O3
8	D	2004	4C2	C9-C10-N3-C11
8	J	2004	4C2	C9-C10-N3-C11
8	D	2004	4C2	C5-C2-S-O2
8	D	2004	4C2	C19-C10-N3-C11
8	J	2004	4C2	C3-C2-S-O3
8	J	2004	4C2	C19-C10-N3-C11
8	D	2004	4C2	C21-C7-N2-C20

There are no ring outliers.

2 monomers are involved in 2 short contacts:

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

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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%)	-0.65	0 100 100	140, 166, 193, 222	0
1	B	289/329 (87%)	-0.65	0 100 100	146, 203, 247, 259	0
1	G	227/329 (68%)	-0.68	0 100 100	189, 214, 238, 246	0
1	H	216/329 (65%)	-0.49	0 100 100	201, 246, 255, 259	0
2	C	1340/1342 (99%)	-0.67	1 (0%) 92 87	115, 159, 222, 268	0
2	I	1340/1342 (99%)	-0.69	0 100 100	153, 185, 240, 340	0
3	D	1163/1407 (82%)	-0.64	0 100 100	121, 156, 213, 257	0
3	J	1152/1407 (81%)	-0.60	1 (0%) 92 87	151, 192, 247, 273	0
4	E	89/91 (97%)	-0.66	0 100 100	174, 192, 209, 216	0
4	K	79/91 (86%)	-0.52	0 100 100	262, 289, 297, 302	0
5	F	468/613 (76%)	-0.54	0 100 100	150, 211, 305, 326	0
5	L	469/613 (76%)	-0.61	0 100 100	163, 215, 294, 309	0
All	All	7067/8222 (85%)	-0.64	2 (0%) 100 100	115, 183, 255, 340	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	1175	LEU	2.5
2	C	206	ALA	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

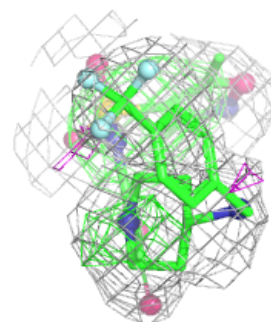
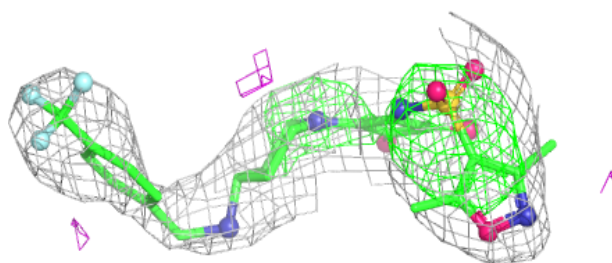
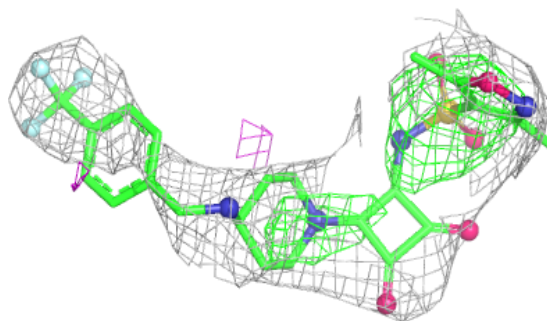
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	MG	J	2001	1/1	0.93	0.08	166,166,166,166	0
6	MG	D	2001	1/1	0.97	0.04	166,166,166,166	0
8	4C2	D	2004	35/35	0.97	0.16	166,166,166,175	0
8	4C2	J	2004	35/35	0.98	0.08	166,166,171,175	0
7	ZN	J	2003	1/1	0.99	0.03	217,217,217,217	0
7	ZN	D	2002	1/1	0.99	0.05	166,166,166,166	0
7	ZN	J	2002	1/1	0.99	0.03	201,201,201,201	0
7	ZN	D	2003	1/1	1.00	0.07	166,166,166,166	0

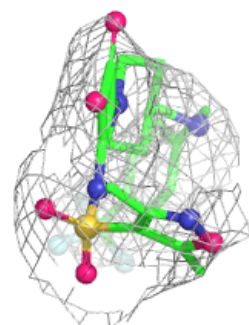
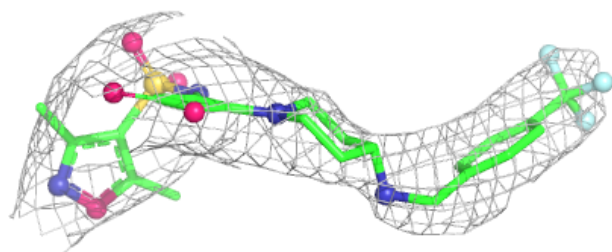
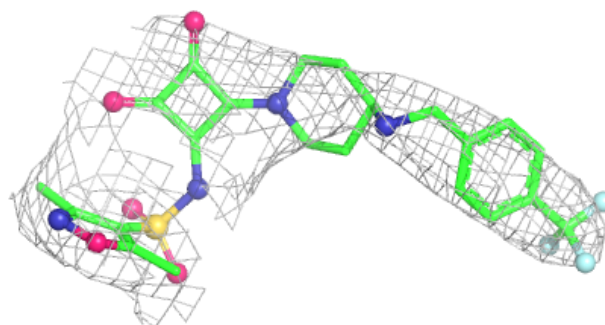
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 4C2 D 2004:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around 4C2 J 2004:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.