



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:45 PM UTC

PDB ID : 4ZH2 / pdb_00004zh2
Title : Crystal structure of Escherichia coli RNA polymerase in complex with CBR703
Authors : Feng, Y.; Ebright, R.H.
Deposited on : 2015-04-24
Resolution : 4.20 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 ⓘ](#)) were used in the production of this report:

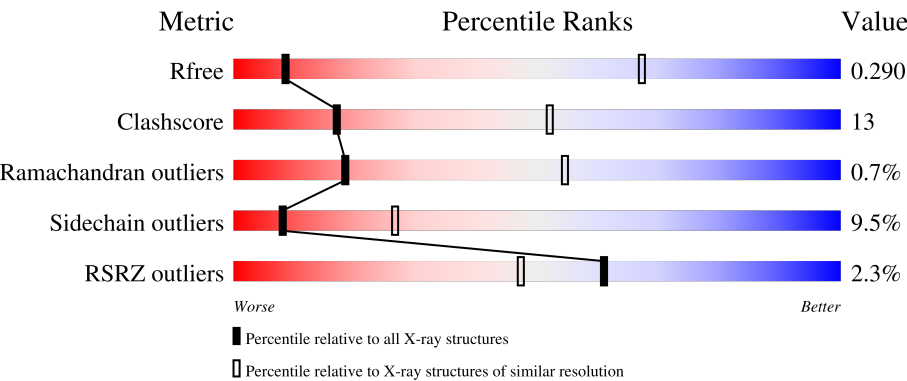
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal 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 4.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1004 (4.52-3.88)
Clashscore	190562	1019 (4.50-3.90)
Ramachandran outliers	187476	1020 (4.56-3.84)
Sidechain outliers	187428	1006 (4.56-3.84)
RSRZ outliers	180081	1001 (4.52-3.88)

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	335	% 61%26%10%
1	B	335	% 39%21%36%
1	G	335	4% 40%24%33%
1	H	335	2% 41%20%36%
2	C	1342	% 67%30%

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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	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	4OB	C	2001	-	-	X	-
6	4OB	I	2001	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 57763 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	302	Total	C	N	O	S	0	0	0
			2328	1456	413	451	8			
1	B	216	Total	C	N	O	S	0	0	0
			1667	1041	294	326	6			
1	G	224	Total	C	N	O	S	0	0	0
			1730	1076	308	340	6			
1	H	216	Total	C	N	O	S	0	0	0
			1662	1038	292	326	6			

There are 28 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	expression tag	UNP P0A7Z4
A	-4	HIS	-	expression tag	UNP P0A7Z4
A	-3	HIS	-	expression tag	UNP P0A7Z4
A	-2	HIS	-	expression tag	UNP P0A7Z4
A	-1	HIS	-	expression tag	UNP P0A7Z4
A	0	HIS	-	expression tag	UNP P0A7Z4
A	1	HIS	-	expression tag	UNP P0A7Z4
B	-5	MET	-	expression tag	UNP P0A7Z4
B	-4	HIS	-	expression tag	UNP P0A7Z4
B	-3	HIS	-	expression tag	UNP P0A7Z4
B	-2	HIS	-	expression tag	UNP P0A7Z4
B	-1	HIS	-	expression tag	UNP P0A7Z4
B	0	HIS	-	expression tag	UNP P0A7Z4
B	1	HIS	-	expression tag	UNP P0A7Z4
G	-5	MET	-	expression tag	UNP P0A7Z4
G	-4	HIS	-	expression tag	UNP P0A7Z4
G	-3	HIS	-	expression tag	UNP P0A7Z4
G	-2	HIS	-	expression tag	UNP P0A7Z4
G	-1	HIS	-	expression tag	UNP P0A7Z4
G	0	HIS	-	expression tag	UNP P0A7Z4
G	1	HIS	-	expression tag	UNP P0A7Z4

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Chain	Residue	Modelled	Actual	Comment	Reference
H	-5	MET	-	expression tag	UNP P0A7Z4
H	-4	HIS	-	expression tag	UNP P0A7Z4
H	-3	HIS	-	expression tag	UNP P0A7Z4
H	-2	HIS	-	expression tag	UNP P0A7Z4
H	-1	HIS	-	expression tag	UNP P0A7Z4
H	0	HIS	-	expression tag	UNP P0A7Z4
H	1	HIS	-	expression tag	UNP P0A7Z4

- 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
			10566	6629	1840	2054	43			

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

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	1166	Total	C	N	O	S	0	0	0
			9107	5723	1634	1704	46			
3	J	1334	Total	C	N	O	S	0	0	0
			10369	6513	1850	1957	49			

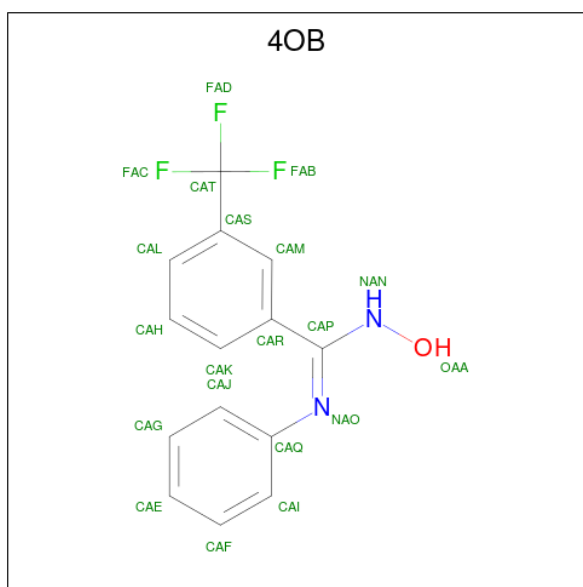
- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

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	542	Total	C	N	O	S	0	0	0
			4204	2625	752	801	26			
5	L	539	Total	C	N	O	S	0	0	0
			4196	2619	749	802	26			

- Molecule 6 is N-hydroxy-N'-phenyl-3-(trifluoromethyl)benzenecarboximidamide (CCD ID: 4OB) (formula: C₁₄H₁₁F₃N₂O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	F	N	O	0	0
			20	14	3	2	1		
6	I	1	Total	C	F	N	O	0	0
			20	14	3	2	1		

- Molecule 7 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

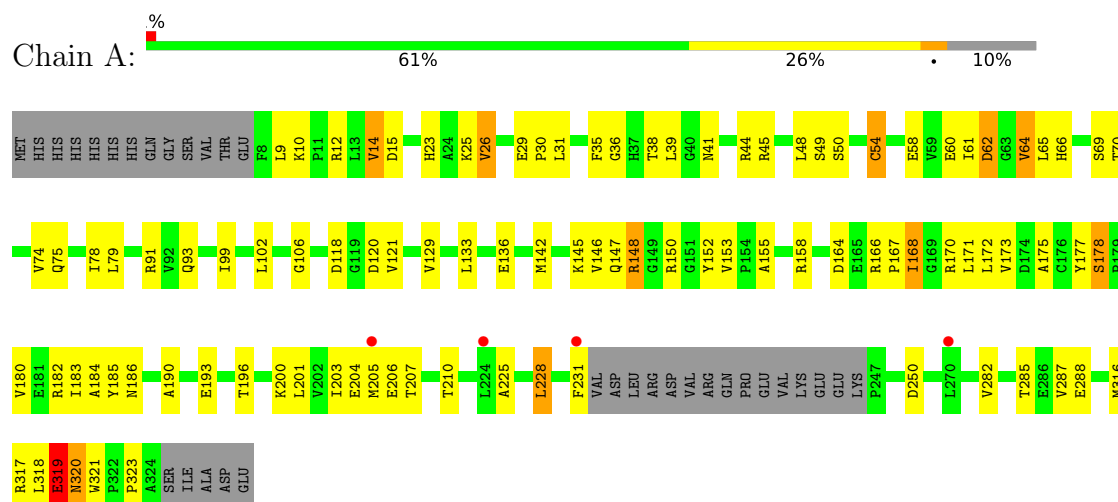
- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

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

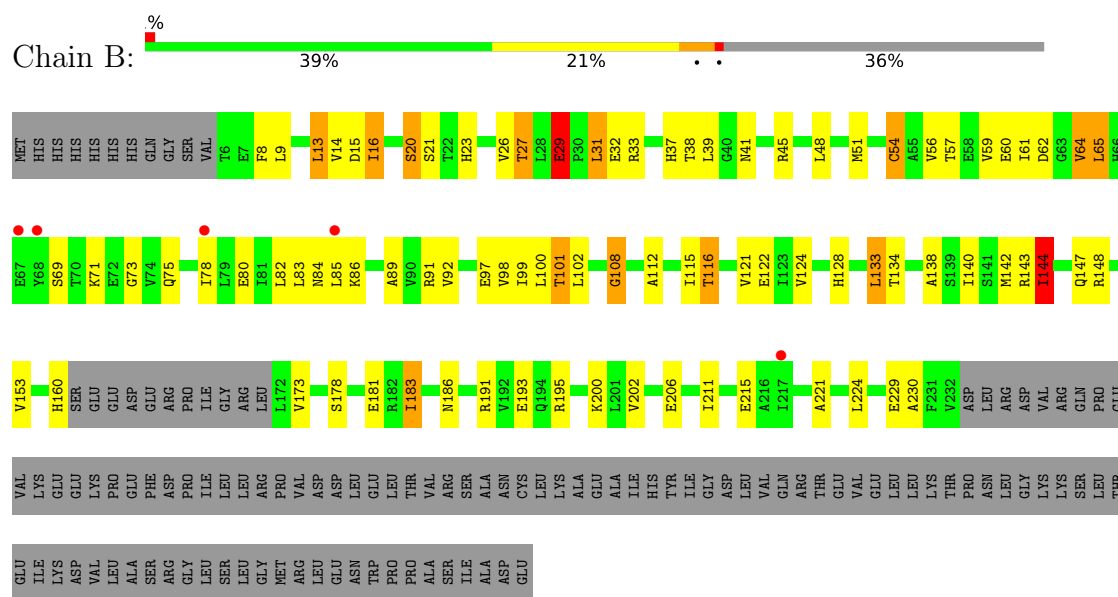
3 Residue-property plots

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

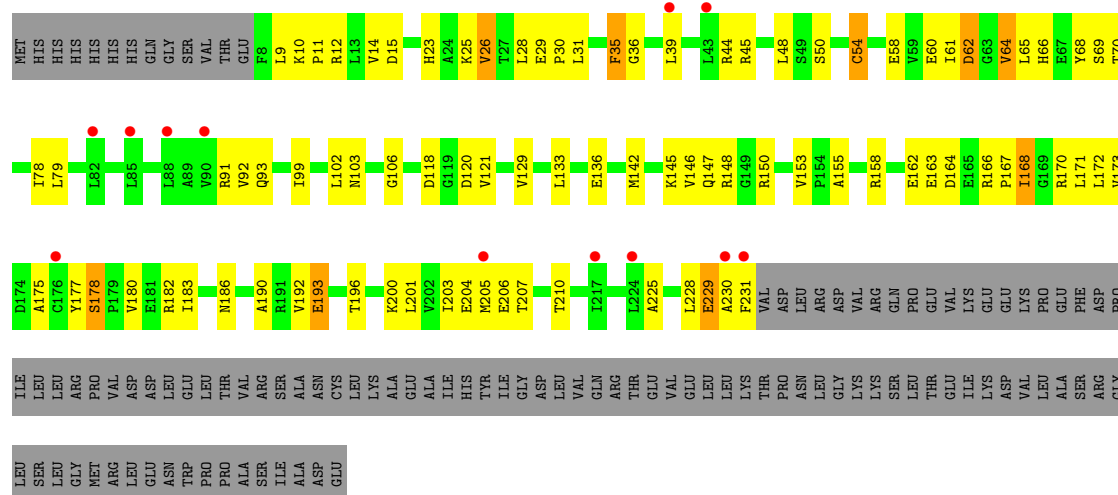


• Molecule 1: DNA-directed RNA polymerase subunit alpha

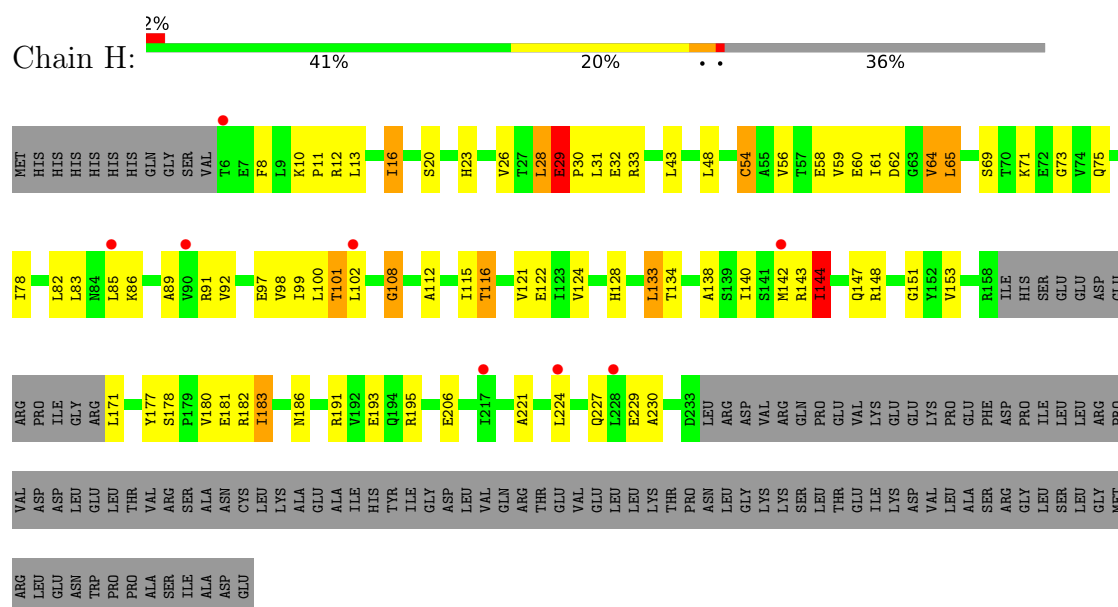


• Molecule 1: DNA-directed RNA polymerase subunit alpha

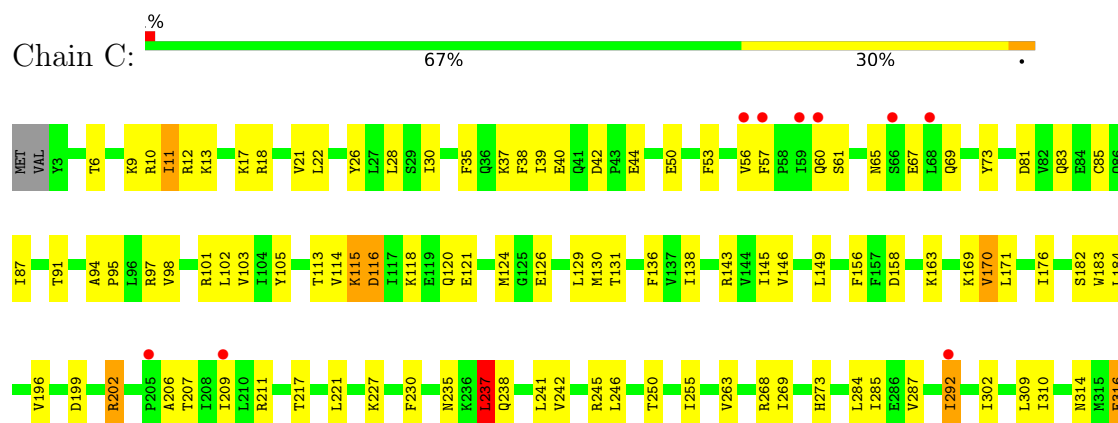


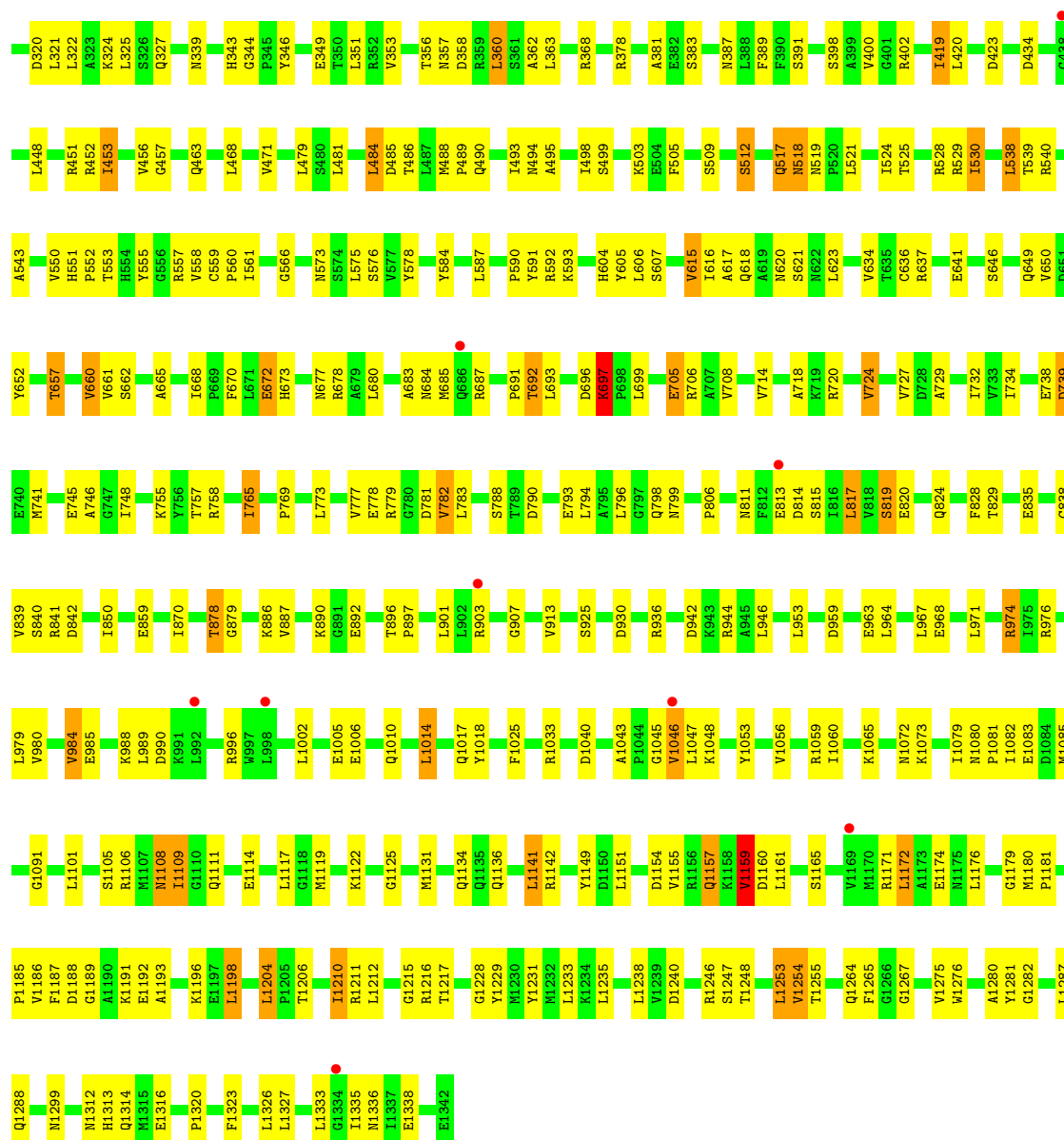


• Molecule 1: DNA-directed RNA polymerase subunit alpha

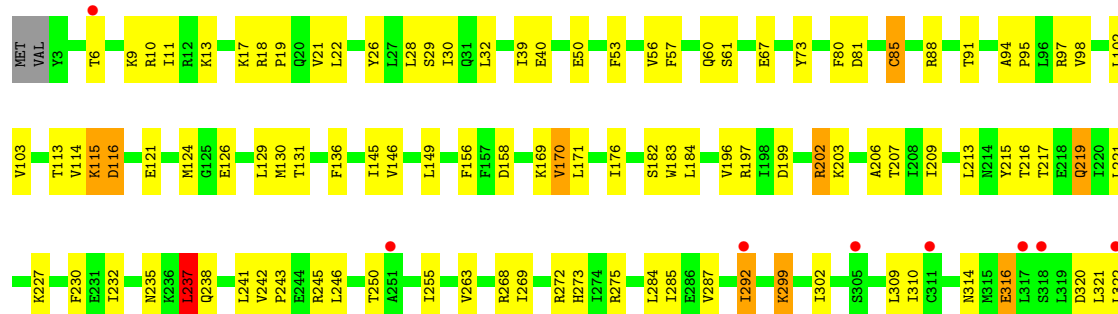


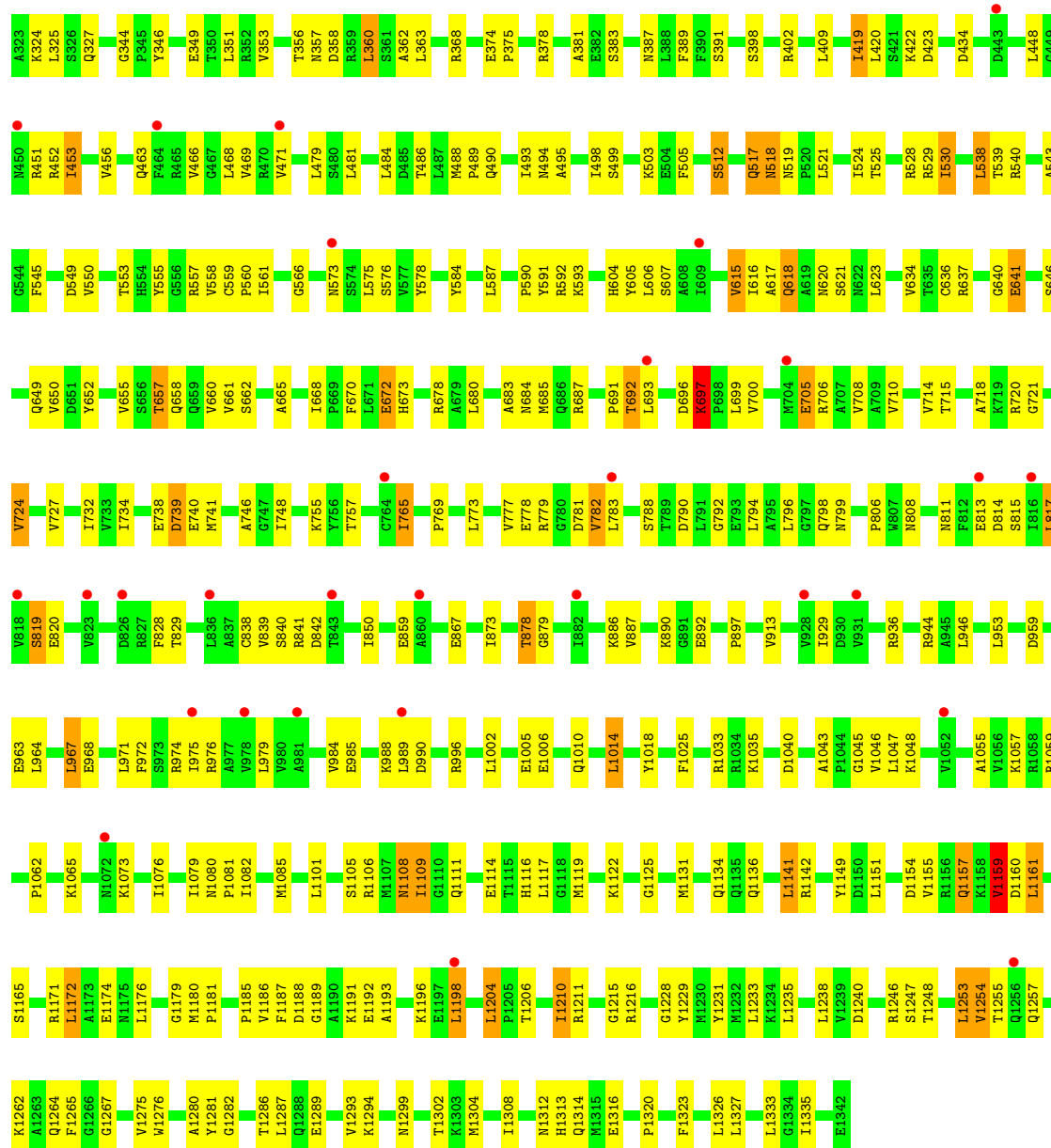
• Molecule 2: DNA-directed RNA polymerase subunit beta



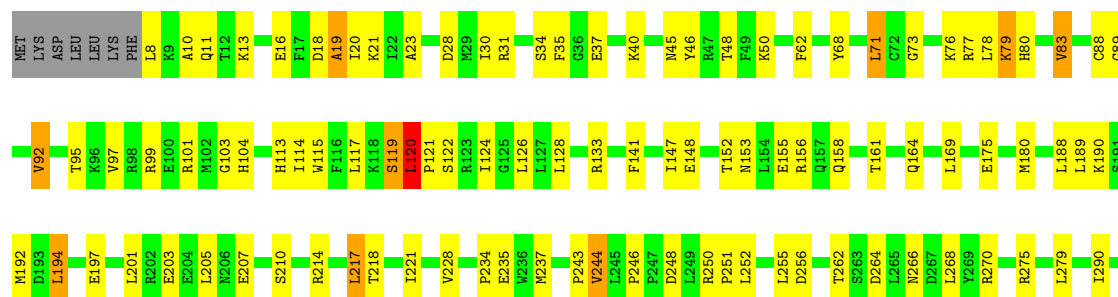


• Molecule 2: DNA-directed RNA polymerase subunit beta



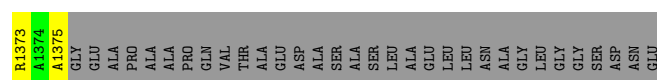


• Molecule 3: DNA-directed RNA polymerase subunit beta'



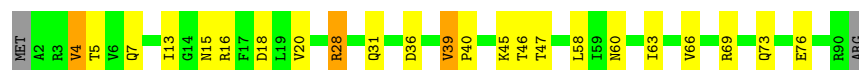


V1280	Y1186	P1096	K972	F892	H777	M698	L587	M484	P379	L279	H192	V92
EL281	M1189	F1100	K973	G993	G776	L701	N593	T487	K384	L282	D193	T95
R1284	I1190	L1101	V974	V894	R780	R706	Q594	N488	E386	L290	L194	K96
K1286	P1191	I1106	I975	H897	K781	V708	K598	I490	L387	L291	E197	V97
K1192	V1193	V1113	H978	C998	L788	M708	I601	V501	R388	N294	L201	R101
I1193	R1194	Q1114	H979	C999	G794	R709	C608	P502	E295	E295	R202	M102
A1288	V1198	I1115	T980	G901	G794	D710	G608	P502	I394	K296	E203	G103
N1289	F1199	S1116	E987	R901	T797	Q712	R610	Q504	E405	M298	E204	H104
E1291	S1117	S1117	V997	A904	R798	K715	L612	V506	V408	D304	H113	H114
E1292	G1118	G1118	V997	R905	R799	Q716	L612	V507	W409	L306	W206	W115
E1293	L1121	L1121	V1017	G906	L800	W717	G613	L508	D410	L307	F116	F116
A1294	A1122	A1122	A1018	H907	D802	W717	L614	Y511	L411	D308	K118	K118
N1295	R1123	R1123	H1019	I908	W801	W717	K615	Y512	L412	R214	S119	S119
V1298	G1207	G1207	H1020	A904	W803	Y723	P616	M513	D413	R214	L120	L120
D1208	P1125	P1125	T1024	R905	D806	R731	T617	T514	E414	R311	P121	P121
V1209	Q1126	Q1126	M1025	I918	L807	G732	A621	R515	V415	R312	T218	T218
T1301	GLU	GLU	M1026	A919	T810	S733	G628	R515	V416	T317	I221	I221
R1304	SER	SER	P1026	A920	E811	A735	F629	V518	R417	N320	V228	V228
L1307	GLY	GLY	V1027	Q921	E811	A735	G628	V518	R417	N320	V228	V228
F1319	GLY	GLY	I1028	S922	E815	Q736	F629	V518	R417	N320	V228	V228
H1227	THR	THR	V1031	I923	G815	W737	A633	E523	E418	N320	V228	V228
S1324	LYS	LYS	V1031	G924	T816	R738	A633	E523	E418	N320	V228	V228
E1327	ASP	ASP	F1034	E925	H817	Q739	A633	E523	E418	N320	V228	V228
T1328	ILE	ILE	R1036	P926	P824	L740	V639	E532	R426	L324	K233	K233
T1328	THR	THR	R1036	G927	P824	A741	G640	E532	R426	L324	K233	K233
T1329	GLY	GLY	F1037	T928	W825	G742	I641	A426	A426	M330	E235	E235
L1332	G1137	G1137	D1042	Q929	I826	W743	M644	R535	P427	K334	W237	W237
T1333	R1140	R1140	Q1043	L930	W831	G745	V645	R535	H430	F338	P243	P243
V1337	E1146	E1146	G1043	T931	L835	L746	P647	R538	E438	Q340	W244	W244
R1341	A1147	A1147	T1045	THR	L835	L746	P647	R538	E438	Q340	W244	W244
D1342	R1148	R1148	I1046	PHE	V639	W750	K650	R547	P439	N341	P247	P247
E1343	I1155	I1155	T1050	HIS	T844	D761	I654	V548	Q448	L342	D248	D248
L1344	L1156	L1156	T1050	ILE	T844	G762	I654	V548	Q448	L342	D248	D248
R1345	A1157	A1157	T1054	GLY	D847	S763	E658	V550	L449	H450	P251	P251
G1346	G1161	G1161	S1057	ALA	W848	W765	A659	K557	P451	V347	L252	L252
L1347	I1162	I1162	S1058	ARG	L849	T767	E660	K557	P451	V347	L252	L252
K1348	V1163	V1163	L1059	ARG	T853	P768	I664	L563	D460	D348	L255	L255
E1349	K1167	K1167	V1061	ALA	L857	W769	E677	S568	F461	T355	D256	D256
N1350	E1168	E1168	L1062	ALA	L857	W769	E677	S568	F461	T355	D256	D256
I1352	T1169	T1169	D1063	GLU	R860	N762	Y679	T572	D463	T356	G257	G257
V1353	K1170	K1170	D1063	GLU	R860	N762	Y679	T572	D463	T356	G257	G257
G1354	G1171	G1171	G1071	S948	L863	F763	V682	T573	D465	L361	T262	T262
I1357	K1172	K1172	K1072	S949	L864	W764	V682	T573	D465	L361	T262	T262
T1361	D1073	D1073	D1073	I950	L864	W764	V682	T573	D465	L361	T262	T262
S1271	A1077	A1077	A1077	I958	Q867	L767	V682	T573	D465	L361	T262	T262
S1272	L1078	L1078	L1078	I959	Q867	L767	V682	T573	D465	L361	T262	T262
F1273	K1079	K1079	K1079	I960	L872	W769	V682	T573	D465	L361	T262	T262
D1368	I1080	I1080	I1080	I963	W877	L774	V682	T573	D465	L361	T262	T262
R1371	D1184	D1184	D1184	V963	W877	L774	V682	T573	D465	L361	T262	T262
R1372	P1185	P1185	M1095	S969	W885	I774	V682	T573	D465	L361	T262	T262



- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain E: 73% 22% . .



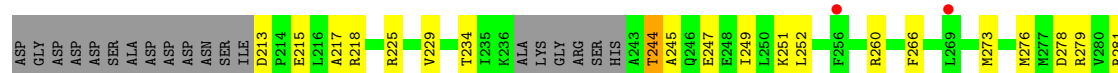
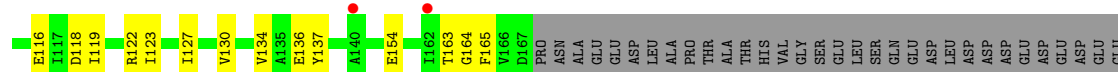
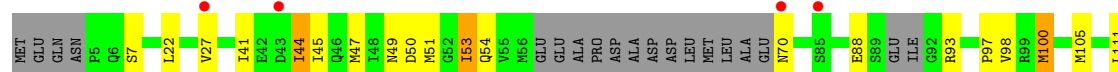
- Molecule 4: DNA-directed RNA polymerase subunit omega

Chain K: 2% 62% 23% 13%



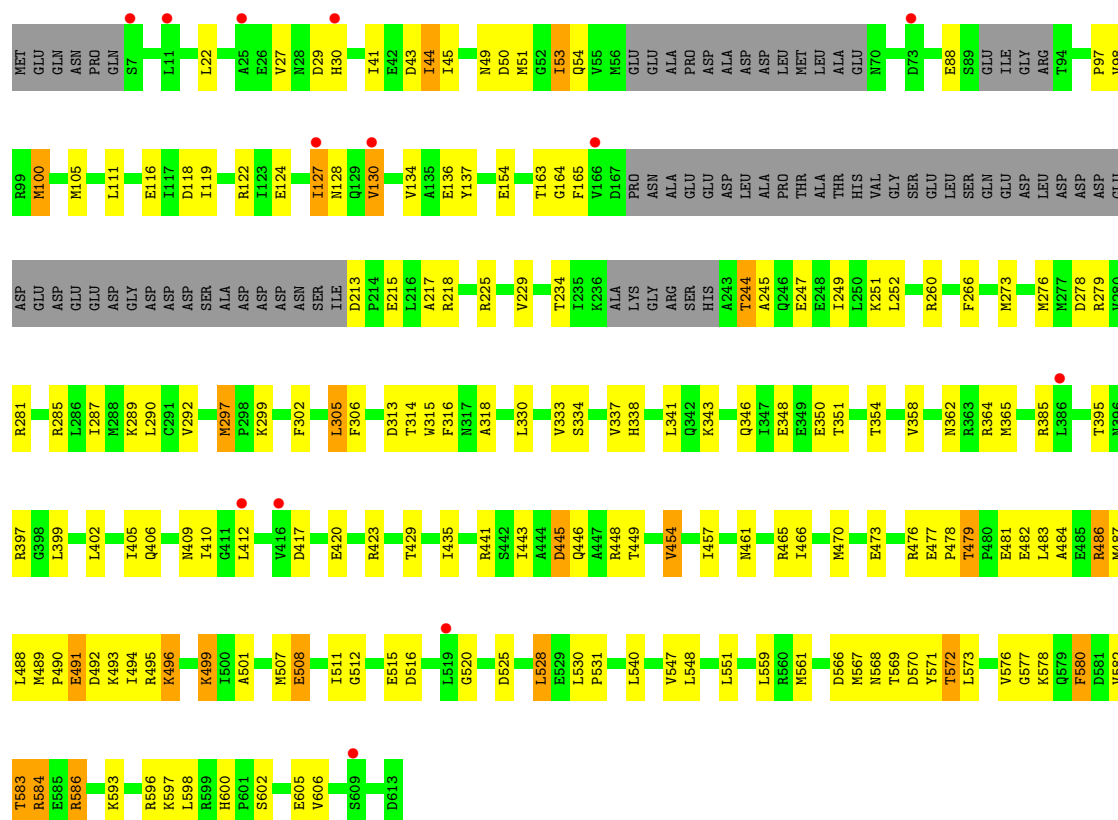
- Molecule 5: RNA polymerase sigma factor RpoD

Chain F: 2% 61% 24% 12%



- Molecule 5: RNA polymerase sigma factor RpoD

Chain L: 2% 59% 25% 12%



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	185.79Å 205.83Å 307.46Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.76 – 4.20 49.76 – 4.20	Depositor EDS
% Data completeness (in resolution range)	94.5 (49.76-4.20) 93.7 (49.76-4.20)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.39 (at 4.14Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.266 , 0.288 0.264 , 0.290	Depositor DCC
R_{free} test set	2581 reflections (2.99%)	wwPDB-VP
Wilson B-factor (Å ²)	152.4	Xtriage
Anisotropy	0.253	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 127.7	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	0.87	EDS
Total number of atoms	57763	wwPDB-VP
Average B, all atoms (Å ²)	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.91% 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: 4OB, ZN, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.41	0/2358	0.92	2/3197 (0.1%)
1	B	0.44	0/1687	0.99	8/2286 (0.3%)
1	G	0.41	0/1751	0.97	0/2373
1	H	0.42	0/1681	1.09	10/2278 (0.4%)
2	C	0.31	0/10739	0.78	9/14489 (0.1%)
2	I	0.30	0/10735	0.77	10/14484 (0.1%)
3	D	0.33	0/9246	0.82	16/12478 (0.1%)
3	J	0.32	0/10525	0.81	12/14212 (0.1%)
4	E	0.33	0/693	0.80	0/935
4	K	0.31	0/629	0.80	0/847
5	F	0.33	0/4254	0.80	7/5731 (0.1%)
5	L	0.33	0/4246	0.80	6/5720 (0.1%)
All	All	0.33	0/58544	0.82	80/79030 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
3	D	0	1
3	J	0	1
All	All	0	2

There are no bond length outliers.

All (80) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	29	GLU	CA-C-N	-15.20	105.42	120.31
1	H	29	GLU	C-N-CA	-15.20	105.42	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	120	LEU	CA-C-N	-10.68	106.49	119.84
3	J	120	LEU	C-N-CA	-10.68	106.49	119.84
3	D	120	LEU	CA-C-N	-9.29	108.22	119.84
3	D	120	LEU	C-N-CA	-9.29	108.22	119.84
3	D	120	LEU	N-CA-C	7.70	126.83	109.81
3	J	120	LEU	N-CA-C	7.45	126.28	109.81
3	D	250	ARG	CA-C-N	7.13	127.10	119.76
3	D	250	ARG	C-N-CA	7.13	127.10	119.76
2	I	1316	GLU	CA-C-N	6.49	125.72	118.97
2	I	1316	GLU	C-N-CA	6.49	125.72	118.97
2	I	1157	GLN	N-CA-C	6.34	118.75	111.02
5	F	51	MET	N-CA-C	6.30	120.28	112.59
5	L	584	ARG	N-CA-C	6.29	117.31	108.00
2	C	1316	GLU	CA-C-N	6.25	125.47	118.97
2	C	1316	GLU	C-N-CA	6.25	125.47	118.97
2	C	1157	GLN	N-CA-C	6.25	118.64	111.02
1	H	108	GLY	CA-C-N	6.24	126.21	119.78
1	H	108	GLY	C-N-CA	6.24	126.21	119.78
5	L	51	MET	N-CA-C	6.23	120.19	112.59
1	B	108	GLY	CA-C-N	6.18	126.15	119.78
1	B	108	GLY	C-N-CA	6.18	126.15	119.78
2	C	237	LEU	N-CA-C	6.17	123.95	110.80
1	H	178	SER	CA-C-N	5.90	125.57	119.56
1	H	178	SER	C-N-CA	5.90	125.57	119.56
2	C	1159	VAL	N-CA-C	5.79	121.38	109.34
3	J	40	LYS	CA-C-N	5.77	125.39	119.56
3	J	40	LYS	C-N-CA	5.77	125.39	119.56
3	D	1210	ILE	N-CA-C	-5.76	107.13	112.83
3	J	1210	ILE	N-CA-C	-5.75	107.13	112.83
2	I	237	LEU	N-CA-C	5.73	123.00	110.80
1	B	181	GLU	N-CA-C	-5.66	105.15	112.68
2	I	1159	VAL	N-CA-C	5.65	121.10	109.34
3	J	1293	GLU	CB-CA-C	-5.63	109.09	115.79
1	H	153	VAL	N-CA-C	5.63	113.72	108.15
3	J	450	HIS	CA-C-N	5.63	125.30	119.05
3	J	450	HIS	C-N-CA	5.63	125.30	119.05
3	D	40	LYS	CA-C-N	5.56	125.17	119.56
3	D	40	LYS	C-N-CA	5.56	125.17	119.56
1	B	29	GLU	CA-C-N	-5.55	114.24	119.85
1	B	29	GLU	C-N-CA	-5.55	114.24	119.85
1	B	153	VAL	N-CA-C	5.46	113.56	108.15
5	F	584	ARG	N-CA-C	5.40	115.99	108.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	ASP	CA-C-N	5.34	125.41	119.32
1	A	250	ASP	C-N-CA	5.34	125.41	119.32
1	H	144	ILE	N-CA-C	5.33	115.53	107.80
3	D	19	ALA	CB-CA-C	-5.33	109.45	115.79
3	D	450	HIS	CA-C-N	5.29	124.93	119.05
3	D	450	HIS	C-N-CA	5.29	124.93	119.05
1	H	181	GLU	N-CA-C	-5.29	105.64	112.68
1	B	20	SER	CB-CA-C	-5.27	110.07	117.23
3	D	246	PRO	CA-C-N	5.25	124.88	119.05
3	D	246	PRO	C-N-CA	5.25	124.88	119.05
1	H	20	SER	CB-CA-C	-5.24	110.11	117.23
2	I	566	GLY	CA-C-N	5.24	125.29	119.32
2	I	566	GLY	C-N-CA	5.24	125.29	119.32
3	J	19	ALA	CB-CA-C	-5.21	109.59	115.79
5	L	53	ILE	N-CA-C	5.17	120.10	109.34
5	L	163	THR	N-CA-C	-5.17	106.82	113.02
2	C	566	GLY	CA-C-N	5.16	125.20	119.32
2	C	566	GLY	C-N-CA	5.16	125.20	119.32
3	D	529	GLY	CA-C-N	5.15	124.94	119.28
3	D	529	GLY	C-N-CA	5.15	124.94	119.28
2	C	398	SER	CB-CA-C	-5.14	109.67	115.79
3	J	246	PRO	CA-C-N	5.13	124.75	119.05
3	J	246	PRO	C-N-CA	5.13	124.75	119.05
1	B	144	ILE	N-CA-C	5.13	115.24	107.80
5	F	383	ASN	N-CA-C	5.12	119.22	112.92
5	F	163	THR	N-CA-C	-5.12	106.88	113.02
5	F	53	ILE	N-CA-C	5.11	119.98	109.34
5	L	213	ASP	CA-C-N	5.11	124.72	119.05
5	L	213	ASP	C-N-CA	5.11	124.72	119.05
2	I	398	SER	CB-CA-C	-5.08	109.75	115.79
3	D	787	ALA	N-CA-C	5.08	116.89	111.36
2	I	618	GLN	N-CA-C	5.05	117.99	109.95
2	I	573	ASN	CB-CA-C	-5.05	109.27	116.34
2	C	573	ASN	CB-CA-C	-5.02	109.32	116.34
5	F	213	ASP	CA-C-N	5.00	124.60	119.05
5	F	213	ASP	C-N-CA	5.00	124.60	119.05

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	120	LEU	Peptide

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Mol	Chain	Res	Type	Group
3	J	120	LEU	Peptide

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	2328	0	2380	65	0
1	B	1667	0	1692	59	0
1	G	1730	0	1756	70	0
1	H	1662	0	1687	58	0
2	C	10570	0	10582	272	0
2	I	10566	0	10576	276	0
3	D	9107	0	9307	283	0
3	J	10369	0	10588	312	0
4	E	691	0	695	17	0
4	K	627	0	634	14	0
5	F	4204	0	4106	105	0
5	L	4196	0	4103	112	0
6	C	20	0	11	8	0
6	I	20	0	11	8	0
7	D	1	0	0	0	0
7	J	1	0	0	0	0
8	D	2	0	0	0	0
8	J	2	0	0	0	0
All	All	57763	0	58128	1468	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 13.

All (1468) 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)
3:J:660:GLU:HB3	3:J:685:ILE:HD12	1.47	0.97
2:I:1105:SER:HB2	3:J:731:ARG:HG2	1.50	0.93
3:D:418:GLU:HG3	4:E:45:LYS:H	1.34	0.92
3:D:660:GLU:HB3	3:D:685:ILE:HD12	1.50	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:555:TYR:HD2	6:C:2001:4OB:H9	1.37	0.90
2:C:1105:SER:HB2	3:D:731:ARG:HG2	1.50	0.89
3:J:133:ARG:HB2	5:L:88:GLU:HA	1.58	0.85
2:I:555:TYR:HD2	6:I:2001:4OB:H9	1.42	0.84
1:A:190:ALA:HB2	1:A:200:LYS:HB2	1.60	0.83
3:J:1044:GLN:HB3	3:J:1071:GLY:HA3	1.59	0.83
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.61	0.83
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.62	0.82
2:I:1312:ASN:HD21	2:I:1314:GLN:HE21	1.28	0.81
1:B:191:ARG:HH22	3:D:409:TRP:HB3	1.45	0.81
2:C:1312:ASN:HD21	2:C:1314:GLN:HE21	1.28	0.81
2:I:525:THR:HG21	2:I:687:ARG:HD2	1.64	0.80
3:J:905:ARG:HH11	4:K:16:ARG:HD2	1.47	0.80
2:C:1065:LYS:HE2	3:D:463:GLY:HA3	1.60	0.80
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.64	0.79
3:D:392:THR:HG21	5:F:606:VAL:HA	1.65	0.78
2:I:1065:LYS:HE2	3:J:463:GLY:HA3	1.63	0.78
2:I:310:ILE:HG21	2:I:325:LEU:HB3	1.66	0.78
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.64	0.78
2:I:806:PRO:HA	2:I:811:ASN:HD21	1.49	0.78
3:D:120:LEU:HD22	3:D:121:PRO:HD3	1.67	0.77
2:C:310:ILE:HG21	2:C:325:LEU:HB3	1.66	0.77
1:G:99:ILE:HG12	1:G:145:LYS:HG2	1.66	0.77
2:C:953:LEU:HD11	2:C:1033:ARG:HG3	1.66	0.77
2:C:673:HIS:HB3	2:C:1109:ILE:HG22	1.68	0.76
2:I:873:ILE:HG13	2:I:944:ARG:HH22	1.50	0.76
1:A:99:ILE:HG12	1:A:145:LYS:HG2	1.67	0.76
2:I:953:LEU:HD11	2:I:1033:ARG:HG3	1.66	0.76
1:G:12:ARG:HG3	1:H:230:ALA:HB1	1.67	0.75
3:D:1280:VAL:HG21	3:D:1304:ARG:HE	1.52	0.75
1:B:101:THR:HG22	1:B:116:THR:HB	1.68	0.75
2:I:215:TYR:HA	2:I:219:GLN:NE2	2.02	0.75
5:F:479:THR:HG22	5:F:482:GLU:HB2	1.69	0.74
3:J:418:GLU:HG3	4:K:45:LYS:H	1.50	0.74
3:D:133:ARG:NH2	5:F:93:ARG:O	2.19	0.74
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.67	0.74
1:H:101:THR:HG22	1:H:116:THR:HB	1.68	0.74
5:L:479:THR:HG22	5:L:482:GLU:HB2	1.69	0.74
1:G:225:ALA:HA	1:G:228:LEU:HD23	1.70	0.74
2:I:673:HIS:HB3	2:I:1109:ILE:HG22	1.69	0.74
2:C:806:PRO:HA	2:C:811:ASN:HD21	1.51	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:NH2	2:C:1215:GLY:O	2.21	0.73
2:I:840:SER:HB2	2:I:850:ILE:HD11	1.69	0.73
3:D:514:THR:HG23	3:D:576:ARG:HG2	1.71	0.72
2:I:452:ARG:NH1	2:I:584:TYR:O	2.22	0.72
2:C:10:ARG:NH2	2:C:790:ASP:OD2	2.23	0.72
2:I:292:ILE:HB	2:I:322:LEU:HD11	1.72	0.72
3:J:155:GLU:HB2	3:J:158:GLN:HB2	1.72	0.72
2:I:10:ARG:NH2	2:I:790:ASP:OD2	2.23	0.72
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.72	0.72
2:C:840:SER:HB2	2:C:850:ILE:HD11	1.69	0.71
3:D:905:ARG:HH11	4:E:16:ARG:HD2	1.54	0.71
3:J:514:THR:HG23	3:J:576:ARG:HG2	1.72	0.71
2:I:1106:ARG:HE	3:J:731:ARG:HH21	1.39	0.71
2:I:555:TYR:CD2	6:I:2001:4OB:H9	2.25	0.71
5:L:470:MET:HA	5:L:473:GLU:HB3	1.72	0.71
2:I:197:ARG:NH2	5:L:29:ASP:OD2	2.24	0.70
1:A:23:HIS:HB2	1:A:205:MET:O	1.91	0.70
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.55	0.70
3:J:342:LEU:HD11	3:J:1324:SER:HB3	1.72	0.70
3:J:1280:VAL:HG21	3:J:1304:ARG:HE	1.54	0.70
1:G:23:HIS:HB2	1:G:205:MET:O	1.91	0.70
5:L:561:MET:HA	5:L:567:MET:HE1	1.72	0.70
3:J:1026:PRO:HB2	3:J:1028:ILE:HG23	1.74	0.70
5:F:470:MET:HA	5:F:473:GLU:HB3	1.72	0.70
2:C:528:ARG:NH2	2:C:576:SER:O	2.25	0.70
2:C:657:THR:HG21	2:C:1188:ASP:HB2	1.73	0.70
2:C:221:LEU:HD11	2:C:314:ASN:HB2	1.72	0.70
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.72	0.70
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.73	0.70
3:J:1035:VAL:HG21	3:J:1121:LEU:HD21	1.74	0.70
2:C:555:TYR:CD2	6:C:2001:4OB:H9	2.25	0.69
5:F:561:MET:HA	5:F:567:MET:HE1	1.73	0.69
2:C:1106:ARG:HE	3:D:731:ARG:HH21	1.40	0.69
2:C:452:ARG:NH1	2:C:584:TYR:O	2.26	0.69
3:D:155:GLU:HB2	3:D:158:GLN:HB2	1.74	0.69
2:I:528:ARG:NH2	2:I:576:SER:O	2.25	0.69
2:I:734:ILE:HD11	2:I:783:LEU:HD11	1.74	0.69
5:F:134:VAL:HG21	5:F:266:PHE:HE1	1.58	0.68
2:C:292:ILE:HB	2:C:322:LEU:HD11	1.74	0.68
1:H:59:VAL:O	1:H:171:LEU:N	2.27	0.68
5:F:602:SER:H	5:F:605:GLU:CD	2.02	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:806:ASP:HA	3:J:1347:LEU:HD13	1.76	0.68
5:L:134:VAL:HG21	5:L:266:PHE:HE1	1.59	0.68
3:D:489:ASN:HA	3:D:904:ALA:HB1	1.76	0.68
2:C:732:ILE:HG21	2:C:783:LEU:HD12	1.76	0.68
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.76	0.67
2:I:657:THR:HG21	2:I:1188:ASP:HB2	1.74	0.67
3:D:806:ASP:HA	3:D:1347:LEU:HD13	1.76	0.67
3:J:489:ASN:HA	3:J:904:ALA:HB1	1.77	0.67
3:J:797:THR:HG22	3:J:924:GLY:HA3	1.76	0.67
3:J:251:PRO:HD2	5:L:507:MET:HE1	1.77	0.67
1:H:29:GLU:HB3	1:H:30:PRO:HD3	1.77	0.66
2:I:221:LEU:HD11	2:I:314:ASN:HB2	1.75	0.66
3:J:532:GLU:HA	3:J:535:ARG:HB3	1.76	0.66
2:C:463:GLN:HG3	2:C:505:PHE:HB2	1.78	0.66
5:F:602:SER:H	5:F:605:GLU:CG	2.08	0.66
2:I:463:GLN:HG3	2:I:505:PHE:HB2	1.78	0.66
3:D:797:THR:HG22	3:D:924:GLY:HA3	1.76	0.66
3:J:749:LYS:HD3	3:J:753:SER:O	1.95	0.66
2:I:88:ARG:NH2	2:I:1035:LYS:O	2.28	0.66
3:D:749:LYS:HD3	3:D:753:SER:O	1.96	0.66
3:D:1310:THR:HG21	5:F:70:ASN:HA	1.76	0.66
1:H:33:ARG:HH11	2:I:1081:PRO:HG3	1.61	0.66
3:D:342:LEU:HD11	3:D:1324:SER:HB3	1.75	0.66
2:I:829:THR:HA	2:I:1059:ARG:HA	1.78	0.65
2:I:732:ILE:HG21	2:I:783:LEU:HD12	1.77	0.65
3:J:664:ILE:HG22	3:J:678:ARG:HG2	1.77	0.65
2:C:18:ARG:NH2	2:C:620:ASN:OD1	2.30	0.65
2:C:734:ILE:HD11	2:C:783:LEU:HD11	1.77	0.65
1:G:166:ARG:O	1:G:168:ILE:N	2.30	0.65
2:I:18:ARG:NH2	2:I:620:ASN:OD1	2.28	0.65
2:C:829:THR:HA	2:C:1059:ARG:HA	1.78	0.65
2:C:1320:PRO:HG2	3:D:1354:GLY:HA3	1.78	0.65
2:C:18:ARG:NH1	2:C:621:SER:O	2.30	0.64
1:A:166:ARG:O	1:A:168:ILE:N	2.30	0.64
2:I:976:ARG:HD2	2:I:989:LEU:HD23	1.78	0.64
3:D:664:ILE:HG22	3:D:678:ARG:HG2	1.79	0.64
1:B:133:LEU:HD11	1:B:140:ILE:HG21	1.79	0.64
3:D:532:GLU:HA	3:D:535:ARG:HB3	1.79	0.64
3:D:1199:PHE:HB2	3:D:1202:GLU:HB2	1.80	0.64
3:J:646:ILE:HD11	3:J:764:ARG:HD2	1.79	0.63
3:J:1199:PHE:HB2	3:J:1202:GLU:HB2	1.81	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:18:ARG:NH1	2:I:621:SER:O	2.31	0.63
1:A:61:ILE:HG22	1:A:62:ASP:H	1.64	0.63
1:G:45:ARG:NH2	2:I:1216:ARG:HA	2.13	0.63
5:L:593:LYS:HE2	5:L:596:ARG:HD3	1.81	0.63
3:D:356:THR:OG1	3:D:357:VAL:N	2.32	0.63
3:D:646:ILE:HD11	3:D:764:ARG:HD2	1.80	0.63
5:F:561:MET:HG2	5:F:576:VAL:HG22	1.81	0.63
1:B:13:LEU:HD12	1:B:29:GLU:HB2	1.79	0.63
3:D:682:VAL:O	3:D:685:ILE:HG12	1.99	0.63
3:J:262:THR:OG1	3:J:266:ASN:ND2	2.32	0.63
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.81	0.62
2:C:814:ASP:OD2	2:C:1106:ARG:NH1	2.29	0.62
2:C:976:ARG:HD2	2:C:989:LEU:HD23	1.80	0.62
2:C:1238:LEU:HD12	2:C:1238:LEU:H	1.64	0.62
1:H:100:LEU:HD21	1:H:121:VAL:HG11	1.81	0.62
2:I:213:LEU:HB3	2:I:422:LYS:HD2	1.79	0.62
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.32	0.62
2:C:897:PRO:HB3	5:F:564:GLY:C	2.25	0.62
5:F:466:ILE:HD11	5:F:487:MET:HE3	1.80	0.62
1:G:39:LEU:HD11	1:H:227:GLN:HB3	1.81	0.62
1:G:61:ILE:HG22	1:G:62:ASP:H	1.63	0.62
1:H:133:LEU:HD11	1:H:140:ILE:HG21	1.79	0.62
2:I:103:VAL:HG12	2:I:116:ASP:HB3	1.81	0.62
3:J:80:HIS:HB3	3:J:83:VAL:HG11	1.82	0.62
5:L:466:ILE:HD11	5:L:487:MET:HE3	1.81	0.62
1:B:100:LEU:HD21	1:B:121:VAL:HG11	1.81	0.62
3:D:1174:ARG:HG2	3:D:1189:MET:HG2	1.81	0.62
2:C:103:VAL:HG12	2:C:116:ASP:HB3	1.82	0.62
2:I:985:GLU:HB3	2:I:988:LYS:HB2	1.82	0.62
3:J:325:LYS:HD3	5:L:508:GLU:HG2	1.80	0.61
3:D:308:ASP:OD2	3:D:311:ARG:NH2	2.32	0.61
1:A:70:THR:HG21	2:C:755:LYS:HE2	1.82	0.61
2:I:1238:LEU:HD12	2:I:1238:LEU:H	1.66	0.61
1:A:31:LEU:HD11	1:A:201:LEU:HB2	1.83	0.61
2:C:136:PHE:O	2:C:143:ARG:N	2.28	0.61
2:I:1157:GLN:HG3	2:I:1159:VAL:HG13	1.81	0.61
1:G:45:ARG:HH22	2:I:1216:ARG:HA	1.66	0.61
2:I:1101:LEU:HD21	3:J:508:LEU:HD22	1.82	0.61
3:J:1174:ARG:HG2	3:J:1189:MET:HG2	1.82	0.61
5:F:105:MET:HE1	5:F:385:ARG:HG2	1.83	0.61
2:I:149:LEU:HD13	2:I:453:ILE:HG13	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:GLY:HA2	1:B:134:THR:HG22	1.83	0.60
2:C:1157:GLN:HG3	2:C:1159:VAL:HG13	1.81	0.60
1:G:14:VAL:HG22	1:G:15:ASP:H	1.64	0.60
3:J:741:ALA:O	3:J:762:ASN:ND2	2.33	0.60
3:J:1172:LYS:HA	3:J:1191:PRO:HA	1.83	0.60
1:B:62:ASP:OD2	1:B:71:LYS:NZ	2.35	0.60
3:D:133:ARG:HB2	5:F:88:GLU:HA	1.83	0.60
1:H:83:LEU:HA	1:H:86:LYS:HE2	1.83	0.60
3:J:650:LYS:HE2	3:J:654:ILE:HD11	1.83	0.60
2:C:120:GLN:HG3	2:C:121:GLU:HG2	1.82	0.60
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.82	0.60
3:D:741:ALA:O	3:D:762:ASN:ND2	2.34	0.60
3:D:1172:LYS:HA	3:D:1191:PRO:HA	1.83	0.60
1:B:33:ARG:HH11	2:C:1081:PRO:HG3	1.66	0.60
3:D:341:ASN:HB2	3:D:1352:ILE:HD13	1.83	0.60
3:D:1238:GLN:NE2	3:D:1248:ILE:O	2.35	0.60
1:H:191:ARG:NH2	3:J:410:ASP:OD2	2.35	0.60
1:A:14:VAL:HG22	1:A:15:ASP:H	1.67	0.60
2:C:746:ALA:HA	2:C:974:ARG:HH21	1.66	0.60
3:D:1140:ARG:HH21	3:D:1236:GLU:HG2	1.67	0.60
3:J:527:LEU:HD23	3:J:532:GLU:HG3	1.84	0.60
5:L:561:MET:HG2	5:L:576:VAL:HG22	1.84	0.60
2:C:1287:LEU:HD13	3:D:1357:ILE:HD11	1.84	0.60
2:C:1108:ASN:OD1	2:C:1111:GLN:NE2	2.34	0.59
3:J:308:ASP:OD2	3:J:311:ARG:NH2	2.34	0.59
1:B:83:LEU:HA	1:B:86:LYS:HE2	1.84	0.59
2:C:841:ARG:HA	2:C:1046:VAL:HA	1.84	0.59
6:C:2001:4OB:H8	3:D:773:PHE:HB3	1.82	0.59
3:D:304:ASP:OD2	3:D:312:ARG:NH2	2.34	0.59
3:J:1050:THR:HG23	3:J:1057:SER:HB3	1.84	0.59
3:J:1157:ALA:HB2	3:J:1210:ILE:HD11	1.84	0.59
2:C:985:GLU:HB3	2:C:988:LYS:HB2	1.83	0.59
3:J:425:ARG:HD2	3:J:459:ALA:HB2	1.84	0.59
5:L:305:LEU:HD13	5:L:315:TRP:HA	1.84	0.59
3:D:80:HIS:HB3	3:D:83:VAL:HG11	1.85	0.59
2:I:269:ILE:HG23	2:I:273:HIS:HB2	1.85	0.59
3:J:682:VAL:O	3:J:685:ILE:HG12	2.02	0.59
4:K:15:ASN:HB3	4:K:18:ASP:HB2	1.84	0.59
5:L:476:ARG:HG2	5:L:477:GLU:HG2	1.84	0.59
4:E:15:ASN:HB3	4:E:18:ASP:HB2	1.84	0.59
4:E:73:GLN:HA	4:E:76:GLU:HB2	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:292:VAL:HG21	5:F:299:LYS:HG3	1.83	0.59
2:I:40:GLU:O	2:I:73:TYR:OH	2.20	0.59
5:L:551:LEU:HD22	5:L:597:LYS:HD2	1.85	0.59
3:D:847:ASP:OD1	3:D:847:ASP:N	2.35	0.59
1:G:25:LYS:HG2	1:G:204:GLU:HG3	1.84	0.59
3:D:425:ARG:HD2	3:D:459:ALA:HB2	1.84	0.59
1:G:45:ARG:NH2	2:I:1215:GLY:O	2.33	0.59
2:I:841:ARG:HA	2:I:1046:VAL:HA	1.84	0.59
2:I:1106:ARG:H	2:I:1106:ARG:HD2	1.67	0.59
3:J:892:PHE:H	3:J:1281:GLU:HG2	1.68	0.59
5:L:292:VAL:HG21	5:L:299:LYS:HG3	1.84	0.59
3:J:1238:GLN:NE2	3:J:1248:ILE:O	2.35	0.59
6:I:2001:4OB:H8	3:J:773:PHE:HB3	1.84	0.59
3:J:317:THR:HG23	3:J:320:ASN:HB3	1.84	0.59
2:C:13:LYS:HZ3	2:C:1151:LEU:HD12	1.66	0.58
3:D:1157:ALA:HB2	3:D:1210:ILE:HD11	1.85	0.58
2:C:269:ILE:HG23	2:C:273:HIS:HB2	1.85	0.58
3:D:194:LEU:HD13	3:D:228:VAL:HG22	1.85	0.58
3:J:304:ASP:OD2	3:J:312:ARG:NH2	2.36	0.58
5:F:551:LEU:HD22	5:F:597:LYS:HD2	1.84	0.58
2:I:494:ASN:OD1	2:I:495:ALA:N	2.34	0.58
5:L:105:MET:HE1	5:L:385:ARG:HG2	1.86	0.58
5:F:305:LEU:HD13	5:F:315:TRP:HA	1.84	0.58
2:C:339:ASN:HB3	2:C:343:HIS:H	1.69	0.58
2:C:897:PRO:HG3	3:D:77:ARG:HH22	1.67	0.58
2:C:1106:ARG:H	2:C:1106:ARG:HD2	1.67	0.58
3:D:650:LYS:HE2	3:D:654:ILE:HD11	1.85	0.58
5:F:461:ASN:O	5:F:465:ARG:HG2	2.04	0.58
1:A:25:LYS:HG2	1:A:204:GLU:HG3	1.85	0.58
1:G:10:LYS:HE2	1:H:229:GLU:HB3	1.84	0.58
3:J:34:SER:OG	3:J:104:HIS:ND1	2.26	0.58
3:J:152:THR:OG1	3:J:153:ASN:N	2.36	0.58
2:C:102:LEU:HB2	2:C:489:PRO:HG3	1.86	0.58
3:D:363:LEU:HD23	3:D:487:THR:HG22	1.86	0.58
1:G:31:LEU:HD11	1:G:201:LEU:HB2	1.84	0.58
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	1.86	0.58
2:C:40:GLU:O	2:C:73:TYR:OH	2.20	0.58
2:I:272:ARG:HA	2:I:275:ARG:HD2	1.86	0.58
2:I:738:GLU:HA	2:I:741:MET:HE2	1.86	0.58
2:I:1293:VAL:HG11	2:I:1304:MET:HE2	1.86	0.58
3:D:398:LYS:HE2	5:F:532:LEU:HD23	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:693:VAL:HG21	3:D:743:MET:HE3	1.86	0.58
5:F:276:MET:SD	5:F:279:ARG:NH1	2.77	0.58
1:H:73:GLY:HA2	1:H:134:THR:HG22	1.84	0.58
1:A:282:VAL:HB	1:A:316:MET:HB2	1.86	0.57
1:H:62:ASP:OD2	1:H:71:LYS:NZ	2.37	0.57
3:J:1140:ARG:HH21	3:J:1236:GLU:HG2	1.68	0.57
1:G:29:GLU:HB3	1:G:30:PRO:HD3	1.86	0.57
3:J:847:ASP:OD1	3:J:847:ASP:N	2.33	0.57
2:C:494:ASN:OD1	2:C:495:ALA:N	2.34	0.57
5:F:278:ASP:OD1	5:F:281:ARG:NH1	2.37	0.57
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.85	0.57
2:I:1108:ASN:OD1	2:I:1111:GLN:NE2	2.37	0.57
3:J:194:LEU:HD13	3:J:228:VAL:HG22	1.87	0.57
2:I:13:LYS:HZ3	2:I:1151:LEU:HD12	1.69	0.57
2:I:1185:PRO:HD2	2:I:1189:GLY:HA2	1.87	0.57
5:F:476:ARG:HG2	5:F:477:GLU:HG2	1.87	0.57
2:C:590:PRO:HG3	2:C:605:TYR:CZ	2.40	0.57
2:C:1142:ARG:HH22	2:C:1165:SER:HB2	1.69	0.57
3:D:1227:HIS:HA	3:D:1230:THR:HG22	1.86	0.57
2:I:94:ALA:HB2	2:I:129:LEU:HD11	1.86	0.57
5:L:225:ARG:O	5:L:229:VAL:HG13	2.04	0.57
3:D:892:PHE:H	3:D:1281:GLU:HG2	1.69	0.57
1:H:182:ARG:NH1	3:J:581:MET:SD	2.78	0.57
2:I:207:THR:HG21	2:I:351:LEU:HG	1.86	0.57
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.19	0.57
2:C:94:ALA:HB2	2:C:129:LEU:HD11	1.86	0.57
3:D:388:ARG:NH1	3:D:414:GLU:OE1	2.38	0.57
5:F:49:ASN:HA	5:F:53:ILE:HA	1.87	0.57
2:C:61:SER:HB3	2:C:479:LEU:HB3	1.86	0.56
2:C:518:ASN:OD1	2:C:518:ASN:N	2.36	0.56
1:H:59:VAL:HG21	1:H:85:LEU:HD13	1.85	0.56
3:J:693:VAL:HG21	3:J:743:MET:HE3	1.86	0.56
5:F:515:GLU:HG2	5:F:516:ASP:H	1.70	0.56
2:I:814:ASP:OD2	2:I:1106:ARG:NH1	2.32	0.56
1:A:60:GLU:HB2	1:A:170:ARG:HG2	1.88	0.56
2:C:1119:MET:HE3	2:C:1204:LEU:HD13	1.87	0.56
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.87	0.56
2:C:1276:TRP:CZ2	3:D:801:VAL:HG21	2.40	0.56
3:D:148:GLU:H	3:D:156:ARG:HG3	1.70	0.56
3:D:527:LEU:HD23	3:D:532:GLU:HG3	1.86	0.56
3:D:854:ALA:HB2	3:J:1372:ARG:HB2	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:102:LEU:HB2	2:I:489:PRO:HG3	1.87	0.56
2:I:518:ASN:OD1	2:I:518:ASN:N	2.37	0.56
2:I:1142:ARG:HH22	2:I:1165:SER:HB2	1.70	0.56
3:J:210:SER:O	3:J:214:ARG:HG2	2.05	0.56
3:J:960:LEU:HB3	3:J:963:VAL:HG11	1.86	0.56
1:B:59:VAL:HG21	1:B:85:LEU:HD13	1.87	0.56
2:C:738:GLU:HA	2:C:741:MET:HE2	1.87	0.56
1:H:32:GLU:OE1	1:H:195:ARG:NH2	2.39	0.56
6:I:2001:4OB:H7	3:J:774:ILE:CG1	2.35	0.56
3:J:148:GLU:H	3:J:156:ARG:HG3	1.69	0.56
3:J:1273:ASP:OD1	3:J:1274:PHE:N	2.38	0.56
2:C:1275:VAL:HG13	2:C:1287:LEU:HD11	1.87	0.56
2:I:560:PRO:O	3:J:780:ARG:NH2	2.30	0.56
2:I:591:TYR:OH	2:I:637:ARG:NH2	2.39	0.56
5:L:49:ASN:HA	5:L:53:ILE:HA	1.87	0.56
5:L:278:ASP:OD1	5:L:281:ARG:NH1	2.38	0.56
1:A:155:ALA:HA	1:A:158:ARG:HG3	1.88	0.56
1:B:29:GLU:HA	1:B:200:LYS:HG3	1.86	0.56
2:C:591:TYR:OH	2:C:637:ARG:NH2	2.38	0.56
3:D:115:TRP:O	3:D:119:SER:HB2	2.06	0.56
3:D:251:PRO:HD2	5:F:507:MET:HE1	1.88	0.56
3:D:1181:ASP:HA	3:J:202:ARG:HD3	1.88	0.56
1:B:32:GLU:OE1	1:B:195:ARG:NH2	2.39	0.56
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.86	0.56
3:J:356:THR:OG1	3:J:357:VAL:N	2.36	0.56
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.88	0.56
3:D:817:HIS:CE1	3:D:860:ARG:HE	2.23	0.56
2:I:30:ILE:HD12	2:I:30:ILE:H	1.70	0.56
5:L:515:GLU:HG2	5:L:516:ASP:H	1.70	0.56
5:L:602:SER:H	5:L:605:GLU:HG3	1.71	0.56
5:F:290:LEU:HB3	5:F:333:VAL:HG21	1.88	0.56
1:G:44:ARG:HG3	1:G:183:ILE:HG22	1.87	0.56
2:C:42:ASP:C	2:C:44:GLU:H	2.14	0.56
2:C:138:ILE:HB	2:C:143:ARG:HD3	1.88	0.56
3:D:1273:ASP:OD1	3:D:1274:PHE:N	2.38	0.56
4:E:39:VAL:HG22	4:E:40:PRO:HD2	1.88	0.56
3:D:141:PHE:HD1	3:D:180:MET:HG3	1.71	0.55
5:F:577:GLY:HA3	5:F:583:THR:HG23	1.89	0.55
2:I:176:ILE:HD12	2:I:184:LEU:HD23	1.88	0.55
2:I:1151:LEU:HD21	2:I:1198:LEU:HD23	1.87	0.55
1:A:29:GLU:HB3	1:A:30:PRO:HD3	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:98:VAL:HG11	1:B:121:VAL:HG22	1.87	0.55
2:C:1151:LEU:HD21	2:C:1198:LEU:HD23	1.87	0.55
3:D:210:SER:O	3:D:214:ARG:HG2	2.07	0.55
3:J:114:ILE:HD12	3:J:304:ASP:HB3	1.87	0.55
1:A:44:ARG:HG3	1:A:183:ILE:HG22	1.88	0.55
2:C:149:LEU:HD13	2:C:453:ILE:HG13	1.87	0.55
3:D:152:THR:OG1	3:D:153:ASN:N	2.38	0.55
1:G:60:GLU:HB2	1:G:170:ARG:HG2	1.87	0.55
3:J:120:LEU:HD22	3:J:121:PRO:HD3	1.88	0.55
4:K:39:VAL:HG22	4:K:40:PRO:HD2	1.88	0.55
2:C:207:THR:HG21	2:C:351:LEU:HG	1.89	0.55
2:C:1101:LEU:HD21	3:D:508:LEU:HD22	1.88	0.55
3:D:474:LEU:HD23	4:E:28:ARG:HG2	1.88	0.55
2:I:1119:MET:HE3	2:I:1204:LEU:HD13	1.89	0.55
3:J:79:LYS:HB2	5:L:569:THR:H	1.70	0.55
3:J:1350:ASN:HA	3:J:1353:VAL:HG12	1.89	0.55
1:H:91:ARG:HG3	1:H:122:GLU:HB3	1.89	0.55
3:J:141:PHE:HD1	3:J:180:MET:HG3	1.69	0.55
5:L:577:GLY:HA3	5:L:583:THR:HG23	1.89	0.55
2:I:1282:GLY:O	3:J:1361:THR:OG1	2.23	0.55
3:D:1293:GLU:H	3:J:1226:VAL:HB	1.71	0.55
2:I:215:TYR:HA	2:I:219:GLN:HE21	1.72	0.55
1:G:11:PRO:HD2	1:H:227:GLN:HA	1.89	0.55
2:I:1320:PRO:HG2	3:J:1354:GLY:HA3	1.88	0.55
3:J:388:ARG:NH1	3:J:414:GLU:OE1	2.39	0.55
5:L:244:THR:O	5:L:247:GLU:HG2	2.06	0.55
2:I:197:ARG:HH12	5:L:29:ASP:HB3	1.71	0.55
3:J:79:LYS:HB2	5:L:569:THR:N	2.22	0.55
2:C:30:ILE:HD12	2:C:30:ILE:H	1.70	0.54
3:D:506:VAL:HG23	3:D:628:GLY:HA3	1.88	0.54
1:H:98:VAL:HG11	1:H:121:VAL:HG22	1.89	0.54
2:I:6:THR:HG21	2:I:782:VAL:HG23	1.89	0.54
2:I:302:ILE:HG22	2:I:309:LEU:HA	1.89	0.54
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.55	0.54
3:J:115:TRP:O	3:J:119:SER:HB2	2.06	0.54
5:L:290:LEU:HB3	5:L:333:VAL:HG21	1.89	0.54
1:B:51:MET:HB3	1:B:178:SER:HA	1.89	0.54
2:C:9:LYS:HA	2:C:1171:ARG:HD2	1.89	0.54
1:B:37:HIS:CE1	2:C:1216:ARG:HD2	2.43	0.54
3:J:817:HIS:CE1	3:J:860:ARG:HE	2.24	0.54
2:C:363:LEU:HB3	2:C:381:ALA:HB1	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:668:ILE:HD11	2:I:683:ALA:HB2	1.89	0.54
1:A:50:SER:HB3	1:A:150:ARG:HD2	1.88	0.54
5:F:111:LEU:HD13	5:F:116:GLU:HG2	1.90	0.54
3:J:1169:THR:HG23	3:J:1192:LYS:HD3	1.88	0.54
3:D:114:ILE:HD12	3:D:304:ASP:HB3	1.89	0.54
3:D:872:LEU:HD22	3:D:877:VAL:HG11	1.90	0.54
1:G:155:ALA:HA	1:G:158:ARG:HG3	1.89	0.54
3:J:733:SER:O	3:J:737:ILE:HG12	2.08	0.54
5:L:276:MET:SD	5:L:279:ARG:NH1	2.80	0.54
3:D:798:ARG:NH1	3:D:802:ASP:OD2	2.41	0.54
2:I:820:GLU:HA	2:I:1079:ILE:HD11	1.90	0.54
3:J:613:GLY:O	3:J:617:THR:OG1	2.26	0.54
5:L:111:LEU:HD13	5:L:116:GLU:HG2	1.90	0.54
5:L:551:LEU:HD11	5:L:598:LEU:HD21	1.88	0.54
1:G:31:LEU:HD13	1:G:36:GLY:HA2	1.90	0.54
2:I:9:LYS:HA	2:I:1171:ARG:HD2	1.89	0.54
2:I:363:LEU:HB3	2:I:381:ALA:HB1	1.90	0.54
3:D:647:PRO:HG3	3:D:697:MET:HB3	1.90	0.53
2:I:1287:LEU:HD13	3:J:1357:ILE:HD11	1.89	0.53
3:J:647:PRO:HG3	3:J:697:MET:HB3	1.90	0.53
2:C:555:TYR:HA	3:D:773:PHE:HE1	1.72	0.53
3:D:474:LEU:HD12	3:D:477:GLN:HE21	1.73	0.53
5:F:479:THR:HG23	5:F:481:GLU:H	1.73	0.53
1:H:23:HIS:ND1	1:H:206:GLU:HG2	2.23	0.53
2:I:61:SER:HB3	2:I:479:LEU:HB3	1.90	0.53
2:I:808:ASN:H	3:J:633:ALA:HB2	1.73	0.53
5:L:479:THR:HG23	5:L:481:GLU:H	1.73	0.53
3:D:683:ILE:HD11	3:D:754:ILE:HG23	1.90	0.53
3:D:853:THR:HG21	3:J:1375:ALA:HB1	1.90	0.53
2:I:124:MET:HB2	2:I:498:ILE:HD13	1.89	0.53
2:I:1275:VAL:HG13	2:I:1287:LEU:HD11	1.88	0.53
3:J:872:LEU:HD22	3:J:877:VAL:HG11	1.91	0.53
2:I:237:LEU:HD22	2:I:237:LEU:H	1.73	0.53
3:J:749:LYS:HB2	3:J:750:PRO:CD	2.38	0.53
3:J:798:ARG:NH1	3:J:802:ASP:OD2	2.42	0.53
5:L:448:ARG:NH1	5:L:501:ALA:O	2.34	0.53
2:C:870:ILE:HB	2:C:944:ARG:HD3	1.91	0.53
3:D:34:SER:OG	3:D:104:HIS:ND1	2.30	0.53
2:I:590:PRO:HG3	2:I:605:TYR:CZ	2.42	0.53
1:A:31:LEU:HD13	1:A:36:GLY:HA2	1.90	0.53
1:A:153:VAL:HB	1:A:175:ALA:HB3	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:77:ARG:HG3	3:D:79:LYS:H	1.74	0.53
2:I:1276:TRP:CZ2	3:J:801:VAL:HG21	2.43	0.53
3:J:363:LEU:HD23	3:J:487:THR:HG22	1.91	0.53
3:D:1169:THR:HG23	3:D:1192:LYS:HD3	1.90	0.53
3:J:506:VAL:HG23	3:J:628:GLY:HA3	1.91	0.53
2:C:1131:MET:HE2	2:C:1141:LEU:HD12	1.89	0.53
3:D:478:LEU:HG	4:E:47:THR:HG23	1.89	0.53
3:D:609:TYR:HB2	3:D:617:THR:HG21	1.89	0.53
1:G:153:VAL:HB	1:G:175:ALA:HB3	1.91	0.53
2:I:344:GLY:HA3	2:I:346:TYR:CZ	2.44	0.53
2:C:668:ILE:HD11	2:C:683:ALA:HB2	1.90	0.53
6:I:2001:4OB:H5	3:J:755:ILE:HG12	1.74	0.53
3:D:1350:ASN:HA	3:D:1353:VAL:HG12	1.90	0.52
3:J:73:GLY:O	3:J:76:LYS:NZ	2.33	0.52
3:J:1227:HIS:HA	3:J:1230:THR:HG22	1.91	0.52
1:B:23:HIS:ND1	1:B:206:GLU:HG2	2.24	0.52
2:C:1192:GLU:O	2:C:1196:LYS:HG2	2.09	0.52
5:F:165:PHE:CE2	5:F:217:ALA:HA	2.44	0.52
3:J:279:LEU:HD11	3:J:296:LYS:HG2	1.92	0.52
3:J:958:ILE:HD11	3:J:1017:VAL:HG11	1.91	0.52
3:D:749:LYS:HB2	3:D:750:PRO:CD	2.39	0.52
5:F:482:GLU:O	5:F:486:ARG:NH2	2.42	0.52
2:C:103:VAL:HB	2:C:113:THR:HG21	1.90	0.52
3:D:613:GLY:O	3:D:617:THR:OG1	2.27	0.52
2:C:734:ILE:HD12	2:C:777:VAL:HG21	1.92	0.52
3:D:28:ASP:OD1	3:D:31:ARG:NH1	2.43	0.52
3:D:585:LYS:HB2	3:D:612:LEU:HD21	1.91	0.52
2:I:718:ALA:HB2	2:I:783:LEU:HD23	1.92	0.52
2:C:95:PRO:HA	2:C:126:GLU:HG2	1.91	0.52
2:I:1131:MET:HE2	2:I:1141:LEU:HD12	1.92	0.52
5:L:165:PHE:CE2	5:L:217:ALA:HA	2.44	0.52
1:A:93:GLN:H	1:A:120:ASP:HB3	1.75	0.52
1:A:285:THR:HG23	1:A:288:GLU:H	1.75	0.52
1:B:64:VAL:HG21	1:B:69:SER:HB3	1.91	0.52
3:D:279:LEU:HD11	3:D:296:LYS:HG2	1.91	0.52
3:D:513:MET:HE1	3:D:579:LEU:HD13	1.91	0.52
5:F:397:ARG:HG2	5:F:443:ILE:HG21	1.92	0.52
1:H:64:VAL:HG21	1:H:69:SER:HB3	1.91	0.52
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.10	0.52
1:A:26:VAL:HG22	1:A:203:ILE:HB	1.92	0.52
1:A:91:ARG:HD3	1:A:210:THR:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ALA:HA	1:A:228:LEU:HD23	1.92	0.52
2:C:344:GLY:HA3	2:C:346:TYR:CZ	2.45	0.52
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.75	0.52
3:D:325:LYS:HD3	5:F:508:GLU:HG2	1.91	0.52
3:D:1233:ILE:O	3:D:1237:VAL:HG12	2.09	0.52
2:I:1246:ARG:NE	3:J:348:ASP:OD1	2.42	0.52
3:J:609:TYR:HB2	3:J:617:THR:HG21	1.92	0.52
2:C:745:GLU:HG3	2:C:1017:GLN:HB3	1.91	0.52
2:C:1176:LEU:HD13	2:C:1180:MET:HG2	1.91	0.52
2:I:95:PRO:HA	2:I:126:GLU:HG2	1.92	0.52
3:J:697:MET:HE1	3:J:737:ILE:HG22	1.91	0.52
5:L:483:LEU:HD12	5:L:483:LEU:H	1.74	0.52
2:I:349:GLU:O	2:I:353:VAL:HG23	2.10	0.51
2:I:1149:TYR:HB3	2:I:1159:VAL:HG11	1.91	0.51
2:C:6:THR:HG21	2:C:782:VAL:HG23	1.90	0.51
2:C:615:VAL:HG13	2:C:650:VAL:HA	1.92	0.51
5:F:134:VAL:HA	5:F:273:MET:HE1	1.91	0.51
1:G:231:PHE:CE1	1:H:28:LEU:HD11	2.45	0.51
2:I:739:ASP:OD1	2:I:739:ASP:N	2.37	0.51
3:J:28:ASP:OD1	3:J:31:ARG:NH1	2.43	0.51
3:J:425:ARG:HG2	3:J:426:ALA:H	1.75	0.51
2:C:903:ARG:O	2:C:907:GLY:N	2.43	0.51
1:G:118:ASP:HB3	1:G:121:VAL:HG23	1.92	0.51
2:I:227:LYS:O	2:I:245:ARG:NH2	2.43	0.51
2:C:488:MET:O	2:C:490:GLN:N	2.37	0.51
1:G:12:ARG:H	1:G:30:PRO:HD2	1.75	0.51
1:H:48:LEU:HD12	1:H:183:ILE:HD11	1.93	0.51
1:H:91:ARG:HG2	1:H:122:GLU:O	2.11	0.51
2:C:817:LEU:HD11	2:C:1080:ASN:HD22	1.75	0.51
1:G:231:PHE:HE1	1:H:28:LEU:HD11	1.74	0.51
3:J:189:LEU:HD22	3:J:234:PRO:HB3	1.91	0.51
3:D:425:ARG:HG2	3:D:426:ALA:H	1.75	0.51
5:F:402:LEU:HA	5:F:405:ILE:HG12	1.93	0.51
5:F:489:MET:HB2	5:F:490:PRO:HD2	1.93	0.51
1:G:11:PRO:HA	1:G:30:PRO:HB2	1.93	0.51
1:G:70:THR:HG21	2:I:755:LYS:HE2	1.93	0.51
1:G:228:LEU:C	1:G:230:ALA:H	2.18	0.51
2:I:149:LEU:HB2	2:I:530:ILE:HG22	1.91	0.51
3:J:478:LEU:HG	4:K:47:THR:HG23	1.91	0.51
2:C:176:ILE:HD12	2:C:184:LEU:HD23	1.92	0.51
2:C:820:GLU:HA	2:C:1079:ILE:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1101:LEU:HD13	3:D:504:GLN:HB2	1.92	0.51
3:D:733:SER:O	3:D:737:ILE:HG12	2.10	0.51
2:I:734:ILE:HD12	2:I:777:VAL:HG21	1.92	0.51
2:I:757:THR:HG23	2:I:765:ILE:HG23	1.91	0.51
5:L:482:GLU:O	5:L:486:ARG:NH2	2.44	0.51
3:D:709:ARG:C	3:D:711:GLY:H	2.19	0.51
5:F:483:LEU:HD12	5:F:483:LEU:H	1.75	0.51
2:I:615:VAL:HG13	2:I:650:VAL:HA	1.92	0.51
3:J:147:ILE:HG22	3:J:188:LEU:HG	1.93	0.51
6:C:2001:4OB:H5	3:D:755:ILE:HG12	1.75	0.51
3:D:77:ARG:HE	5:F:569:THR:HA	1.75	0.51
1:H:100:LEU:HD11	1:H:121:VAL:HG21	1.92	0.51
2:I:324:LYS:O	2:I:327:GLN:NE2	2.43	0.51
3:J:585:LYS:HB2	3:J:612:LEU:HD21	1.92	0.51
3:J:1170:LYS:C	3:J:1172:LYS:H	2.19	0.51
3:J:1267:VAL:HB	3:J:1301:THR:OG1	2.10	0.51
5:L:487:MET:HA	5:L:487:MET:HE2	1.93	0.51
1:B:91:ARG:HG3	1:B:122:GLU:HB3	1.92	0.51
2:C:718:ALA:HB2	2:C:783:LEU:HD23	1.93	0.51
2:C:758:ARG:NH1	2:C:835:GLU:OE1	2.43	0.51
2:I:103:VAL:HB	2:I:113:THR:HG21	1.92	0.51
3:J:341:ASN:HB2	3:J:1352:ILE:HD13	1.93	0.51
2:C:757:THR:HG23	2:C:765:ILE:HG23	1.92	0.50
2:I:97:ARG:HB3	2:I:121:GLU:HB2	1.93	0.50
2:I:136:PHE:CE2	2:I:456:VAL:HG11	2.45	0.50
2:I:819:SER:HB2	2:I:1085:MET:HG3	1.92	0.50
2:C:936:ARG:NH2	2:C:1043:ALA:O	2.44	0.50
2:C:227:LYS:O	2:C:245:ARG:NH2	2.45	0.50
2:C:560:PRO:CB	3:D:776:THR:HG21	2.42	0.50
5:F:441:ARG:NH1	5:F:445:ASP:OD1	2.45	0.50
5:L:397:ARG:HG2	5:L:443:ILE:HG21	1.92	0.50
2:C:672:GLU:HG2	2:C:1187:PHE:HA	1.93	0.50
3:D:682:VAL:HA	3:D:685:ILE:CD1	2.41	0.50
2:I:241:LEU:HD21	2:I:246:LEU:HD11	1.94	0.50
2:I:488:MET:O	2:I:490:GLN:N	2.39	0.50
2:I:1191:LYS:HD3	2:I:1193:ALA:H	1.75	0.50
3:J:77:ARG:HE	5:L:569:THR:HA	1.76	0.50
3:J:750:PRO:HA	3:J:777:HIS:CE1	2.47	0.50
3:J:752:GLY:O	3:J:754:ILE:N	2.45	0.50
5:L:489:MET:HB2	5:L:490:PRO:HD2	1.93	0.50
2:C:324:LYS:O	2:C:327:GLN:NE2	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1227:HIS:CG	3:J:1293:GLU:HG2	2.47	0.50
2:I:968:GLU:HG3	2:I:1018:TYR:HE1	1.76	0.50
3:J:1233:ILE:O	3:J:1237:VAL:HG12	2.12	0.50
5:L:134:VAL:HA	5:L:273:MET:HE1	1.92	0.50
5:L:511:ILE:HG13	5:L:512:GLY:H	1.76	0.50
1:A:118:ASP:HB3	1:A:121:VAL:HG23	1.92	0.50
2:C:685:MET:SD	2:C:1073:LYS:HG2	2.51	0.50
1:G:26:VAL:HG22	1:G:203:ILE:HB	1.93	0.50
1:G:182:ARG:O	1:G:206:GLU:N	2.44	0.50
2:I:21:VAL:HG11	2:I:592:ARG:HD2	1.94	0.50
1:A:45:ARG:HG2	1:B:38:THR:HB	1.93	0.50
3:D:189:LEU:HD22	3:D:234:PRO:HB3	1.92	0.50
1:G:93:GLN:H	1:G:120:ASP:HB3	1.76	0.50
2:I:26:TYR:HE2	2:I:32:LEU:HD12	1.77	0.50
2:I:517:GLN:O	2:I:517:GLN:HG2	2.12	0.50
3:J:1162:ILE:HG23	3:J:1178:THR:HB	1.94	0.50
5:L:119:ILE:HA	5:L:122:ARG:HD3	1.94	0.50
3:D:712:GLN:H	3:D:712:GLN:CD	2.19	0.50
3:D:824:PRO:HD3	3:D:835:LEU:HB2	1.94	0.50
5:F:487:MET:HE2	5:F:487:MET:HA	1.94	0.50
5:L:137:TYR:HD2	5:L:273:MET:HE2	1.76	0.50
1:B:100:LEU:HD11	1:B:121:VAL:HG21	1.93	0.50
2:C:896:THR:HB	2:C:897:PRO:HD2	1.93	0.50
3:D:697:MET:HE1	3:D:737:ILE:HG22	1.93	0.50
5:F:119:ILE:HA	5:F:122:ARG:HD3	1.93	0.50
5:F:511:ILE:HG13	5:F:512:GLY:H	1.77	0.50
1:H:64:VAL:HG12	1:H:65:LEU:H	1.77	0.50
2:I:213:LEU:HD13	2:I:422:LYS:HG2	1.93	0.50
3:J:683:ILE:HD11	3:J:754:ILE:HG23	1.94	0.50
2:C:26:TYR:CZ	2:C:28:LEU:HB2	2.47	0.49
2:C:538:LEU:HD22	2:C:543:ALA:HB2	1.94	0.49
3:D:789:LYS:HA	3:D:792:ASN:HB2	1.93	0.49
2:I:692:THR:OG1	2:I:693:LEU:N	2.45	0.49
5:L:164:GLY:O	5:L:260:ARG:HB2	2.11	0.49
2:C:349:GLU:O	2:C:353:VAL:HG23	2.12	0.49
3:D:1170:LYS:C	3:D:1172:LYS:H	2.19	0.49
5:F:137:TYR:HD2	5:F:273:MET:HE2	1.77	0.49
3:J:794:GLY:O	3:J:797:THR:OG1	2.26	0.49
3:J:1343:GLU:HB3	3:J:1345:ARG:HD3	1.93	0.49
1:B:91:ARG:HG2	1:B:122:GLU:O	2.12	0.49
3:J:368:LEU:HD22	3:J:373:ALA:HB2	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:ARG:HD3	2:C:1083:GLU:HB3	1.93	0.49
2:C:50:GLU:HG2	2:C:73:TYR:HE1	1.78	0.49
2:C:1149:TYR:HB3	2:C:1159:VAL:HG11	1.95	0.49
1:H:61:ILE:HB	1:H:64:VAL:O	2.12	0.49
2:I:387:ASN:HA	2:I:391:SER:HB2	1.94	0.49
3:J:124:ILE:HG23	3:J:189:LEU:HD11	1.95	0.49
3:J:709:ARG:C	3:J:711:GLY:H	2.20	0.49
3:J:1077:ALA:HB2	3:J:1100:PHE:CD1	2.47	0.49
3:J:1191:PRO:HB2	3:J:1194:ARG:HD3	1.93	0.49
1:B:64:VAL:HG12	1:B:65:LEU:H	1.78	0.49
2:C:968:GLU:HG3	2:C:1018:TYR:HE1	1.77	0.49
2:C:1281:TYR:CD1	3:D:484:MET:HG2	2.47	0.49
3:D:1135:THR:OG1	3:D:1136:GLY:N	2.46	0.49
2:I:545:PHE:CZ	3:J:781:LYS:HG3	2.47	0.49
3:J:68:TYR:HA	3:J:92:VAL:HG23	1.95	0.49
3:J:1198:VAL:HG23	3:J:1204:VAL:HG11	1.94	0.49
2:C:250:THR:HA	2:C:268:ARG:HA	1.94	0.49
2:C:387:ASN:HA	2:C:391:SER:HB2	1.95	0.49
2:C:878:THR:OG1	2:C:879:GLY:N	2.45	0.49
3:D:1162:ILE:HG23	3:D:1178:THR:HB	1.94	0.49
2:I:685:MET:SD	2:I:1073:LYS:HG2	2.53	0.49
2:I:878:THR:OG1	2:I:879:GLY:N	2.45	0.49
3:J:268:LEU:HB3	3:J:306:LEU:HD23	1.94	0.49
3:J:474:LEU:HD12	3:J:477:GLN:HE21	1.77	0.49
2:C:124:MET:HB2	2:C:498:ILE:HD13	1.94	0.49
3:D:708:ASN:HB3	3:D:712:GLN:O	2.12	0.49
3:D:1341:ARG:HH22	3:D:1373:ARG:HH21	1.59	0.49
5:F:164:GLY:O	5:F:260:ARG:HB2	2.12	0.49
1:G:229:GLU:O	1:G:229:GLU:HG2	2.13	0.49
5:L:41:ILE:HA	5:L:44:ILE:HG23	1.94	0.49
2:C:255:ILE:HB	2:C:263:VAL:HB	1.95	0.49
2:C:517:GLN:HG2	2:C:517:GLN:O	2.11	0.49
2:C:1122:LYS:HG2	2:C:1229:TYR:CE1	2.47	0.49
2:C:1246:ARG:NE	3:D:348:ASP:OD1	2.35	0.49
6:C:2001:4OB:FAD	3:D:750:PRO:HD3	2.02	0.49
3:D:1286:LYS:O	3:D:1290:ARG:HB2	2.13	0.49
1:G:66:HIS:HA	1:G:171:LEU:HD11	1.95	0.49
2:I:672:GLU:HG2	2:I:1187:PHE:HA	1.95	0.49
1:A:182:ARG:O	1:A:206:GLU:N	2.45	0.49
2:C:149:LEU:HB2	2:C:530:ILE:HG22	1.95	0.49
3:D:298:MET:SD	5:F:402:LEU:HB3	2.53	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:26:TYR:CZ	2:I:28:LEU:HB2	2.47	0.49
5:L:548:LEU:HD21	5:L:559:LEU:HD23	1.95	0.49
3:D:268:LEU:HB3	3:D:306:LEU:HD23	1.94	0.49
1:G:50:SER:HB3	1:G:150:ARG:HD2	1.95	0.49
6:I:2001:4OB:FAD	3:J:750:PRO:HD3	2.03	0.49
3:J:800:LEU:HB3	3:J:920:ALA:HB1	1.94	0.49
3:J:1024:THR:HG22	3:J:1026:PRO:HD3	1.93	0.49
5:L:402:LEU:HA	5:L:405:ILE:HG12	1.94	0.49
2:C:146:VAL:HG13	2:C:529:ARG:HB3	1.95	0.48
2:C:242:VAL:HB	2:C:245:ARG:HD2	1.94	0.48
2:C:1254:VAL:HG13	2:C:1255:THR:H	1.78	0.48
3:D:275:ARG:HD3	3:D:298:MET:HB3	1.95	0.48
3:D:1280:VAL:HG11	3:D:1304:ARG:HH21	1.77	0.48
1:G:91:ARG:HD3	1:G:210:THR:O	2.13	0.48
2:I:216:THR:O	2:I:219:GLN:HB2	2.13	0.48
3:J:1286:LYS:O	3:J:1290:ARG:HB2	2.12	0.48
1:B:61:ILE:HB	1:B:64:VAL:O	2.13	0.48
2:C:28:LEU:HD21	2:C:524:ILE:HG13	1.95	0.48
2:C:692:THR:OG1	2:C:693:LEU:N	2.45	0.48
3:D:73:GLY:O	3:D:76:LYS:NZ	2.31	0.48
5:F:281:ARG:O	5:F:285:ARG:HG3	2.13	0.48
1:H:54:CYS:SG	1:H:148:ARG:HG2	2.54	0.48
2:I:255:ILE:HB	2:I:263:VAL:HB	1.94	0.48
5:F:466:ILE:HD13	5:F:486:ARG:HB3	1.94	0.48
1:G:50:SER:HB3	1:H:8:PHE:HE1	1.76	0.48
1:H:182:ARG:HD2	3:J:581:MET:HE1	1.95	0.48
3:J:189:LEU:HB3	3:J:234:PRO:HB2	1.96	0.48
3:J:978:ARG:HB2	3:J:1199:PHE:HZ	1.78	0.48
2:C:241:LEU:HD21	2:C:246:LEU:HD11	1.95	0.48
2:C:842:ASP:N	2:C:1045:GLY:O	2.47	0.48
3:D:218:THR:HA	3:D:221:ILE:HG22	1.96	0.48
3:D:1267:VAL:HB	3:D:1301:THR:OG1	2.14	0.48
1:G:177:TYR:O	1:G:178:SER:HB2	2.12	0.48
1:A:66:HIS:CE1	1:A:69:SER:HB3	2.49	0.48
2:C:145:ILE:HB	2:C:456:VAL:HG22	1.96	0.48
2:C:646:SER:HB3	2:C:649:GLN:HG3	1.95	0.48
2:C:677:ASN:OD1	3:D:779:ALA:HB1	2.12	0.48
3:D:103:GLY:HA3	3:D:244:VAL:HG22	1.95	0.48
3:D:1191:PRO:HB2	3:D:1194:ARG:HD3	1.94	0.48
2:I:50:GLU:HG2	2:I:73:TYR:HE1	1.78	0.48
2:I:897:PRO:HG3	3:J:77:ARG:HH22	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:45:ASN:HB3	3:J:48:THR:O	2.13	0.48
1:B:211:ILE:HD11	1:B:215:GLU:OE2	2.13	0.48
3:D:1280:VAL:HG21	3:D:1304:ARG:NE	2.25	0.48
1:H:48:LEU:HD21	3:J:535:ARG:HG3	1.95	0.48
1:H:97:GLU:OE1	1:H:147:GLN:HG3	2.14	0.48
2:I:646:SER:HB3	2:I:649:GLN:HG3	1.95	0.48
2:I:971:LEU:HG	2:I:1014:LEU:HD23	1.96	0.48
2:I:1176:LEU:HD13	2:I:1180:MET:HG2	1.96	0.48
3:J:650:LYS:O	3:J:654:ILE:HG13	2.14	0.48
5:L:281:ARG:O	5:L:285:ARG:HG3	2.13	0.48
1:A:228:LEU:HD11	1:B:221:ALA:HB1	1.96	0.48
1:A:316:MET:HG2	5:F:600:HIS:CE1	2.49	0.48
1:B:31:LEU:HD11	1:B:39:LEU:HD12	1.96	0.48
1:B:54:CYS:SG	1:B:148:ARG:HG2	2.53	0.48
2:C:1282:GLY:O	3:D:1361:THR:OG1	2.29	0.48
3:D:751:ASP:OD2	3:D:752:GLY:N	2.46	0.48
5:F:448:ARG:NH1	5:F:501:ALA:O	2.35	0.48
3:J:950:ILE:HG13	3:J:1020:TRP:CH2	2.48	0.48
3:D:752:GLY:O	3:D:754:ILE:N	2.47	0.48
3:D:1198:VAL:HG23	3:D:1204:VAL:HG11	1.94	0.48
2:I:115:LYS:HE3	2:I:116:ASP:H	1.78	0.48
2:I:538:LEU:HD22	2:I:543:ALA:HB2	1.95	0.48
2:I:842:ASP:N	2:I:1045:GLY:O	2.46	0.48
3:J:474:LEU:HD23	4:K:28:ARG:HG2	1.96	0.48
3:J:1167:LYS:HE3	3:J:1168:GLU:H	1.78	0.48
3:D:368:LEU:HD22	3:D:373:ALA:HB2	1.95	0.48
5:F:602:SER:N	5:F:605:GLU:OE2	2.46	0.48
2:I:202:ARG:HH22	2:I:368:ARG:HH12	1.61	0.48
2:I:799:ASN:HA	2:I:1231:TYR:HA	1.95	0.48
3:J:16:GLU:HG3	3:J:17:PHE:HD2	1.78	0.48
3:J:863:LEU:HD11	3:J:901:ARG:HB3	1.96	0.48
5:L:316:PHE:HZ	5:L:334:SER:HA	1.79	0.48
3:D:749:LYS:HE2	3:D:753:SER:HB3	1.96	0.48
2:I:1065:LYS:HD2	2:I:1235:LEU:HD12	1.96	0.48
2:I:1254:VAL:HG13	2:I:1255:THR:H	1.78	0.48
3:J:275:ARG:HD3	3:J:298:MET:HB3	1.95	0.48
1:A:66:HIS:HA	1:A:171:LEU:HD11	1.97	0.47
1:A:102:LEU:HD12	1:A:142:MET:HE3	1.95	0.47
2:C:819:SER:HB2	2:C:1085:MET:HG3	1.96	0.47
3:D:45:ASN:HB3	3:D:48:THR:O	2.14	0.47
3:D:189:LEU:HB3	3:D:234:PRO:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:73:GLY:HA3	1:H:138:ALA:HB1	1.96	0.47
2:I:820:GLU:N	2:I:1080:ASN:O	2.47	0.47
2:I:850:ILE:HG13	2:I:1048:LYS:HE2	1.95	0.47
3:J:218:THR:HA	3:J:221:ILE:HG22	1.96	0.47
3:J:568:SER:OG	3:J:569:LEU:N	2.47	0.47
3:J:1078:LEU:HD13	3:J:1121:LEU:HD22	1.96	0.47
5:L:461:ASN:O	5:L:465:ARG:HG2	2.13	0.47
5:L:573:LEU:HD23	5:L:573:LEU:H	1.79	0.47
2:C:850:ILE:HG13	2:C:1048:LYS:HE2	1.95	0.47
3:D:161:THR:HG22	3:D:164:GLN:CD	2.39	0.47
3:D:422:LEU:HD13	3:D:471:PRO:HG3	1.97	0.47
3:D:1167:LYS:HE3	3:D:1168:GLU:H	1.77	0.47
4:E:60:ASN:HD21	4:E:63:ILE:HD13	1.78	0.47
2:I:936:ARG:NH2	2:I:1043:ALA:O	2.47	0.47
3:J:513:MET:HE1	3:J:579:LEU:HD13	1.95	0.47
1:A:54:CYS:HA	1:A:148:ARG:HG3	1.96	0.47
2:C:1085:MET:HE2	2:C:1085:MET:HA	1.95	0.47
3:D:694:SER:OG	3:D:738:ARG:NE	2.39	0.47
3:D:800:LEU:HB3	3:D:920:ALA:HB1	1.97	0.47
3:J:975:ILE:HD13	3:J:980:THR:HG21	1.95	0.47
1:A:102:LEU:HB3	1:A:142:MET:HG2	1.95	0.47
1:A:282:VAL:O	1:A:316:MET:N	2.46	0.47
2:C:820:GLU:N	2:C:1080:ASN:O	2.48	0.47
5:F:244:THR:O	5:F:247:GLU:HG2	2.15	0.47
5:F:583:THR:HG22	5:F:584:ARG:H	1.80	0.47
3:J:338:PHE:CB	3:J:343:LEU:HB2	2.44	0.47
3:J:385:LEU:HD11	3:J:408:VAL:HG12	1.97	0.47
3:J:1295:ASN:HB2	3:J:1298:VAL:HB	1.95	0.47
3:J:824:PRO:HD3	3:J:835:LEU:HB2	1.96	0.47
3:J:839:VAL:HG12	3:J:864:LEU:HD12	1.97	0.47
3:J:1280:VAL:HG21	3:J:1304:ARG:NE	2.27	0.47
2:C:115:LYS:HE3	2:C:116:ASP:H	1.78	0.47
2:C:1336:ASN:N	3:D:23:ALA:O	2.35	0.47
3:D:712:GLN:CD	3:D:712:GLN:N	2.71	0.47
5:F:165:PHE:HE2	5:F:217:ALA:HA	1.79	0.47
5:F:316:PHE:HZ	5:F:334:SER:HA	1.80	0.47
5:F:532:LEU:O	5:F:536:THR:HG23	2.14	0.47
5:F:573:LEU:H	5:F:573:LEU:HD23	1.79	0.47
1:H:101:THR:H	1:H:116:THR:HG22	1.80	0.47
2:I:402:ARG:NH2	2:I:419:ILE:O	2.47	0.47
3:J:749:LYS:HE2	3:J:753:SER:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:844:THR:OG1	3:J:860:ARG:O	2.31	0.47
3:J:1349:GLU:OE2	3:J:1349:GLU:N	2.35	0.47
2:C:97:ARG:HB3	2:C:121:GLU:HB2	1.95	0.47
2:C:402:ARG:NH2	2:C:419:ILE:O	2.47	0.47
3:D:147:ILE:HG22	3:D:188:LEU:HG	1.96	0.47
3:D:425:ARG:HE	3:D:427:PRO:HD2	1.80	0.47
5:F:41:ILE:HA	5:F:44:ILE:HG23	1.97	0.47
1:G:102:LEU:HD12	1:G:142:MET:HE3	1.95	0.47
2:I:242:VAL:HB	2:I:245:ARG:HD2	1.95	0.47
3:J:282:LEU:HD21	5:L:410:ILE:HG12	1.96	0.47
3:J:425:ARG:HH12	3:J:464:ASP:CG	2.21	0.47
5:L:466:ILE:HD13	5:L:486:ARG:HB3	1.97	0.47
3:D:615:LYS:HB2	3:D:616:PRO:HD3	1.97	0.47
3:D:905:ARG:HH21	3:D:907:HIS:CB	2.28	0.47
5:F:137:TYR:HE1	5:F:351:THR:HB	1.80	0.47
1:G:66:HIS:CD2	2:I:929:ILE:HG22	2.50	0.47
1:G:182:ARG:C	1:G:183:ILE:HD12	2.40	0.47
1:G:231:PHE:CE2	1:H:43:LEU:HD21	2.50	0.47
2:I:250:THR:HA	2:I:268:ARG:HA	1.96	0.47
2:I:817:LEU:HD11	2:I:1080:ASN:HD22	1.79	0.47
5:L:580:PHE:C	5:L:582:VAL:H	2.23	0.47
1:A:48:LEU:HA	1:A:180:VAL:HG21	1.97	0.47
2:C:400:VAL:HG21	2:C:452:ARG:NH1	2.30	0.47
6:C:2001:4OB:H7	3:D:774:ILE:HG13	1.97	0.47
3:D:839:VAL:HG12	3:D:864:LEU:HD12	1.96	0.47
3:D:1227:HIS:HB2	3:J:1293:GLU:HG2	1.96	0.47
5:F:489:MET:HE2	5:F:493:LYS:HD2	1.96	0.47
2:C:202:ARG:HH22	2:C:368:ARG:HH12	1.62	0.47
2:C:238:GLN:HB3	2:C:284:LEU:HD11	1.97	0.47
3:D:568:SER:OG	3:D:569:LEU:N	2.47	0.47
2:I:1122:LYS:HG2	2:I:1229:TYR:CE1	2.49	0.47
3:J:205:LEU:HD23	3:J:217:LEU:HB3	1.97	0.47
3:J:425:ARG:HE	3:J:427:PRO:HD2	1.80	0.47
3:D:205:LEU:HD23	3:D:217:LEU:HB3	1.97	0.46
3:D:425:ARG:HH12	3:D:464:ASP:CG	2.23	0.46
3:D:1239:ASP:OD1	3:D:1242:ARG:NH2	2.47	0.46
2:I:578:TYR:HB3	2:I:590:PRO:HG2	1.97	0.46
5:L:299:LYS:HA	5:L:302:PHE:HB3	1.97	0.46
5:L:489:MET:HE2	5:L:493:LYS:HD2	1.96	0.46
1:B:97:GLU:OE1	1:B:147:GLN:HG3	2.14	0.46
2:C:21:VAL:HG11	2:C:592:ARG:HD2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:591:TYR:HD2	2:C:606:LEU:HD13	1.80	0.46
2:C:799:ASN:HA	2:C:1231:TYR:HA	1.96	0.46
2:C:971:LEU:HG	2:C:1014:LEU:HD23	1.96	0.46
1:H:16:ILE:HG13	1:H:26:VAL:HG22	1.95	0.46
2:I:206:ALA:O	2:I:209:ILE:HG22	2.15	0.46
5:L:492:ASP:HB2	5:L:495:ARG:HH12	1.80	0.46
1:A:10:LYS:HE2	1:B:229:GLU:HB3	1.98	0.46
3:J:103:GLY:HA3	3:J:244:VAL:HG22	1.96	0.46
3:J:695:LYS:HA	3:J:695:LYS:HD3	1.73	0.46
4:K:73:GLN:HA	4:K:76:GLU:HB3	1.97	0.46
5:L:287:ILE:HG12	5:L:337:VAL:HG13	1.97	0.46
2:C:217:THR:HG23	2:C:351:LEU:HD13	1.97	0.46
2:C:724:VAL:HG11	2:C:727:VAL:HG22	1.97	0.46
2:C:813:GLU:HB2	3:D:461:PHE:HB2	1.97	0.46
2:C:1280:ALA:HB1	3:D:918:ILE:HG22	1.97	0.46
3:D:1319:PHE:CE2	3:D:1342:ASP:HB2	2.50	0.46
2:I:1085:MET:HA	2:I:1085:MET:HE2	1.96	0.46
3:J:35:PHE:HD1	3:J:101:ARG:HD3	1.80	0.46
3:J:77:ARG:HG3	3:J:79:LYS:H	1.80	0.46
3:J:587:LEU:HD11	3:J:608:CYS:HA	1.96	0.46
3:J:1060:VAL:HG22	3:J:1106:ILE:HG23	1.97	0.46
5:L:137:TYR:HE1	5:L:351:THR:HB	1.81	0.46
3:D:405:GLU:O	3:D:408:VAL:HG22	2.16	0.46
3:D:412:LEU:HA	3:D:415:VAL:HG22	1.97	0.46
3:D:548:VAL:HG12	3:D:550:VAL:HG13	1.98	0.46
3:D:860:ARG:HB3	3:D:861:ASN:H	1.53	0.46
1:H:56:VAL:HG22	1:H:144:ILE:HD11	1.96	0.46
3:J:120:LEU:HD12	5:L:43:ASP:HB3	1.96	0.46
3:J:325:LYS:HD3	5:L:508:GLU:CG	2.45	0.46
1:A:79:LEU:HD11	2:C:693:LEU:HD21	1.98	0.46
2:C:680:LEU:O	2:C:684:ASN:HB2	2.16	0.46
3:D:1230:THR:OG1	3:D:1257:VAL:HG11	2.16	0.46
5:F:580:PHE:C	5:F:582:VAL:H	2.23	0.46
3:J:502:PRO:HB2	3:J:507:VAL:HG12	1.98	0.46
5:L:362:ASN:HB2	5:L:365:MET:HE2	1.96	0.46
1:A:54:CYS:O	1:A:146:VAL:HG13	2.16	0.46
3:D:35:PHE:HD1	3:D:101:ARG:HD3	1.80	0.46
3:D:115:TRP:CE2	3:D:1329:THR:HG23	2.51	0.46
5:F:287:ILE:HG12	5:F:337:VAL:HG13	1.98	0.46
1:G:79:LEU:CD1	2:I:693:LEU:HD21	2.45	0.46
1:G:102:LEU:HB3	1:G:142:MET:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:ARG:C	1:A:183:ILE:HD12	2.40	0.46
1:B:56:VAL:HG22	1:B:144:ILE:HD11	1.98	0.46
1:B:73:GLY:HA3	1:B:138:ALA:HB1	1.96	0.46
2:C:149:LEU:HD11	2:C:451:ARG:HB3	1.97	0.46
2:C:509:SER:HB3	2:C:512:SER:HB3	1.97	0.46
4:E:60:ASN:ND2	4:E:63:ILE:HD13	2.30	0.46
1:G:172:LEU:HD12	1:G:172:LEU:H	1.81	0.46
3:J:266:ASN:O	3:J:270:ARG:HB2	2.15	0.46
1:A:177:TYR:O	1:A:178:SER:HB2	2.14	0.46
3:D:68:TYR:HA	3:D:92:VAL:HG23	1.96	0.46
3:D:735:ALA:O	3:D:738:ARG:HB3	2.16	0.46
3:D:1295:ASN:HB2	3:D:1298:VAL:HB	1.98	0.46
5:F:313:ASP:OD1	5:F:338:HIS:NE2	2.49	0.46
2:I:10:ARG:NH1	2:I:697:LYS:HD3	2.31	0.46
2:I:705:GLU:HB2	2:I:794:LEU:HB3	1.98	0.46
3:J:79:LYS:HG3	3:J:80:HIS:N	2.31	0.46
3:J:422:LEU:HD13	3:J:471:PRO:HG3	1.98	0.46
5:L:165:PHE:HE2	5:L:217:ALA:HA	1.79	0.46
5:L:493:LYS:HA	5:L:496:LYS:HE2	1.98	0.46
1:A:93:GLN:HB2	1:A:120:ASP:OD2	2.16	0.46
1:B:48:LEU:HD12	1:B:183:ILE:HD11	1.98	0.46
2:C:170:VAL:HG23	2:C:171:LEU:N	2.31	0.46
2:C:578:TYR:HB3	2:C:590:PRO:HG2	1.97	0.46
2:C:1336:ASN:O	3:D:23:ALA:N	2.46	0.46
3:D:120:LEU:HD23	5:F:47:MET:SD	2.55	0.46
3:D:385:LEU:HD11	3:D:408:VAL:HG12	1.96	0.46
1:G:10:LYS:HB3	1:G:10:LYS:HE3	1.71	0.46
2:I:146:VAL:HG13	2:I:529:ARG:HB3	1.97	0.46
2:I:1308:ILE:HG21	3:J:379:PRO:HB2	1.98	0.46
2:I:1312:ASN:OD1	2:I:1314:GLN:HG3	2.16	0.46
3:J:50:LYS:HB3	3:J:71:LEU:HD21	1.98	0.46
2:C:840:SER:O	2:C:1047:LEU:N	2.49	0.45
2:C:1159:VAL:HB	2:C:1160:ASP:H	1.59	0.45
2:I:217:THR:HG23	2:I:351:LEU:HD13	1.97	0.45
2:I:448:LEU:HB2	2:I:553:THR:HB	1.97	0.45
2:I:697:LYS:HE2	2:I:697:LYS:HB3	1.82	0.45
3:J:1286:LYS:HD2	3:J:1290:ARG:NH2	2.31	0.45
2:C:206:ALA:O	2:C:209:ILE:HG22	2.16	0.45
2:C:448:LEU:HB2	2:C:553:THR:HB	1.97	0.45
5:F:493:LYS:HA	5:F:496:LYS:HE2	1.97	0.45
5:F:572:THR:O	5:F:576:VAL:HG23	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:68:TYR:OH	2:I:1057:LYS:HB2	2.16	0.45
2:I:453:ILE:HD12	2:I:587:LEU:HD21	1.98	0.45
2:I:1281:TYR:CD1	3:J:484:MET:HG2	2.51	0.45
3:J:246:PRO:HA	3:J:247:PRO:HD3	1.80	0.45
3:J:950:ILE:HB	3:J:1018:ALA:HB3	1.99	0.45
3:J:1095:MET:HA	3:J:1096:PRO:HD3	1.83	0.45
3:J:1244:GLN:HE21	3:J:1244:GLN:HB3	1.58	0.45
1:B:101:THR:H	1:B:116:THR:HG22	1.80	0.45
1:B:221:ALA:O	1:B:224:LEU:HB3	2.16	0.45
6:C:2001:4OB:H1	3:D:774:ILE:HG12	1.97	0.45
3:D:190:LYS:HD3	3:D:235:GLU:HG2	1.98	0.45
2:I:28:LEU:HD21	2:I:524:ILE:HG13	1.98	0.45
3:J:102:MET:HE3	3:J:246:PRO:HD3	1.98	0.45
3:J:735:ALA:O	3:J:738:ARG:HB3	2.16	0.45
5:L:561:MET:HG3	5:L:571:TYR:CD2	2.51	0.45
5:L:572:THR:O	5:L:576:VAL:HG23	2.16	0.45
1:B:78:ILE:O	1:B:82:LEU:HG	2.16	0.45
2:C:56:VAL:HG11	2:C:468:LEU:HB3	1.97	0.45
3:D:133:ARG:HD3	5:F:88:GLU:O	2.16	0.45
3:D:268:LEU:HD13	3:D:306:LEU:HA	1.98	0.45
3:D:598:LYS:O	3:D:601:ILE:HG22	2.16	0.45
3:D:611:ILE:HG22	3:D:612:LEU:HD12	1.98	0.45
3:D:885:VAL:HG12	3:D:894:VAL:HG11	1.98	0.45
2:I:838:CYS:SG	2:I:886:LYS:HD3	2.56	0.45
3:J:258:GLY:HA3	5:L:499:LYS:HD3	1.98	0.45
5:L:97:PRO:HA	5:L:100:MET:HG3	1.98	0.45
1:A:64:VAL:HG11	1:A:78:ILE:HG21	1.99	0.45
3:D:113:HIS:CE1	3:D:307:LEU:HD13	2.52	0.45
3:D:124:ILE:HG23	3:D:189:LEU:HD11	1.97	0.45
3:D:266:ASN:O	3:D:270:ARG:HB2	2.17	0.45
3:D:587:LEU:HD11	3:D:608:CYS:HA	1.99	0.45
3:J:190:LYS:HD3	3:J:235:GLU:HG2	1.98	0.45
4:K:60:ASN:HD21	4:K:63:ILE:HD13	1.81	0.45
2:C:1065:LYS:HD2	2:C:1235:LEU:HD12	1.97	0.45
2:C:1288:GLN:HE21	3:D:1355:ARG:HA	1.81	0.45
3:D:62:PHE:O	3:D:101:ARG:HD2	2.17	0.45
3:D:502:PRO:HB2	3:D:507:VAL:HG12	1.99	0.45
5:F:569:THR:OG1	5:F:570:ASP:N	2.48	0.45
1:G:64:VAL:HG11	1:G:78:ILE:HG21	1.99	0.45
2:I:678:ARG:HG3	2:I:1108:ASN:HD22	1.80	0.45
2:I:1125:GLY:HA3	2:I:1179:GLY:HA2	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:115:TRP:CE2	3:J:1329:THR:HG23	2.51	0.45
3:J:198:CYS:O	3:J:202:ARG:HG3	2.16	0.45
3:J:1025:MET:SD	3:J:1124:ILE:HD12	2.57	0.45
1:A:172:LEU:HD12	1:A:172:LEU:H	1.82	0.45
2:C:557:ARG:HH21	2:C:607:SER:C	2.24	0.45
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.98	0.45
3:D:1233:ILE:HG12	3:D:1260:MET:HE1	1.99	0.45
3:D:1287:ILE:O	3:D:1291:GLU:HG3	2.16	0.45
1:G:228:LEU:CD1	1:H:221:ALA:HB1	2.45	0.45
2:I:183:TRP:HB2	2:I:199:ASP:HA	1.99	0.45
3:J:298:MET:SD	5:L:402:LEU:HB3	2.57	0.45
5:L:313:ASP:OD1	5:L:338:HIS:NE2	2.50	0.45
5:L:582:VAL:HG22	5:L:586:ARG:HG2	1.98	0.45
2:C:724:VAL:HA	2:C:734:ILE:HD13	1.99	0.45
3:D:50:LYS:HB3	3:D:71:LEU:HD21	1.99	0.45
3:D:1227:HIS:CD2	3:J:1293:GLU:HG2	2.52	0.45
2:I:746:ALA:HB3	2:I:971:LEU:HA	1.98	0.45
3:J:334:LYS:HD2	3:J:334:LYS:HA	1.57	0.45
3:J:405:GLU:O	3:J:408:VAL:HG22	2.16	0.45
3:J:611:ILE:HG22	3:J:612:LEU:HD12	1.99	0.45
3:J:1078:LEU:HB3	3:J:1121:LEU:HD13	1.98	0.45
4:K:60:ASN:ND2	4:K:63:ILE:HD13	2.32	0.45
2:C:196:VAL:HG12	2:C:206:ALA:HA	1.99	0.45
1:G:54:CYS:HA	1:G:148:ARG:HG3	1.98	0.45
1:G:106:GLY:HA2	1:G:136:GLU:O	2.16	0.45
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.97	0.45
3:J:62:PHE:O	3:J:101:ARG:HD2	2.17	0.45
3:J:598:LYS:O	3:J:601:ILE:HG22	2.17	0.45
3:J:950:ILE:HG13	3:J:1020:TRP:HH2	1.82	0.45
3:J:1046:ILE:HD12	3:J:1059:LEU:HB3	1.99	0.45
5:L:130:VAL:HB	5:L:365:MET:HG3	1.99	0.45
1:A:319:GLU:O	1:A:320:ASN:HB2	2.16	0.45
2:C:136:PHE:CE2	2:C:456:VAL:HG11	2.52	0.45
3:D:418:GLU:H	4:E:45:LYS:NZ	2.15	0.45
3:D:708:ASN:OD1	3:D:708:ASN:N	2.50	0.45
3:D:1146:GLU:HB3	3:D:1148:ARG:HG3	1.99	0.45
2:I:732:ILE:HD11	2:I:769:PRO:HB3	1.99	0.45
3:J:548:VAL:HG12	3:J:550:VAL:HG13	1.99	0.45
3:J:1280:VAL:HG11	3:J:1304:ARG:HH21	1.82	0.45
1:A:106:GLY:HA2	1:A:136:GLU:O	2.17	0.44
3:D:770:LEU:H	3:D:770:LEU:HD22	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:48:LEU:HA	1:G:180:VAL:HG21	2.00	0.44
2:I:1286:THR:N	3:J:479:GLU:OE2	2.44	0.44
3:J:294:ASN:HD22	5:L:406:GLN:NE2	2.15	0.44
5:L:412:LEU:HD13	5:L:435:ILE:HD11	1.98	0.44
5:L:547:VAL:HG12	5:L:598:LEU:HD22	1.99	0.44
3:D:37:GLU:HB2	3:D:104:HIS:CE1	2.52	0.44
5:F:605:GLU:H	5:F:605:GLU:HG3	1.53	0.44
1:H:221:ALA:O	1:H:224:LEU:HB3	2.16	0.44
2:I:316:GLU:H	2:I:316:GLU:CD	2.25	0.44
3:J:35:PHE:CD1	3:J:101:ARG:HD3	2.53	0.44
3:J:430:HIS:HA	3:J:921:GLN:HB3	1.98	0.44
3:J:694:SER:OG	3:J:738:ARG:NE	2.40	0.44
3:J:1233:ILE:HG12	3:J:1260:MET:HE1	1.97	0.44
5:L:234:THR:O	5:L:245:ALA:HB2	2.17	0.44
5:L:569:THR:OG1	5:L:570:ASP:N	2.50	0.44
3:D:16:GLU:HG3	3:D:1369:ARG:NH2	2.33	0.44
3:D:1286:LYS:HD2	3:D:1290:ARG:NH2	2.32	0.44
5:F:492:ASP:HB2	5:F:495:ARG:HH12	1.81	0.44
1:H:108:GLY:O	1:H:133:LEU:HB2	2.16	0.44
2:I:56:VAL:HG11	2:I:468:LEU:HB3	2.00	0.44
2:I:1323:PHE:CE1	3:J:1353:VAL:HG23	2.52	0.44
6:I:2001:4OB:H7	3:J:774:ILE:HG12	1.99	0.44
3:J:615:LYS:HB2	3:J:616:PRO:HD3	1.99	0.44
1:A:12:ARG:H	1:A:30:PRO:HD2	1.82	0.44
2:I:808:ASN:OD1	2:I:1216:ARG:NH2	2.50	0.44
3:J:412:LEU:HA	3:J:415:VAL:HG22	2.00	0.44
3:J:421:VAL:HG13	3:J:439:PRO:HG3	1.99	0.44
1:A:231:PHE:HE1	1:B:39:LEU:HD13	1.81	0.44
2:C:389:PHE:HB3	2:C:420:LEU:HD12	1.99	0.44
5:F:299:LYS:HA	5:F:302:PHE:HB3	1.98	0.44
5:F:602:SER:H	5:F:605:GLU:HG3	1.80	0.44
2:I:591:TYR:HD2	2:I:606:LEU:HD13	1.81	0.44
3:J:122:SER:O	3:J:126:LEU:HG	2.18	0.44
3:J:264:ASP:OD2	3:J:264:ASP:N	2.50	0.44
3:J:679:TYR:CZ	3:J:683:ILE:HD12	2.53	0.44
3:J:1287:ILE:O	3:J:1291:GLU:HG3	2.18	0.44
5:L:297:MET:HE3	5:L:330:LEU:HD11	1.99	0.44
2:C:1314:GLN:HG2	4:E:28:ARG:CZ	2.48	0.44
3:D:1193:TRP:HB2	3:D:1194:ARG:NH1	2.32	0.44
3:D:1280:VAL:O	3:D:1284:ARG:HB3	2.18	0.44
3:D:1343:GLU:HB3	3:D:1345:ARG:HD3	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:113:HIS:CE1	3:J:307:LEU:HD13	2.52	0.44
3:J:1239:ASP:OD1	3:J:1242:ARG:NH2	2.49	0.44
2:C:10:ARG:NH1	2:C:697:LYS:HD3	2.32	0.44
2:C:383:SER:O	2:C:387:ASN:HB2	2.18	0.44
2:C:678:ARG:HG3	2:C:1108:ASN:HD22	1.82	0.44
2:C:901:LEU:HB2	5:F:565:ILE:HD11	1.99	0.44
3:D:290:ILE:HD12	3:D:290:ILE:H	1.82	0.44
3:D:863:LEU:HD11	3:D:901:ARG:HB3	1.98	0.44
5:F:44:ILE:HA	5:F:47:MET:HB2	1.99	0.44
1:G:58:GLU:HB2	1:G:145:LYS:HB3	1.98	0.44
1:G:229:GLU:OE1	1:H:10:LYS:HD3	2.17	0.44
2:I:26:TYR:CE2	2:I:32:LEU:HD12	2.52	0.44
2:I:113:THR:OG1	2:I:116:ASP:OD2	2.25	0.44
2:I:549:ASP:OD2	3:J:777:HIS:ND1	2.49	0.44
2:I:660:VAL:HG11	3:J:769:VAL:HG13	1.99	0.44
2:I:680:LEU:O	2:I:684:ASN:HB2	2.17	0.44
2:I:724:VAL:HG11	2:I:727:VAL:HG22	1.99	0.44
2:I:782:VAL:HG11	2:I:792:GLY:HA2	2.00	0.44
2:I:1333:LEU:C	2:I:1335:ILE:H	2.25	0.44
3:J:268:LEU:HD13	3:J:306:LEU:HA	1.99	0.44
3:D:349:TYR:HE2	3:D:379:PRO:HG2	1.83	0.44
3:D:421:VAL:HG13	3:D:439:PRO:HG3	1.99	0.44
5:F:249:ILE:O	5:F:252:LEU:HB3	2.17	0.44
2:I:299:LYS:HB2	2:I:299:LYS:HE2	1.61	0.44
3:J:1156:LEU:HB3	3:J:1207:GLY:HA2	2.00	0.44
3:J:1319:PHE:CE2	3:J:1342:ASP:HB2	2.53	0.44
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.50	0.44
3:D:77:ARG:NE	5:F:569:THR:HA	2.33	0.44
3:D:614:LEU:HD23	4:E:7:GLN:HB2	2.00	0.44
3:D:905:ARG:HH21	3:D:907:HIS:HB3	1.83	0.44
3:D:1205:GLU:O	3:D:1208:ASP:HB2	2.18	0.44
5:F:234:THR:O	5:F:245:ALA:HB2	2.18	0.44
1:G:39:LEU:HD23	1:G:39:LEU:HA	1.84	0.44
5:L:249:ILE:O	5:L:252:LEU:HB3	2.17	0.44
5:L:346:GLN:O	5:L:350:GLU:HG3	2.18	0.44
1:B:102:LEU:HD23	1:B:115:ILE:HG23	2.00	0.43
3:D:264:ASP:OD2	3:D:264:ASP:N	2.51	0.43
3:D:930:LEU:HD11	3:D:1241:TYR:CE2	2.53	0.43
3:D:1293:GLU:HB3	3:D:1294:ALA:H	1.69	0.43
2:I:60:GLN:HB3	2:I:67:GLU:HG3	2.00	0.43
2:I:1159:VAL:HB	2:I:1160:ASP:H	1.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:751:ASP:OD2	3:J:752:GLY:N	2.51	0.43
3:J:756:GLU:H	3:J:756:GLU:HG2	1.55	0.43
3:J:885:VAL:HG12	3:J:894:VAL:HG11	1.99	0.43
3:J:1205:GLU:O	3:J:1208:ASP:HB2	2.17	0.43
2:C:453:ILE:HD12	2:C:587:LEU:HD21	2.00	0.43
2:C:670:PHE:HZ	2:C:1117:LEU:HD13	1.83	0.43
2:C:1282:GLY:O	3:D:1361:THR:N	2.50	0.43
3:D:557:LYS:HE3	3:D:557:LYS:HB2	1.79	0.43
5:F:346:GLN:O	5:F:350:GLU:HG3	2.18	0.43
3:J:128:LEU:HD23	3:J:192:MET:HE3	2.00	0.43
3:J:511:TYR:OH	3:J:515:ARG:NH1	2.52	0.43
1:A:152:TYR:CG	2:C:824:GLN:HG2	2.54	0.43
2:C:98:VAL:HG21	2:C:124:MET:HE3	2.01	0.43
2:C:942:ASP:OD2	2:C:1048:LYS:NZ	2.34	0.43
3:D:122:SER:O	3:D:126:LEU:HG	2.18	0.43
3:D:810:THR:HG23	3:D:811:GLU:H	1.83	0.43
5:F:362:ASN:HB2	5:F:365:MET:HE2	1.98	0.43
5:F:559:LEU:HD12	5:F:559:LEU:HA	1.83	0.43
2:I:170:VAL:HG23	2:I:171:LEU:N	2.32	0.43
2:I:778:GLU:O	2:I:781:ASP:HB2	2.18	0.43
5:L:136:GLU:OE1	5:L:364:ARG:NH2	2.51	0.43
1:B:100:LEU:HB2	1:B:144:ILE:HG23	2.01	0.43
2:C:237:LEU:H	2:C:237:LEU:HD22	1.83	0.43
2:C:887:VAL:HB	2:C:913:VAL:CG2	2.48	0.43
2:C:996:ARG:HD3	2:C:996:ARG:HA	1.90	0.43
3:D:430:HIS:HA	3:D:921:GLN:HB3	2.00	0.43
2:I:17:LYS:HE3	2:I:1154:ASP:HB3	2.00	0.43
2:I:524:ILE:HG21	2:I:708:VAL:HG13	2.00	0.43
2:I:1253:LEU:HA	5:L:525:ASP:HB2	2.01	0.43
2:I:1267:GLY:HA3	3:J:347:VAL:O	2.18	0.43
3:J:30:ILE:HG23	3:J:243:PRO:HG3	1.99	0.43
3:J:1193:TRP:HB2	3:J:1194:ARG:NH1	2.33	0.43
3:J:1341:ARG:HH22	3:J:1373:ARG:HH21	1.65	0.43
1:A:58:GLU:HB2	1:A:145:LYS:HB3	2.00	0.43
1:B:41:ASN:ND2	2:C:1217:THR:HA	2.32	0.43
1:B:108:GLY:O	1:B:133:LEU:HB2	2.18	0.43
2:C:17:LYS:HE3	2:C:1154:ASP:HB3	2.00	0.43
2:C:739:ASP:OD1	2:C:739:ASP:N	2.38	0.43
2:C:1333:LEU:C	2:C:1335:ILE:H	2.25	0.43
3:D:30:ILE:HG23	3:D:243:PRO:HG3	1.98	0.43
5:F:215:GLU:HG2	5:F:218:ARG:HH21	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:561:MET:SD	5:F:576:VAL:HG13	2.59	0.43
1:H:102:LEU:HD12	1:H:142:MET:HG2	2.00	0.43
2:I:557:ARG:HH21	2:I:607:SER:C	2.27	0.43
3:J:426:ALA:HB3	3:J:427:PRO:HD3	2.00	0.43
3:J:709:ARG:O	3:J:711:GLY:N	2.51	0.43
3:J:800:LEU:O	3:J:803:VAL:HG12	2.18	0.43
2:C:10:ARG:HA	2:C:1172:LEU:HD23	2.01	0.43
2:C:705:GLU:HB2	2:C:794:LEU:HB3	2.00	0.43
2:C:1323:PHE:CE1	3:D:1353:VAL:HG23	2.53	0.43
3:D:355:ILE:HD13	3:D:466:MET:HG3	2.00	0.43
3:D:872:LEU:O	3:D:877:VAL:HG12	2.18	0.43
3:D:1156:LEU:HB3	3:D:1207:GLY:HA2	1.99	0.43
1:H:78:ILE:O	1:H:82:LEU:HG	2.19	0.43
1:H:99:ILE:HD11	1:H:143:ARG:HB3	2.00	0.43
2:I:26:TYR:O	2:I:29:SER:HB2	2.18	0.43
2:I:640:GLY:C	2:I:641:GLU:HG2	2.43	0.43
2:I:700:VAL:HG13	2:I:1117:LEU:HD22	2.00	0.43
2:I:1247:SER:HB3	3:J:375:GLU:O	2.19	0.43
2:I:1280:ALA:HB1	3:J:918:ILE:HG22	2.00	0.43
3:J:1034:PHE:HA	3:J:1114:GLN:HA	2.01	0.43
3:J:1280:VAL:O	3:J:1284:ARG:HB3	2.19	0.43
5:L:289:LYS:HE2	5:L:289:LYS:HB3	1.88	0.43
1:A:12:ARG:HG3	1:B:230:ALA:HB1	2.01	0.43
1:A:39:LEU:HD23	1:A:39:LEU:HA	1.83	0.43
2:C:316:GLU:CD	2:C:316:GLU:H	2.26	0.43
2:C:524:ILE:HG21	2:C:708:VAL:HG13	1.99	0.43
2:C:778:GLU:O	2:C:781:ASP:HB2	2.19	0.43
2:C:1122:LYS:HG2	2:C:1229:TYR:CZ	2.54	0.43
3:D:77:ARG:HD2	3:D:78:LEU:H	1.84	0.43
1:G:102:LEU:HD22	1:G:103:ASN:H	1.84	0.43
2:I:1289:GLU:OE2	3:J:473:THR:HG22	2.19	0.43
2:I:1302:THR:HG22	5:L:531:PRO:HB3	2.01	0.43
3:J:367:GLY:HA3	3:J:448:GLN:HB2	2.01	0.43
3:J:810:THR:HG23	3:J:811:GLU:H	1.83	0.43
2:C:838:CYS:SG	2:C:886:LYS:HD3	2.59	0.43
2:C:887:VAL:HB	2:C:913:VAL:HG21	2.00	0.43
3:D:35:PHE:CD1	3:D:101:ARG:HD3	2.53	0.43
3:D:426:ALA:HB3	3:D:427:PRO:HD3	2.01	0.43
3:D:757:THR:O	3:D:757:THR:OG1	2.25	0.43
3:D:1163:VAL:HG23	3:D:1177:ILE:HA	2.01	0.43
5:F:297:MET:HE3	5:F:330:LEU:HD11	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:10:ARG:HA	2:I:1172:LEU:HD23	2.01	0.43
2:I:657:THR:OG1	2:I:1187:PHE:HB2	2.18	0.43
3:J:484:MET:HB3	3:J:484:MET:HE2	1.78	0.43
5:L:482:GLU:HG2	5:L:486:ARG:HH22	1.84	0.43
1:B:80:GLU:HG3	3:D:551:ARG:NH2	2.33	0.43
3:D:800:LEU:O	3:D:803:VAL:HG12	2.18	0.43
1:G:66:HIS:CE1	1:G:69:SER:HB3	2.54	0.43
2:I:518:ASN:O	2:I:691:PRO:HD3	2.19	0.43
2:I:670:PHE:HZ	2:I:1117:LEU:HD13	1.83	0.43
2:I:1122:LYS:HG2	2:I:1229:TYR:CZ	2.53	0.43
2:C:69:GLN:HE21	2:C:69:GLN:HB3	1.67	0.43
2:C:758:ARG:HD3	2:C:835:GLU:HB2	2.01	0.43
2:C:897:PRO:CG	3:D:77:ARG:HH22	2.31	0.43
5:F:136:GLU:OE1	5:F:364:ARG:NH2	2.52	0.43
2:I:383:SER:O	2:I:387:ASN:HB2	2.19	0.43
3:J:203:GLU:O	3:J:207:GLU:HG2	2.19	0.43
3:J:697:MET:O	3:J:701:LEU:HB2	2.19	0.43
3:J:701:LEU:HD13	3:J:723:TYR:HB2	2.01	0.43
3:J:1230:THR:OG1	3:J:1257:VAL:HG11	2.19	0.43
5:L:470:MET:HE3	5:L:478:PRO:HB3	2.00	0.43
5:L:507:MET:HG2	5:L:520:GLY:HA3	2.00	0.43
1:A:38:THR:OG1	1:B:45:ARG:NH1	2.48	0.42
1:A:79:LEU:CD1	2:C:693:LEU:HD21	2.49	0.42
1:B:99:ILE:HD11	1:B:143:ARG:HB3	2.01	0.42
3:D:394:ILE:CG2	5:F:536:THR:HA	2.49	0.42
3:D:701:LEU:HD13	3:D:723:TYR:HB2	2.00	0.42
1:G:35:PHE:HD1	1:G:35:PHE:HA	1.70	0.42
1:H:11:PRO:HB3	1:H:30:PRO:O	2.18	0.42
2:I:149:LEU:HB2	2:I:530:ILE:CG2	2.49	0.42
2:I:1282:GLY:HA3	4:K:17:PHE:CE1	2.54	0.42
3:J:438:GLU:HA	3:J:439:PRO:HD3	1.85	0.42
3:J:573:THR:OG1	3:J:576:ARG:HG3	2.19	0.42
3:D:497:GLU:HA	3:D:498:PRO:HD3	1.85	0.42
2:I:98:VAL:HG21	2:I:124:MET:HE3	2.01	0.42
3:J:349:TYR:HE2	3:J:379:PRO:HG2	1.84	0.42
3:J:708:ASN:OD1	3:J:708:ASN:N	2.50	0.42
5:L:582:VAL:CG2	5:L:586:ARG:HG2	2.49	0.42
5:L:583:THR:HB	5:L:584:ARG:HG2	2.01	0.42
1:B:64:VAL:HG21	1:B:69:SER:CB	2.49	0.42
3:D:418:GLU:HB2	4:E:45:LYS:HB2	2.01	0.42
3:D:557:LYS:HA	3:D:563:LEU:HA	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:709:ARG:O	3:D:711:GLY:N	2.50	0.42
3:D:1226:VAL:HB	3:J:1293:GLU:H	1.83	0.42
3:D:1287:ILE:HG13	3:D:1288:ALA:N	2.35	0.42
3:D:1293:GLU:HG2	3:J:1227:HIS:HB2	2.01	0.42
1:H:48:LEU:HA	1:H:180:VAL:HG21	2.01	0.42
2:I:196:VAL:HG12	2:I:206:ALA:HA	2.00	0.42
2:I:238:GLN:HB3	2:I:284:LEU:HD11	2.00	0.42
2:I:360:LEU:HB2	2:I:378:ARG:HH21	1.84	0.42
2:I:389:PHE:HB3	2:I:420:LEU:HD12	2.00	0.42
2:I:634:VAL:HG13	2:I:636:CYS:SG	2.59	0.42
2:I:710:VAL:HA	2:I:715:THR:HG21	2.01	0.42
3:J:987:GLU:H	3:J:987:GLU:HG3	1.64	0.42
3:J:1348:LYS:HD2	3:J:1348:LYS:HA	1.85	0.42
3:J:1368:ASP:OD1	3:J:1371:ARG:NH2	2.52	0.42
2:C:38:PHE:HB2	2:C:457:GLY:CA	2.48	0.42
2:C:83:GLN:O	2:C:87:ILE:HG13	2.19	0.42
2:C:660:VAL:HG11	3:D:769:VAL:HG13	2.01	0.42
4:E:66:VAL:HG22	4:E:69:ARG:HH21	1.84	0.42
5:F:22:LEU:H	5:F:54:GLN:CB	2.33	0.42
2:I:519:ASN:HD21	2:I:796:LEU:HD23	1.84	0.42
2:I:964:LEU:HD22	2:I:1025:PHE:CG	2.54	0.42
2:I:1101:LEU:HD13	3:J:504:GLN:HB2	2.01	0.42
4:K:66:VAL:HG22	4:K:69:ARG:HH21	1.85	0.42
5:L:215:GLU:HG2	5:L:218:ARG:HH21	1.82	0.42
1:B:61:ILE:HG21	1:B:78:ILE:HD13	2.02	0.42
2:C:360:LEU:HB2	2:C:378:ARG:HH21	1.85	0.42
2:C:499:SER:O	2:C:503:LYS:HB2	2.20	0.42
2:C:720:ARG:HA	2:C:779:ARG:HG3	2.01	0.42
2:C:964:LEU:HD22	2:C:1025:PHE:CG	2.54	0.42
3:D:505:ASP:HB2	3:D:629:PHE:HE1	1.85	0.42
5:F:412:LEU:HD13	5:F:435:ILE:HD11	2.00	0.42
5:F:565:ILE:HG22	5:F:566:ASP:CG	2.45	0.42
2:I:18:ARG:HA	2:I:19:PRO:HD3	1.92	0.42
2:I:203:LYS:CB	5:L:29:ASP:HB2	2.49	0.42
2:I:538:LEU:H	2:I:538:LEU:HG	1.64	0.42
2:I:887:VAL:HB	2:I:913:VAL:CG2	2.49	0.42
2:I:1294:LYS:HD3	3:J:472:LEU:HG	2.00	0.42
5:L:399:LEU:HD12	5:L:399:LEU:HA	1.85	0.42
1:B:84:ASN:O	1:B:128:HIS:HE1	2.03	0.42
1:B:89:ALA:HB3	1:B:124:VAL:HG12	2.02	0.42
1:B:112:ALA:HB2	1:B:128:HIS:HB3	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1125:GLY:HA3	2:C:1179:GLY:HA2	2.00	0.42
3:D:334:LYS:HD2	3:D:334:LYS:HA	1.58	0.42
3:D:697:MET:O	3:D:701:LEU:HB2	2.19	0.42
1:H:100:LEU:HB2	1:H:144:ILE:HG23	2.01	0.42
1:H:151:GLY:O	1:H:177:TYR:HD2	2.03	0.42
2:I:660:VAL:HG13	2:I:661:VAL:HG13	2.00	0.42
2:I:806:PRO:O	3:J:633:ALA:HA	2.19	0.42
3:J:1198:VAL:HB	3:J:1210:ILE:HA	2.01	0.42
2:C:211:ARG:NH1	2:C:357:ASN:O	2.52	0.42
2:C:518:ASN:O	2:C:691:PRO:HD3	2.19	0.42
1:G:182:ARG:HB3	1:G:206:GLU:HB3	2.02	0.42
2:I:616:ILE:HG13	2:I:652:TYR:HB2	2.01	0.42
2:I:1276:TRP:HE1	3:J:1348:LYS:NZ	2.18	0.42
3:J:355:ILE:HD13	3:J:466:MET:HG3	2.01	0.42
5:L:314:THR:O	5:L:318:ALA:HB3	2.20	0.42
1:A:228:LEU:HD21	1:B:224:LEU:HD23	2.01	0.42
2:C:60:GLN:HB3	2:C:67:GLU:HG3	2.01	0.42
2:C:1080:ASN:HA	2:C:1081:PRO:HD3	1.96	0.42
2:C:1247:SER:O	3:D:348:ASP:HB3	2.20	0.42
2:C:1267:GLY:HA3	3:D:347:VAL:O	2.20	0.42
3:D:490:ILE:HA	3:D:500:ILE:HD11	2.02	0.42
2:I:156:PHE:CE2	2:I:158:ASP:HB2	2.54	0.42
2:I:232:ILE:HG12	2:I:237:LEU:HD13	2.02	0.42
3:J:901:ARG:HD2	3:J:906:GLY:O	2.19	0.42
3:J:1163:VAL:HG23	3:J:1177:ILE:HA	2.02	0.42
5:L:441:ARG:NH1	5:L:445:ASP:OD1	2.50	0.42
1:A:41:ASN:HB2	1:A:185:TYR:OH	2.19	0.42
2:C:1276:TRP:HE1	3:D:1348:LYS:NZ	2.17	0.42
2:C:1338:GLU:N	3:D:21:LYS:O	2.34	0.42
3:D:13:LYS:HA	3:D:13:LYS:HD3	1.72	0.42
3:D:450:HIS:HA	3:D:451:PRO:HD3	1.85	0.42
5:F:484:ALA:HB1	5:F:491:GLU:HB2	2.02	0.42
5:F:507:MET:HG2	5:F:520:GLY:HA3	2.01	0.42
2:I:169:LYS:O	2:I:170:VAL:HG22	2.20	0.42
2:I:720:ARG:HA	2:I:779:ARG:HG3	2.01	0.42
3:J:644:MET:HE3	3:J:644:MET:HB2	1.89	0.42
3:J:1036:ARG:HG2	3:J:1037:PHE:H	1.85	0.42
5:L:124:GLU:O	5:L:128:ASN:HB2	2.20	0.42
5:L:454:VAL:HA	5:L:457:ILE:HD12	2.02	0.42
2:C:156:PHE:CE2	2:C:158:ASP:HB2	2.55	0.42
2:C:519:ASN:HD21	2:C:796:LEU:HD23	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:128:LEU:HD23	3:D:192:MET:HE3	2.00	0.42
3:D:355:ILE:HG22	3:D:447:ILE:HB	2.01	0.42
3:D:385:LEU:HD23	3:D:385:LEU:HA	1.92	0.42
3:D:901:ARG:HD2	3:D:906:GLY:O	2.20	0.42
2:I:661:VAL:HB	2:I:665:ALA:HB3	2.01	0.42
2:I:887:VAL:HB	2:I:913:VAL:HG21	2.01	0.42
2:I:929:ILE:HD13	2:I:1055:ALA:HB2	2.01	0.42
3:J:290:ILE:H	3:J:290:ILE:HD12	1.85	0.42
3:J:974:VAL:HG21	3:J:1118:GLY:HA2	2.02	0.42
3:J:1287:ILE:HG13	3:J:1288:ALA:N	2.34	0.42
2:C:660:VAL:HG13	2:C:661:VAL:HG13	2.02	0.41
2:C:1059:ARG:HB2	2:C:1060:ILE:H	1.74	0.41
3:D:527:LEU:HD22	3:D:533:ALA:HA	2.02	0.41
5:F:470:MET:HE3	5:F:478:PRO:HB3	2.02	0.41
1:G:31:LEU:CD1	1:G:201:LEU:HB2	2.50	0.41
2:I:356:THR:HG21	2:I:362:ALA:HA	2.02	0.41
2:I:617:ALA:HA	2:I:636:CYS:SG	2.60	0.41
2:I:1161:LEU:HD12	2:I:1161:LEU:HA	1.70	0.41
3:J:872:LEU:O	3:J:877:VAL:HG12	2.19	0.41
3:J:1146:GLU:HB3	3:J:1148:ARG:HG3	2.01	0.41
3:D:338:PHE:CB	3:D:343:LEU:HB2	2.50	0.41
3:D:794:GLY:O	3:D:797:THR:OG1	2.26	0.41
3:D:1198:VAL:HB	3:D:1210:ILE:HA	2.02	0.41
5:F:119:ILE:O	5:F:123:ILE:HG13	2.20	0.41
2:I:32:LEU:HD23	2:I:32:LEU:HA	1.91	0.41
2:I:996:ARG:HD3	2:I:996:ARG:HA	1.89	0.41
2:I:1257:GLN:OE1	3:J:340:GLN:NE2	2.53	0.41
3:J:557:LYS:HA	3:J:563:LEU:HA	2.02	0.41
3:J:1027:VAL:HG21	3:J:1122:ALA:HB3	2.02	0.41
5:L:528:LEU:HD23	5:L:528:LEU:HA	1.92	0.41
2:C:593:LYS:HD3	2:C:652:TYR:CZ	2.56	0.41
3:D:1216:ALA:HA	3:D:1217:PRO:HD3	1.89	0.41
3:D:1349:GLU:OE2	3:D:1349:GLU:N	2.38	0.41
3:D:1355:ARG:NH1	3:D:1369:ARG:HH12	2.18	0.41
5:F:289:LYS:HE2	5:F:289:LYS:HB3	1.88	0.41
5:F:343:LYS:HD2	5:F:343:LYS:H	1.85	0.41
2:I:26:TYR:CE2	2:I:28:LEU:HB2	2.56	0.41
2:I:840:SER:O	2:I:1047:LEU:N	2.53	0.41
2:I:1010:GLN:O	2:I:1014:LEU:HD12	2.20	0.41
3:J:478:LEU:HB3	4:K:20:VAL:HG13	2.02	0.41
3:J:770:LEU:HD22	3:J:770:LEU:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:LEU:HD12	1:B:142:MET:HG2	2.02	0.41
2:C:12:ARG:HH21	2:C:793:GLU:CD	2.28	0.41
2:C:101:ARG:HH21	2:C:118:LYS:HE3	1.85	0.41
2:C:357:ASN:ND2	2:C:358:ASP:OD2	2.53	0.41
2:C:561:ILE:HD11	2:C:665:ALA:HB1	2.01	0.41
2:C:616:ILE:HG13	2:C:652:TYR:HB2	2.02	0.41
3:D:482:ALA:HB3	4:E:20:VAL:HG22	2.03	0.41
3:D:1194:ARG:HD2	3:D:1194:ARG:N	2.36	0.41
5:F:561:MET:HG3	5:F:571:TYR:CD2	2.55	0.41
1:G:102:LEU:HD22	1:G:103:ASN:N	2.36	0.41
2:I:499:SER:O	2:I:503:LYS:HB2	2.19	0.41
2:I:1062:PRO:HA	2:I:1076:ILE:HG23	2.02	0.41
3:J:450:HIS:HA	3:J:451:PRO:HD3	1.85	0.41
3:J:474:LEU:HD12	3:J:474:LEU:HA	1.90	0.41
4:K:49:ILE:HA	4:K:52:ARG:HD3	2.02	0.41
5:L:420:GLU:OE1	5:L:423:ARG:NH2	2.50	0.41
2:C:183:TRP:HB2	2:C:199:ASP:HA	2.02	0.41
2:C:468:LEU:HA	2:C:471:VAL:HG12	2.02	0.41
2:C:617:ALA:HA	2:C:636:CYS:SG	2.61	0.41
2:C:925:SER:O	2:C:1056:VAL:HG13	2.21	0.41
3:D:203:GLU:O	3:D:207:GLU:HG2	2.20	0.41
3:D:418:GLU:H	4:E:45:LYS:HZ3	1.68	0.41
3:D:1236:GLU:O	3:D:1240:VAL:HG23	2.21	0.41
4:E:4:VAL:HG22	4:E:5:THR:HG23	2.03	0.41
5:F:97:PRO:HA	5:F:100:MET:HG3	2.02	0.41
2:I:230:PHE:HE1	2:I:287:VAL:HG21	1.85	0.41
3:J:197:GLU:O	3:J:201:LEU:HG	2.20	0.41
3:J:654:ILE:O	3:J:658:GLU:HB2	2.21	0.41
5:L:245:ALA:O	5:L:249:ILE:HG13	2.20	0.41
1:A:31:LEU:CD1	1:A:201:LEU:HB2	2.48	0.41
2:C:959:ASP:O	2:C:963:GLU:HG2	2.21	0.41
2:C:1210:ILE:HG22	2:C:1211:ARG:H	1.85	0.41
3:D:661:VAL:HG11	3:D:686:TRP:NE1	2.35	0.41
5:F:225:ARG:O	5:F:229:VAL:HG13	2.21	0.41
2:I:242:VAL:HA	2:I:243:PRO:HD3	1.93	0.41
2:I:555:TYR:HA	3:J:773:PHE:HE2	1.86	0.41
2:I:1210:ILE:HG22	2:I:1211:ARG:H	1.85	0.41
3:J:119:SER:O	3:J:121:PRO:HD2	2.21	0.41
3:J:361:LEU:HD22	3:J:365:GLN:HG3	2.01	0.41
3:J:572:THR:OG1	3:J:573:THR:N	2.52	0.41
3:J:759:ILE:HG22	3:J:761:ALA:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:SER:OG	1:B:21:SER:N	2.53	0.41
2:C:53:PHE:O	2:C:57:PHE:HB2	2.21	0.41
2:C:169:LYS:O	2:C:170:VAL:HG22	2.21	0.41
2:C:634:VAL:HG13	2:C:636:CYS:SG	2.60	0.41
2:C:1080:ASN:HB3	2:C:1085:MET:HE3	2.03	0.41
2:C:1109:ILE:HD12	2:C:1109:ILE:HA	1.86	0.41
3:D:372:MET:HE2	3:D:372:MET:HB3	1.98	0.41
3:D:579:LEU:HD12	3:D:582:ILE:HD12	2.03	0.41
5:F:462:LYS:O	5:F:466:ILE:HG13	2.20	0.41
1:G:11:PRO:HD3	1:H:227:GLN:OE1	2.21	0.41
1:G:230:ALA:HB2	1:H:12:ARG:HA	2.03	0.41
1:H:64:VAL:HG21	1:H:69:SER:CB	2.50	0.41
1:H:65:LEU:HD13	1:H:65:LEU:O	2.21	0.41
1:H:89:ALA:HB3	1:H:124:VAL:HG12	2.01	0.41
2:I:53:PHE:O	2:I:57:PHE:HB2	2.21	0.41
2:I:357:ASN:ND2	2:I:358:ASP:OD2	2.53	0.41
2:I:374:GLU:HA	2:I:375:PRO:HD3	1.93	0.41
2:I:590:PRO:HB2	2:I:655:VAL:HG21	2.01	0.41
3:J:262:THR:C	5:L:507:MET:HB2	2.46	0.41
3:J:1237:VAL:HG13	3:J:1253:ILE:HD13	2.02	0.41
3:J:1319:PHE:CD2	3:J:1342:ASP:HB2	2.56	0.41
1:B:133:LEU:HD12	1:B:133:LEU:HA	1.92	0.41
2:C:551:HIS:CG	2:C:552:PRO:HD2	2.56	0.41
2:C:980:VAL:HG13	2:C:984:VAL:HB	2.02	0.41
3:D:844:THR:OG1	3:D:860:ARG:O	2.32	0.41
2:I:149:LEU:HD11	2:I:451:ARG:HB3	2.03	0.41
2:I:593:LYS:HD3	2:I:652:TYR:CZ	2.55	0.41
2:I:658:GLN:O	2:I:661:VAL:HG22	2.21	0.41
3:J:70:CYS:SG	3:J:71:LEU:N	2.94	0.41
3:J:137:ARG:HG2	3:J:143:SER:HB2	2.03	0.41
3:J:274:ASN:ND2	5:L:446:GLN:HB2	2.36	0.41
3:J:527:LEU:HD22	3:J:533:ALA:HA	2.02	0.41
5:L:127:ILE:O	5:L:130:VAL:HG22	2.20	0.41
1:A:10:LYS:HB3	1:A:10:LYS:HE3	1.79	0.41
1:A:75:GLN:HA	2:C:729:ALA:N	2.36	0.41
1:B:57:THR:O	1:B:173:VAL:HB	2.20	0.41
1:B:191:ARG:HH22	3:D:409:TRP:CB	2.25	0.41
2:C:11:ILE:HD13	2:C:11:ILE:HA	1.88	0.41
2:C:171:LEU:HD23	2:C:171:LEU:HA	1.92	0.41
2:C:559:CYS:HA	2:C:560:PRO:HD3	1.89	0.41
2:C:1010:GLN:O	2:C:1014:LEU:HD12	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1179:GLY:O	2:C:1181:PRO:HD3	2.21	0.41
2:C:1211:ARG:O	2:C:1212:LEU:HD12	2.21	0.41
2:C:1313:HIS:HB2	3:D:474:LEU:HD13	2.02	0.41
3:D:19:ALA:HB2	3:D:1373:ARG:HH22	1.86	0.41
3:D:653:ILE:HD13	3:D:692:ARG:HB3	2.03	0.41
3:D:1319:PHE:CD2	3:D:1342:ASP:HB2	2.56	0.41
5:F:314:THR:O	5:F:318:ALA:HB3	2.21	0.41
1:G:54:CYS:O	1:G:146:VAL:HG13	2.21	0.41
1:G:164:ASP:C	1:G:166:ARG:H	2.28	0.41
2:I:145:ILE:HG13	2:I:512:SER:HB2	2.03	0.41
2:I:213:LEU:HB3	2:I:422:LYS:CD	2.49	0.41
2:I:724:VAL:HA	2:I:734:ILE:HD13	2.02	0.41
2:I:1262:LYS:HD3	2:I:1262:LYS:HA	1.83	0.41
3:J:384:LYS:HD2	3:J:387:LEU:HD23	2.03	0.41
3:J:901:ARG:HA	3:J:908:ILE:HA	2.03	0.41
3:J:930:LEU:HD11	3:J:1241:TYR:CE2	2.56	0.41
3:J:1077:ALA:HA	3:J:1100:PHE:HA	2.02	0.41
5:L:343:LYS:H	5:L:343:LYS:HD2	1.85	0.41
5:L:580:PHE:HD1	5:L:580:PHE:HA	1.71	0.41
1:A:145:LYS:NZ	1:A:147:GLN:OE1	2.54	0.41
1:B:27:THR:HG22	1:B:202:VAL:HG13	2.03	0.41
2:C:230:PHE:HE1	2:C:287:VAL:HG21	1.85	0.41
2:C:560:PRO:HB2	3:D:776:THR:HG21	2.03	0.41
3:D:528:THR:HG22	3:D:532:GLU:CD	2.46	0.41
3:D:573:THR:OG1	3:D:576:ARG:HG3	2.20	0.41
3:D:743:MET:HE2	3:D:743:MET:HB3	1.95	0.41
3:D:853:THR:HG22	3:D:854:ALA:H	1.86	0.41
5:F:559:LEU:O	5:F:563:PHE:HD2	2.03	0.41
1:G:93:GLN:HB2	1:G:120:ASP:OD2	2.21	0.41
1:H:29:GLU:HB3	1:H:30:PRO:CD	2.48	0.41
1:H:102:LEU:HD23	1:H:115:ILE:HG23	2.02	0.41
2:I:409:LEU:HD23	2:I:409:LEU:HA	1.93	0.41
3:J:579:LEU:HD12	3:J:582:ILE:HD12	2.01	0.41
1:A:49:SER:HB3	2:C:1083:GLU:CD	2.46	0.40
1:A:164:ASP:C	1:A:166:ARG:H	2.28	0.40
1:B:16:ILE:HG13	1:B:26:VAL:HG22	2.03	0.40
2:C:26:TYR:CE2	2:C:28:LEU:HB2	2.56	0.40
2:C:37:LYS:HD3	2:C:37:LYS:HA	1.79	0.40
2:C:65:ASN:HB3	2:C:105:TYR:HB2	2.03	0.40
2:C:732:ILE:HD11	2:C:769:PRO:HB3	2.03	0.40
3:D:197:GLU:O	3:D:201:LEU:HG	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:572:THR:OG1	3:D:573:THR:N	2.54	0.40
5:F:482:GLU:HG2	5:F:486:ARG:HH22	1.86	0.40
5:F:511:ILE:HD12	5:F:511:ILE:HA	1.86	0.40
2:I:80:PHE:HB2	2:I:85:CYS:SG	2.62	0.40
2:I:468:LEU:HA	2:I:471:VAL:HG12	2.03	0.40
2:I:561:ILE:HD11	2:I:665:ALA:HB1	2.02	0.40
2:I:867:GLU:H	2:I:867:GLU:HG3	1.65	0.40
2:I:972:PHE:CD2	2:I:975:ILE:HD12	2.56	0.40
2:I:1287:LEU:HD22	3:J:1357:ILE:HD11	2.03	0.40
6:I:2001:4OB:H7	3:J:774:ILE:HG13	2.02	0.40
3:J:505:ASP:HB2	3:J:629:PHE:HE1	1.87	0.40
3:J:740:LEU:HD12	3:J:740:LEU:HA	1.91	0.40
5:L:22:LEU:H	5:L:54:GLN:CB	2.34	0.40
5:L:29:ASP:OD1	5:L:30:HIS:N	2.54	0.40
5:L:348:GLU:HG2	5:L:354:THR:HA	2.04	0.40
5:L:484:ALA:HB1	5:L:491:GLU:HB2	2.02	0.40
2:C:163:LYS:HE3	2:C:163:LYS:HB3	1.89	0.40
2:C:356:THR:HG21	2:C:362:ALA:HA	2.03	0.40
3:D:657:ALA:O	3:D:661:VAL:HG13	2.21	0.40
1:G:145:LYS:NZ	1:G:147:GLN:OE1	2.54	0.40
2:I:130:MET:HB2	2:I:136:PHE:CZ	2.56	0.40
2:I:721:GLY:N	2:I:740:GLU:OE1	2.50	0.40
3:J:37:GLU:HB2	3:J:104:HIS:CE1	2.56	0.40
3:J:291:ILE:HD13	5:L:409:ASN:HB3	2.03	0.40
3:J:708:ASN:HB3	3:J:712:GLN:O	2.21	0.40
5:L:525:ASP:CG	5:L:528:LEU:HB2	2.46	0.40
2:C:35:PHE:CD2	2:C:130:MET:HB3	2.57	0.40
2:C:484:LEU:HD12	2:C:485:ASP:H	1.86	0.40
2:C:552:PRO:HG3	6:C:2001:4OB:CAL	2.51	0.40
5:F:399:LEU:HA	5:F:399:LEU:HD12	1.86	0.40
5:F:465:ARG:HA	5:F:468:ARG:HH12	1.86	0.40
1:G:92:VAL:HA	1:G:120:ASP:O	2.21	0.40
1:G:162:GLU:HB3	1:G:163:GLU:H	1.72	0.40
1:H:33:ARG:NH1	2:I:1081:PRO:HG3	2.32	0.40
2:I:466:VAL:O	2:I:469:VAL:HG22	2.21	0.40
2:I:521:LEU:HD23	2:I:708:VAL:HG11	2.03	0.40
2:I:658:GLN:O	2:I:660:VAL:N	2.54	0.40
2:I:813:GLU:HB2	3:J:461:PHE:HB2	2.03	0.40
2:I:959:ASP:O	2:I:963:GLU:HG2	2.21	0.40
3:J:233:LYS:HA	3:J:234:PRO:HD3	1.93	0.40
3:J:682:VAL:HA	3:J:685:ILE:CD1	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:354:THR:O	5:L:358:VAL:HG23	2.21	0.40
1:B:33:ARG:HH12	2:C:820:GLU:CD	2.29	0.40
1:B:65:LEU:HD13	1:B:65:LEU:O	2.22	0.40
2:C:498:ILE:HD12	2:C:498:ILE:H	1.87	0.40
2:C:521:LEU:HD23	2:C:708:VAL:HG11	2.03	0.40
2:C:930:ASP:HB3	2:C:1053:TYR:HB2	2.03	0.40
2:C:1253:LEU:O	3:D:99:ARG:NH2	2.55	0.40
3:D:756:GLU:H	3:D:756:GLU:HG2	1.57	0.40
3:D:870:ASP:O	3:D:874:GLU:HG2	2.21	0.40
3:D:901:ARG:HA	3:D:908:ILE:HA	2.02	0.40
5:F:602:SER:N	5:F:605:GLU:CD	2.76	0.40
2:I:967:LEU:HD12	2:I:967:LEU:HA	1.93	0.40
2:I:1179:GLY:O	2:I:1181:PRO:HD3	2.21	0.40
3:J:34:SER:HG	3:J:104:HIS:CG	2.29	0.40
3:J:97:VAL:HG12	3:J:101:ARG:HG3	2.04	0.40
3:J:706:VAL:HG12	3:J:715:LYS:HB3	2.04	0.40
3:J:905:ARG:NH1	4:K:16:ARG:HD2	2.26	0.40
3:J:969:SER:HB3	3:J:1116:SER:HB2	2.03	0.40
3:J:1061:VAL:HG21	3:J:1101:LEU:HB2	2.03	0.40
3:D:905:ARG:HE	3:D:907:HIS:HB2	1.86	0.40
3:D:1162:ILE:HA	3:D:1203:ARG:HA	2.04	0.40
3:D:1368:ASP:OD1	3:D:1371:ARG:NH2	2.55	0.40
5:F:348:GLU:HG2	5:F:354:THR:HA	2.03	0.40
1:G:192:VAL:O	1:G:193:GLU:C	2.65	0.40
1:H:112:ALA:HB2	1:H:128:HIS:HB3	2.02	0.40
3:J:925:GLU:HB3	3:J:926:PRO:HD3	2.03	0.40
3:J:1031:VAL:HG23	3:J:1080:ILE:HG21	2.04	0.40
3:J:1194:ARG:HD2	3:J:1194:ARG:N	2.36	0.40
5:L:561:MET:HG3	5:L:571:TYR:HD2	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	298/335 (89%)	270 (91%)	19 (6%)	9 (3%)	3	23
1	B	212/335 (63%)	190 (90%)	20 (9%)	2 (1%)	14	49
1	G	222/335 (66%)	196 (88%)	20 (9%)	6 (3%)	4	26
1	H	212/335 (63%)	193 (91%)	17 (8%)	2 (1%)	14	49
2	C	1338/1342 (100%)	1234 (92%)	98 (7%)	6 (0%)	30	66
2	I	1338/1342 (100%)	1232 (92%)	100 (8%)	6 (0%)	30	66
3	D	1162/1407 (83%)	1045 (90%)	105 (9%)	12 (1%)	12	47
3	J	1328/1407 (94%)	1195 (90%)	122 (9%)	11 (1%)	16	52
4	E	87/91 (96%)	81 (93%)	6 (7%)	0	100	100
4	K	77/91 (85%)	73 (95%)	4 (5%)	0	100	100
5	F	532/613 (87%)	481 (90%)	50 (9%)	1 (0%)	43	77
5	L	529/613 (86%)	480 (91%)	49 (9%)	0	100	100
All	All	7335/8246 (89%)	6670 (91%)	610 (8%)	55 (1%)	18	54

All (55) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	319	GLU
1	A	320	ASN
2	C	237	LEU
3	D	120	LEU
3	D	751	ASP
2	I	237	LEU
3	J	120	LEU
3	J	751	ASP
1	A	193	GLU
1	A	323	PRO
1	B	15	ASP
2	C	170	VAL
3	D	10	ALA
3	D	89	GLY
3	D	753	SER
1	G	193	GLU
2	I	170	VAL
3	J	89	GLY
3	J	753	SER
1	A	62	ASP
3	D	756	GLU
5	F	7	SER

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Mol	Chain	Res	Type
1	G	62	ASP
3	J	756	GLU
1	A	196	THR
2	C	1136	GLN
3	D	710	ASP
1	G	196	THR
1	G	229	GLU
1	H	29	GLU
2	I	1136	GLN
3	J	710	ASP
1	A	167	PRO
2	C	697	LYS
3	D	777	HIS
1	G	167	PRO
1	G	178	SER
2	I	697	LYS
1	A	178	SER
1	B	193	GLU
2	C	1186	VAL
3	D	778	GLY
3	D	831	VAL
1	H	193	GLU
2	I	1186	VAL
3	J	831	VAL
3	D	758	PRO
3	J	749	LYS
3	J	778	GLY
3	J	758	PRO
1	A	14	VAL
2	C	1159	VAL
3	D	749	LYS
2	I	1159	VAL
3	J	752	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	257/292 (88%)	237 (92%)	20 (8%)	11	33
1	B	184/292 (63%)	163 (89%)	21 (11%)	5	21
1	G	191/292 (65%)	178 (93%)	13 (7%)	14	37
1	H	183/292 (63%)	166 (91%)	17 (9%)	8	27
2	C	1155/1157 (100%)	1053 (91%)	102 (9%)	9	30
2	I	1154/1157 (100%)	1051 (91%)	103 (9%)	9	29
3	D	975/1168 (84%)	871 (89%)	104 (11%)	6	22
3	J	1117/1168 (96%)	1005 (90%)	112 (10%)	7	24
4	E	72/75 (96%)	64 (89%)	8 (11%)	6	21
4	K	67/75 (89%)	60 (90%)	7 (10%)	7	23
5	F	426/540 (79%)	384 (90%)	42 (10%)	7	25
5	L	428/540 (79%)	386 (90%)	42 (10%)	7	25
All	All	6209/7048 (88%)	5618 (90%)	591 (10%)	8	26

All (591) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	26	VAL
1	A	35	PHE
1	A	54	CYS
1	A	64	VAL
1	A	65	LEU
1	A	74	VAL
1	A	129	VAL
1	A	133	LEU
1	A	148	ARG
1	A	168	ILE
1	A	173	VAL
1	A	186	ASN
1	A	207	THR
1	A	228	LEU
1	A	287	VAL
1	A	317	ARG
1	A	318	LEU
1	A	319	GLU
1	A	321	TRP
1	B	8	PHE
1	B	9	LEU

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Mol	Chain	Res	Type
1	B	13	LEU
1	B	14	VAL
1	B	16	ILE
1	B	27	THR
1	B	29	GLU
1	B	31	LEU
1	B	54	CYS
1	B	60	GLU
1	B	64	VAL
1	B	65	LEU
1	B	75	GLN
1	B	92	VAL
1	B	101	THR
1	B	116	THR
1	B	133	LEU
1	B	144	ILE
1	B	160	HIS
1	B	183	ILE
1	B	186	ASN
2	C	11	ILE
2	C	22	LEU
2	C	39	ILE
2	C	81	ASP
2	C	85	CYS
2	C	91	THR
2	C	114	VAL
2	C	115	LYS
2	C	116	ASP
2	C	131	THR
2	C	182	SER
2	C	202	ARG
2	C	235	ASN
2	C	285	ILE
2	C	292	ILE
2	C	316	GLU
2	C	320	ASP
2	C	321	LEU
2	C	360	LEU
2	C	419	ILE
2	C	423	ASP
2	C	434	ASP
2	C	453	ILE

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Mol	Chain	Res	Type
2	C	481	LEU
2	C	484	LEU
2	C	486	THR
2	C	493	ILE
2	C	512	SER
2	C	517	GLN
2	C	518	ASN
2	C	530	ILE
2	C	538	LEU
2	C	539	THR
2	C	540	ARG
2	C	550	VAL
2	C	558	VAL
2	C	575	LEU
2	C	604	HIS
2	C	615	VAL
2	C	618	GLN
2	C	623	LEU
2	C	641	GLU
2	C	657	THR
2	C	660	VAL
2	C	672	GLU
2	C	692	THR
2	C	697	LYS
2	C	699	LEU
2	C	705	GLU
2	C	706	ARG
2	C	714	VAL
2	C	724	VAL
2	C	739	ASP
2	C	748	ILE
2	C	765	ILE
2	C	773	LEU
2	C	782	VAL
2	C	788	SER
2	C	815	SER
2	C	817	LEU
2	C	819	SER
2	C	828	PHE
2	C	839	VAL
2	C	859	GLU
2	C	878	THR

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Mol	Chain	Res	Type
2	C	890	LYS
2	C	892	GLU
2	C	946	LEU
2	C	967	LEU
2	C	974	ARG
2	C	979	LEU
2	C	984	VAL
2	C	990	ASP
2	C	1002	LEU
2	C	1005	GLU
2	C	1006	GLU
2	C	1014	LEU
2	C	1040	ASP
2	C	1046	VAL
2	C	1082	ILE
2	C	1108	ASN
2	C	1109	ILE
2	C	1114	GLU
2	C	1134	GLN
2	C	1141	LEU
2	C	1155	VAL
2	C	1161	LEU
2	C	1172	LEU
2	C	1174	GLU
2	C	1198	LEU
2	C	1204	LEU
2	C	1210	ILE
2	C	1233	LEU
2	C	1240	ASP
2	C	1248	THR
2	C	1253	LEU
2	C	1254	VAL
2	C	1264	GLN
2	C	1265	PHE
2	C	1299	ASN
2	C	1326	LEU
2	C	1327	LEU
3	D	8	LEU
3	D	11	GLN
3	D	18	ASP
3	D	20	ILE
3	D	46	TYR

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Mol	Chain	Res	Type
3	D	71	LEU
3	D	79	LYS
3	D	83	VAL
3	D	88	CYS
3	D	92	VAL
3	D	95	THR
3	D	97	VAL
3	D	117	LEU
3	D	119	SER
3	D	120	LEU
3	D	169	LEU
3	D	175	GLU
3	D	194	LEU
3	D	217	LEU
3	D	237	MET
3	D	244	VAL
3	D	248	ASP
3	D	252	LEU
3	D	255	LEU
3	D	256	ASP
3	D	311	ARG
3	D	324	LEU
3	D	330	MET
3	D	339	ARG
3	D	356	THR
3	D	374	LEU
3	D	394	ILE
3	D	416	ILE
3	D	474	LEU
3	D	501	VAL
3	D	506	VAL
3	D	507	VAL
3	D	523	GLU
3	D	536	LEU
3	D	547	ARG
3	D	568	SER
3	D	593	ASN
3	D	594	GLN
3	D	615	LYS
3	D	641	ILE
3	D	660	GLU
3	D	677	GLU

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Mol	Chain	Res	Type
3	D	678	ARG
3	D	683	ILE
3	D	685	ILE
3	D	697	MET
3	D	698	MET
3	D	701	LEU
3	D	707	ILE
3	D	708	ASN
3	D	710	ASP
3	D	712	GLN
3	D	717	VAL
3	D	740	LEU
3	D	746	LEU
3	D	749	LYS
3	D	754	ILE
3	D	756	GLU
3	D	760	THR
3	D	767	LEU
3	D	783	LEU
3	D	810	THR
3	D	826	ILE
3	D	847	ASP
3	D	848	VAL
3	D	849	LEU
3	D	853	THR
3	D	857	LEU
3	D	860	ARG
3	D	867	GLN
3	D	890	THR
3	D	897	HIS
3	D	908	ILE
3	D	913	GLU
3	D	918	ILE
3	D	928	THR
3	D	931	THR
3	D	1155	ILE
3	D	1163	VAL
3	D	1167	LYS
3	D	1177	ILE
3	D	1186	TYR
3	D	1202	GLU
3	D	1209	VAL

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Mol	Chain	Res	Type
3	D	1215	GLU
3	D	1244	GLN
3	D	1251	LYS
3	D	1255	VAL
3	D	1272	SER
3	D	1274	PHE
3	D	1281	GLU
3	D	1284	ARG
3	D	1285	VAL
3	D	1289	ASN
3	D	1307	LEU
3	D	1327	GLU
3	D	1332	LEU
3	D	1333	THR
3	D	1343	GLU
4	E	4	VAL
4	E	13	ILE
4	E	28	ARG
4	E	31	GLN
4	E	36	ASP
4	E	39	VAL
4	E	46	THR
4	E	58	LEU
5	F	27	VAL
5	F	44	ILE
5	F	45	ILE
5	F	50	ASP
5	F	98	VAL
5	F	100	MET
5	F	118	ASP
5	F	127	ILE
5	F	130	VAL
5	F	154	GLU
5	F	244	THR
5	F	251	LYS
5	F	297	MET
5	F	305	LEU
5	F	306	PHE
5	F	341	LEU
5	F	395	THR
5	F	417	ASP
5	F	429	THR

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Mol	Chain	Res	Type
5	F	445	ASP
5	F	449	THR
5	F	454	VAL
5	F	479	THR
5	F	486	ARG
5	F	488	LEU
5	F	491	GLU
5	F	494	ILE
5	F	496	LYS
5	F	499	LYS
5	F	508	GLU
5	F	528	LEU
5	F	530	LEU
5	F	540	LEU
5	F	566	ASP
5	F	568	ASN
5	F	572	THR
5	F	578	LYS
5	F	580	PHE
5	F	583	THR
5	F	586	ARG
5	F	600	HIS
5	F	606	VAL
1	G	9	LEU
1	G	26	VAL
1	G	28	LEU
1	G	35	PHE
1	G	54	CYS
1	G	64	VAL
1	G	65	LEU
1	G	129	VAL
1	G	133	LEU
1	G	168	ILE
1	G	173	VAL
1	G	186	ASN
1	G	207	THR
1	H	13	LEU
1	H	16	ILE
1	H	28	LEU
1	H	31	LEU
1	H	54	CYS
1	H	58	GLU

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Mol	Chain	Res	Type
1	H	60	GLU
1	H	64	VAL
1	H	65	LEU
1	H	75	GLN
1	H	92	VAL
1	H	101	THR
1	H	116	THR
1	H	133	LEU
1	H	144	ILE
1	H	183	ILE
1	H	186	ASN
2	I	11	ILE
2	I	22	LEU
2	I	39	ILE
2	I	81	ASP
2	I	85	CYS
2	I	91	THR
2	I	114	VAL
2	I	115	LYS
2	I	116	ASP
2	I	131	THR
2	I	182	SER
2	I	202	ARG
2	I	219	GLN
2	I	235	ASN
2	I	285	ILE
2	I	292	ILE
2	I	299	LYS
2	I	316	GLU
2	I	320	ASP
2	I	321	LEU
2	I	360	LEU
2	I	419	ILE
2	I	423	ASP
2	I	434	ASP
2	I	453	ILE
2	I	481	LEU
2	I	484	LEU
2	I	486	THR
2	I	493	ILE
2	I	512	SER
2	I	517	GLN

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Mol	Chain	Res	Type
2	I	518	ASN
2	I	530	ILE
2	I	538	LEU
2	I	539	THR
2	I	540	ARG
2	I	550	VAL
2	I	558	VAL
2	I	575	LEU
2	I	604	HIS
2	I	615	VAL
2	I	618	GLN
2	I	623	LEU
2	I	641	GLU
2	I	657	THR
2	I	672	GLU
2	I	692	THR
2	I	697	LYS
2	I	699	LEU
2	I	705	GLU
2	I	706	ARG
2	I	714	VAL
2	I	724	VAL
2	I	739	ASP
2	I	748	ILE
2	I	765	ILE
2	I	773	LEU
2	I	782	VAL
2	I	788	SER
2	I	815	SER
2	I	817	LEU
2	I	819	SER
2	I	828	PHE
2	I	839	VAL
2	I	859	GLU
2	I	878	THR
2	I	890	LYS
2	I	892	GLU
2	I	946	LEU
2	I	967	LEU
2	I	974	ARG
2	I	979	LEU
2	I	984	VAL

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Mol	Chain	Res	Type
2	I	990	ASP
2	I	1002	LEU
2	I	1005	GLU
2	I	1006	GLU
2	I	1014	LEU
2	I	1040	ASP
2	I	1082	ILE
2	I	1108	ASN
2	I	1109	ILE
2	I	1114	GLU
2	I	1134	GLN
2	I	1141	LEU
2	I	1155	VAL
2	I	1161	LEU
2	I	1172	LEU
2	I	1174	GLU
2	I	1198	LEU
2	I	1204	LEU
2	I	1210	ILE
2	I	1233	LEU
2	I	1240	ASP
2	I	1248	THR
2	I	1253	LEU
2	I	1254	VAL
2	I	1264	GLN
2	I	1265	PHE
2	I	1299	ASN
2	I	1313	HIS
2	I	1326	LEU
2	I	1327	LEU
3	J	18	ASP
3	J	20	ILE
3	J	46	TYR
3	J	71	LEU
3	J	79	LYS
3	J	83	VAL
3	J	88	CYS
3	J	92	VAL
3	J	95	THR
3	J	97	VAL
3	J	117	LEU
3	J	119	SER

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Mol	Chain	Res	Type
3	J	120	LEU
3	J	169	LEU
3	J	175	GLU
3	J	194	LEU
3	J	217	LEU
3	J	237	MET
3	J	244	VAL
3	J	248	ASP
3	J	252	LEU
3	J	255	LEU
3	J	256	ASP
3	J	311	ARG
3	J	324	LEU
3	J	330	MET
3	J	339	ARG
3	J	356	THR
3	J	374	LEU
3	J	394	ILE
3	J	416	ILE
3	J	474	LEU
3	J	501	VAL
3	J	506	VAL
3	J	507	VAL
3	J	523	GLU
3	J	536	LEU
3	J	547	ARG
3	J	568	SER
3	J	593	ASN
3	J	594	GLN
3	J	615	LYS
3	J	641	ILE
3	J	660	GLU
3	J	677	GLU
3	J	678	ARG
3	J	683	ILE
3	J	685	ILE
3	J	697	MET
3	J	698	MET
3	J	701	LEU
3	J	707	ILE
3	J	708	ASN
3	J	710	ASP

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Mol	Chain	Res	Type
3	J	712	GLN
3	J	717	VAL
3	J	740	LEU
3	J	746	LEU
3	J	749	LYS
3	J	754	ILE
3	J	756	GLU
3	J	760	THR
3	J	767	LEU
3	J	788	LEU
3	J	810	THR
3	J	826	ILE
3	J	847	ASP
3	J	848	VAL
3	J	849	LEU
3	J	853	THR
3	J	857	LEU
3	J	860	ARG
3	J	867	GLN
3	J	897	HIS
3	J	908	ILE
3	J	913	GLU
3	J	918	ILE
3	J	928	THR
3	J	931	THR
3	J	972	LYS
3	J	987	GLU
3	J	997	VAL
3	J	1017	VAL
3	J	1025	MET
3	J	1042	ASP
3	J	1062	LEU
3	J	1063	ASP
3	J	1073	ASP
3	J	1113	VAL
3	J	1115	ILE
3	J	1155	ILE
3	J	1163	VAL
3	J	1167	LYS
3	J	1177	ILE
3	J	1186	TYR
3	J	1202	GLU

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Mol	Chain	Res	Type
3	J	1209	VAL
3	J	1215	GLU
3	J	1244	GLN
3	J	1251	LYS
3	J	1255	VAL
3	J	1272	SER
3	J	1274	PHE
3	J	1281	GLU
3	J	1284	ARG
3	J	1285	VAL
3	J	1289	ASN
3	J	1307	LEU
3	J	1327	GLU
3	J	1332	LEU
3	J	1333	THR
3	J	1343	GLU
4	K	13	ILE
4	K	28	ARG
4	K	31	GLN
4	K	36	ASP
4	K	39	VAL
4	K	46	THR
4	K	58	LEU
5	L	27	VAL
5	L	44	ILE
5	L	45	ILE
5	L	50	ASP
5	L	98	VAL
5	L	100	MET
5	L	118	ASP
5	L	127	ILE
5	L	130	VAL
5	L	154	GLU
5	L	244	THR
5	L	251	LYS
5	L	297	MET
5	L	305	LEU
5	L	306	PHE
5	L	341	LEU
5	L	395	THR
5	L	417	ASP
5	L	429	THR

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Mol	Chain	Res	Type
5	L	445	ASP
5	L	449	THR
5	L	454	VAL
5	L	479	THR
5	L	486	ARG
5	L	488	LEU
5	L	491	GLU
5	L	494	ILE
5	L	496	LYS
5	L	499	LYS
5	L	508	GLU
5	L	528	LEU
5	L	530	LEU
5	L	540	LEU
5	L	566	ASP
5	L	568	ASN
5	L	572	THR
5	L	578	LYS
5	L	580	PHE
5	L	583	THR
5	L	586	ARG
5	L	600	HIS
5	L	606	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (68) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	75	GLN
1	A	128	HIS
1	A	283	GLN
1	A	294	ASN
1	A	320	ASN
2	C	510	GLN
2	C	513	GLN
2	C	684	ASN
2	C	1017	GLN
2	C	1108	ASN
2	C	1111	GLN
2	C	1116	HIS
2	C	1288	GLN
2	C	1314	GLN

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Mol	Chain	Res	Type
3	D	158	GLN
3	D	196	GLN
3	D	340	GLN
3	D	364	HIS
3	D	419	HIS
3	D	435	GLN
3	D	469	HIS
3	D	560	ASN
3	D	593	ASN
3	D	665	GLN
3	D	667	GLN
3	D	792	ASN
3	D	897	HIS
3	D	1295	ASN
3	D	1367	GLN
4	E	61	ASN
5	F	131	GLN
5	F	345	GLN
5	F	406	GLN
5	F	461	ASN
5	F	545	HIS
5	F	600	HIS
1	G	66	HIS
1	G	128	HIS
2	I	343	HIS
2	I	513	GLN
2	I	684	ASN
2	I	1017	GLN
2	I	1108	ASN
2	I	1111	GLN
2	I	1116	HIS
2	I	1257	GLN
2	I	1314	GLN
2	I	1324	ASN
3	J	196	GLN
3	J	340	GLN
3	J	364	HIS
3	J	419	HIS
3	J	435	GLN
3	J	560	ASN
3	J	593	ASN
3	J	665	GLN

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Mol	Chain	Res	Type
3	J	667	GLN
3	J	792	ASN
3	J	897	HIS
3	J	954	ASN
3	J	1126	GLN
3	J	1367	GLN
4	K	60	ASN
4	K	61	ASN
5	L	345	GLN
5	L	406	GLN
5	L	461	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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
6	4OB	C	2001	-	21,21,21	2.45	5 (23%)	28,29,29	1.43	5 (17%)
6	4OB	I	2001	-	21,21,21	2.45	5 (23%)	28,29,29	1.43	5 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	4OB	C	2001	-	-	1/15/16/16	0/2/2/2
6	4OB	I	2001	-	-	1/15/16/16	0/2/2/2

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	2001	4OB	CAQ-NAO	-6.52	1.31	1.42
6	C	2001	4OB	CAQ-NAO	-6.51	1.31	1.42
6	I	2001	4OB	CAT-CAS	-6.26	1.37	1.49
6	C	2001	4OB	CAT-CAS	-6.24	1.37	1.49
6	C	2001	4OB	CAR-CAP	-4.35	1.39	1.47
6	I	2001	4OB	CAR-CAP	-4.35	1.39	1.47
6	C	2001	4OB	CAP-NAO	3.31	1.33	1.28
6	I	2001	4OB	CAP-NAO	3.29	1.33	1.28
6	I	2001	4OB	OAA-NAN	3.14	1.47	1.40
6	C	2001	4OB	OAA-NAN	3.14	1.47	1.40

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	I	2001	4OB	CAM-CAS-CAT	3.27	123.89	119.57
6	C	2001	4OB	CAM-CAS-CAT	3.26	123.87	119.57
6	I	2001	4OB	CAL-CAS-CAT	-2.73	115.56	119.96
6	C	2001	4OB	CAL-CAS-CAT	-2.73	115.57	119.96
6	C	2001	4OB	OAA-NAN-CAP	-2.39	113.26	119.72
6	I	2001	4OB	OAA-NAN-CAP	-2.38	113.29	119.72
6	I	2001	4OB	CAK-CAR-CAP	-2.33	116.69	120.83
6	C	2001	4OB	CAK-CAR-CAP	-2.33	116.69	120.83
6	C	2001	4OB	CAQ-NAO-CAP	2.31	125.52	120.49
6	I	2001	4OB	CAQ-NAO-CAP	2.30	125.50	120.49

There are no chirality outliers.

All (2) torsion outliers are listed below:

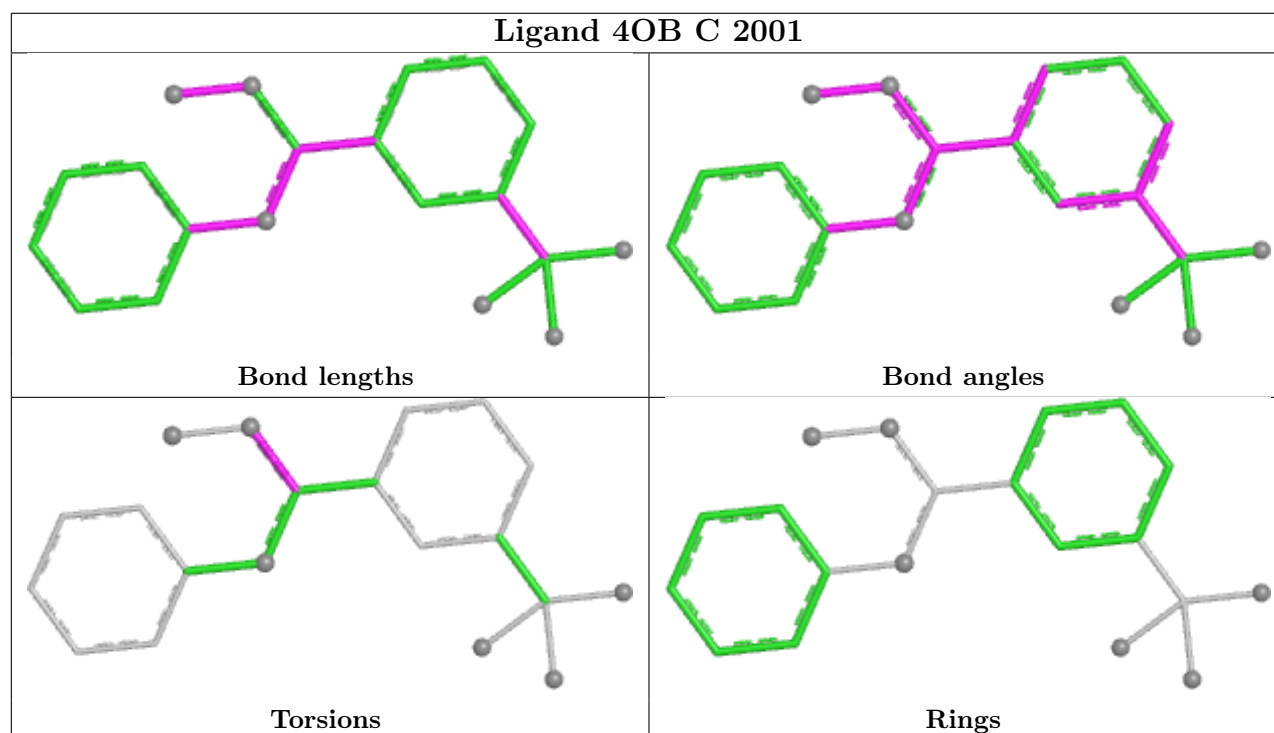
Mol	Chain	Res	Type	Atoms
6	C	2001	4OB	CAR-CAP-NAN-OAA
6	I	2001	4OB	CAR-CAP-NAN-OAA

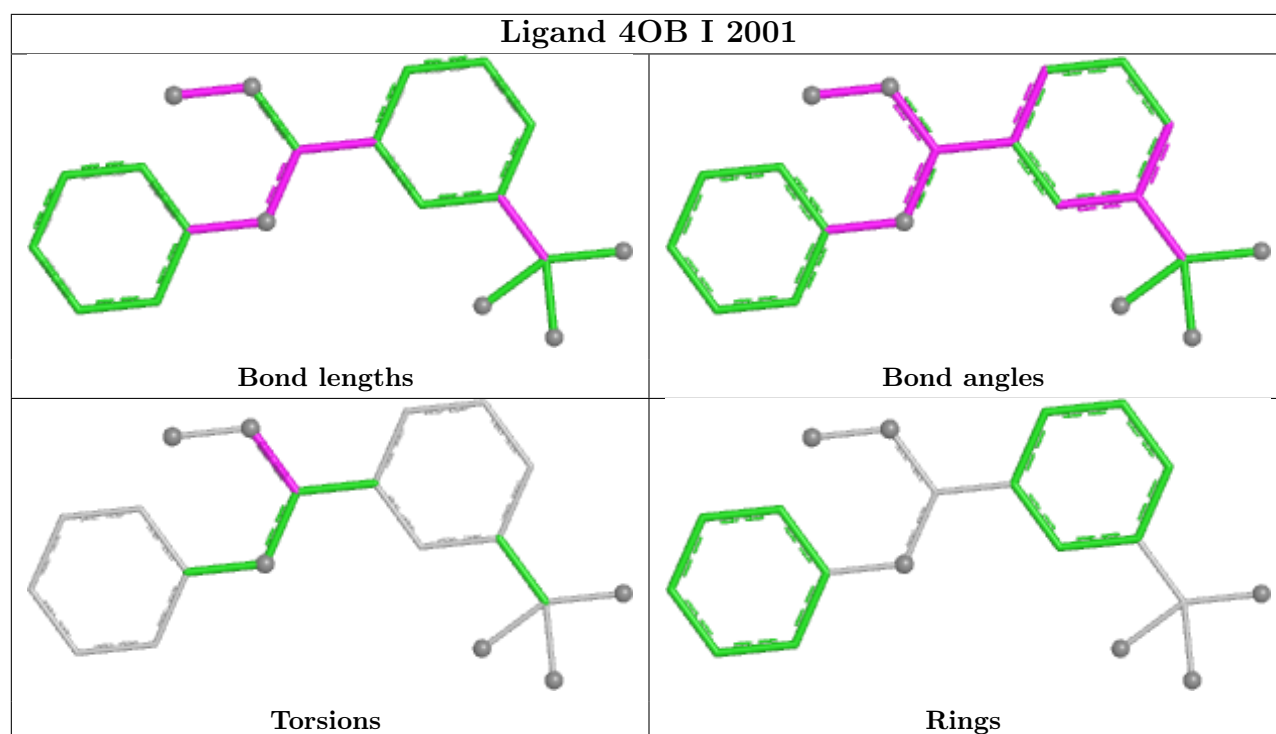
There are no ring outliers.

2 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	2001	4OB	8	0
6	I	2001	4OB	8	0

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





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	302/335 (90%)	0.06	4 (1%) 75 59	28, 105, 237, 409	0
1	B	216/335 (64%)	0.17	5 (2%) 61 47	28, 127, 210, 290	0
1	G	224/335 (66%)	0.18	12 (5%) 31 29	59, 127, 200, 244	0
1	H	216/335 (64%)	0.18	8 (3%) 45 36	49, 145, 220, 274	0
2	C	1340/1342 (99%)	0.10	18 (1%) 75 59	15, 95, 231, 320	0
2	I	1340/1342 (99%)	0.19	37 (2%) 55 42	21, 132, 241, 336	0
3	D	1166/1407 (82%)	0.09	25 (2%) 63 49	13, 70, 178, 278	0
3	J	1334/1407 (94%)	0.08	30 (2%) 62 48	16, 95, 214, 287	0
4	E	89/91 (97%)	-0.26	0 100 100	16, 93, 132, 215	0
4	K	79/91 (86%)	-0.08	2 (2%) 58 45	54, 120, 204, 224	0
5	F	542/613 (88%)	0.12	14 (2%) 57 43	31, 145, 251, 341	0
5	L	539/613 (87%)	0.14	13 (2%) 59 46	34, 147, 248, 314	0
All	All	7387/8246 (89%)	0.11	168 (2%) 61 47	13, 110, 229, 409	0

All (168) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	78	ILE	7.1
1	B	67	GLU	5.8
3	D	826	ILE	4.9
2	I	322	LEU	4.7
2	I	317	LEU	4.7
2	C	56	VAL	4.6
5	F	575	GLU	4.5
2	I	609	ILE	4.4
3	D	682	VAL	4.3
1	G	85	LEU	4.3
3	J	340	GLN	4.2

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Mol	Chain	Res	Type	RSRZ
2	I	471	VAL	4.1
3	J	341	ASN	4.0
1	G	231	PHE	4.0
2	C	209	ILE	4.0
1	G	82	LEU	3.9
3	D	604	MET	3.9
2	C	1334	GLY	3.7
5	F	463	LEU	3.7
5	L	412	LEU	3.7
2	I	251	ALA	3.7
5	F	579	GLN	3.5
5	F	140	ALA	3.5
2	I	443	ASP	3.5
3	J	1248	ILE	3.4
2	C	1046	VAL	3.4
3	J	1054	THR	3.4
3	J	1184	ASP	3.3
2	C	59	ILE	3.2
1	H	217	ILE	3.2
3	D	533	ALA	3.1
5	L	11	LEU	3.1
2	I	931	VAL	3.1
5	F	553	ALA	3.1
2	I	1256	GLN	3.1
1	A	231	PHE	3.1
3	J	160	LEU	3.1
1	A	224	LEU	3.1
5	F	27	VAL	3.1
1	A	205	MET	3.1
2	I	836	LEU	3.0
3	J	518	VAL	3.0
3	J	894	VAL	3.0
3	J	693	VAL	3.0
2	C	57	PHE	2.9
2	C	292	ILE	2.9
5	L	130	VAL	2.9
2	I	764	CYS	2.9
3	J	176	PHE	2.9
2	C	813	GLU	2.9
1	G	39	LEU	2.9
3	J	899	TYR	2.8
5	F	85	SER	2.8

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Mol	Chain	Res	Type	RSRZ
3	D	686	TRP	2.8
1	G	217	ILE	2.8
3	J	744	ARG	2.8
1	A	270	LEU	2.8
3	D	577	ALA	2.8
2	C	998	LEU	2.8
1	B	217	ILE	2.7
1	H	228	LEU	2.7
3	D	704	GLU	2.7
5	L	30	HIS	2.7
2	I	823	VAL	2.7
2	I	975	ILE	2.7
2	C	1169	VAL	2.7
1	G	230	ALA	2.7
3	D	596	LEU	2.7
3	D	678	ARG	2.6
3	J	923	ILE	2.6
1	G	224	LEU	2.6
3	J	621	ALA	2.6
2	I	6	THR	2.6
2	I	305	SER	2.6
5	F	256	PHE	2.6
5	F	269	LEU	2.6
3	J	317	THR	2.6
1	G	90	VAL	2.5
3	J	1237	VAL	2.5
2	I	450	ASN	2.5
3	J	815	GLY	2.5
2	I	818	VAL	2.5
3	J	538	ARG	2.5
2	I	882	ILE	2.5
2	I	1072	ASN	2.5
1	H	224	LEU	2.5
3	J	490	ILE	2.5
2	I	978	VAL	2.5
1	H	102	LEU	2.5
2	C	992	LEU	2.5
2	I	813	GLU	2.5
2	I	989	LEU	2.5
3	J	885	VAL	2.4
1	G	205	MET	2.4
5	L	609	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	H	142	MET	2.4
1	G	88	LEU	2.4
3	J	282	LEU	2.4
1	H	6	THR	2.4
1	G	176	CYS	2.4
5	L	166	VAL	2.4
3	D	460	ASP	2.3
3	D	528	THR	2.3
1	H	85	LEU	2.3
3	J	1161	GLY	2.3
2	I	843	THR	2.3
2	I	1052	VAL	2.3
3	D	681	LYS	2.3
3	J	1337	VAL	2.3
2	I	981	ALA	2.3
1	H	90	VAL	2.3
2	C	66	SER	2.3
2	I	318	SER	2.3
2	I	826	ASP	2.3
3	D	310	GLY	2.3
2	C	68	LEU	2.3
3	D	431	ARG	2.3
3	J	807	LEU	2.3
5	F	591	GLU	2.3
3	D	423	LEU	2.3
2	I	573	ASN	2.2
3	D	1319	PHE	2.2
3	D	482	ALA	2.2
5	L	519	LEU	2.2
2	I	816	ILE	2.2
2	C	903	ARG	2.2
5	L	7	SER	2.2
5	F	162	ILE	2.2
5	F	70	ASN	2.2
2	I	783	LEU	2.2
2	I	1198	LEU	2.2
3	J	682	VAL	2.2
2	C	205	PRO	2.2
1	G	43	LEU	2.2
2	C	60	GLN	2.2
3	D	483	LEU	2.2
5	L	73	ASP	2.2

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Mol	Chain	Res	Type	RSRZ
2	I	928	VAL	2.2
3	D	1180	VAL	2.2
3	D	1161	GLY	2.2
3	D	1265	THR	2.2
3	D	814	CYS	2.2
3	J	639	VAL	2.2
3	J	1095	MET	2.2
3	D	1228	ALA	2.1
5	L	416	VAL	2.1
3	D	302	ALA	2.1
5	F	43	ASP	2.1
2	C	686	GLN	2.1
2	I	464	PHE	2.1
2	I	311	CYS	2.1
2	I	860	ALA	2.1
5	L	25	ALA	2.1
1	B	68	TYR	2.1
4	K	13	ILE	2.1
2	I	704	MET	2.1
4	K	18	ASP	2.1
5	F	590	ILE	2.1
3	J	1271	SER	2.1
2	I	693	LEU	2.0
5	L	386	LEU	2.0
2	C	438	GLY	2.0
1	B	85	LEU	2.0
2	I	292	ILE	2.0
5	L	127	ILE	2.0
3	D	743	MET	2.0
3	J	218	THR	2.0
3	J	816	THR	2.0

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

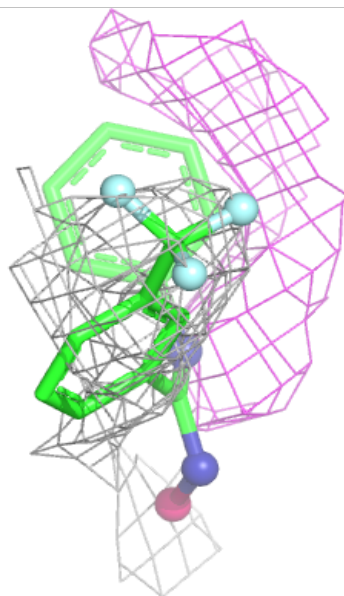
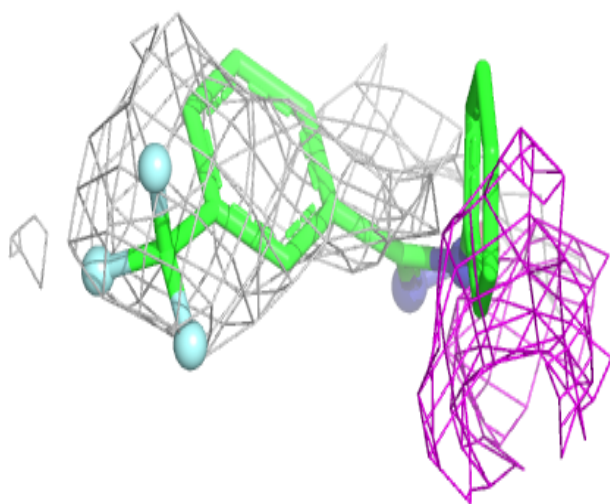
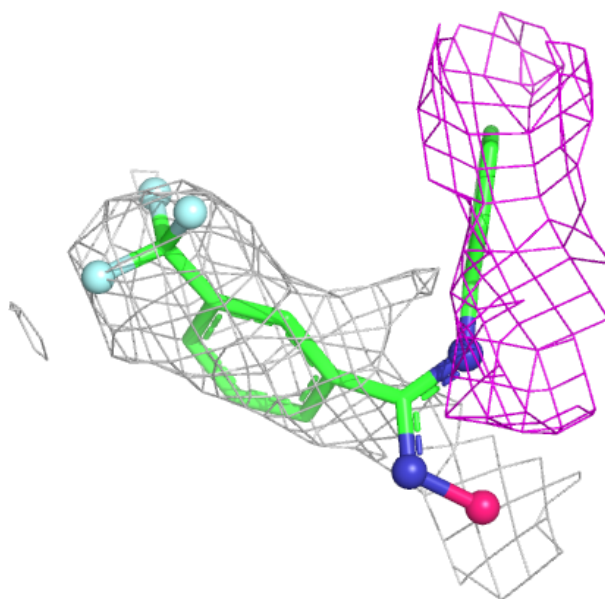
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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
7	MG	D	1501	1/1	0.52	0.38	72,72,72,72	0
6	4OB	I	2001	20/20	0.71	0.14	90,112,127,136	0
6	4OB	C	2001	20/20	0.85	0.10	50,73,98,99	0
7	MG	J	1501	1/1	0.86	0.23	33,33,33,33	0
8	ZN	D	1502	1/1	0.98	0.07	90,90,90,90	0
8	ZN	J	1502	1/1	0.98	0.06	79,79,79,79	0
8	ZN	D	1503	1/1	0.99	0.25	138,138,138,138	0
8	ZN	J	1503	1/1	1.00	0.08	31,31,31,31	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.

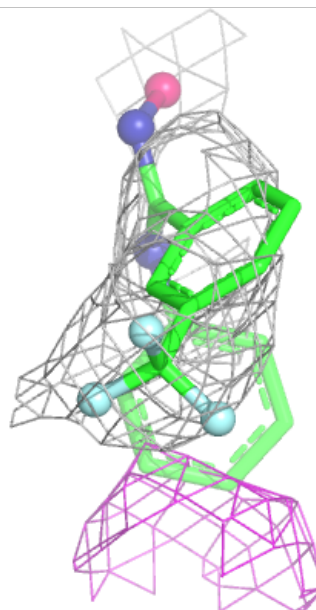
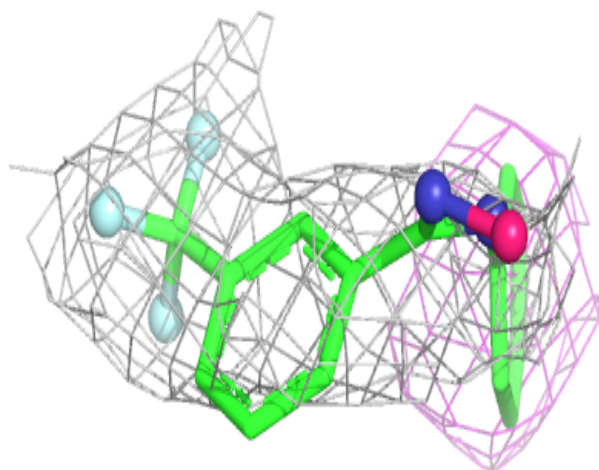
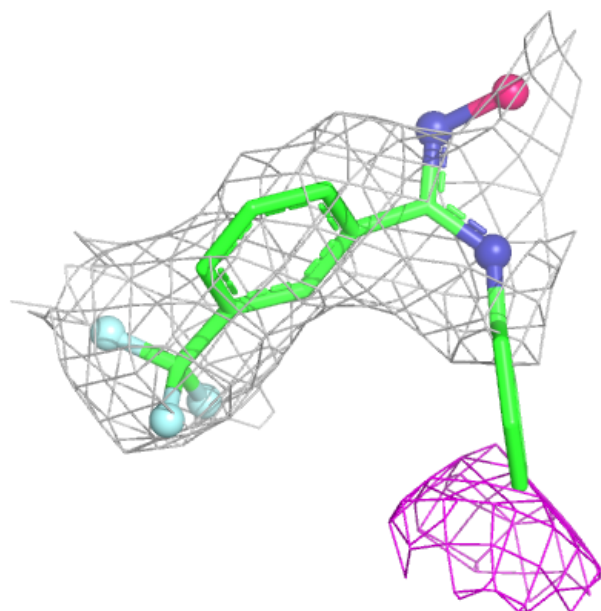
Electron density around 4OB I 2001:

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



Electron density around 4OB C 2001:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.