



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 09:27 PM GMT

PDB ID : 4ZH4
Title : Crystal structure of Escherichia coli RNA polymerase in complex with CBRP18
Authors : Feng, Y.; Ebright, R.H.
Deposited on : 2015-04-24
Resolution : 3.99 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026982
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20026982

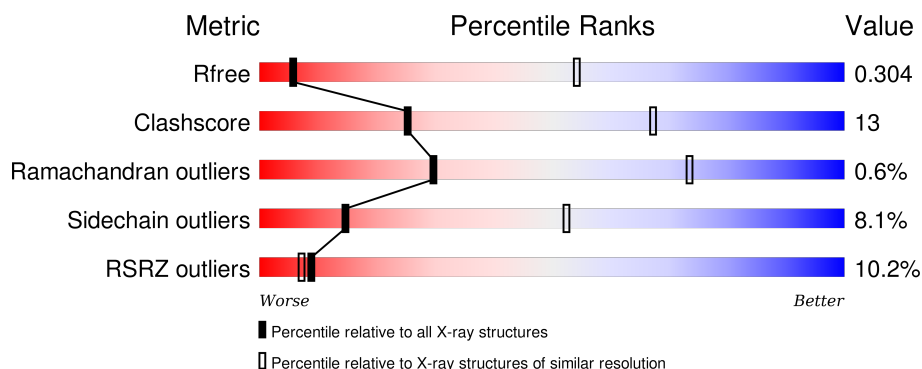
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.99 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}	91344	1010 (4.42-3.56)
Clashscore	102246	1052 (4.40-3.60)
Ramachandran outliers	100387	1005 (4.40-3.60)
Sidechain outliers	100360	1013 (4.42-3.58)
RSRZ outliers	91569	1013 (4.42-3.56)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	335	<div> <div>7%</div> <div>60%</div> <div>26%</div> <div>10%</div> </div>
1	B	335	<div> <div>6%</div> <div>38%</div> <div>24%</div> <div>36%</div> </div>
1	G	335	<div> <div>5%</div> <div>41%</div> <div>24%</div> <div>33%</div> </div>
1	H	335	<div> <div>11%</div> <div>38%</div> <div>24%</div> <div>36%</div> </div>
2	C	1342	<div> <div>9%</div> <div>66%</div> <div>31%</div> <div>•</div> </div>

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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	4OE	C	2001	-	-	-	X
6	4OE	I	2001	-	-	-	X

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 57539 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	1151	Total	C	N	O	S	0	0	0
			8992	5653	1608	1686	45			
3	J	1319	Total	C	N	O	S	0	0	0
			10254	6443	1824	1939	48			

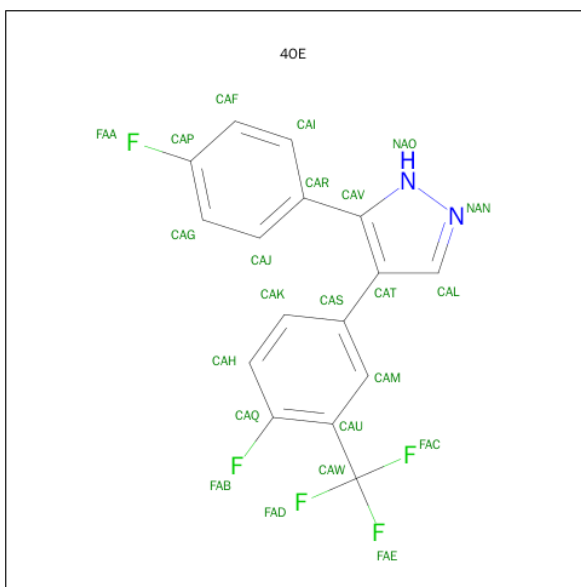
- Molecule 4 is a protein called DNA-directed RNA polymerase subunit omega.

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 5-(4-fluorophenyl)-4-[4-fluoro-3-(trifluoromethyl)phenyl]-1H-pyrazole (three-letter code: 4OE) (formula: C₁₆H₉F₅N₂).



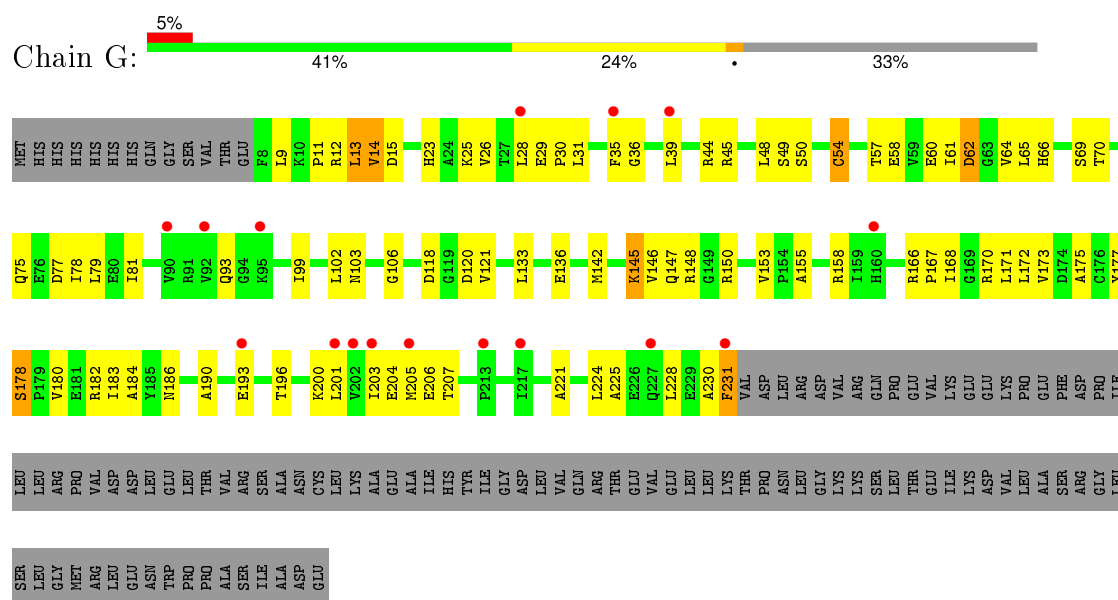
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	F	N	0	0
			23	16	5	2		
6	I	1	Total	C	F	N	0	0
			23	16	5	2		

- Molecule 7 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

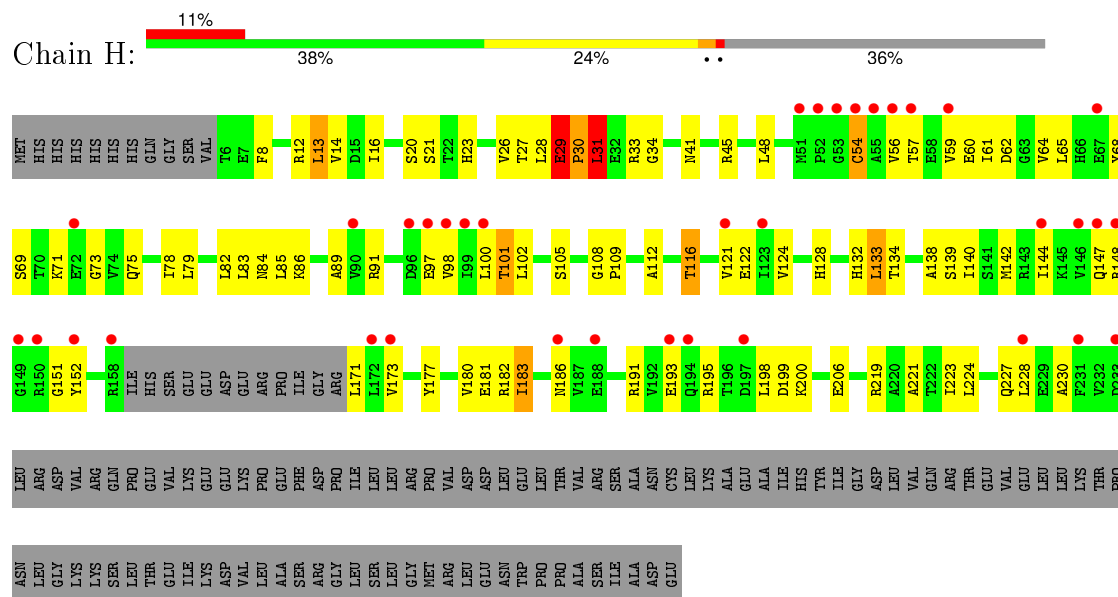
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	J	1	Total	Mg	0	0
			1	1		
7	D	1	Total	Mg	0	0
			1	1		

- Molecule 8 is ZINC ION (three-letter code: ZN) (formula: Zn).

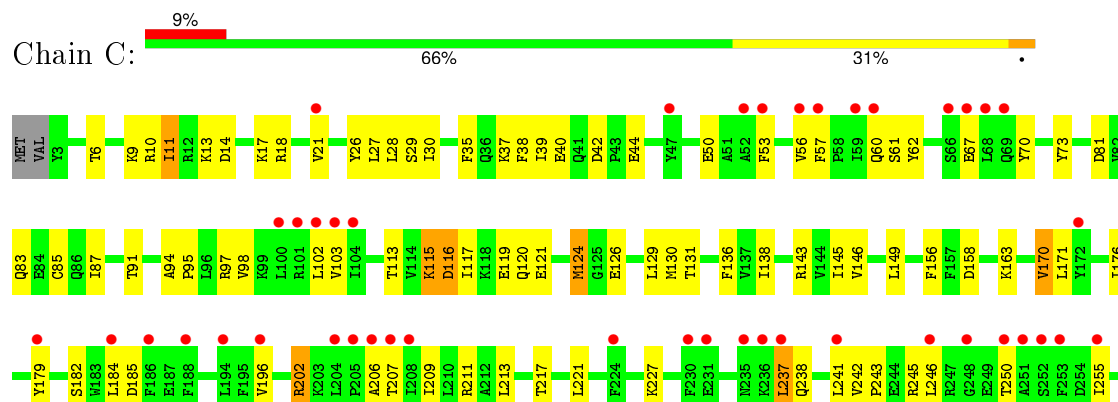
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	J	2	Total	Zn	0	0
			2	2		
8	D	2	Total	Zn	0	0
			2	2		

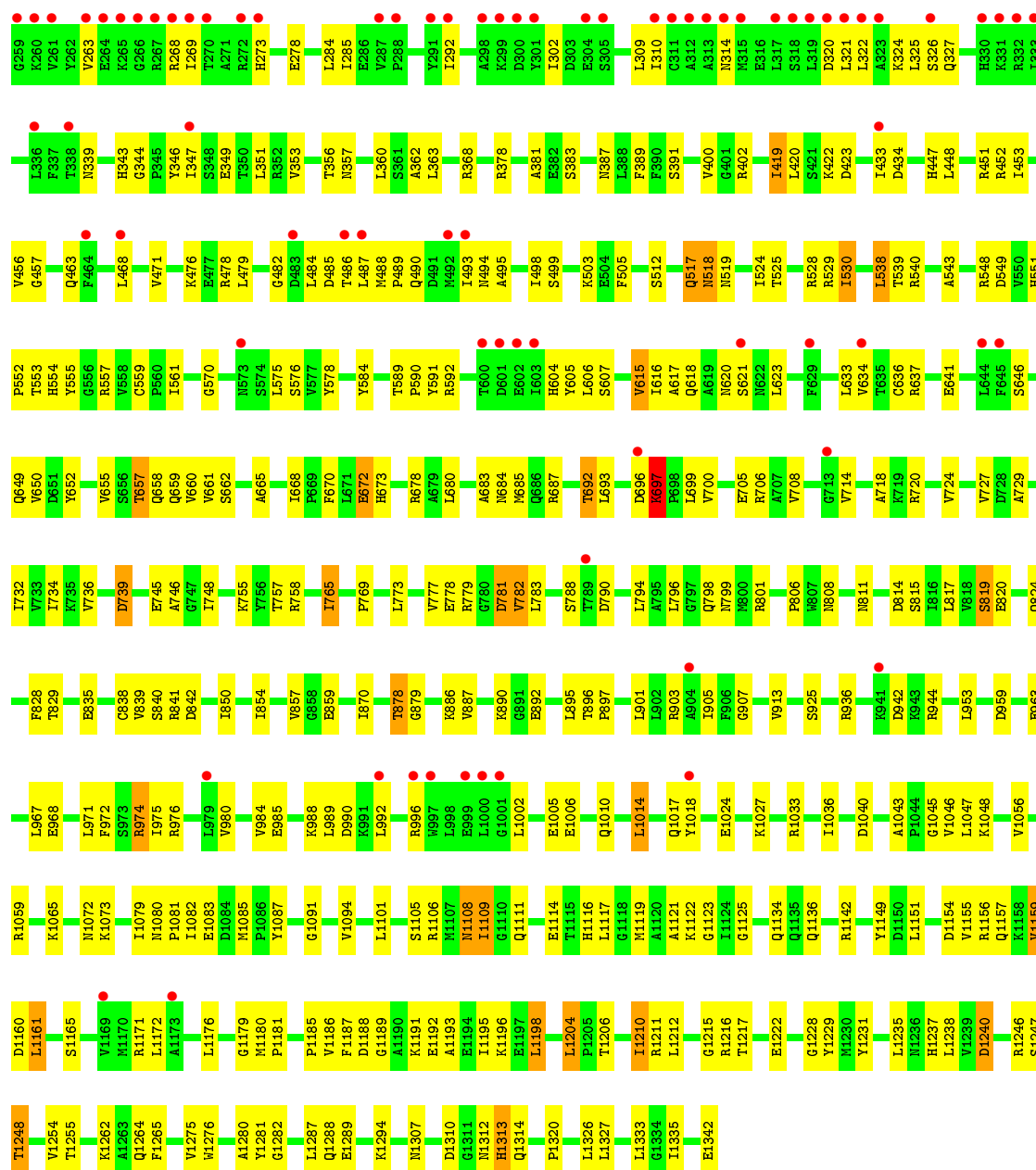


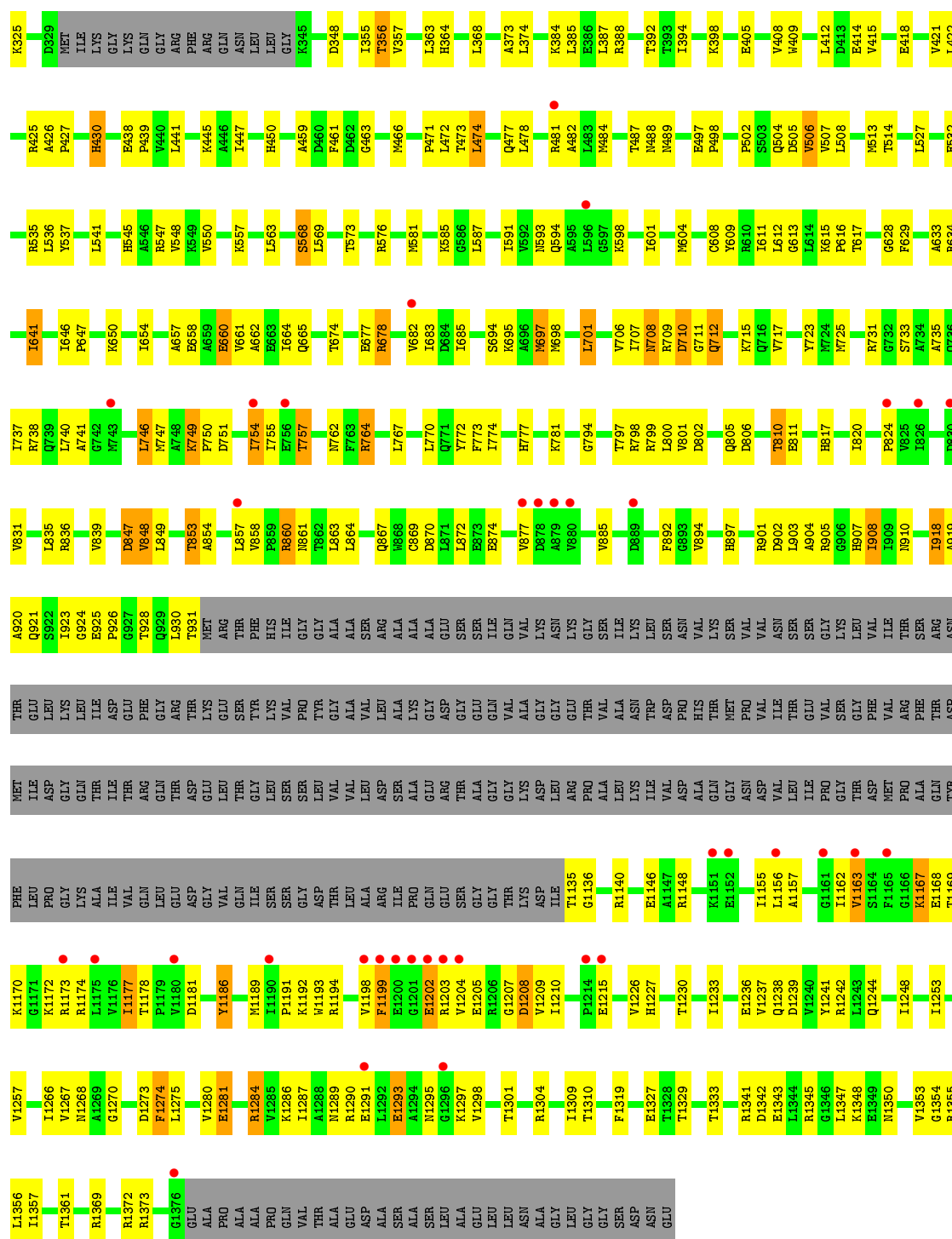
• Molecule 1: DNA-directed RNA polymerase subunit alpha



• Molecule 2: DNA-directed RNA polymerase subunit beta





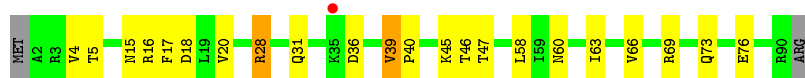
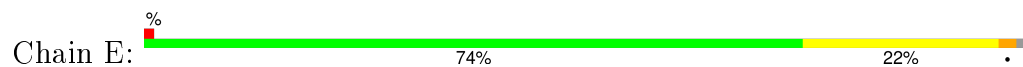


• Molecule 3: DNA-directed RNA polymerase subunit beta'



R1345	G1346	D1239	G1161	L1078	V1011	L849	V747	A562	L563	P471	Q365	L279	L189	V92
G1347	Y1240	Y1241	G1162	R1079	A1012	R850	A748	E563	S588	L474	C366	L282	K190	T95
K1348	R1242	R1243	V1163	I1080	G1013	T853	K750	I664	L569	P750	L368	A287	M192	V97
E1349	Q1244	Q1243	K1167	A1083	V1017	A854	D751	Q668	K570	Q477	A373	I230	D193	R101
M1350			E1168	A1084	A1018	L857	I754	Q669	D571	L478	E375	I230	E197	M102
V1353	I1248		T1169	ARG	W1019	P858	I755	S670	T572	P479	L374	I291	C198	G103
G1354	E1254		K1170	ALA	W1020	P859	E756	R678	V574	R481	E375	V292	G198	H104
I1357			R1171	ALA		R860	I757	R678	G575	M484	P379	K296	L201	
T1361	V1257		R1172	GLU	T1024	L863	N762	K681	R576			K296	L201	
			R1173	S948	M1025	L864	F763	V682				R297	R202	I114
			L1175	S949	P1026		R764	I683	L579			M298	E203	H115
D1368	I1266		V1176	I950	V1027	Q887	L767	D684	M580			E204	L205	F116
	V1267		I1177	P951	I1028	L872		I685	M581			D304	L387	L117
R1371	N1268		T1178	P952	T1029	L873		M686	I582			A305	M206	K118
A1269	A1269		P1179	R955	S1032			A689	K585	P602		L306	M206	S119
R1373	G1270		V1180	Q956	G1033	V877		S584	G586	S503		I307	T208	L120
A1374			D1181	S957	F1034			K695	L587	P506		D308	M209	P121
	D1273			F1100	F1035	S884		A696	P588				S210	P122
	F1274		Y1186	L1101	R1036	V885		M697	I591			R311	R214	G125
GLY	L1275		E1187	G1103	F1037			M698	V592			R312	R214	I124
ALA			M1188			C888	H777		M593			T317	L217	L126
PRO	V1280		E1189	I1106	M1040	D889			Q594				T218	L127
ALA	E1281			Y1107	I1041	T880	R780	L701				N320	T221	L128
			P1191	Q1108	I1042	D891	K781							R133
R1284			K1192	S965	G1043	F892		V706	K598			L324	I221	
V1285	K1286		W1193	G1044	T1045	G893	G794	I707				K325	V228	
VAL			R1194	Q1045	Q1046	H894		N708	I601					R137
					I1047	C895	I797	R709	M604			D329	P234	
T1289			Q1195	I1114	T1048	A896	R798	D710				MET	E235	
R1290			I1115	T1115	K1048	R897	R799	G711				ILE	E142	F141
			S1117	S1117	Q1049	C898	L800	Q712				LYS	P243	E142
E1293			G1118	S977	T1050			E713				GLY	A426	S143
ALA	A1294		F1199	G1118	T1050			E522				LYS	V244	
SER	N1295			D1119	D1051	R901	D802	E714				LYS	D248	I147
ALA	G1296		E1202	T1120	E1052	D902	V803	K715				GLN	E148	
			R1203	L1121	L1053	L903		Q716				GLY		
R1297			V1204	A1122	G1054	A904	D806					ARG	L252	
V1298			E1205	R1123	G1055	R905		S718				PHE	V253	T152
	T1301		G1207	I1124	L1056	G906		F719				ARG	P254	N153
GLU	Y1302		D1208	P1125	S1057	H907	E311					GLN	L255	A154
S1303				Q1126	S1058	I908		Y723				ASN	D256	E155
R1304				GLU	L1059		H817					LEU	G257	R156
ASN				SER	V1060	I918		R731				LEU	G258	Q158
					V1061	A919		G732				GLY		
GLY	I1309		E1215	GLY	T1062	A920		S539				K345	T262	T161
LEU				THR	L1063	R991		G540				R346	S263	
GLY	S1318		P1217	THR	S1064	Q921	P824	A734				V347	D264	Q164
GLY	F1319			LYS	A1065			A735				D348	L285	
SER				ASP		G924		Q736				Y349	N286	L169
ASP	E1327		V1226	ILE				I737					D287	
ASN	T1328		H1227	THR	T1068	T928		R738				I355	L288	E175
GLU	T1329			GLY	A1069	Q929	L835	Q739				T356	F176	D177
					G1070	L930		L740				R270	G259	A178
	T1333		T1230		K1071	T931		A741					R270	
					G1072	MET		G742						K179
			I1233		D1073	ARG	V843	N743				L361	I273	
R1341					L1074	THR		R744				R362	N274	M180
D1342			E1236			PHE		G745					R275	
E1343			V1237											
L1344			Q1238		A1157			L746						

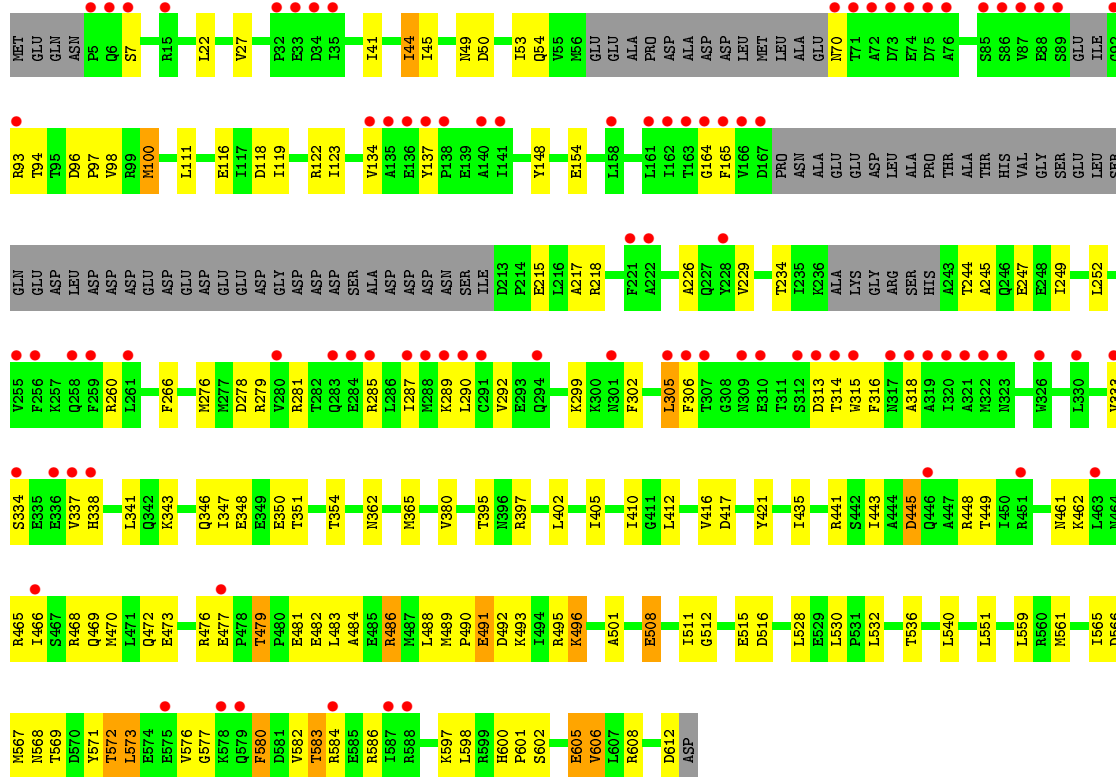
- Molecule 4: DNA-directed RNA polymerase subunit omega



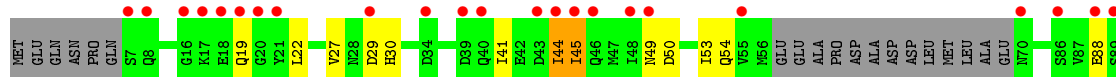
- Molecule 4: DNA-directed RNA polymerase subunit omega



- Molecule 5: RNA polymerase sigma factor RpoD



- Molecule 5: RNA polymerase sigma factor RpoD



D526	D528	L529	L530	L540	V547	L548	L551	L559	R560	M561	D566	M567	M568	T569	D570	Y571	T572	L573	V576	G577	F580	D581	V582	T583	R584	E585	R586	Q589	K593	R596	K597	L598	R599	H600	F601	S602	E605	V606	L607	R608	S609	F610	D613								
D444	D445	Q446	A447	R448	T449	P453	V454	I457	M461	R465	I466	R468	S467	Q469	M470	E473	R476	E477	P478	T479	P480	E481	E482	L483	A484	E485	R486	M487	M489	P490	E491	D492	K493	L494	R495	K496	V497	L498	K499	I500	A501	M507	E508	I511	G512	E515	D516	G520			
I320	A321	P325	M326	S327	E328	K329	L330	V333	S334	V337	H338	L341	Q342	K343	L344	Q345	I346	E347	E348	E349	E350	T351	T354	N362	R363	R364	M365	T395	N396	R397	G398	L399	Q400	F401	L402	I405	N409	I410	G411	L412	D417	Y421	T429	I435	I436	I438	I443				
E248	I249	L252	S253	F256	K257	Q258	F259	R260	K264	Q265	F266	M273	M276	D278	R279	V280	R281	T282	Q283	E284	R285	L286	I287	M288	K289	L290	C291	V292	E293	Q294	C295	K296	K299	F302	I303	L304	L305	F306	T307	G308	N309	E310	T311	S312	D313	T314	M315	F316	M317	A318	A319
VAL	GLY	SER	GLU	LEU	SER	GLN	GLU	ASP	LEU	ASP	ASP	GLU	ASP	ASP	GLY	ASP	ASP	ASP	SER	ALA	ASP	ASP	ASN	SER	ILE	D213	P214	E215	L216	A217	R218	F221	R225	Y228	V229	T234	I235	K236	ALA	LYS	GLY	ARG	SER	LEU	ALA	PRO	THR	ALA	THR	HIS	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	185.58Å 204.10Å 308.04Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.20 – 3.99 49.79 – 3.99	Depositor EDS
% Data completeness (in resolution range)	93.1 (49.20-3.99) 92.3 (49.79-3.99)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.00 (at 4.00Å)	Xtriage
Refinement program	PHENIX	Depositor
R, R_{free}	0.250 , 0.283 0.287 , 0.304	Depositor DCC
R_{free} test set	1978 reflections (2.19%)	DCC
Wilson B-factor (Å ²)	156.4	Xtriage
Anisotropy	0.091	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 88.8	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 98970 reflections	Xtriage
F_o, F_c correlation	0.88	EDS
Total number of atoms	57539	wwPDB-VP
Average B, all atoms (Å ²)	116.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.57% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, MG, 4OE

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	0.39	1/2358 (0.0%)	0.67	2/3197 (0.1%)
1	B	0.39	0/1687	0.73	1/2286 (0.0%)
1	G	0.33	0/1751	0.66	0/2373
1	H	0.37	0/1681	0.70	2/2278 (0.1%)
2	C	0.28	0/10739	0.49	0/14489
2	I	0.28	1/10735 (0.0%)	0.47	0/14484
3	D	0.29	0/9130	0.50	1/12325 (0.0%)
3	J	0.27	0/10409	0.48	1/14059 (0.0%)
4	E	0.29	0/693	0.49	0/935
4	K	0.26	0/629	0.48	0/847
5	F	0.31	2/4254 (0.0%)	0.51	1/5731 (0.0%)
5	L	0.28	0/4246	0.49	0/5720
All	All	0.30	4/58312 (0.0%)	0.52	8/78724 (0.0%)

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

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	954	LYS	CD-CE	-6.99	1.33	1.51
5	F	605	GLU	CD-OE2	5.91	1.32	1.25
1	A	231	PHE	CD2-CE2	-5.76	1.27	1.39
5	F	605	GLU	CD-OE1	5.01	1.31	1.25

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	250	ASP	CB-CG-OD1	-9.38	109.86	118.30
5	F	605	GLU	OE1-CD-OE2	9.01	134.11	123.30
1	B	29	GLU	C-N-CD	8.36	145.96	128.40
1	H	13	LEU	CA-CB-CG	6.42	130.07	115.30
3	D	120	LEU	N-CA-C	5.85	126.80	111.00
3	J	120	LEU	N-CA-C	5.43	125.66	111.00
1	H	31	LEU	CA-CB-CG	5.41	127.75	115.30
1	A	317	ARG	CD-NE-CZ	5.02	130.62	123.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	D	120	LEU	Peptide
3	J	120	LEU	Peptide

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2328	0	2380	72	0
1	B	1667	0	1692	63	0
1	G	1730	0	1756	69	0
1	H	1662	0	1687	67	0
2	C	10570	0	10582	277	0
2	I	10566	0	10576	262	0
3	D	8992	0	9180	271	0
3	J	10254	0	10461	313	0
4	E	691	0	695	14	0
4	K	627	0	634	19	0
5	F	4204	0	4106	95	0
5	L	4196	0	4103	103	0
6	C	23	0	9	5	0
6	I	23	0	9	4	0
7	D	1	0	0	0	0
7	J	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	D	2	0	0	0	0
8	J	2	0	0	0	0
All	All	57539	0	57870	1457	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 (1457) 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:D:660:GLU:HB3	3:D:685:ILE:HD12	1.41	1.01
3:J:660:GLU:HB3	3:J:685:ILE:HD12	1.46	0.97
1:H:29:GLU:HB3	1:H:30:PRO:HD3	1.48	0.95
3:D:1280:VAL:HG21	3:D:1304:ARG:HE	1.39	0.88
2:C:1105:SER:HB2	3:D:731:ARG:HG2	1.56	0.87
1:A:190:ALA:HB2	1:A:200:LYS:HB2	1.58	0.86
1:G:190:ALA:HB2	1:G:200:LYS:HB2	1.58	0.85
3:D:418:GLU:HG3	4:E:45:LYS:H	1.42	0.85
2:I:1065:LYS:HE2	3:J:463:GLY:HA3	1.58	0.84
3:J:1044:GLN:HB3	3:J:1071:GLY:HA3	1.59	0.83
2:I:1105:SER:HB2	3:J:731:ARG:HG2	1.61	0.83
2:I:525:THR:HG21	2:I:687:ARG:HD2	1.61	0.83
1:H:28:LEU:HB3	1:H:31:LEU:HD21	1.61	0.82
3:D:755:ILE:HD13	3:D:774:ILE:HD11	1.59	0.82
2:C:525:THR:HG21	2:C:687:ARG:HD2	1.63	0.81
2:C:310:ILE:HG21	2:C:325:LEU:HB3	1.61	0.80
3:J:1280:VAL:HG21	3:J:1304:ARG:HE	1.45	0.80
2:C:1065:LYS:HE2	3:D:463:GLY:HA3	1.62	0.79
3:J:418:GLU:HG3	4:K:45:LYS:H	1.46	0.79
1:A:231:PHE:HE2	1:B:43:LEU:HD21	1.46	0.79
2:I:673:HIS:HB3	2:I:1109:ILE:HG22	1.65	0.79
2:I:10:ARG:HD3	2:I:1181:PRO:HG2	1.64	0.78
2:C:10:ARG:HD3	2:C:1181:PRO:HG2	1.64	0.78
2:C:953:LEU:HD11	2:C:1033:ARG:HG3	1.65	0.78
3:D:392:THR:HG21	5:F:606:VAL:HA	1.64	0.78
2:I:953:LEU:HD11	2:I:1033:ARG:HG3	1.64	0.77
3:J:155:GLU:HB2	3:J:158:GLN:HB2	1.66	0.77
2:I:310:ILE:HG21	2:I:325:LEU:HB3	1.67	0.77
5:F:561:MET:HA	5:F:567:MET:HE1	1.66	0.76
2:I:840:SER:HB2	2:I:850:ILE:HD11	1.68	0.76
1:A:99:ILE:HG12	1:A:145:LYS:HG2	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1312:ASN:HD21	2:I:1314:GLN:HE21	1.34	0.75
5:L:479:THR:HG22	5:L:482:GLU:HB2	1.68	0.75
3:J:755:ILE:HD13	3:J:774:ILE:HD11	1.69	0.74
3:J:755:ILE:HG22	3:J:757:THR:H	1.51	0.74
5:F:479:THR:HG22	5:F:482:GLU:HB2	1.69	0.74
1:G:99:ILE:HG12	1:G:145:LYS:HG2	1.69	0.74
2:I:873:ILE:HG13	2:I:944:ARG:HH22	1.52	0.73
1:H:101:THR:HG22	1:H:116:THR:HB	1.68	0.73
3:J:282:LEU:HD21	5:L:410:ILE:HG12	1.71	0.73
2:C:559:CYS:HB2	2:C:662:SER:HB3	1.70	0.73
2:I:292:ILE:HB	2:I:322:LEU:HD11	1.71	0.73
1:H:59:VAL:O	1:H:171:LEU:N	2.22	0.73
1:B:101:THR:HG22	1:B:116:THR:HB	1.71	0.73
2:C:696:ASP:HB2	2:C:798:GLN:HG2	1.69	0.73
2:C:673:HIS:HB3	2:C:1109:ILE:HG22	1.70	0.72
1:A:45:ARG:HH22	2:C:1216:ARG:HA	1.54	0.72
6:I:2001:4OE:H9	3:J:774:ILE:HB	1.71	0.72
2:C:1312:ASN:HD21	2:C:1314:GLN:HE21	1.36	0.72
2:I:10:ARG:NH2	2:I:790:ASP:OD2	2.23	0.72
2:I:696:ASP:HB2	2:I:798:GLN:HG2	1.70	0.72
3:D:489:ASN:HA	3:D:904:ALA:HB1	1.72	0.72
1:G:23:HIS:HB2	1:G:205:MET:O	1.90	0.71
3:J:514:THR:HG23	3:J:576:ARG:HG2	1.72	0.71
1:A:23:HIS:HB2	1:A:205:MET:O	1.90	0.71
3:J:1035:VAL:HG21	3:J:1121:LEU:HD21	1.72	0.71
2:C:18:ARG:NH2	2:C:620:ASN:OD1	2.23	0.71
2:C:10:ARG:NH2	2:C:790:ASP:OD2	2.24	0.71
1:H:29:GLU:HB3	1:H:30:PRO:CD	2.20	0.71
2:I:203:LYS:HB2	5:L:29:ASP:HB2	1.72	0.71
3:D:155:GLU:HB2	3:D:158:GLN:HB2	1.72	0.71
2:C:840:SER:HB2	2:C:850:ILE:HD11	1.71	0.70
2:I:452:ARG:NH1	2:I:584:TYR:O	2.24	0.70
5:L:561:MET:HA	5:L:567:MET:HE1	1.72	0.70
2:I:559:CYS:HB2	2:I:662:SER:HB3	1.72	0.70
2:C:814:ASP:OD2	2:C:1106:ARG:NH1	2.23	0.70
5:L:470:MET:HA	5:L:473:GLU:HB3	1.73	0.70
2:I:734:ILE:HD11	2:I:783:LEU:HD11	1.72	0.70
1:A:45:ARG:NH2	2:C:1215:GLY:O	2.23	0.70
2:C:806:PRO:HA	2:C:811:ASN:HD21	1.54	0.70
2:I:806:PRO:HA	2:I:811:ASN:HD21	1.56	0.70
2:I:528:ARG:NH2	2:I:576:SER:O	2.24	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:514:THR:HG23	3:D:576:ARG:HG2	1.74	0.70
3:D:120:LEU:HD22	3:D:121:PRO:HD3	1.73	0.69
3:J:1026:PRO:HB2	3:J:1028:ILE:HG23	1.75	0.69
1:B:133:LEU:HD11	1:B:140:ILE:HG21	1.73	0.69
2:I:814:ASP:OD2	2:I:1106:ARG:NH1	2.21	0.69
1:G:45:ARG:NH2	2:I:1215:GLY:O	2.22	0.69
2:C:732:ILE:HG21	2:C:783:LEU:HD12	1.74	0.69
3:D:797:THR:HG22	3:D:924:GLY:HA3	1.74	0.69
2:I:1106:ARG:HE	3:J:731:ARG:HH21	1.40	0.68
3:D:133:ARG:NH2	5:F:93:ARG:O	2.25	0.68
3:J:797:THR:HG22	3:J:924:GLY:HA3	1.74	0.68
1:H:133:LEU:HD11	1:H:140:ILE:HG21	1.75	0.68
2:C:528:ARG:NH2	2:C:576:SER:O	2.27	0.68
2:C:1238:LEU:HD12	2:C:1238:LEU:H	1.59	0.68
2:I:18:ARG:NH1	2:I:621:SER:O	2.27	0.67
2:I:18:ARG:NH2	2:I:620:ASN:OD1	2.27	0.67
5:F:602:SER:H	5:F:605:GLU:HG3	1.59	0.67
5:F:470:MET:HA	5:F:473:GLU:HB3	1.74	0.67
1:A:166:ARG:O	1:A:168:ILE:N	2.27	0.67
2:C:452:ARG:NH1	2:C:584:TYR:O	2.28	0.67
2:C:221:LEU:HD11	2:C:314:ASN:HB2	1.75	0.67
1:H:191:ARG:NH2	3:J:410:ASP:OD2	2.27	0.67
1:B:62:ASP:OD2	1:B:71:LYS:NZ	2.28	0.67
5:L:134:VAL:HG21	5:L:266:PHE:HE1	1.60	0.67
1:A:184:ALA:HB2	2:C:1091:GLY:HA3	1.75	0.67
3:J:80:HIS:HB3	3:J:83:VAL:HG11	1.78	0.66
2:I:657:THR:HG21	2:I:1188:ASP:HB2	1.76	0.66
2:I:808:ASN:H	3:J:633:ALA:HB2	1.60	0.66
2:I:221:LEU:HD11	2:I:314:ASN:HB2	1.76	0.66
3:J:664:ILE:HG22	3:J:678:ARG:HG2	1.77	0.66
2:I:1116:HIS:HE1	3:J:641:ILE:H	1.44	0.66
3:D:356:THR:OG1	3:D:357:VAL:N	2.29	0.66
2:C:657:THR:HG21	2:C:1188:ASP:HB2	1.77	0.66
3:J:489:ASN:HA	3:J:904:ALA:HB1	1.78	0.66
3:D:317:THR:HG23	3:D:320:ASN:HB3	1.76	0.66
1:A:225:ALA:HA	1:A:228:LEU:HD23	1.78	0.66
2:C:18:ARG:NH1	2:C:621:SER:O	2.29	0.65
3:D:806:ASP:HA	3:D:1347:LEU:HD13	1.78	0.65
1:G:39:LEU:HD11	1:H:227:GLN:HB3	1.77	0.65
5:F:134:VAL:HG21	5:F:266:PHE:HE1	1.61	0.65
3:D:425:ARG:HD2	3:D:459:ALA:HB2	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:853:THR:HG21	3:J:1375:ALA:HB1	1.78	0.65
1:G:166:ARG:O	1:G:168:ILE:N	2.30	0.65
1:A:61:ILE:HG22	1:A:62:ASP:H	1.61	0.65
2:I:732:ILE:HG21	2:I:783:LEU:HD12	1.77	0.65
2:C:1106:ARG:HE	3:D:731:ARG:HH21	1.44	0.65
2:C:292:ILE:HB	2:C:322:LEU:HD11	1.77	0.65
3:D:755:ILE:HG22	3:D:757:THR:H	1.60	0.64
3:J:532:GLU:HA	3:J:535:ARG:HB3	1.78	0.64
1:A:231:PHE:HE2	1:B:43:LEU:CD2	2.10	0.64
2:I:88:ARG:NH2	2:I:1035:LYS:O	2.30	0.64
3:J:905:ARG:HH11	4:K:16:ARG:HD2	1.60	0.64
2:I:103:VAL:HG12	2:I:116:ASP:HB3	1.79	0.64
2:C:302:ILE:HG22	2:C:309:LEU:HA	1.80	0.64
2:I:197:ARG:HH12	5:L:29:ASP:HB3	1.62	0.64
3:J:1199:PHE:HB2	3:J:1202:GLU:HB2	1.80	0.64
2:I:829:THR:HA	2:I:1059:ARG:HA	1.80	0.64
3:J:806:ASP:HA	3:J:1347:LEU:HD13	1.80	0.64
3:J:748:ALA:O	3:J:777:HIS:HD2	1.80	0.64
3:J:425:ARG:HD2	3:J:459:ALA:HB2	1.80	0.64
1:G:61:ILE:HG22	1:G:62:ASP:H	1.62	0.64
5:F:461:ASN:O	5:F:465:ARG:HG2	1.98	0.64
2:I:1157:GLN:HG3	2:I:1159:VAL:HG13	1.79	0.64
5:F:292:VAL:HG21	5:F:299:LYS:HG3	1.80	0.63
2:C:463:GLN:HG3	2:C:505:PHE:HB2	1.80	0.63
5:L:593:LYS:HE2	5:L:596:ARG:HD3	1.79	0.63
3:D:1280:VAL:HG11	3:D:1304:ARG:HH21	1.63	0.63
2:C:746:ALA:HA	2:C:974:ARG:HH21	1.63	0.63
3:D:746:LEU:HD22	3:D:754:ILE:HD11	1.80	0.63
3:D:664:ILE:HG22	3:D:678:ARG:HG2	1.81	0.63
3:J:356:THR:OG1	3:J:357:VAL:N	2.32	0.63
3:J:646:ILE:HD11	3:J:764:ARG:HD2	1.79	0.63
1:H:100:LEU:HD21	1:H:121:VAL:HG11	1.81	0.63
3:D:77:ARG:HE	5:F:569:THR:HA	1.64	0.63
3:D:304:ASP:OD2	3:D:312:ARG:NH2	2.31	0.63
2:C:976:ARG:HD2	2:C:989:LEU:HD23	1.81	0.62
5:F:561:MET:HG2	5:F:576:VAL:HG22	1.81	0.62
2:C:734:ILE:HD11	2:C:783:LEU:HD11	1.80	0.62
5:L:292:VAL:HG21	5:L:299:LYS:HG3	1.80	0.62
1:B:51:MET:HB3	1:B:178:SER:HA	1.81	0.62
1:H:73:GLY:HA3	1:H:138:ALA:HB1	1.82	0.62
1:G:12:ARG:HG3	1:H:230:ALA:HB1	1.82	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:532:GLU:HA	3:D:535:ARG:HB3	1.81	0.62
3:D:262:THR:OG1	3:D:266:ASN:ND2	2.32	0.62
3:D:1199:PHE:HB2	3:D:1202:GLU:HB2	1.82	0.62
2:I:985:GLU:HB3	2:I:988:LYS:HB2	1.82	0.62
2:C:1142:ARG:HH22	2:C:1165:SER:HB2	1.65	0.61
1:H:29:GLU:CB	1:H:30:PRO:HD3	2.25	0.61
1:H:73:GLY:HA2	1:H:134:THR:HG22	1.81	0.61
3:D:1174:ARG:HG2	3:D:1189:MET:HG2	1.82	0.61
1:A:31:LEU:HD11	1:A:201:LEU:HB2	1.81	0.61
2:I:1142:ARG:HH22	2:I:1165:SER:HB2	1.65	0.61
5:F:276:MET:SD	5:F:279:ARG:NH1	2.74	0.61
2:I:976:ARG:HD2	2:I:989:LEU:HD23	1.81	0.61
2:I:1151:LEU:HD21	2:I:1198:LEU:HD23	1.82	0.61
2:C:13:LYS:HZ3	2:C:1151:LEU:HD12	1.63	0.61
6:C:2001:4OE:H8	3:D:773:PHE:HB3	1.83	0.61
1:H:14:VAL:HG11	1:H:29:GLU:HG2	1.83	0.61
2:C:1106:ARG:H	2:C:1106:ARG:HD2	1.64	0.61
2:I:207:THR:HG21	2:I:351:LEU:HG	1.82	0.61
5:L:225:ARG:O	5:L:229:VAL:HG13	2.00	0.61
2:C:757:THR:HG23	2:C:765:ILE:HG23	1.82	0.61
3:D:749:LYS:HG3	3:D:751:ASP:HB3	1.82	0.61
1:B:73:GLY:HA2	1:B:134:THR:HG22	1.82	0.61
1:A:231:PHE:CE2	1:B:43:LEU:HD21	2.32	0.61
3:J:304:ASP:OD2	3:J:312:ARG:NH2	2.34	0.61
3:D:817:HIS:CE1	3:D:860:ARG:HE	2.17	0.61
2:C:61:SER:HB3	2:C:479:LEU:HB3	1.83	0.60
1:G:31:LEU:HD11	1:G:201:LEU:HB2	1.83	0.60
2:I:176:ILE:HD12	2:I:184:LEU:HD23	1.83	0.60
1:A:50:SER:HB3	1:A:150:ARG:HD2	1.81	0.60
2:C:1157:GLN:HG3	2:C:1159:VAL:HG13	1.82	0.60
1:A:155:ALA:HA	1:A:158:ARG:HG3	1.84	0.60
3:D:325:LYS:HD3	5:F:508:GLU:HG2	1.84	0.60
3:D:905:ARG:HH11	4:E:16:ARG:HD2	1.64	0.60
5:L:305:LEU:HD13	5:L:315:TRP:HA	1.83	0.60
3:D:1280:VAL:HG21	3:D:1304:ARG:NE	2.14	0.60
5:F:49:ASN:HA	5:F:53:ILE:HA	1.83	0.60
2:I:149:LEU:HD13	2:I:453:ILE:HG13	1.84	0.60
1:A:250:ASP:HB2	5:F:605:GLU:HG2	1.83	0.60
3:J:388:ARG:NH1	3:J:414:GLU:OE1	2.34	0.60
5:F:602:SER:H	5:F:605:GLU:CG	2.15	0.60
4:E:73:GLN:HA	4:E:76:GLU:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:262:THR:OG1	3:J:266:ASN:ND2	2.35	0.60
6:C:2001:4OE:H9	3:D:774:ILE:HB	1.82	0.60
1:G:12:ARG:HG2	1:G:13:LEU:H	1.66	0.60
3:D:1293:GLU:H	3:J:1226:VAL:HB	1.66	0.60
3:J:527:LEU:HD23	3:J:532:GLU:HG3	1.84	0.59
3:J:650:LYS:HE2	3:J:654:ILE:HD11	1.82	0.59
2:I:1108:ASN:OD1	2:I:1111:GLN:NE2	2.35	0.59
3:D:741:ALA:O	3:D:762:ASN:ND2	2.35	0.59
5:F:602:SER:H	5:F:605:GLU:CD	2.05	0.59
3:J:817:HIS:CE1	3:J:860:ARG:HE	2.19	0.59
2:I:463:GLN:HG3	2:I:505:PHE:HB2	1.84	0.59
3:J:148:GLU:H	3:J:156:ARG:HG3	1.66	0.59
3:J:1174:ARG:HG2	3:J:1189:MET:HG2	1.84	0.59
3:J:308:ASP:OD2	3:J:311:ARG:NH2	2.34	0.59
3:D:1310:THR:HG21	5:F:70:ASN:HA	1.85	0.59
3:D:585:LYS:HB2	3:D:612:LEU:HD21	1.84	0.59
2:C:363:LEU:HB3	2:C:381:ALA:HB1	1.84	0.59
3:D:872:LEU:HD22	3:D:877:VAL:HG11	1.85	0.59
3:J:1140:ARG:HH21	3:J:1236:GLU:HG2	1.67	0.59
3:D:363:LEU:HD23	3:D:487:THR:HG22	1.84	0.59
2:I:856:ASN:HB3	5:L:613:ASP:HA	1.84	0.59
2:C:94:ALA:HB2	2:C:129:LEU:HD11	1.83	0.59
2:C:1185:PRO:HD2	2:C:1189:GLY:HA2	1.84	0.59
2:C:136:PHE:O	2:C:143:ARG:N	2.29	0.59
3:D:114:ILE:HD12	3:D:304:ASP:HB3	1.84	0.59
2:C:1196:LYS:HD2	2:C:1206:THR:HG23	1.85	0.59
3:J:317:THR:HG23	3:J:320:ASN:HB3	1.83	0.59
2:I:1238:LEU:HD12	2:I:1238:LEU:H	1.68	0.59
6:I:2001:4OE:H8	3:J:773:PHE:HB3	1.85	0.59
1:A:45:ARG:HG2	1:B:38:THR:HB	1.85	0.59
2:C:40:GLU:O	2:C:73:TYR:OH	2.20	0.58
2:C:841:ARG:HA	2:C:1046:VAL:HA	1.85	0.58
3:J:210:SER:O	3:J:214:ARG:HG2	2.03	0.58
3:D:115:TRP:O	3:D:119:SER:HB2	2.03	0.58
3:D:1172:LYS:HA	3:D:1191:PRO:HA	1.84	0.58
3:J:1172:LYS:HA	3:J:1191:PRO:HA	1.86	0.58
1:G:70:THR:HG21	2:I:755:LYS:HE2	1.84	0.58
2:C:103:VAL:HG12	2:C:116:ASP:HB3	1.85	0.58
1:B:61:ILE:HB	1:B:64:VAL:O	2.03	0.58
5:F:111:LEU:HD13	5:F:116:GLU:HG2	1.85	0.58
3:J:960:LEU:HB3	3:J:963:VAL:HG11	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1275:VAL:HG13	2:I:1287:LEU:HD11	1.84	0.58
2:C:829:THR:HA	2:C:1059:ARG:HA	1.84	0.58
2:C:820:GLU:HA	2:C:1079:ILE:HD11	1.85	0.58
5:F:305:LEU:HD13	5:F:315:TRP:HA	1.84	0.58
3:D:708:ASN:HB3	3:D:712:GLN:O	2.03	0.58
5:L:111:LEU:HD13	5:L:116:GLU:HG2	1.85	0.58
4:K:15:ASN:HB3	4:K:18:ASP:HB2	1.85	0.58
2:C:269:ILE:HG23	2:C:273:HIS:HB2	1.85	0.58
1:A:310:ARG:O	5:F:608:ARG:NH1	2.37	0.58
2:I:1119:MET:HB2	2:I:1228:GLY:HA2	1.85	0.58
2:C:120:GLN:HG3	2:C:121:GLU:HG2	1.84	0.58
1:A:12:ARG:HG2	1:A:13:LEU:H	1.69	0.58
1:G:12:ARG:H	1:G:30:PRO:HD2	1.67	0.58
5:L:476:ARG:HG2	5:L:477:GLU:HG2	1.85	0.58
2:I:1101:LEU:HD21	3:J:508:LEU:HD22	1.84	0.58
3:J:141:PHE:HD1	3:J:180:MET:HG3	1.67	0.58
5:F:577:GLY:HA3	5:F:583:THR:HG23	1.86	0.58
3:J:1157:ALA:HB2	3:J:1210:ILE:HD11	1.86	0.58
2:I:591:TYR:OH	2:I:637:ARG:NH2	2.37	0.58
2:C:1320:PRO:HG2	3:D:1354:GLY:HA3	1.85	0.58
3:J:1350:ASN:HA	3:J:1353:VAL:HG12	1.86	0.58
3:J:189:LEU:HD22	3:J:234:PRO:HB3	1.86	0.58
2:C:102:LEU:HB2	2:C:489:PRO:HG3	1.86	0.58
1:H:83:LEU:HA	1:H:86:LYS:HE2	1.86	0.58
3:J:1273:ASP:OD1	3:J:1274:PHE:N	2.36	0.58
3:D:1227:HIS:HA	3:D:1230:THR:HG22	1.85	0.57
2:C:30:ILE:H	2:C:30:ILE:HD12	1.68	0.57
3:J:325:LYS:HD3	5:L:508:GLU:HG2	1.86	0.57
3:D:1140:ARG:HH21	3:D:1236:GLU:HG2	1.70	0.57
3:J:1280:VAL:HG21	3:J:1304:ARG:NE	2.17	0.57
2:C:718:ALA:HB2	2:C:783:LEU:HD23	1.87	0.57
3:D:1297:LYS:HB3	3:J:1303:SER:HA	1.87	0.57
3:J:1169:THR:HG23	3:J:1192:LYS:HD3	1.85	0.57
2:C:739:ASP:OD1	2:C:739:ASP:N	2.36	0.57
3:D:824:PRO:HD3	3:D:835:LEU:HB2	1.86	0.57
2:I:30:ILE:H	2:I:30:ILE:HD12	1.69	0.57
3:J:892:PHE:H	3:J:1281:GLU:HG2	1.68	0.57
2:C:149:LEU:HD13	2:C:453:ILE:HG13	1.85	0.57
2:I:13:LYS:HZ3	2:I:1151:LEU:HD12	1.69	0.57
3:D:646:ILE:HD11	3:D:764:ARG:HD2	1.85	0.57
2:C:590:PRO:HG3	2:C:605:TYR:CZ	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:152:THR:OG1	3:D:153:ASN:N	2.37	0.57
1:H:100:LEU:HD11	1:H:121:VAL:HG21	1.87	0.57
1:H:98:VAL:HG11	1:H:121:VAL:HG22	1.86	0.57
3:D:854:ALA:HB2	3:J:1372:ARG:HB2	1.86	0.57
3:D:282:LEU:HD21	5:F:410:ILE:HG12	1.87	0.57
4:E:15:ASN:HB3	4:E:18:ASP:HB2	1.86	0.57
5:L:515:GLU:HG2	5:L:516:ASP:H	1.69	0.57
3:D:650:LYS:HE2	3:D:654:ILE:HD11	1.87	0.57
2:I:494:ASN:OD1	2:I:495:ALA:N	2.36	0.57
3:D:892:PHE:H	3:D:1281:GLU:HG2	1.69	0.57
6:I:2001:4OE:NAN	3:J:755:ILE:HG12	2.19	0.57
5:L:561:MET:HG2	5:L:576:VAL:HG22	1.87	0.57
3:D:527:LEU:HD23	3:D:532:GLU:HG3	1.85	0.57
2:I:102:LEU:HB2	2:I:489:PRO:HG3	1.87	0.57
1:G:11:PRO:HD2	1:H:227:GLN:HA	1.86	0.56
2:C:494:ASN:OD1	2:C:495:ALA:N	2.36	0.56
1:G:44:ARG:HG3	1:G:183:ILE:HG22	1.87	0.56
1:A:25:LYS:HG2	1:A:204:GLU:HG3	1.87	0.56
3:J:114:ILE:HD12	3:J:304:ASP:HB3	1.86	0.56
3:D:279:LEU:HD11	3:D:296:LYS:HG2	1.87	0.56
2:I:61:SER:HB3	2:I:479:LEU:HB3	1.87	0.56
2:I:40:GLU:O	2:I:73:TYR:OH	2.23	0.56
5:F:278:ASP:OD1	5:F:281:ARG:NH1	2.37	0.56
5:F:551:LEU:HD22	5:F:597:LYS:HD2	1.86	0.56
5:L:49:ASN:HA	5:L:53:ILE:HA	1.87	0.56
2:I:518:ASN:N	2:I:518:ASN:OD1	2.36	0.56
1:B:191:ARG:HH22	3:D:409:TRP:HB3	1.71	0.56
2:C:1276:TRP:CZ2	3:D:801:VAL:HG21	2.41	0.56
5:F:515:GLU:HG2	5:F:516:ASP:H	1.71	0.56
2:C:324:LYS:O	2:C:327:GLN:NE2	2.38	0.56
3:D:847:ASP:N	3:D:847:ASP:OD1	2.38	0.56
3:D:1273:ASP:OD1	3:D:1274:PHE:N	2.38	0.56
2:I:1106:ARG:HD2	2:I:1106:ARG:H	1.69	0.56
2:C:1151:LEU:HD21	2:C:1198:LEU:HD23	1.87	0.56
5:L:585:GLU:O	5:L:589:GLN:HG3	2.05	0.56
1:G:228:LEU:HD11	1:H:221:ALA:HB1	1.87	0.56
1:A:14:VAL:HG22	1:A:15:ASP:H	1.71	0.56
2:I:841:ARG:HA	2:I:1046:VAL:HA	1.87	0.56
2:I:6:THR:HG21	2:I:782:VAL:HG23	1.88	0.56
3:D:682:VAL:O	3:D:685:ILE:HG12	2.05	0.56
3:J:363:LEU:HD23	3:J:487:THR:HG22	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:476:ARG:HG2	5:F:477:GLU:HG2	1.88	0.56
5:L:551:LEU:HD22	5:L:597:LYS:HD2	1.88	0.56
2:C:538:LEU:HD22	2:C:543:ALA:HB2	1.88	0.56
3:D:80:HIS:HB3	3:D:83:VAL:HG11	1.88	0.56
3:J:258:GLY:HA3	5:L:499:LYS:HD3	1.88	0.56
5:L:244:THR:O	5:L:247:GLU:HG2	2.05	0.56
3:J:1238:GLN:NE2	3:J:1248:ILE:O	2.38	0.56
5:F:483:LEU:H	5:F:483:LEU:HD12	1.70	0.56
3:D:210:SER:O	3:D:214:ARG:HG2	2.06	0.55
3:J:474:LEU:HD23	4:K:28:ARG:HG2	1.88	0.55
2:C:488:MET:O	2:C:490:GLN:N	2.34	0.55
2:C:1254:VAL:HG13	2:C:1255:THR:H	1.71	0.55
1:B:59:VAL:HG21	1:B:85:LEU:HD13	1.88	0.55
2:I:269:ILE:HG23	2:I:273:HIS:HB2	1.88	0.55
3:J:478:LEU:HG	4:K:47:THR:HG23	1.88	0.55
2:C:1287:LEU:HD13	3:D:1357:ILE:HD11	1.89	0.55
2:I:448:LEU:HB2	2:I:553:THR:HB	1.88	0.55
3:J:847:ASP:N	3:J:847:ASP:OD1	2.36	0.55
2:I:560:PRO:O	3:J:780:ARG:NH2	2.33	0.55
1:B:100:LEU:HD21	1:B:121:VAL:HG11	1.88	0.55
3:J:120:LEU:HD22	3:J:121:PRO:HD3	1.88	0.55
2:C:985:GLU:HB3	2:C:988:LYS:HB2	1.87	0.55
3:D:141:PHE:HD1	3:D:180:MET:HG3	1.72	0.55
3:J:647:PRO:HG3	3:J:697:MET:HB3	1.89	0.55
1:B:48:LEU:HD12	1:B:183:ILE:HD11	1.88	0.55
3:J:1280:VAL:HG11	3:J:1304:ARG:HH21	1.71	0.55
5:L:482:GLU:O	5:L:486:ARG:NH2	2.39	0.55
2:I:124:MET:HB2	2:I:498:ILE:HD13	1.89	0.55
1:H:48:LEU:HD12	1:H:183:ILE:HD11	1.89	0.55
2:C:745:GLU:HG3	2:C:1017:GLN:HB3	1.88	0.55
2:I:95:PRO:HA	2:I:126:GLU:HG2	1.89	0.55
3:J:115:TRP:O	3:J:119:SER:HB2	2.07	0.54
2:I:590:PRO:HG3	2:I:605:TYR:CZ	2.42	0.54
5:F:479:THR:HG23	5:F:481:GLU:H	1.72	0.54
3:D:474:LEU:HD12	3:D:477:GLN:HE21	1.72	0.54
3:D:647:PRO:HG3	3:D:697:MET:HB3	1.90	0.54
5:F:290:LEU:HB3	5:F:333:VAL:HG21	1.89	0.54
2:I:1320:PRO:HG2	3:J:1354:GLY:HA3	1.87	0.54
3:D:1157:ALA:HB2	3:D:1210:ILE:HD11	1.89	0.54
2:I:363:LEU:HB3	2:I:381:ALA:HB1	1.90	0.54
3:J:268:LEU:HD13	3:J:306:LEU:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1196:LYS:HD2	2:I:1206:THR:HG23	1.88	0.54
3:D:709:ARG:C	3:D:711:GLY:H	2.08	0.54
1:G:45:ARG:HH22	2:I:1216:ARG:HA	1.72	0.54
1:H:48:LEU:HD22	3:J:539:SER:HB3	1.89	0.54
5:F:165:PHE:CE2	5:F:217:ALA:HA	2.42	0.54
2:I:551:HIS:CG	2:I:552:PRO:HD2	2.41	0.54
5:F:482:GLU:O	5:F:486:ARG:NH2	2.41	0.54
2:I:672:GLU:HG2	2:I:1187:PHE:HA	1.90	0.54
2:C:1119:MET:HB2	2:C:1228:GLY:HA2	1.88	0.54
5:L:278:ASP:OD1	5:L:281:ARG:NH1	2.40	0.54
3:D:28:ASP:OD1	3:D:31:ARG:NH1	2.41	0.54
3:D:1238:GLN:NE2	3:D:1248:ILE:O	2.41	0.54
1:G:45:ARG:NH2	2:I:1216:ARG:HA	2.23	0.54
2:I:9:LYS:HA	2:I:1171:ARG:HD2	1.89	0.54
1:A:285:THR:HG23	1:A:288:GLU:H	1.73	0.54
2:C:591:TYR:OH	2:C:637:ARG:NH2	2.40	0.54
2:C:615:VAL:HG13	2:C:650:VAL:HA	1.89	0.54
2:C:617:ALA:HA	2:C:636:CYS:SG	2.48	0.54
5:L:602:SER:H	5:L:605:GLU:HG3	1.73	0.54
2:I:1149:TYR:HB3	2:I:1159:VAL:HG11	1.90	0.54
5:F:511:ILE:HG13	5:F:512:GLY:H	1.73	0.54
3:J:45:ASN:HB3	3:J:48:THR:O	2.08	0.54
2:I:166:SER:OG	5:L:19:GLN:O	2.20	0.54
5:L:276:MET:SD	5:L:279:ARG:NH1	2.80	0.54
1:G:14:VAL:HG22	1:G:15:ASP:H	1.73	0.54
2:I:615:VAL:HG13	2:I:650:VAL:HA	1.90	0.54
1:H:61:ILE:HB	1:H:64:VAL:O	2.08	0.54
1:G:25:LYS:HG2	1:G:204:GLU:HG3	1.90	0.54
1:G:50:SER:HB3	1:H:8:PHE:HE1	1.72	0.54
2:C:942:ASP:OD2	2:C:1048:LYS:NZ	2.32	0.54
3:J:79:LYS:HG3	3:J:80:HIS:N	2.23	0.54
1:G:230:ALA:HB1	1:H:12:ARG:HA	1.90	0.54
1:B:98:VAL:HG11	1:B:121:VAL:HG22	1.89	0.54
3:D:694:SER:OG	3:D:738:ARG:NE	2.36	0.54
1:G:184:ALA:HB2	2:I:1091:GLY:HA3	1.89	0.54
1:A:45:ARG:NH2	2:C:1216:ARG:HA	2.22	0.53
2:I:718:ALA:HB2	2:I:783:LEU:HD23	1.90	0.53
3:J:189:LEU:HB3	3:J:234:PRO:HB2	1.91	0.53
2:C:1108:ASN:OD1	2:C:1111:GLN:NE2	2.41	0.53
2:C:56:VAL:HG11	2:C:468:LEU:HB3	1.90	0.53
2:I:1251:TYR:OH	3:J:348:ASP:OD2	2.18	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:817:LEU:HD11	2:C:1080:ASN:HD22	1.73	0.53
3:J:568:SER:OG	3:J:569:LEU:N	2.41	0.53
3:J:958:ILE:HD11	3:J:1017:VAL:HG11	1.91	0.53
1:A:60:GLU:HB2	1:A:170:ARG:HG2	1.90	0.53
3:D:405:GLU:O	3:D:408:VAL:HG22	2.09	0.53
3:D:1233:ILE:O	3:D:1237:VAL:HG12	2.08	0.53
2:C:344:GLY:HA3	2:C:346:TYR:CZ	2.42	0.53
2:C:518:ASN:OD1	2:C:518:ASN:N	2.40	0.53
1:B:13:LEU:HB3	1:B:29:GLU:CB	2.38	0.53
3:D:148:GLU:H	3:D:156:ARG:HG3	1.73	0.53
1:B:11:PRO:HA	1:B:30:PRO:HD2	1.90	0.53
5:L:569:THR:OG1	5:L:570:ASP:N	2.37	0.53
3:D:662:ALA:HA	3:D:665:GLN:HB3	1.90	0.53
3:J:1050:THR:HG23	3:J:1057:SER:HB3	1.89	0.53
5:F:489:MET:HB2	5:F:490:PRO:HD2	1.90	0.53
2:C:551:HIS:CG	2:C:552:PRO:HD2	2.44	0.53
3:J:733:SER:O	3:J:737:ILE:HG12	2.09	0.53
2:C:217:THR:HG23	2:C:351:LEU:HD13	1.91	0.53
1:A:44:ARG:HG3	1:A:183:ILE:HG22	1.90	0.53
3:D:194:LEU:HD13	3:D:228:VAL:HG22	1.90	0.53
3:J:474:LEU:HD12	3:J:477:GLN:HE21	1.72	0.53
3:J:79:LYS:HB2	5:L:569:THR:H	1.74	0.53
3:J:1286:LYS:HD2	3:J:1290:ARG:NH2	2.23	0.53
1:H:91:ARG:HG3	1:H:122:GLU:HB3	1.91	0.53
1:A:153:VAL:HB	1:A:175:ALA:HB3	1.91	0.53
3:J:133:ARG:HB2	5:L:88:GLU:HA	1.91	0.53
2:C:1246:ARG:NE	3:D:348:ASP:OD1	2.36	0.53
2:C:1065:LYS:HD2	2:C:1235:LEU:HD12	1.89	0.53
5:F:466:ILE:HD13	5:F:486:ARG:HB3	1.90	0.53
3:J:741:ALA:O	3:J:762:ASN:ND2	2.42	0.53
1:H:64:VAL:HG21	1:H:69:SER:HB3	1.89	0.53
2:C:1191:LYS:HD3	2:C:1193:ALA:H	1.74	0.53
3:J:124:ILE:HG23	3:J:189:LEU:HD11	1.91	0.53
1:A:48:LEU:HA	1:A:180:VAL:HG21	1.91	0.53
3:J:682:VAL:O	3:J:685:ILE:HG12	2.09	0.53
2:I:971:LEU:HG	2:I:1014:LEU:HD23	1.91	0.53
1:A:93:GLN:H	1:A:120:ASP:HB3	1.74	0.53
3:J:683:ILE:HD11	3:J:754:ILE:HG12	1.91	0.53
5:L:290:LEU:HB3	5:L:333:VAL:HG21	1.91	0.53
2:C:732:ILE:HD11	2:C:769:PRO:HB3	1.90	0.52
2:I:344:GLY:HA3	2:I:346:TYR:CZ	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:609:TYR:HB2	3:J:617:THR:HG21	1.92	0.52
3:J:35:PHE:HD1	3:J:101:ARG:HD3	1.74	0.52
2:C:980:VAL:HG13	2:C:984:VAL:HB	1.91	0.52
2:C:146:VAL:HG13	2:C:529:ARG:HB3	1.91	0.52
3:D:425:ARG:HG2	3:D:426:ALA:H	1.74	0.52
2:C:1192:GLU:O	2:C:1196:LYS:HG2	2.09	0.52
2:C:241:LEU:HD21	2:C:246:LEU:HD11	1.91	0.52
3:J:1060:VAL:HG22	3:J:1106:ILE:HG23	1.91	0.52
1:G:60:GLU:HB2	1:G:170:ARG:HG2	1.90	0.52
1:H:23:HIS:ND1	1:H:206:GLU:HG2	2.24	0.52
2:I:1185:PRO:HD2	2:I:1189:GLY:HA2	1.91	0.52
3:J:978:ARG:HB2	3:J:1199:PHE:HZ	1.74	0.52
1:A:12:ARG:H	1:A:30:PRO:HD2	1.73	0.52
1:H:59:VAL:HG21	1:H:85:LEU:HD13	1.90	0.52
1:B:64:VAL:HG21	1:B:69:SER:HB3	1.91	0.52
5:F:281:ARG:O	5:F:285:ARG:HG3	2.10	0.52
3:D:709:ARG:O	3:D:711:GLY:N	2.40	0.52
3:D:1169:THR:HG23	3:D:1192:LYS:HD3	1.91	0.52
5:L:397:ARG:HG2	5:L:443:ILE:HG21	1.90	0.52
2:C:95:PRO:HA	2:C:126:GLU:HG2	1.91	0.52
3:D:1135:THR:OG1	3:D:1136:GLY:N	2.43	0.52
2:I:1276:TRP:CZ2	3:J:801:VAL:HG21	2.44	0.52
1:G:225:ALA:HA	1:G:228:LEU:HD23	1.92	0.52
2:C:6:THR:HG21	2:C:782:VAL:HG23	1.90	0.52
2:C:618:GLN:HG3	3:D:770:LEU:HD21	1.92	0.52
2:C:339:ASN:HB3	2:C:343:HIS:H	1.75	0.52
3:D:1350:ASN:HA	3:D:1353:VAL:HG12	1.91	0.52
3:J:425:ARG:HG2	3:J:426:ALA:H	1.75	0.52
3:D:77:ARG:HG3	3:D:79:LYS:H	1.75	0.52
3:J:279:LEU:HD11	3:J:296:LYS:HG2	1.92	0.52
2:I:302:ILE:HG22	2:I:309:LEU:HA	1.92	0.52
4:E:60:ASN:HD21	4:E:63:ILE:HD13	1.74	0.52
3:J:872:LEU:HD22	3:J:877:VAL:HG11	1.92	0.52
3:D:124:ILE:HG23	3:D:189:LEU:HD11	1.90	0.52
1:G:118:ASP:HB3	1:G:121:VAL:HG23	1.91	0.52
5:L:511:ILE:HG13	5:L:512:GLY:H	1.75	0.52
4:E:60:ASN:ND2	4:E:63:ILE:HD13	2.25	0.52
5:F:402:LEU:HA	5:F:405:ILE:HG12	1.92	0.52
3:D:798:ARG:NH1	3:D:802:ASP:OD2	2.43	0.52
2:I:97:ARG:HB3	2:I:121:GLU:HB2	1.92	0.52
3:D:777:HIS:CE1	3:D:781:LYS:HB2	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:79:LYS:HB2	5:L:569:THR:N	2.25	0.52
3:D:697:MET:SD	3:D:741:ALA:HB3	2.50	0.52
3:D:839:VAL:HG12	3:D:864:LEU:HD12	1.92	0.52
3:J:298:MET:SD	5:L:402:LEU:HB3	2.49	0.52
5:L:577:GLY:HA3	5:L:583:THR:HG23	1.92	0.52
3:J:1227:HIS:HA	3:J:1230:THR:HG22	1.92	0.51
2:C:138:ILE:HB	2:C:143:ARG:HD3	1.92	0.51
3:D:368:LEU:HD22	3:D:373:ALA:HB2	1.91	0.51
3:J:591:ILE:HG13	3:J:604:MET:HE2	1.92	0.51
3:J:585:LYS:HB2	3:J:612:LEU:HD21	1.91	0.51
3:D:820:ILE:HG22	3:D:1227:HIS:ND1	2.26	0.51
3:D:388:ARG:NH1	3:D:414:GLU:OE1	2.43	0.51
3:D:478:LEU:HG	4:E:47:THR:HG23	1.91	0.51
2:I:136:PHE:CE2	2:I:456:VAL:HG11	2.45	0.51
3:J:1233:ILE:O	3:J:1237:VAL:HG12	2.10	0.51
5:F:119:ILE:HA	5:F:122:ARG:HD3	1.92	0.51
3:J:147:ILE:HG22	3:J:188:LEU:HG	1.92	0.51
1:A:118:ASP:HB3	1:A:121:VAL:HG23	1.92	0.51
3:J:748:ALA:HA	3:J:755:ILE:HD12	1.91	0.51
2:I:968:GLU:HG3	2:I:1018:TYR:HE1	1.74	0.51
2:I:206:ALA:O	2:I:209:ILE:HG22	2.10	0.51
1:B:83:LEU:HA	1:B:86:LYS:HE2	1.91	0.51
3:J:614:LEU:HD23	4:K:7:GLN:HB2	1.91	0.51
2:C:672:GLU:HG2	2:C:1187:PHE:HA	1.92	0.51
2:I:646:SER:HB3	2:I:649:GLN:HG3	1.91	0.51
2:C:1314:GLN:HG2	4:E:28:ARG:CZ	2.41	0.51
3:D:275:ARG:HD3	3:D:298:MET:HB3	1.92	0.51
3:J:824:PRO:HD3	3:J:835:LEU:HB2	1.91	0.51
5:F:532:LEU:O	5:F:536:THR:HG23	2.11	0.51
3:D:506:VAL:HG23	3:D:628:GLY:HA3	1.91	0.51
1:B:91:ARG:HG3	1:B:122:GLU:HB3	1.93	0.51
5:L:165:PHE:CE2	5:L:217:ALA:HA	2.45	0.51
5:L:479:THR:HG23	5:L:481:GLU:H	1.76	0.51
4:E:39:VAL:HG22	4:E:40:PRO:HD2	1.93	0.51
2:C:1281:TYR:CD1	3:D:484:MET:HG2	2.45	0.51
3:D:613:GLY:O	3:D:617:THR:OG1	2.27	0.51
2:C:641:GLU:OE2	3:D:749:LYS:NZ	2.42	0.51
2:C:9:LYS:HA	2:C:1171:ARG:HD2	1.92	0.51
2:I:237:LEU:HD22	2:I:237:LEU:H	1.75	0.51
1:A:45:ARG:HD3	2:C:1083:GLU:HB3	1.91	0.51
3:J:794:GLY:O	3:J:797:THR:OG1	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:103:VAL:HB	2:C:113:THR:HG21	1.92	0.51
2:I:1119:MET:HE3	2:I:1204:LEU:HD13	1.93	0.51
3:D:189:LEU:HD22	3:D:234:PRO:HB3	1.92	0.51
1:A:70:THR:HG21	2:C:755:LYS:HE2	1.91	0.51
2:I:1191:LYS:HD3	2:I:1193:ALA:H	1.74	0.51
5:L:97:PRO:HA	5:L:100:MET:HG3	1.92	0.51
1:H:29:GLU:OE2	1:H:200:LYS:HE3	2.11	0.51
2:C:50:GLU:HG2	2:C:73:TYR:HE1	1.76	0.51
3:D:298:MET:SD	5:F:402:LEU:HB3	2.51	0.51
1:B:91:ARG:HG2	1:B:122:GLU:O	2.11	0.51
1:A:79:LEU:HD11	2:C:693:LEU:HD21	1.93	0.51
5:L:489:MET:HB2	5:L:490:PRO:HD2	1.92	0.51
5:L:119:ILE:HA	5:L:122:ARG:HD3	1.92	0.51
5:L:448:ARG:NH1	5:L:501:ALA:O	2.36	0.51
3:D:611:ILE:HG22	3:D:612:LEU:HD12	1.93	0.50
2:C:971:LEU:HG	2:C:1014:LEU:HD23	1.93	0.50
2:I:21:VAL:HG11	2:I:592:ARG:HD2	1.93	0.50
5:L:41:ILE:HA	5:L:44:ILE:HG23	1.93	0.50
3:D:1239:ASP:OD1	3:D:1242:ARG:NH2	2.43	0.50
2:I:349:GLU:O	2:I:353:VAL:HG23	2.11	0.50
5:L:483:LEU:H	5:L:483:LEU:HD12	1.75	0.50
1:B:64:VAL:HG11	1:B:69:SER:OG	2.11	0.50
3:D:35:PHE:HD1	3:D:101:ARG:HD3	1.76	0.50
2:I:26:TYR:CZ	2:I:28:LEU:HB2	2.46	0.50
2:C:692:THR:OG1	2:C:693:LEU:N	2.43	0.50
2:I:878:THR:OG1	2:I:879:GLY:N	2.44	0.50
1:G:153:VAL:HB	1:G:175:ALA:HB3	1.93	0.50
1:G:177:TYR:O	1:G:178:SER:HB2	2.10	0.50
3:D:872:LEU:O	3:D:877:VAL:HG12	2.11	0.50
4:K:39:VAL:HG22	4:K:40:PRO:HD2	1.93	0.50
2:I:227:LYS:O	2:I:245:ARG:NH2	2.44	0.50
1:H:101:THR:H	1:H:116:THR:HG22	1.77	0.50
4:K:4:VAL:HG22	4:K:5:THR:HG23	1.94	0.50
2:I:692:THR:OG1	2:I:693:LEU:N	2.45	0.50
1:B:154:PRO:HG3	3:D:541:LEU:HD13	1.93	0.50
2:I:241:LEU:HD21	2:I:246:LEU:HD11	1.94	0.50
1:A:66:HIS:CE1	1:A:69:SER:HB3	2.47	0.50
2:C:202:ARG:HH22	2:C:368:ARG:HH12	1.58	0.50
1:G:182:ARG:O	1:G:206:GLU:N	2.45	0.50
1:G:230:ALA:CB	1:H:12:ARG:HA	2.42	0.50
3:J:115:TRP:CE2	3:J:1329:THR:HG23	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:397:ARG:HG2	5:F:443:ILE:HG21	1.94	0.50
2:C:678:ARG:HG3	2:C:1108:ASN:HD22	1.77	0.50
3:J:1286:LYS:O	3:J:1290:ARG:HB2	2.11	0.50
3:D:609:TYR:HB2	3:D:617:THR:HG21	1.92	0.50
2:C:1101:LEU:HD13	3:D:504:GLN:HB2	1.93	0.50
2:I:488:MET:O	2:I:490:GLN:N	2.39	0.50
2:I:94:ALA:HB2	2:I:129:LEU:HD11	1.93	0.50
3:D:205:LEU:HD23	3:D:217:LEU:HB3	1.93	0.50
2:C:402:ARG:NH2	2:C:419:ILE:O	2.45	0.50
5:L:582:VAL:HG22	5:L:586:ARG:HG2	1.94	0.50
3:J:1167:LYS:HE3	3:J:1168:GLU:H	1.76	0.50
2:I:10:ARG:HA	2:I:1172:LEU:HD23	1.94	0.50
1:G:228:LEU:CD1	1:H:221:ALA:HB1	2.42	0.50
2:I:26:TYR:HE2	2:I:32:LEU:HD12	1.77	0.50
5:L:164:GLY:O	5:L:260:ARG:HB2	2.11	0.50
1:B:151:GLY:O	1:B:177:TYR:HB2	2.12	0.50
1:B:23:HIS:ND1	1:B:206:GLU:HG2	2.26	0.50
1:G:66:HIS:HA	1:G:171:LEU:HD11	1.94	0.50
5:L:29:ASP:OD1	5:L:30:HIS:N	2.45	0.50
1:G:155:ALA:HA	1:G:158:ARG:HG3	1.93	0.50
2:C:1122:LYS:HG2	2:C:1229:TYR:CE1	2.47	0.50
4:K:60:ASN:HD21	4:K:63:ILE:HD13	1.77	0.50
5:F:573:LEU:H	5:F:573:LEU:HD23	1.76	0.50
2:I:103:VAL:HB	2:I:113:THR:HG21	1.93	0.49
5:L:551:LEU:HD11	5:L:598:LEU:HD21	1.93	0.49
2:C:98:VAL:HG21	2:C:124:MET:HE3	1.94	0.49
2:I:1313:HIS:ND1	4:K:31:GLN:OE1	2.45	0.49
3:J:16:GLU:HG3	3:J:17:PHE:HD2	1.76	0.49
3:J:367:GLY:HA3	3:J:448:GLN:HB2	1.94	0.49
5:F:165:PHE:HE2	5:F:217:ALA:HA	1.77	0.49
3:J:198:CYS:O	3:J:202:ARG:HG3	2.11	0.49
3:D:45:ASN:HB3	3:D:48:THR:O	2.11	0.49
2:C:685:MET:SD	2:C:1073:LYS:HG2	2.52	0.49
3:J:435:GLN:HB2	3:J:457:TYR:OH	2.12	0.49
3:D:683:ILE:HD11	3:D:754:ILE:HG12	1.95	0.49
2:I:1192:GLU:O	2:I:1196:LYS:HG2	2.13	0.49
1:A:91:ARG:HD3	1:A:210:THR:O	2.12	0.49
2:C:448:LEU:HB2	2:C:553:THR:HB	1.93	0.49
2:C:1282:GLY:O	3:D:1361:THR:N	2.44	0.49
3:D:1341:ARG:HH22	3:D:1373:ARG:HH21	1.60	0.49
5:L:137:TYR:HE1	5:L:351:THR:HB	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:D:1191:PRO:HB2	3:D:1194:ARG:HD3	1.94	0.49
2:C:968:GLU:HG3	2:C:1018:TYR:HE1	1.76	0.49
3:J:194:LEU:HD13	3:J:228:VAL:HG22	1.94	0.49
2:C:255:ILE:HB	2:C:263:VAL:HB	1.95	0.49
3:J:748:ALA:O	3:J:777:HIS:CD2	2.64	0.49
4:K:60:ASN:ND2	4:K:63:ILE:HD13	2.28	0.49
3:J:950:ILE:HG13	3:J:1020:TRP:CH2	2.47	0.49
1:A:287:VAL:HG12	1:A:291:LYS:HE3	1.93	0.49
2:I:517:GLN:O	2:I:517:GLN:HG2	2.12	0.49
1:B:73:GLY:HA3	1:B:138:ALA:HB1	1.95	0.49
2:C:1294:LYS:HD3	3:D:472:LEU:HG	1.95	0.49
2:C:668:ILE:HD11	2:C:683:ALA:HB2	1.95	0.49
1:A:177:TYR:O	1:A:178:SER:HB2	2.12	0.49
1:A:41:ASN:HB2	1:A:185:TYR:OH	2.12	0.49
5:L:493:LYS:HA	5:L:496:LYS:HE2	1.94	0.49
2:C:349:GLU:O	2:C:353:VAL:HG23	2.12	0.49
2:I:819:SER:HB2	2:I:1085:MET:HG3	1.93	0.49
1:H:91:ARG:HG2	1:H:122:GLU:O	2.13	0.49
3:J:798:ARG:NH1	3:J:802:ASP:OD2	2.46	0.49
2:I:838:CYS:SG	2:I:886:LYS:HD3	2.53	0.49
3:J:28:ASP:OD1	3:J:31:ARG:NH1	2.45	0.49
3:J:975:ILE:HD13	3:J:980:THR:HG21	1.93	0.49
2:C:207:THR:HG21	2:C:351:LEU:HG	1.95	0.49
2:I:242:VAL:HB	2:I:245:ARG:HD2	1.94	0.49
2:C:115:LYS:HE3	2:C:116:ASP:H	1.77	0.49
3:J:35:PHE:CD1	3:J:101:ARG:HD3	2.48	0.49
3:D:1162:ILE:HG23	3:D:1178:THR:HB	1.95	0.49
1:G:93:GLN:H	1:G:120:ASP:HB3	1.78	0.49
2:I:734:ILE:HD12	2:I:777:VAL:HG21	1.94	0.49
3:J:613:GLY:O	3:J:617:THR:OG1	2.25	0.49
2:I:213:LEU:HD13	2:I:422:LYS:HG2	1.95	0.49
2:C:517:GLN:HG2	2:C:517:GLN:O	2.12	0.49
2:I:1314:GLN:HG2	4:K:28:ARG:CZ	2.43	0.48
5:L:482:GLU:HG2	5:L:486:ARG:HH22	1.78	0.48
1:G:228:LEU:HD13	1:G:231:PHE:HD2	1.76	0.48
3:J:1267:VAL:HB	3:J:1301:THR:OG1	2.13	0.48
2:I:357:ASN:ND2	2:I:358:ASP:OD2	2.45	0.48
2:C:901:LEU:HB2	5:F:565:ILE:HD11	1.94	0.48
5:L:299:LYS:HA	5:L:302:PHE:HB3	1.95	0.48
1:H:221:ALA:O	1:H:224:LEU:HB3	2.12	0.48
3:D:568:SER:OG	3:D:569:LEU:N	2.45	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:448:ARG:NH1	5:F:501:ALA:O	2.36	0.48
3:J:885:VAL:HG12	3:J:894:VAL:HG11	1.95	0.48
3:J:1078:LEU:HD13	3:J:1121:LEU:HD22	1.96	0.48
3:J:950:ILE:HB	3:J:1018:ALA:HB3	1.96	0.48
3:D:355:ILE:HD13	3:D:466:MET:HG3	1.94	0.48
3:J:800:LEU:HB3	3:J:920:ALA:HB1	1.95	0.48
2:I:324:LYS:O	2:I:327:GLN:NE2	2.46	0.48
2:I:685:MET:SD	2:I:1073:LYS:HG2	2.53	0.48
3:J:152:THR:OG1	3:J:153:ASN:N	2.44	0.48
2:C:170:VAL:HG23	2:C:171:LEU:N	2.28	0.48
1:G:45:ARG:HD3	2:I:1083:GLU:HB3	1.95	0.48
3:D:733:SER:O	3:D:737:ILE:HG12	2.13	0.48
2:I:202:ARG:HH22	2:I:368:ARG:HH12	1.61	0.48
3:J:405:GLU:O	3:J:408:VAL:HG22	2.12	0.48
3:D:474:LEU:HD23	4:E:28:ARG:HG2	1.96	0.48
2:C:528:ARG:NH2	2:C:575:LEU:HD23	2.29	0.48
1:B:13:LEU:HB3	1:B:29:GLU:HB3	1.95	0.48
1:H:97:GLU:OE1	1:H:147:GLN:HG3	2.14	0.48
2:I:203:LYS:CB	5:L:29:ASP:HB2	2.43	0.48
3:D:1198:VAL:HG23	3:D:1204:VAL:HG11	1.94	0.48
5:L:281:ARG:O	5:L:285:ARG:HG3	2.13	0.48
2:I:387:ASN:HA	2:I:391:SER:HB2	1.95	0.48
3:D:218:THR:HA	3:D:221:ILE:HG22	1.95	0.48
1:A:38:THR:OG1	1:B:45:ARG:NH1	2.45	0.48
1:B:33:ARG:HH11	2:C:1081:PRO:HG3	1.78	0.48
2:C:1176:LEU:HD13	2:C:1180:MET:HG2	1.96	0.48
3:J:1341:ARG:HH22	3:J:1373:ARG:HH21	1.60	0.48
3:J:1162:ILE:HG23	3:J:1178:THR:HB	1.96	0.48
1:H:108:GLY:O	1:H:133:LEU:HB2	2.14	0.48
3:J:1191:PRO:HB2	3:J:1194:ARG:HD3	1.95	0.48
1:A:321:TRP:HA	1:A:322:PRO:HA	1.73	0.48
2:C:799:ASN:HA	2:C:1231:TYR:HA	1.95	0.48
3:D:863:LEU:HD11	3:D:901:ARG:HB3	1.94	0.48
3:D:1167:LYS:HE3	3:D:1168:GLU:H	1.77	0.48
5:L:466:ILE:HD13	5:L:486:ARG:HB3	1.96	0.48
2:C:870:ILE:HB	2:C:944:ARG:HD3	1.96	0.48
1:H:182:ARG:NH1	3:J:581:MET:SD	2.87	0.48
2:I:1287:LEU:HD13	3:J:1357:ILE:HD11	1.96	0.48
2:I:1101:LEU:HD13	3:J:504:GLN:HB2	1.96	0.48
2:I:50:GLU:HG2	2:I:73:TYR:HE1	1.79	0.48
2:I:641:GLU:OE2	3:J:749:LYS:NZ	2.36	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1223:ARG:NH2	3:J:719:PHE:O	2.47	0.48
2:C:878:THR:OG1	2:C:879:GLY:N	2.44	0.48
5:L:316:PHE:HZ	5:L:334:SER:HA	1.78	0.48
2:I:1065:LYS:HD2	2:I:1235:LEU:HD12	1.96	0.48
3:J:777:HIS:CE1	3:J:781:LYS:HD2	2.49	0.48
2:C:1185:PRO:HB2	2:C:1188:ASP:HB3	1.96	0.48
1:B:56:VAL:HG22	1:B:144:ILE:HD11	1.96	0.48
2:C:1116:HIS:HE1	3:D:641:ILE:H	1.61	0.48
3:D:398:LYS:HE2	5:F:532:LEU:HD23	1.94	0.48
1:A:66:HIS:HA	1:A:171:LEU:HD11	1.96	0.48
2:I:668:ILE:HD11	2:I:683:ALA:HB2	1.95	0.48
3:D:128:LEU:HA	3:D:192:MET:HE1	1.96	0.48
3:J:68:TYR:HA	3:J:92:VAL:HG23	1.96	0.48
1:H:102:LEU:HD12	1:H:142:MET:HG2	1.95	0.48
3:J:1170:LYS:C	3:J:1172:LYS:H	2.18	0.47
3:D:1227:HIS:CG	3:J:1293:GLU:HG2	2.48	0.47
3:D:1287:ILE:O	3:D:1291:GLU:HG3	2.13	0.47
3:D:189:LEU:HB3	3:D:234:PRO:HB2	1.96	0.47
3:J:218:THR:HA	3:J:221:ILE:HG22	1.96	0.47
2:I:842:ASP:N	2:I:1045:GLY:O	2.47	0.47
3:J:481:ARG:NH1	4:K:3:ARG:O	2.47	0.47
1:A:282:VAL:O	1:A:316:MET:N	2.47	0.47
3:D:885:VAL:HG12	3:D:894:VAL:HG11	1.96	0.47
1:B:182:ARG:NH1	3:D:581:MET:SD	2.87	0.47
2:C:903:ARG:O	2:C:907:GLY:N	2.46	0.47
1:G:66:HIS:CE1	1:G:69:SER:HB3	2.49	0.47
3:J:1295:ASN:HB2	3:J:1298:VAL:HB	1.94	0.47
1:H:62:ASP:OD2	1:H:71:LYS:NZ	2.43	0.47
3:D:30:ILE:HG23	3:D:243:PRO:HG3	1.94	0.47
3:D:355:ILE:HG22	3:D:447:ILE:HB	1.95	0.47
1:B:97:GLU:OE1	1:B:147:GLN:HG3	2.14	0.47
2:I:146:VAL:HG13	2:I:529:ARG:HB3	1.94	0.47
3:J:412:LEU:HA	3:J:415:VAL:HG22	1.96	0.47
2:C:28:LEU:HD21	2:C:524:ILE:HG13	1.95	0.47
2:C:1275:VAL:HG13	2:C:1287:LEU:HD11	1.95	0.47
2:I:590:PRO:HB2	2:I:655:VAL:HG21	1.95	0.47
2:I:661:VAL:HB	2:I:665:ALA:HB3	1.96	0.47
3:J:1077:ALA:HB2	3:J:1100:PHE:CD1	2.49	0.47
2:C:211:ARG:NH1	2:C:357:ASN:O	2.47	0.47
2:I:929:ILE:HD13	2:I:1055:ALA:HB2	1.95	0.47
2:C:149:LEU:HB2	2:C:530:ILE:HG22	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:616:ILE:HG13	2:C:652:TYR:HB2	1.97	0.47
2:I:250:THR:HA	2:I:268:ARG:HA	1.95	0.47
2:C:850:ILE:HG13	2:C:1048:LYS:HE2	1.96	0.47
3:J:697:MET:SD	3:J:741:ALA:HB3	2.55	0.47
3:J:548:VAL:HG12	3:J:550:VAL:HG13	1.96	0.47
2:C:250:THR:HA	2:C:268:ARG:HA	1.96	0.47
3:D:1280:VAL:O	3:D:1284:ARG:HB3	2.14	0.47
5:F:572:THR:O	5:F:576:VAL:HG23	2.15	0.47
1:G:28:LEU:HB2	1:G:201:LEU:HB3	1.95	0.47
1:G:31:LEU:HD13	1:G:36:GLY:HA2	1.97	0.47
1:G:230:ALA:HB2	1:H:12:ARG:HG2	1.95	0.47
2:C:842:ASP:N	2:C:1045:GLY:O	2.48	0.47
2:C:227:LYS:O	2:C:245:ARG:NH2	2.48	0.47
2:C:896:THR:HB	2:C:897:PRO:HD2	1.95	0.47
3:J:895:CYS:SG	3:J:898:CYS:HB2	2.55	0.47
1:B:44:ARG:NH1	1:B:44:ARG:HB3	2.30	0.47
3:D:800:LEU:HB3	3:D:920:ALA:HB1	1.97	0.47
3:J:839:VAL:HG12	3:J:864:LEU:HD12	1.96	0.47
3:D:68:TYR:HA	3:D:92:VAL:HG23	1.95	0.47
2:I:1254:VAL:HG13	2:I:1255:THR:H	1.79	0.47
3:J:1343:GLU:HB3	3:J:1345:ARG:HD3	1.97	0.47
2:I:806:PRO:O	3:J:633:ALA:HA	2.14	0.47
2:C:145:ILE:HB	2:C:456:VAL:HG22	1.97	0.47
2:C:97:ARG:HB3	2:C:121:GLU:HB2	1.96	0.47
2:I:746:ALA:HB3	2:I:971:LEU:HA	1.96	0.47
2:I:26:TYR:O	2:I:29:SER:HB2	2.15	0.47
2:C:901:LEU:O	2:C:905:ILE:HG13	2.15	0.47
1:A:282:VAL:HB	1:A:316:MET:HB2	1.95	0.47
5:L:287:ILE:HG12	5:L:337:VAL:HG13	1.97	0.47
2:I:617:ALA:HA	2:I:636:CYS:SG	2.54	0.47
2:I:739:ASP:N	2:I:739:ASP:OD1	2.40	0.47
2:C:149:LEU:HD11	2:C:451:ARG:HB3	1.96	0.47
1:A:182:ARG:O	1:A:183:ILE:HD12	2.14	0.47
2:C:658:GLN:O	2:C:660:VAL:N	2.48	0.47
3:J:205:LEU:HD23	3:J:217:LEU:HB3	1.97	0.47
3:D:122:SER:O	3:D:126:LEU:HG	2.14	0.47
2:I:389:PHE:HB3	2:I:420:LEU:HD12	1.96	0.47
3:J:1046:ILE:HD12	3:J:1059:LEU:HB3	1.97	0.47
3:D:1226:VAL:HG23	3:J:1296:GLY:HA2	1.96	0.47
3:D:1295:ASN:HB2	3:D:1298:VAL:HB	1.96	0.47
3:D:1297:LYS:HG2	3:J:1302:TYR:H	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:GLN:HB2	1:A:120:ASP:OD2	2.15	0.47
2:C:1289:GLU:OE2	3:D:473:THR:HG22	2.14	0.47
3:D:1205:GLU:O	3:D:1208:ASP:HB2	2.14	0.47
1:A:102:LEU:HB3	1:A:142:MET:HG2	1.96	0.47
3:J:709:ARG:C	3:J:711:GLY:H	2.18	0.47
2:I:820:GLU:HA	2:I:1079:ILE:HD11	1.97	0.47
3:D:708:ASN:N	3:D:708:ASN:OD1	2.47	0.46
3:D:35:PHE:CD1	3:D:101:ARG:HD3	2.50	0.46
1:G:79:LEU:CD1	2:I:693:LEU:HD21	2.45	0.46
3:J:103:GLY:HA3	3:J:244:VAL:HG22	1.97	0.46
3:J:73:GLY:O	3:J:76:LYS:NZ	2.36	0.46
2:I:255:ILE:HB	2:I:263:VAL:HB	1.96	0.46
3:D:103:GLY:HA3	3:D:244:VAL:HG22	1.97	0.46
1:B:39:LEU:O	1:B:43:LEU:HB2	2.16	0.46
1:H:64:VAL:HG12	1:H:65:LEU:H	1.80	0.46
2:C:468:LEU:HA	2:C:471:VAL:HG12	1.97	0.46
2:I:1280:ALA:HB1	3:J:918:ILE:HG22	1.97	0.46
3:D:1286:LYS:O	3:D:1290:ARG:HB2	2.15	0.46
1:A:54:CYS:HA	1:A:148:ARG:HG3	1.97	0.46
3:D:682:VAL:HA	3:D:685:ILE:CD1	2.46	0.46
3:J:1024:THR:HG22	3:J:1026:PRO:HD3	1.96	0.46
2:C:820:GLU:N	2:C:1080:ASN:O	2.49	0.46
2:I:28:LEU:HD21	2:I:524:ILE:HG13	1.96	0.46
2:C:387:ASN:HA	2:C:391:SER:HB2	1.97	0.46
2:C:646:SER:HB3	2:C:649:GLN:HG3	1.97	0.46
3:D:930:LEU:HD11	3:D:1241:TYR:CE2	2.50	0.46
1:B:108:GLY:O	1:B:133:LEU:HB2	2.15	0.46
2:I:1313:HIS:N	4:K:31:GLN:OE1	2.49	0.46
5:F:316:PHE:HZ	5:F:334:SER:HA	1.80	0.46
5:F:441:ARG:NH1	5:F:445:ASP:OD1	2.48	0.46
5:L:548:LEU:HD21	5:L:559:LEU:HD23	1.98	0.46
3:D:598:LYS:HA	3:D:601:ILE:HG22	1.96	0.46
2:C:196:VAL:HG12	2:C:206:ALA:HA	1.98	0.46
3:D:147:ILE:HG22	3:D:188:LEU:HG	1.97	0.46
1:A:106:GLY:HA2	1:A:136:GLU:O	2.15	0.46
5:L:573:LEU:H	5:L:573:LEU:HD23	1.80	0.46
2:C:724:VAL:HA	2:C:734:ILE:HD13	1.97	0.46
3:D:357:VAL:HG22	3:D:461:PHE:CE1	2.51	0.46
2:C:136:PHE:CE2	2:C:456:VAL:HG11	2.51	0.46
3:D:654:ILE:O	3:D:658:GLU:HB2	2.15	0.46
1:A:182:ARG:C	1:A:183:ILE:HD12	2.35	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:MET:HB3	1:A:316:MET:HE3	1.84	0.46
1:G:221:ALA:HB1	1:H:228:LEU:HD13	1.98	0.46
3:D:848:VAL:HG22	3:D:858:VAL:CG2	2.45	0.46
3:J:888:CYS:SG	3:J:890:THR:HB	2.56	0.46
3:J:253:VAL:HA	3:J:254:PRO:HD3	1.78	0.46
1:A:54:CYS:O	1:A:146:VAL:HG13	2.15	0.46
2:I:757:THR:HG23	2:I:765:ILE:HG23	1.97	0.46
5:F:164:GLY:O	5:F:260:ARG:HB2	2.15	0.46
2:I:705:GLU:HB2	2:I:794:LEU:HB3	1.97	0.46
2:I:1176:LEU:HD13	2:I:1180:MET:HG2	1.98	0.46
1:H:56:VAL:HG22	1:H:144:ILE:HD11	1.97	0.46
2:C:26:TYR:CZ	2:C:28:LEU:HB2	2.51	0.46
3:D:1163:VAL:HG23	3:D:1177:ILE:HA	1.98	0.46
2:I:799:ASN:HA	2:I:1231:TYR:HA	1.96	0.46
5:L:492:ASP:HB2	5:L:495:ARG:HH12	1.81	0.46
3:J:421:VAL:HG13	3:J:439:PRO:HG3	1.97	0.46
3:D:9:LYS:HE2	3:D:11:GLN:HA	1.98	0.46
1:A:172:LEU:H	1:A:172:LEU:HD12	1.81	0.46
2:I:197:ARG:NH2	5:L:29:ASP:OD2	2.49	0.46
5:L:572:THR:O	5:L:576:VAL:HG23	2.16	0.46
5:F:299:LYS:HA	5:F:302:PHE:HB3	1.97	0.46
3:D:712:GLN:CD	3:D:712:GLN:H	2.14	0.46
5:F:551:LEU:HD21	5:F:598:LEU:HD21	1.98	0.46
1:G:50:SER:HB3	1:G:150:ARG:HD2	1.98	0.46
1:B:151:GLY:O	1:B:177:TYR:HD2	1.99	0.46
3:D:901:ARG:HA	3:D:908:ILE:HA	1.96	0.46
5:L:561:MET:HG3	5:L:571:TYR:CD2	2.51	0.46
5:F:583:THR:HG22	5:F:584:ARG:H	1.81	0.46
3:J:950:ILE:HG13	3:J:1020:TRP:HH2	1.81	0.46
3:J:735:ALA:O	3:J:738:ARG:HB3	2.15	0.46
3:J:128:LEU:HA	3:J:192:MET:HE1	1.98	0.46
3:D:482:ALA:HB3	4:E:20:VAL:HG22	1.98	0.46
3:J:1025:MET:SD	3:J:1124:ILE:HD12	2.56	0.46
5:F:362:ASN:HB2	5:F:365:MET:HE2	1.98	0.46
5:F:41:ILE:HA	5:F:44:ILE:HG23	1.98	0.46
3:D:425:ARG:HE	3:D:427:PRO:HD2	1.80	0.46
2:C:578:TYR:HB3	2:C:590:PRO:HG2	1.97	0.46
3:J:872:LEU:O	3:J:877:VAL:HG12	2.16	0.46
2:C:524:ILE:HG21	2:C:708:VAL:HG13	1.98	0.46
5:L:313:ASP:OD1	5:L:338:HIS:NE2	2.49	0.46
2:I:215:TYR:HA	2:I:219:GLN:NE2	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:197:GLU:O	3:J:201:LEU:HG	2.16	0.46
3:J:426:ALA:HB3	3:J:427:PRO:HD3	1.98	0.45
5:L:402:LEU:HA	5:L:405:ILE:HG12	1.97	0.45
2:C:557:ARG:HH21	2:C:607:SER:C	2.19	0.45
2:I:820:GLU:N	2:I:1080:ASN:O	2.48	0.45
1:A:319:GLU:O	1:A:320:ASN:HB2	2.15	0.45
2:I:1286:THR:N	3:J:479:GLU:OE2	2.42	0.45
3:D:591:ILE:HG13	3:D:604:MET:HE2	1.97	0.45
4:K:73:GLN:HA	4:K:76:GLU:HB3	1.98	0.45
2:C:819:SER:HB2	2:C:1085:MET:HG3	1.97	0.45
1:G:26:VAL:HG22	1:G:203:ILE:HB	1.97	0.45
3:D:16:GLU:HG3	3:D:1369:ARG:NH2	2.31	0.45
1:G:28:LEU:HD22	1:G:201:LEU:HD23	1.99	0.45
5:L:165:PHE:HE2	5:L:217:ALA:HA	1.80	0.45
3:J:709:ARG:O	3:J:711:GLY:N	2.48	0.45
2:C:206:ALA:O	2:C:209:ILE:HG22	2.16	0.45
1:G:106:GLY:HA2	1:G:136:GLU:O	2.16	0.45
3:D:1267:VAL:HB	3:D:1301:THR:OG1	2.17	0.45
2:I:854:ILE:HB	2:I:857:VAL:HG21	1.99	0.45
5:F:493:LYS:HA	5:F:496:LYS:HE2	1.98	0.45
2:C:21:VAL:HG11	2:C:592:ARG:HD2	1.99	0.45
3:D:77:ARG:NE	5:F:569:THR:HA	2.32	0.45
2:I:578:TYR:HB3	2:I:590:PRO:HG2	1.97	0.45
2:I:680:LEU:O	2:I:684:ASN:HB2	2.16	0.45
2:I:1125:GLY:HA3	2:I:1179:GLY:HA2	1.98	0.45
3:J:425:ARG:HE	3:J:427:PRO:HD2	1.81	0.45
3:D:770:LEU:H	3:D:770:LEU:HD22	1.82	0.45
3:J:291:ILE:HD13	5:L:409:ASN:HB3	1.99	0.45
5:L:130:VAL:HB	5:L:365:MET:HG3	1.97	0.45
1:A:28:LEU:HB2	1:A:201:LEU:HB3	1.99	0.45
2:I:149:LEU:HB2	2:I:530:ILE:HG22	1.97	0.45
3:J:1198:VAL:HG23	3:J:1204:VAL:HG11	1.98	0.45
5:L:465:ARG:HA	5:L:468:ARG:HH12	1.82	0.45
2:I:710:VAL:HA	2:I:715:THR:HG21	1.98	0.45
3:J:361:LEU:HD22	3:J:365:GLN:HG3	1.97	0.45
3:J:290:ILE:HD12	3:J:290:ILE:H	1.81	0.45
5:F:601:PRO:HB2	5:F:605:GLU:OE2	2.17	0.45
3:D:905:ARG:HH21	3:D:907:HIS:CB	2.29	0.45
2:I:149:LEU:HD11	2:I:451:ARG:HB3	1.99	0.45
3:D:1227:HIS:HD2	3:J:1293:GLU:H	1.65	0.45
2:I:553:THR:O	2:I:557:ARG:HD2	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:275:ARG:HD3	3:J:298:MET:HB3	1.97	0.45
3:D:62:PHE:O	3:D:101:ARG:HD2	2.17	0.45
3:D:198:CYS:O	3:D:202:ARG:HG3	2.17	0.45
3:J:122:SER:O	3:J:126:LEU:HG	2.17	0.45
2:C:840:SER:O	2:C:1047:LEU:N	2.50	0.45
3:D:115:TRP:CE2	3:D:1329:THR:HG23	2.52	0.45
2:C:590:PRO:HB2	2:C:655:VAL:HG21	1.98	0.45
2:C:1101:LEU:HD21	3:D:508:LEU:HD22	1.97	0.45
5:L:461:ASN:O	5:L:465:ARG:HG2	2.16	0.45
2:C:389:PHE:HB3	2:C:420:LEU:HD12	1.97	0.45
5:F:287:ILE:HG12	5:F:337:VAL:HG13	1.99	0.45
1:B:89:ALA:HB3	1:B:124:VAL:HG12	1.98	0.45
3:J:1205:GLU:O	3:J:1208:ASP:HB2	2.16	0.45
2:I:778:GLU:O	2:I:781:ASP:HB2	2.17	0.45
3:D:587:LEU:HD11	3:D:608:CYS:HA	1.99	0.45
2:C:734:ILE:HD12	2:C:777:VAL:HG21	1.98	0.45
3:J:266:ASN:O	3:J:270:ARG:HB2	2.17	0.45
1:B:64:VAL:HG12	1:B:65:LEU:H	1.81	0.45
1:B:78:ILE:O	1:B:82:LEU:HG	2.16	0.45
3:D:712:GLN:N	3:D:712:GLN:CD	2.69	0.45
2:C:1282:GLY:HA3	4:E:17:PHE:CE1	2.51	0.45
3:D:925:GLU:HB3	3:D:926:PRO:HD3	1.99	0.45
2:I:402:ARG:NH2	2:I:419:ILE:O	2.50	0.45
3:J:1319:PHE:CE2	3:J:1342:ASP:HB2	2.52	0.45
3:J:810:THR:HG23	3:J:811:GLU:H	1.81	0.45
5:F:492:ASP:HB2	5:F:495:ARG:HH12	1.81	0.45
1:B:54:CYS:SG	1:B:148:ARG:HG2	2.57	0.45
2:C:680:LEU:O	2:C:684:ASN:HB2	2.17	0.45
3:J:1078:LEU:HB3	3:J:1121:LEU:HD13	1.98	0.45
2:I:115:LYS:HE3	2:I:116:ASP:H	1.82	0.45
2:C:1159:VAL:HB	2:C:1160:ASP:H	1.60	0.45
2:I:1282:GLY:O	3:J:1361:THR:N	2.49	0.45
3:J:368:LEU:HD22	3:J:373:ALA:HB2	1.99	0.45
3:J:901:ARG:HD2	3:J:906:GLY:O	2.16	0.45
2:I:1240:ASP:HB3	3:J:445:LYS:HD2	1.98	0.45
3:D:421:VAL:HG13	3:D:439:PRO:HG3	1.98	0.45
1:G:58:GLU:HB2	1:G:145:LYS:HB3	1.98	0.45
1:B:37:HIS:CE1	2:C:1216:ARG:HD2	2.52	0.45
2:I:26:TYR:CE2	2:I:32:LEU:HD12	2.52	0.45
3:D:1286:LYS:HD2	3:D:1290:ARG:NH2	2.32	0.45
2:C:60:GLN:HB3	2:C:67:GLU:HG3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:42:ASP:OD2	2:I:46:GLN:HB3	2.17	0.45
1:H:54:CYS:SG	1:H:148:ARG:HG2	2.57	0.45
3:J:668:PHE:HB2	3:J:678:ARG:HG3	1.99	0.44
3:J:1280:VAL:O	3:J:1284:ARG:HB3	2.17	0.44
1:B:100:LEU:HD11	1:B:121:VAL:HG21	1.97	0.44
2:C:242:VAL:HB	2:C:245:ARG:HD2	1.98	0.44
3:D:598:LYS:O	3:D:601:ILE:HG22	2.17	0.44
5:F:346:GLN:O	5:F:350:GLU:HG3	2.17	0.44
3:J:1036:ARG:HG2	3:J:1037:PHE:H	1.81	0.44
5:F:380:VAL:HG22	5:F:416:VAL:HG21	1.98	0.44
3:J:1368:ASP:OD1	3:J:1371:ARG:NH2	2.49	0.44
2:C:1072:ASN:OD1	2:C:1072:ASN:N	2.49	0.44
3:D:1230:THR:OG1	3:D:1257:VAL:HG11	2.17	0.44
2:I:232:ILE:HG12	2:I:237:LEU:HD13	1.99	0.44
2:C:10:ARG:NH1	2:C:697:LYS:HD3	2.32	0.44
3:D:573:THR:OG1	3:D:576:ARG:HG3	2.16	0.44
2:I:1185:PRO:HB2	2:I:1188:ASP:HB3	1.98	0.44
5:F:465:ARG:HA	5:F:468:ARG:HH12	1.83	0.44
2:I:678:ARG:HG3	2:I:1108:ASN:HD22	1.81	0.44
5:F:412:LEU:HD13	5:F:435:ILE:HD11	1.98	0.44
3:D:657:ALA:O	3:D:661:VAL:HG13	2.17	0.44
1:B:99:ILE:HD11	1:B:143:ARG:HB3	1.99	0.44
3:J:70:CYS:SG	3:J:71:LEU:N	2.90	0.44
2:I:618:GLN:HG3	3:J:770:LEU:HD21	1.99	0.44
3:J:1244:GLN:HE21	3:J:1244:GLN:HB3	1.59	0.44
2:C:1313:HIS:HB2	3:D:474:LEU:HD13	1.99	0.44
3:D:425:ARG:NH1	3:D:459:ALA:HA	2.33	0.44
3:D:860:ARG:HB3	3:D:861:ASN:H	1.56	0.44
3:D:1193:TRP:HB2	3:D:1194:ARG:NH1	2.32	0.44
1:G:182:ARG:C	1:G:183:ILE:HD12	2.38	0.44
5:F:244:THR:O	5:F:247:GLU:HG2	2.18	0.44
2:I:936:ARG:NH2	2:I:1043:ALA:O	2.51	0.44
2:I:828:PHE:CE2	2:I:1234:LYS:HB2	2.52	0.44
2:C:808:ASN:H	3:D:633:ALA:HB2	1.82	0.44
2:C:35:PHE:CD2	2:C:130:MET:HB3	2.53	0.44
3:D:1170:LYS:C	3:D:1172:LYS:H	2.20	0.44
2:C:124:MET:HB2	2:C:498:ILE:HD13	2.00	0.44
2:C:213:LEU:HD13	2:C:422:LYS:HG2	1.98	0.44
3:J:203:GLU:O	3:J:207:GLU:HG2	2.18	0.44
2:I:130:MET:SD	2:I:134:GLY:HA2	2.58	0.44
2:I:238:GLN:HB3	2:I:284:LEU:HD11	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:J:505:ASP:HB2	3:J:629:PHE:HE1	1.83	0.44
3:J:706:VAL:HG12	3:J:715:LYS:HB3	2.00	0.44
3:D:615:LYS:HB2	3:D:616:PRO:HD3	1.99	0.44
5:F:559:LEU:HA	5:F:559:LEU:HD12	1.80	0.44
3:J:660:GLU:O	3:J:664:ILE:HG12	2.17	0.44
2:I:850:ILE:HG13	2:I:1048:LYS:HE2	1.98	0.44
1:G:182:ARG:HB3	1:G:206:GLU:HB3	2.00	0.44
3:J:50:LYS:HB3	3:J:71:LEU:HD21	2.00	0.44
3:D:412:LEU:HA	3:D:415:VAL:HG22	1.99	0.44
2:I:356:THR:HG21	2:I:362:ALA:HA	1.99	0.44
1:A:51:MET:HE3	1:A:51:MET:HB3	1.91	0.44
5:L:127:ILE:O	5:L:130:VAL:HG22	2.18	0.44
2:C:1142:ARG:HH12	2:C:1165:SER:HA	1.82	0.44
3:J:701:LEU:HD13	3:J:723:TYR:HB2	2.00	0.44
3:J:587:LEU:HD11	3:J:608:CYS:HA	1.99	0.44
3:J:506:VAL:HG23	3:J:628:GLY:HA3	2.00	0.44
5:F:313:ASP:OD1	5:F:338:HIS:NE2	2.50	0.44
3:J:708:ASN:N	3:J:708:ASN:OD1	2.49	0.44
3:D:266:ASN:O	3:D:270:ARG:HB2	2.17	0.44
3:J:697:MET:O	3:J:701:LEU:HB2	2.18	0.44
1:G:102:LEU:HB3	1:G:142:MET:HG2	1.99	0.44
5:L:136:GLU:OE1	5:L:364:ARG:NH2	2.51	0.44
3:D:497:GLU:HA	3:D:498:PRO:HD3	1.84	0.44
3:J:598:LYS:O	3:J:601:ILE:HG22	2.18	0.44
5:F:215:GLU:HG2	5:F:218:ARG:HH21	1.82	0.44
2:C:237:LEU:HD22	2:C:237:LEU:H	1.82	0.44
1:G:39:LEU:HD23	1:G:39:LEU:HA	1.86	0.44
3:D:701:LEU:HD13	3:D:723:TYR:HB2	1.99	0.44
3:D:156:ARG:NH2	3:D:191:SER:OG	2.46	0.44
3:J:438:GLU:HA	3:J:439:PRO:HD3	1.86	0.44
1:G:48:LEU:HA	1:G:180:VAL:HG21	2.00	0.44
1:G:54:CYS:HA	1:G:148:ARG:HG3	1.98	0.44
2:I:1267:GLY:HA3	3:J:347:VAL:O	2.18	0.44
2:C:176:ILE:HD12	2:C:184:LEU:HD23	1.99	0.44
2:I:316:GLU:CD	2:I:316:GLU:H	2.21	0.44
1:B:221:ALA:O	1:B:224:LEU:HB3	2.18	0.43
3:J:385:LEU:HD11	3:J:408:VAL:HG12	2.00	0.43
3:J:694:SER:OG	3:J:738:ARG:NE	2.42	0.43
2:C:53:PHE:O	2:C:57:PHE:HB2	2.19	0.43
2:I:1103:VAL:HG11	2:I:1112:ILE:HD11	1.99	0.43
2:I:1211:ARG:O	2:I:1212:LEU:HD12	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:499:SER:O	2:C:503:LYS:HB2	2.18	0.43
2:C:838:CYS:SG	2:C:886:LYS:HD3	2.58	0.43
3:J:1349:GLU:N	3:J:1349:GLU:OE2	2.38	0.43
1:B:61:ILE:HG21	1:B:78:ILE:HD13	1.99	0.43
1:H:89:ALA:HB3	1:H:124:VAL:HG12	1.99	0.43
3:D:197:GLU:O	3:D:201:LEU:HG	2.17	0.43
5:F:580:PHE:C	5:F:582:VAL:H	2.21	0.43
2:C:1149:TYR:HB3	2:C:1159:VAL:HG11	2.01	0.43
2:C:14:ASP:N	2:C:1157:GLN:OE1	2.33	0.43
2:I:813:GLU:HA	3:J:504:GLN:NE2	2.33	0.43
3:J:268:LEU:HB3	3:J:306:LEU:HD23	2.00	0.43
3:J:611:ILE:HG22	3:J:612:LEU:HD12	2.00	0.43
1:A:79:LEU:CD1	2:C:693:LEU:HD21	2.49	0.43
3:J:190:LYS:HD3	3:J:235:GLU:HG2	2.00	0.43
3:D:548:VAL:HG12	3:D:550:VAL:HG13	1.99	0.43
3:D:384:LYS:HD2	3:D:387:LEU:HD23	1.99	0.43
3:D:308:ASP:OD2	3:D:311:ARG:NH2	2.43	0.43
2:C:356:THR:HG21	2:C:362:ALA:HA	1.99	0.43
1:B:57:THR:HG22	1:B:58:GLU:HG2	2.00	0.43
3:D:441:LEU:HD13	3:D:441:LEU:HA	1.85	0.43
6:C:2001:4OE:CAL	3:D:755:ILE:HG12	2.48	0.43
5:F:561:MET:HG3	5:F:571:TYR:CD2	2.54	0.43
5:F:462:LYS:O	5:F:466:ILE:HG13	2.17	0.43
3:J:1048:ARG:NH2	3:J:1057:SER:HB2	2.33	0.43
3:D:777:HIS:CE1	3:D:781:LYS:HD2	2.53	0.43
3:D:268:LEU:HB3	3:D:306:LEU:HD23	2.00	0.43
2:C:1210:ILE:HG22	2:C:1211:ARG:H	1.83	0.43
2:I:720:ARG:HA	2:I:779:ARG:HG3	2.00	0.43
1:H:16:ILE:HG13	1:H:26:VAL:HG22	2.00	0.43
2:C:17:LYS:HE3	2:C:1154:ASP:HB3	2.00	0.43
5:L:289:LYS:HE2	5:L:289:LYS:HB3	1.88	0.43
2:C:996:ARG:HD3	2:C:996:ARG:HA	1.91	0.43
2:I:808:ASN:OD1	2:I:1216:ARG:NH2	2.52	0.43
3:D:426:ALA:HB3	3:D:427:PRO:HD3	2.00	0.43
3:J:1348:LYS:HA	3:J:1348:LYS:HD2	1.84	0.43
5:F:137:TYR:HE1	5:F:351:THR:HB	1.83	0.43
3:D:799:ARG:HB3	3:D:1309:ILE:HD12	2.00	0.43
2:C:360:LEU:HB2	2:C:378:ARG:HH21	1.83	0.43
3:J:422:LEU:HD13	3:J:471:PRO:HG3	2.00	0.43
3:D:697:MET:HE1	3:D:737:ILE:HG22	2.01	0.43
2:C:1121:ALA:HB1	2:C:1180:MET:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:60:GLN:HB3	2:I:67:GLU:HG3	2.01	0.43
3:J:34:SER:OG	3:J:104:HIS:ND1	2.30	0.43
2:C:238:GLN:HB3	2:C:284:LEU:HD11	2.00	0.43
2:I:170:VAL:HG23	2:I:171:LEU:N	2.32	0.43
3:J:264:ASP:OD2	3:J:264:ASP:N	2.52	0.43
2:C:724:VAL:HG11	2:C:727:VAL:HG22	2.00	0.43
3:J:820:ILE:HG22	3:J:1227:HIS:ND1	2.34	0.43
2:C:758:ARG:NH1	2:C:835:GLU:OE1	2.51	0.43
4:K:49:ILE:HA	4:K:52:ARG:HD3	2.01	0.43
3:J:969:SER:HB3	3:J:1116:SER:HB2	2.01	0.43
2:C:83:GLN:O	2:C:87:ILE:HG13	2.19	0.43
3:J:799:ARG:HB3	3:J:1309:ILE:HD12	1.99	0.43
2:C:37:LYS:HA	2:C:37:LYS:HD3	1.83	0.43
2:C:552:PRO:HG3	6:C:2001:4OE:CAQ	2.49	0.43
2:C:953:LEU:HD12	2:C:1036:ILE:HD12	2.00	0.43
5:F:511:ILE:HA	5:F:511:ILE:HD12	1.84	0.43
2:I:499:SER:O	2:I:503:LYS:HB2	2.18	0.43
2:C:1247:SER:OG	2:C:1248:THR:N	2.52	0.43
2:C:700:VAL:HG13	2:C:1117:LEU:HD22	2.00	0.43
2:I:721:GLY:N	2:I:740:GLU:OE1	2.47	0.43
2:I:906:PHE:CE2	5:L:608:ARG:HG3	2.54	0.43
3:D:264:ASP:N	3:D:264:ASP:OD2	2.52	0.43
3:J:1230:THR:OG1	3:J:1257:VAL:HG11	2.19	0.43
3:J:1193:TRP:HB2	3:J:1194:ARG:NH1	2.34	0.43
2:I:551:HIS:ND1	2:I:552:PRO:HD2	2.34	0.43
3:J:62:PHE:O	3:J:101:ARG:HD2	2.19	0.43
2:I:692:THR:OG1	2:I:827:ARG:O	2.34	0.43
2:I:56:VAL:HG11	2:I:468:LEU:HB3	2.01	0.43
2:C:478:ARG:HH12	2:C:482:GLY:HA2	1.82	0.43
3:J:848:VAL:HG22	3:J:858:VAL:CG2	2.48	0.43
5:L:234:THR:O	5:L:245:ALA:HB2	2.18	0.43
2:I:1122:LYS:HG2	2:I:1229:TYR:CE1	2.53	0.43
2:C:705:GLU:HB2	2:C:794:LEU:HB3	2.00	0.43
3:D:430:HIS:HA	3:D:921:GLN:HB3	2.01	0.43
3:J:1095:MET:HA	3:J:1096:PRO:HD3	1.83	0.43
3:J:987:GLU:HG3	3:J:987:GLU:H	1.61	0.43
2:I:10:ARG:NH1	2:I:697:LYS:HD3	2.34	0.43
1:B:100:LEU:HB2	1:B:144:ILE:HG23	2.01	0.43
2:C:634:VAL:HG13	2:C:636:CYS:SG	2.59	0.43
3:J:479:GLU:HG3	4:K:20:VAL:HG11	2.00	0.43
5:F:582:VAL:HG22	5:F:586:ARG:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:68:LEU:HD11	2:I:100:LEU:HB3	2.00	0.43
3:J:274:ASN:ND2	5:L:446:GLN:HB2	2.34	0.43
2:C:936:ARG:NH2	2:C:1043:ALA:O	2.51	0.43
5:F:22:LEU:H	5:F:54:GLN:CB	2.32	0.43
3:D:1146:GLU:HB3	3:D:1148:ARG:HG3	2.01	0.43
1:B:101:THR:HG23	1:B:103:ASN:H	1.84	0.42
2:I:976:ARG:NH2	2:I:990:ASP:OD2	2.52	0.42
3:D:1293:GLU:HG2	3:J:1227:HIS:HB2	2.01	0.42
3:D:854:ALA:HB2	3:J:1372:ARG:CB	2.47	0.42
2:I:26:TYR:CE2	2:I:28:LEU:HB2	2.54	0.42
2:C:383:SER:O	2:C:387:ASN:HB2	2.19	0.42
3:J:1319:PHE:CD2	3:J:1342:ASP:HB2	2.54	0.42
3:J:287:ALA:HB3	3:J:292:VAL:HG13	2.01	0.42
5:F:469:GLN:O	5:F:472:GLN:NE2	2.53	0.42
2:I:17:LYS:HE3	2:I:1154:ASP:HB3	2.01	0.42
1:B:16:ILE:HG13	1:B:26:VAL:HG22	2.00	0.42
2:I:538:LEU:H	2:I:538:LEU:HG	1.62	0.42
5:L:124:GLU:O	5:L:128:ASN:HB2	2.19	0.42
2:I:299:LYS:HB2	2:I:299:LYS:HE2	1.78	0.42
1:A:231:PHE:CE2	1:B:43:LEU:CD2	2.96	0.42
2:C:10:ARG:HA	2:C:1172:LEU:HD23	2.01	0.42
1:A:58:GLU:HB2	1:A:145:LYS:HB3	2.00	0.42
6:I:2001:4OE:CAL	3:J:755:ILE:HG12	2.49	0.42
1:A:31:LEU:HD13	1:A:36:GLY:HA2	2.00	0.42
3:D:1194:ARG:N	3:D:1194:ARG:HD2	2.34	0.42
2:I:658:GLN:O	2:I:660:VAL:N	2.52	0.42
5:F:348:GLU:HG2	5:F:354:THR:HA	2.00	0.42
2:I:742:TYR:O	2:I:974:ARG:NH2	2.52	0.42
3:D:1319:PHE:CE2	3:D:1342:ASP:HB2	2.54	0.42
2:I:528:ARG:NH2	2:I:575:LEU:HD23	2.34	0.42
3:J:425:ARG:HH12	3:J:464:ASP:CG	2.21	0.42
2:I:1142:ARG:HH12	2:I:1165:SER:HA	1.84	0.42
2:C:1149:TYR:CD1	2:C:1159:VAL:HG11	2.54	0.42
2:C:1276:TRP:HE1	3:D:1348:LYS:NZ	2.17	0.42
3:J:863:LEU:HD11	3:J:901:ARG:HB3	2.01	0.42
2:C:1117:LEU:HD12	2:C:1195:ILE:HG12	2.02	0.42
2:I:538:LEU:HD22	2:I:543:ALA:HB2	2.00	0.42
2:C:778:GLU:O	2:C:781:ASP:HB2	2.20	0.42
1:H:33:ARG:HH11	2:I:1081:PRO:HG3	1.84	0.42
1:H:100:LEU:HB2	1:H:144:ILE:HG23	2.01	0.42
2:I:1123:GLY:HA3	2:I:1204:LEU:HD11	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:547:VAL:HG12	5:L:598:LEU:HD22	2.01	0.42
1:B:48:LEU:HA	1:B:180:VAL:HG21	2.01	0.42
1:H:64:VAL:HG21	1:H:69:SER:CB	2.48	0.42
2:C:980:VAL:HA	2:C:984:VAL:HA	2.00	0.42
3:J:385:LEU:HD23	3:J:385:LEU:HA	1.92	0.42
2:I:383:SER:O	2:I:387:ASN:HB2	2.19	0.42
2:I:1121:ALA:HB1	2:I:1180:MET:O	2.20	0.42
2:C:561:ILE:HD11	2:C:665:ALA:HB1	2.00	0.42
5:L:348:GLU:HG2	5:L:354:THR:HA	2.02	0.42
2:C:887:VAL:HB	2:C:913:VAL:CG2	2.49	0.42
2:C:1333:LEU:C	2:C:1335:ILE:H	2.23	0.42
3:J:349:TYR:HE2	3:J:379:PRO:HG2	1.84	0.42
2:C:548:ARG:O	2:C:570:GLY:HA3	2.19	0.42
2:C:1087:TYR:HE1	2:C:1215:GLY:HA2	1.85	0.42
3:J:572:THR:OG1	3:J:573:THR:N	2.52	0.42
1:G:12:ARG:HG2	1:G:13:LEU:N	2.34	0.42
3:D:27:PRO:O	3:D:31:ARG:HG3	2.20	0.42
2:C:591:TYR:HD2	2:C:606:LEU:HD13	1.83	0.42
5:L:511:ILE:HA	5:L:511:ILE:HD12	1.87	0.42
1:G:224:LEU:HD13	1:H:228:LEU:HD11	2.00	0.42
3:D:1355:ARG:NH1	3:D:1369:ARG:HH12	2.17	0.42
2:C:661:VAL:HB	2:C:665:ALA:HB3	2.01	0.42
2:I:466:VAL:O	2:I:469:VAL:HG22	2.19	0.42
5:L:412:LEU:HD13	5:L:435:ILE:HD11	2.01	0.42
1:B:84:ASN:O	1:B:128:HIS:HE1	2.02	0.42
2:C:959:ASP:O	2:C:963:GLU:HG2	2.19	0.42
2:C:972:PHE:CD2	2:C:975:ILE:HD12	2.55	0.42
3:D:1343:GLU:HB3	3:D:1345:ARG:HD3	2.01	0.42
2:C:720:ARG:HE	2:C:736:VAL:HG11	1.83	0.42
2:I:559:CYS:HA	2:I:560:PRO:HD3	1.87	0.42
5:L:130:VAL:O	5:L:134:VAL:HG23	2.20	0.42
1:B:149:GLY:HA3	1:B:177:TYR:CD2	2.54	0.42
3:D:1270:GLY:HA3	3:D:1298:VAL:HG22	2.02	0.42
5:F:148:TYR:OH	5:F:218:ARG:HA	2.20	0.42
2:C:1024:GLU:HA	2:C:1027:LYS:HG2	2.00	0.42
3:J:1034:PHE:HA	3:J:1114:GLN:HA	2.02	0.42
2:I:1146:GLN:NE2	2:I:1160:ASP:OD1	2.52	0.42
3:J:1156:LEU:HB3	3:J:1207:GLY:HA2	2.02	0.42
1:A:75:GLN:HA	2:C:729:ALA:N	2.35	0.42
4:K:51:LEU:HD23	4:K:51:LEU:HA	1.93	0.42
2:I:1312:ASN:OD1	2:I:1314:GLN:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:1276:TRP:HE1	3:J:1348:LYS:NZ	2.17	0.42
3:J:1318:SER:OG	3:J:1342:ASP:OD2	2.27	0.42
1:G:54:CYS:O	1:G:146:VAL:HG13	2.19	0.42
2:I:1281:TYR:CD1	3:J:484:MET:HG2	2.54	0.42
5:F:249:ILE:O	5:F:252:LEU:HB3	2.19	0.42
3:D:919:ALA:O	3:D:923:ILE:HG13	2.20	0.42
3:D:836:ARG:HG3	3:D:869:CYS:HB3	2.00	0.42
1:A:39:LEU:HD11	1:B:227:GLN:HB3	2.00	0.42
5:L:22:LEU:H	5:L:54:GLN:CB	2.32	0.42
3:D:106:GLU:OE2	3:D:241:VAL:HG22	2.19	0.42
3:D:695:LYS:HA	3:D:695:LYS:HD3	1.69	0.42
2:I:657:THR:HG1	2:I:1187:PHE:HB2	1.85	0.42
3:D:394:ILE:CG2	5:F:536:THR:HA	2.50	0.42
1:G:79:LEU:HD11	2:I:693:LEU:HD21	2.01	0.42
2:C:1101:LEU:HD23	3:D:725:MET:SD	2.60	0.42
2:I:211:ARG:NH1	2:I:357:ASN:O	2.53	0.42
3:J:1270:GLY:HA3	3:J:1298:VAL:HG22	2.02	0.42
3:J:557:LYS:HA	3:J:563:LEU:HA	2.02	0.42
2:C:1280:ALA:HB1	3:D:918:ILE:HG22	2.01	0.42
3:D:1372:ARG:HG3	3:J:853:THR:HB	2.01	0.42
5:F:343:LYS:H	5:F:343:LYS:HD2	1.85	0.42
5:F:343:LYS:O	5:F:347:ILE:HG13	2.20	0.42
3:D:557:LYS:HA	3:D:563:LEU:HA	2.02	0.42
3:D:422:LEU:HD13	3:D:471:PRO:HG3	2.02	0.42
1:B:102:LEU:HD23	1:B:115:ILE:HG23	2.02	0.42
5:F:97:PRO:HA	5:F:100:MET:HG3	2.00	0.42
2:I:1179:GLY:O	2:I:1181:PRO:HD3	2.20	0.42
1:G:145:LYS:NZ	1:G:147:GLN:OE1	2.53	0.42
3:D:77:ARG:HD2	3:D:78:LEU:H	1.85	0.42
2:I:176:ILE:HB	2:I:184:LEU:HB3	2.02	0.42
3:D:505:ASP:HB2	3:D:629:PHE:HE1	1.85	0.42
1:A:221:ALA:HB1	1:B:228:LEU:HD22	2.01	0.42
3:D:203:GLU:O	3:D:207:GLU:HG2	2.20	0.42
3:D:1156:LEU:HB3	3:D:1207:GLY:HA2	2.00	0.42
2:I:183:TRP:HB2	2:I:199:ASP:HA	2.02	0.42
5:F:234:THR:O	5:F:245:ALA:HB2	2.19	0.42
1:H:34:GLY:N	1:H:199:ASP:OD2	2.51	0.42
2:I:967:LEU:HA	2:I:967:LEU:HD12	1.91	0.42
1:A:43:LEU:HD23	1:A:43:LEU:HA	1.91	0.42
1:A:228:LEU:CD1	1:B:221:ALA:HB1	2.49	0.42
1:H:181:GLU:HA	3:J:535:ARG:NH2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1116:HIS:O	2:C:1119:MET:HB3	2.20	0.42
2:C:553:THR:O	2:C:557:ARG:HD2	2.20	0.42
2:C:26:TYR:CE2	2:C:28:LEU:HB2	2.55	0.42
5:F:496:LYS:HB2	5:F:496:LYS:HE3	1.88	0.42
3:J:708:ASN:HB3	3:J:712:GLN:O	2.20	0.42
2:C:360:LEU:HB2	2:C:378:ARG:NH2	2.35	0.42
5:L:253:SER:O	5:L:257:LYS:HG3	2.20	0.42
3:D:674:THR:OG1	3:D:677:GLU:HB2	2.20	0.42
2:C:519:ASN:HD21	2:C:796:LEU:HD23	1.84	0.42
2:C:156:PHE:CE2	2:C:158:ASP:HB2	2.55	0.42
3:D:1268:ASN:HB2	3:J:1268:ASN:HD22	1.85	0.42
5:L:580:PHE:HA	5:L:580:PHE:HD1	1.70	0.42
2:I:697:LYS:HE2	2:I:697:LYS:HB3	1.88	0.41
2:C:817:LEU:HD11	2:C:1080:ASN:ND2	2.35	0.41
2:I:196:VAL:HG12	2:I:206:ALA:HA	2.01	0.41
1:B:50:SER:HA	1:B:151:GLY:HA2	2.01	0.41
5:L:559:LEU:HA	5:L:559:LEU:HD12	1.77	0.41
3:J:853:THR:HG22	3:J:854:ALA:H	1.84	0.41
3:D:557:LYS:HE3	3:D:557:LYS:HB2	1.80	0.41
2:I:670:PHE:HZ	2:I:1117:LEU:HD13	1.84	0.41
4:E:66:VAL:HG22	4:E:69:ARG:HH21	1.84	0.41
3:D:537:TYR:OH	3:D:634:ARG:NH2	2.53	0.41
3:D:137:ARG:HG2	3:D:143:SER:HB2	2.01	0.41
3:D:870:ASP:O	3:D:874:GLU:HG2	2.20	0.41
2:I:812:PHE:HZ	3:J:503:SER:HB2	1.85	0.41
2:C:42:ASP:C	2:C:44:GLU:H	2.22	0.41
3:J:843:VAL:HG11	3:J:897:HIS:O	2.20	0.41
2:I:724:VAL:HG11	2:I:727:VAL:HG22	2.02	0.41
1:G:77:ASP:O	1:G:81:ILE:HG13	2.20	0.41
2:I:197:ARG:NH1	2:I:201:ARG:O	2.52	0.41
1:B:64:VAL:HG21	1:B:69:SER:CB	2.50	0.41
3:J:963:VAL:HB	3:J:980:THR:HG23	2.02	0.41
3:D:19:ALA:HB2	3:D:1373:ARG:HH22	1.85	0.41
5:F:380:VAL:HG13	5:F:412:LEU:HD23	2.02	0.41
2:C:1222:GLU:OE2	3:D:537:TYR:OH	2.28	0.41
3:D:37:GLU:HB2	3:D:104:HIS:CE1	2.55	0.41
3:J:579:LEU:HD12	3:J:582:ILE:HD12	2.01	0.41
3:J:137:ARG:HG2	3:J:143:SER:HB2	2.02	0.41
1:H:152:TYR:CE2	3:J:536:LEU:HD21	2.56	0.41
1:A:219:ARG:HE	1:A:219:ARG:HB2	1.74	0.41
2:I:699:LEU:HA	2:I:699:LEU:HD22	1.95	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:F:482:GLU:HG2	5:F:486:ARG:HH22	1.85	0.41
2:C:1307:ASN:HB3	2:C:1312:ASN:O	2.20	0.41
2:I:30:ILE:HD11	2:I:575:LEU:HD22	2.02	0.41
3:J:119:SER:O	3:J:121:PRO:HD2	2.21	0.41
3:J:746:LEU:H	3:J:746:LEU:HD12	1.85	0.41
3:J:746:LEU:HD22	3:J:754:ILE:HD11	2.02	0.41
2:C:498:ILE:HD12	2:C:498:ILE:H	1.85	0.41
3:D:1177:ILE:HD12	3:D:1186:TYR:HB3	2.02	0.41
2:C:670:PHE:HZ	2:C:1117:LEU:HD13	1.85	0.41
1:H:78:ILE:O	1:H:82:LEU:HG	2.21	0.41
5:F:484:ALA:HB1	5:F:491:GLU:HB2	2.02	0.41
1:H:41:ASN:O	1:H:45:ARG:HG3	2.19	0.41
3:J:1031:VAL:HG23	3:J:1080:ILE:HG21	2.03	0.41
3:D:385:LEU:HD23	3:D:385:LEU:HA	1.93	0.41
2:C:11:ILE:HA	2:C:11:ILE:HD13	1.87	0.41
2:I:732:ILE:HD11	2:I:769:PRO:HB3	2.02	0.41
2:C:322:LEU:O	2:C:326:SER:OG	2.34	0.41
3:J:1194:ARG:HD2	3:J:1194:ARG:N	2.35	0.41
2:I:73:TYR:HB2	2:I:98:VAL:HG22	2.02	0.41
2:I:782:VAL:HG11	2:I:792:GLY:HA2	2.03	0.41
1:G:64:VAL:HG11	1:G:78:ILE:HG21	2.02	0.41
3:D:1295:ASN:CB	3:D:1298:VAL:HB	2.50	0.41
2:C:819:SER:HB2	2:C:1085:MET:SD	2.60	0.41
2:C:720:ARG:HA	2:C:779:ARG:HG3	2.01	0.41
3:J:1268:ASN:OD1	3:J:1269:ALA:N	2.50	0.41
3:D:190:LYS:HD3	3:D:235:GLU:HG2	2.02	0.41
3:J:930:LEU:HD11	3:J:1241:TYR:CE2	2.55	0.41
3:J:615:LYS:HB2	3:J:616:PRO:HD3	2.02	0.41
3:J:1163:VAL:HG23	3:J:1177:ILE:HA	2.02	0.41
3:J:56:LEU:HD11	3:J:273:ILE:HD12	2.02	0.41
3:J:997:VAL:HA	3:J:998:PRO:HD3	1.85	0.41
1:A:318:LEU:H	1:A:318:LEU:HD22	1.84	0.41
2:C:1240:ASP:HB3	3:D:445:LYS:HD2	2.02	0.41
2:C:718:ALA:HB2	2:C:783:LEU:CD2	2.49	0.41
5:L:362:ASN:HB2	5:L:365:MET:HE2	2.02	0.41
1:G:29:GLU:HB3	1:G:30:PRO:HD3	2.03	0.41
2:I:28:LEU:HD22	2:I:527:LYS:HD2	2.02	0.41
5:L:507:MET:HG2	5:L:520:GLY:HA3	2.02	0.41
1:H:109:PRO:HA	1:H:132:HIS:HA	2.02	0.41
3:J:1216:ALA:HA	3:J:1217:PRO:HD3	1.90	0.41
1:B:34:GLY:N	1:B:199:ASP:OD2	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:409:LEU:HD23	2:I:409:LEU:HA	1.94	0.41
3:J:441:LEU:HA	3:J:441:LEU:HD13	1.91	0.41
5:L:299:LYS:O	5:L:303:ILE:HG12	2.21	0.41
3:D:735:ALA:O	3:D:738:ARG:HB3	2.20	0.41
5:L:401:PHE:O	5:L:405:ILE:HG23	2.21	0.41
3:J:800:LEU:O	3:J:803:VAL:HG12	2.20	0.41
1:A:102:LEU:HD22	1:A:103:ASN:H	1.86	0.41
3:D:202:ARG:HD3	3:J:1181:ASP:HA	2.02	0.41
3:D:438:GLU:HA	3:D:439:PRO:HD3	1.80	0.41
3:J:37:GLU:HB2	3:J:104:HIS:CE1	2.55	0.41
2:I:1117:LEU:HD12	2:I:1195:ILE:HG12	2.03	0.41
3:J:384:LYS:HD2	3:J:387:LEU:HD23	2.02	0.41
2:C:1123:GLY:HA3	2:C:1204:LEU:HD11	2.03	0.41
3:D:502:PRO:HB2	3:D:507:VAL:HG12	2.03	0.41
5:F:314:THR:O	5:F:318:ALA:HB3	2.20	0.41
3:J:355:ILE:HD13	3:J:466:MET:HG3	2.02	0.41
3:J:740:LEU:HA	3:J:740:LEU:HD12	1.89	0.41
2:C:967:LEU:HA	2:C:967:LEU:HD12	1.85	0.41
3:J:695:LYS:HA	3:J:695:LYS:HD3	1.69	0.41
2:C:1161:LEU:HA	2:C:1161:LEU:HD12	1.66	0.41
3:D:794:GLY:O	3:D:797:THR:OG1	2.28	0.41
3:J:588:PRO:O	3:J:591:ILE:HG22	2.20	0.41
5:L:41:ILE:O	5:L:45:ILE:HG22	2.21	0.41
2:C:27:LEU:HB2	2:C:524:ILE:HD11	2.02	0.41
2:I:91:THR:HG21	2:I:503:LYS:NZ	2.36	0.41
2:I:1247:SER:HB3	3:J:375:GLU:O	2.21	0.41
2:I:62:TYR:CZ	2:I:476:LYS:HB3	2.56	0.41
2:C:854:ILE:HB	2:C:857:VAL:HG21	2.03	0.41
5:L:346:GLN:O	5:L:350:GLU:HG3	2.21	0.41
1:H:20:SER:OG	1:H:21:SER:N	2.53	0.41
1:G:75:GLN:HA	2:I:729:ALA:N	2.36	0.41
5:F:289:LYS:HB3	5:F:289:LYS:HE2	1.88	0.41
3:D:746:LEU:H	3:D:746:LEU:HD12	1.86	0.41
3:D:905:ARG:NH1	3:D:910:ASN:OD1	2.54	0.41
3:D:1291:GLU:HG2	3:D:1297:LYS:HD3	2.02	0.41
1:G:69:SER:O	1:G:78:ILE:HG12	2.21	0.41
2:C:170:VAL:HG23	2:C:171:LEU:H	1.85	0.41
1:G:102:LEU:HD22	1:G:103:ASN:H	1.86	0.41
1:G:75:GLN:O	2:I:729:ALA:HB2	2.20	0.41
1:H:219:ARG:O	1:H:223:ILE:HG13	2.21	0.41
1:A:152:TYR:CG	2:C:824:GLN:HG2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:549:ASP:OD1	3:D:750:PRO:HG2	2.20	0.41
1:B:20:SER:OG	1:B:21:SER:N	2.53	0.41
3:J:974:VAL:HG21	3:J:1118:GLY:HA2	2.02	0.41
3:D:253:VAL:HA	3:D:254:PRO:HD3	1.81	0.41
2:C:38:PHE:HB2	2:C:457:GLY:CA	2.50	0.41
3:J:24:LEU:HA	3:J:24:LEU:HD13	1.97	0.41
2:C:684:ASN:HA	2:C:687:ARG:NH1	2.35	0.41
3:J:1266:ILE:HB	3:J:1274:PHE:O	2.21	0.41
3:D:1237:VAL:HG13	3:D:1253:ILE:HD13	2.03	0.41
2:C:1010:GLN:O	2:C:1014:LEU:HD12	2.21	0.41
3:J:198:CYS:HA	3:J:221:ILE:HD13	2.03	0.41
2:I:720:ARG:HE	2:I:736:VAL:HG11	1.85	0.41
5:F:94:THR:HG23	5:F:96:ASP:OD1	2.20	0.41
2:I:1253:LEU:HA	5:L:525:ASP:HB2	2.03	0.41
2:C:62:TYR:CZ	2:C:476:LYS:HB3	2.56	0.41
1:H:151:GLY:O	1:H:177:TYR:HD2	2.04	0.41
2:I:157:PHE:CZ	2:I:431:LYS:HG2	2.56	0.41
3:J:884:SER:OG	3:J:1254:GLU:OE1	2.23	0.41
1:H:112:ALA:HB2	1:H:128:HIS:HB3	2.01	0.41
5:L:99:ARG:HA	5:L:99:ARG:HD3	1.74	0.41
2:C:163:LYS:HB3	2:C:163:LYS:HE3	1.90	0.41
1:H:84:ASN:O	1:H:128:HIS:HE1	2.04	0.41
5:L:249:ILE:O	5:L:252:LEU:HB3	2.21	0.41
5:L:454:VAL:HA	5:L:457:ILE:HD12	2.03	0.41
4:E:4:VAL:HG22	4:E:5:THR:HG23	2.03	0.41
2:C:801:ARG:HG2	2:C:1094:VAL:HG23	2.03	0.41
2:I:548:ARG:O	2:I:570:GLY:HA3	2.21	0.41
2:I:840:SER:O	2:I:1047:LEU:N	2.54	0.41
3:D:1266:ILE:HD12	3:D:1273:ASP:O	2.20	0.41
1:G:49:SER:OG	1:G:50:SER:N	2.54	0.41
3:D:1181:ASP:HA	3:J:202:ARG:HD3	2.02	0.41
3:J:481:ARG:O	3:J:488:ASN:ND2	2.54	0.41
2:I:42:ASP:HA	2:I:43:PRO:HD3	1.84	0.41
2:I:169:LYS:O	2:I:170:VAL:HG22	2.21	0.41
3:D:481:ARG:O	3:D:488:ASN:ND2	2.54	0.41
3:D:902:ASP:OD1	3:D:903:LEU:N	2.54	0.41
3:J:511:TYR:OH	3:J:515:ARG:NH1	2.54	0.41
5:F:226:ALA:HA	5:F:229:VAL:HG22	2.03	0.41
2:C:555:TYR:HD2	6:C:2001:4OE:FAA	1.94	0.40
3:J:573:THR:OG1	3:J:576:ARG:HG3	2.21	0.40
2:I:718:ALA:HB2	2:I:783:LEU:CD2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:I:18:ARG:HA	2:I:19:PRO:HD3	1.92	0.40
1:B:73:GLY:CA	1:B:134:THR:HG22	2.51	0.40
3:D:1198:VAL:HB	3:D:1210:ILE:HA	2.03	0.40
2:C:478:ARG:NH1	2:C:482:GLY:HA2	2.36	0.40
2:C:1125:GLY:HA3	2:C:1179:GLY:HA2	2.02	0.40
3:J:902:ASP:OD1	3:J:903:LEU:N	2.54	0.40
5:L:484:ALA:HB1	5:L:491:GLU:HB2	2.02	0.40
3:J:502:PRO:HB2	3:J:507:VAL:HG12	2.04	0.40
3:J:30:ILE:HG23	3:J:243:PRO:HG3	2.02	0.40
1:G:172:LEU:HD12	1:G:172:LEU:H	1.85	0.40
2:C:1262:LYS:HA	2:C:1262:LYS:HD3	1.82	0.40
2:C:589:THR:HA	2:C:590:PRO:HD3	1.94	0.40
1:G:228:LEU:C	1:G:230:ALA:H	2.23	0.40
1:H:48:LEU:HA	1:H:180:VAL:HG21	2.03	0.40
5:L:583:THR:HG22	5:L:584:ARG:H	1.85	0.40
2:C:171:LEU:HA	2:C:171:LEU:HD23	1.92	0.40
3:J:770:LEU:HD22	3:J:770:LEU:H	1.86	0.40
3:D:1319:PHE:CD2	3:D:1342:ASP:HB2	2.56	0.40
3:D:190:LYS:HE2	3:D:190:LYS:HB2	1.89	0.40
1:B:41:ASN:CG	2:C:1217:THR:HA	2.41	0.40
3:J:1040:MET:HE3	3:J:1101:LEU:HD12	2.03	0.40
1:H:57:THR:O	1:H:173:VAL:HB	2.21	0.40
2:C:925:SER:O	2:C:1056:VAL:HG13	2.22	0.40
5:L:399:LEU:HA	5:L:399:LEU:HD12	1.88	0.40
3:D:697:MET:O	3:D:701:LEU:HB2	2.21	0.40
1:H:68:TYR:O	1:H:69:SER:OG	2.36	0.40
2:I:634:VAL:HG13	2:I:636:CYS:SG	2.61	0.40
3:J:901:ARG:HA	3:J:908:ILE:HA	2.03	0.40
2:I:812:PHE:CZ	3:J:503:SER:HB2	2.56	0.40
2:C:1288:GLN:HB2	3:D:1356:LEU:HD23	2.03	0.40
2:C:347:ILE:HD11	2:C:433:ILE:HD11	2.04	0.40
1:A:57:THR:O	1:A:173:VAL:HG22	2.21	0.40
5:L:215:GLU:HG2	5:L:218:ARG:HH21	1.85	0.40
3:J:418:GLU:HG3	4:K:45:LYS:N	2.25	0.40
5:F:561:MET:HG3	5:F:571:TYR:HD2	1.86	0.40
2:C:400:VAL:HG21	2:C:452:ARG:NH1	2.36	0.40
1:H:73:GLY:CA	1:H:134:THR:HG22	2.50	0.40
1:A:31:LEU:CD1	1:A:201:LEU:HB2	2.49	0.40
2:I:1323:PHE:CE1	3:J:1353:VAL:HG23	2.56	0.40
1:G:225:ALA:O	1:G:228:LEU:HB2	2.21	0.40
2:I:1272:GLU:HG2	2:I:1276:TRP:CE2	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:L:582:VAL:CG2	5:L:586:ARG:HG2	2.51	0.40
3:D:1162:ILE:HA	3:D:1203:ARG:HA	2.04	0.40
3:J:749:LYS:HG3	3:J:751:ASP:HB3	2.04	0.40
1:A:313:SER:O	1:A:316:MET:HG3	2.21	0.40
2:I:1212:LEU:HD22	2:I:1225:VAL:HG21	2.02	0.40
2:I:742:TYR:CD2	2:I:743:PRO:HD2	2.57	0.40
5:F:96:ASP:HA	5:F:97:PRO:HD2	1.93	0.40
3:D:34:SER:OG	3:D:104:HIS:ND1	2.29	0.40
3:J:263:SER:HB2	5:L:507:MET:HE2	2.02	0.40
3:J:430:HIS:HA	3:J:921:GLN:HB3	2.02	0.40
2:I:972:PHE:CD2	2:I:975:ILE:HD12	2.56	0.40
3:D:810:THR:HG23	3:D:811:GLU:H	1.86	0.40
3:J:161:THR:H	3:J:164:GLN:HB2	1.86	0.40
2:C:243:PRO:HB2	2:C:278:GLU:HG3	2.03	0.40
2:I:453:ILE:HD12	2:I:587:LEU:HD21	2.04	0.40
3:D:363:LEU:HD12	3:D:450:HIS:CE1	2.56	0.40
2:C:117:ILE:HG21	2:C:488:MET:HG2	2.04	0.40
3:J:119:SER:O	3:J:121:PRO:N	2.55	0.40
3:J:97:VAL:HG12	3:J:101:ARG:HG3	2.04	0.40
5:F:119:ILE:O	5:F:123:ILE:HG13	2.21	0.40
2:I:242:VAL:HA	2:I:243:PRO:HD3	1.94	0.40
2:C:447:HIS:CE1	2:C:553:THR:HG21	2.56	0.40
3:J:598:LYS:HA	3:J:601:ILE:HG22	2.03	0.40
2:C:1211:ARG:O	2:C:1212:LEU:HD12	2.21	0.40
3:J:557:LYS:HB2	3:J:557:LYS:HE3	1.80	0.40
1:H:151:GLY:O	1:H:177:TYR:HB2	2.21	0.40
5:L:343:LYS:O	5:L:347:ILE:HG13	2.22	0.40
3:J:1239:ASP:OD1	3:J:1242:ARG:NH2	2.54	0.40
1:G:57:THR:O	1:G:173:VAL:HG22	2.22	0.40
1:H:195:ARG:HB2	1:H:198:LEU:HD21	2.03	0.40
1:A:207:THR:HG22	1:A:208:ASN:H	1.86	0.40
3:D:706:VAL:HG12	3:D:715:LYS:HB3	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

of similar resolution.

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	298/335 (89%)	269 (90%)	20 (7%)	9 (3%)	5	45
1	B	212/335 (63%)	191 (90%)	18 (8%)	3 (1%)	14	59
1	G	222/335 (66%)	200 (90%)	16 (7%)	6 (3%)	6	47
1	H	212/335 (63%)	192 (91%)	17 (8%)	3 (1%)	14	59
2	C	1338/1342 (100%)	1236 (92%)	95 (7%)	7 (0%)	34	76
2	I	1338/1342 (100%)	1234 (92%)	98 (7%)	6 (0%)	39	79
3	D	1145/1407 (81%)	1050 (92%)	90 (8%)	5 (0%)	39	79
3	J	1311/1407 (93%)	1196 (91%)	112 (8%)	3 (0%)	52	86
4	E	87/91 (96%)	79 (91%)	8 (9%)	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%)	52	86
5	L	529/613 (86%)	481 (91%)	48 (9%)	0	100	100
All	All	7301/8246 (88%)	6682 (92%)	576 (8%)	43 (1%)	30	73

All (43) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	193	GLU
1	A	319	GLU
1	A	320	ASN
1	B	29	GLU
2	C	237	LEU
3	D	10	ALA
3	D	120	LEU
1	G	193	GLU
2	I	237	LEU
3	J	120	LEU
1	A	323	PRO
2	C	170	VAL
2	I	170	VAL
1	A	62	ASP
5	F	7	SER
1	G	62	ASP
1	H	29	GLU
1	H	30	PRO

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Mol	Chain	Res	Type
1	A	196	THR
1	B	13	LEU
1	B	15	ASP
2	C	659	GLN
2	C	1136	GLN
3	D	710	ASP
1	G	196	THR
2	I	659	GLN
2	I	1136	GLN
3	J	710	ASP
1	A	167	PRO
1	A	178	SER
2	C	697	LYS
3	D	747	MET
1	G	167	PRO
1	G	178	SER
1	H	193	GLU
2	I	697	LYS
2	C	1186	VAL
3	D	831	VAL
2	I	1186	VAL
3	J	831	VAL
1	A	14	VAL
1	G	14	VAL
2	C	1159	VAL

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%)	243 (95%)	14 (5%)	27	67
1	B	184/292 (63%)	166 (90%)	18 (10%)	10	43
1	G	191/292 (65%)	181 (95%)	10 (5%)	29	68
1	H	183/292 (63%)	168 (92%)	15 (8%)	14	51
2	C	1155/1157 (100%)	1064 (92%)	91 (8%)	15	54

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	I	1154/1157 (100%)	1062 (92%)	92 (8%)	15	53
3	D	964/1168 (82%)	877 (91%)	87 (9%)	12	47
3	J	1106/1168 (95%)	1012 (92%)	94 (8%)	13	51
4	E	72/75 (96%)	66 (92%)	6 (8%)	14	51
4	K	67/75 (89%)	60 (90%)	7 (10%)	9	40
5	F	426/540 (79%)	392 (92%)	34 (8%)	15	53
5	L	428/540 (79%)	393 (92%)	35 (8%)	14	51
All	All	6187/7048 (88%)	5684 (92%)	503 (8%)	15	52

All (503) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	LEU
1	A	13	LEU
1	A	35	PHE
1	A	54	CYS
1	A	65	LEU
1	A	133	LEU
1	A	145	LYS
1	A	186	ASN
1	A	207	THR
1	A	231	PHE
1	A	317	ARG
1	A	318	LEU
1	A	319	GLU
1	A	321	TRP
1	B	8	PHE
1	B	9	LEU
1	B	12	ARG
1	B	13	LEU
1	B	31	LEU
1	B	43	LEU
1	B	54	CYS
1	B	60	GLU
1	B	65	LEU
1	B	75	GLN
1	B	79	LEU
1	B	101	THR
1	B	116	THR
1	B	133	LEU

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Mol	Chain	Res	Type
1	B	158	ARG
1	B	160	HIS
1	B	183	ILE
1	B	186	ASN
2	C	11	ILE
2	C	29	SER
2	C	39	ILE
2	C	70	TYR
2	C	81	ASP
2	C	85	CYS
2	C	91	THR
2	C	115	LYS
2	C	116	ASP
2	C	119	GLU
2	C	124	MET
2	C	131	THR
2	C	179	TYR
2	C	182	SER
2	C	185	ASP
2	C	202	ARG
2	C	285	ILE
2	C	320	ASP
2	C	321	LEU
2	C	419	ILE
2	C	423	ASP
2	C	434	ASP
2	C	484	LEU
2	C	485	ASP
2	C	486	THR
2	C	487	LEU
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	554	HIS
2	C	604	HIS
2	C	615	VAL
2	C	623	LEU

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Mol	Chain	Res	Type
2	C	633	LEU
2	C	657	THR
2	C	672	GLU
2	C	692	THR
2	C	697	LYS
2	C	699	LEU
2	C	706	ARG
2	C	714	VAL
2	C	739	ASP
2	C	748	ILE
2	C	765	ILE
2	C	773	LEU
2	C	781	ASP
2	C	782	VAL
2	C	788	SER
2	C	815	SER
2	C	819	SER
2	C	828	PHE
2	C	839	VAL
2	C	859	GLU
2	C	878	THR
2	C	890	LYS
2	C	892	GLU
2	C	895	LEU
2	C	974	ARG
2	C	990	ASP
2	C	992	LEU
2	C	1002	LEU
2	C	1005	GLU
2	C	1006	GLU
2	C	1014	LEU
2	C	1040	ASP
2	C	1082	ILE
2	C	1108	ASN
2	C	1109	ILE
2	C	1114	GLU
2	C	1134	GLN
2	C	1155	VAL
2	C	1156	ARG
2	C	1161	LEU
2	C	1198	LEU
2	C	1204	LEU

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Mol	Chain	Res	Type
2	C	1210	ILE
2	C	1237	HIS
2	C	1240	ASP
2	C	1248	THR
2	C	1264	GLN
2	C	1265	PHE
2	C	1310	ASP
2	C	1313	HIS
2	C	1326	LEU
2	C	1327	LEU
2	C	1342	GLU
3	D	11	GLN
3	D	18	ASP
3	D	20	ILE
3	D	46	TYR
3	D	79	LYS
3	D	92	VAL
3	D	95	THR
3	D	117	LEU
3	D	119	SER
3	D	120	LEU
3	D	169	LEU
3	D	175	GLU
3	D	176	PHE
3	D	217	LEU
3	D	248	ASP
3	D	252	LEU
3	D	255	LEU
3	D	256	ASP
3	D	264	ASP
3	D	311	ARG
3	D	324	LEU
3	D	356	THR
3	D	364	HIS
3	D	374	LEU
3	D	430	HIS
3	D	474	LEU
3	D	506	VAL
3	D	513	MET
3	D	536	LEU
3	D	545	HIS
3	D	547	ARG

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Mol	Chain	Res	Type
3	D	568	SER
3	D	593	ASN
3	D	594	GLN
3	D	641	ILE
3	D	660	GLU
3	D	678	ARG
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	757	THR
3	D	764	ARG
3	D	767	LEU
3	D	772	TYR
3	D	805	GLN
3	D	810	THR
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	897	HIS
3	D	908	ILE
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	1173	ARG
3	D	1177	ILE
3	D	1186	TYR

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Mol	Chain	Res	Type
3	D	1199	PHE
3	D	1202	GLU
3	D	1208	ASP
3	D	1209	VAL
3	D	1215	GLU
3	D	1244	GLN
3	D	1274	PHE
3	D	1275	LEU
3	D	1281	GLU
3	D	1284	ARG
3	D	1289	ASN
3	D	1293	GLU
3	D	1327	GLU
3	D	1333	THR
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	154	GLU
5	F	305	LEU
5	F	306	PHE
5	F	341	LEU
5	F	395	THR
5	F	417	ASP
5	F	421	TYR
5	F	445	ASP
5	F	449	THR
5	F	479	THR
5	F	486	ARG
5	F	488	LEU
5	F	491	GLU
5	F	496	LYS
5	F	508	GLU

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Mol	Chain	Res	Type
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	573	LEU
5	F	580	PHE
5	F	583	THR
5	F	600	HIS
5	F	606	VAL
5	F	612	ASP
1	G	9	LEU
1	G	13	LEU
1	G	35	PHE
1	G	54	CYS
1	G	65	LEU
1	G	133	LEU
1	G	145	LYS
1	G	186	ASN
1	G	207	THR
1	G	231	PHE
1	H	13	LEU
1	H	27	THR
1	H	29	GLU
1	H	31	LEU
1	H	54	CYS
1	H	60	GLU
1	H	75	GLN
1	H	79	LEU
1	H	101	THR
1	H	105	SER
1	H	116	THR
1	H	133	LEU
1	H	139	SER
1	H	183	ILE
1	H	186	ASN
2	I	11	ILE
2	I	29	SER
2	I	39	ILE
2	I	70	TYR
2	I	81	ASP

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Mol	Chain	Res	Type
2	I	85	CYS
2	I	91	THR
2	I	115	LYS
2	I	116	ASP
2	I	119	GLU
2	I	131	THR
2	I	179	TYR
2	I	182	SER
2	I	185	ASP
2	I	202	ARG
2	I	285	ILE
2	I	320	ASP
2	I	321	LEU
2	I	419	ILE
2	I	423	ASP
2	I	434	ASP
2	I	453	ILE
2	I	484	LEU
2	I	485	ASP
2	I	486	THR
2	I	487	LEU
2	I	493	ILE
2	I	512	SER
2	I	517	GLN
2	I	518	ASN
2	I	530	ILE
2	I	538	LEU
2	I	539	THR
2	I	540	ARG
2	I	554	HIS
2	I	604	HIS
2	I	615	VAL
2	I	623	LEU
2	I	633	LEU
2	I	657	THR
2	I	672	GLU
2	I	692	THR
2	I	697	LYS
2	I	699	LEU
2	I	706	ARG
2	I	714	VAL
2	I	739	ASP

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Mol	Chain	Res	Type
2	I	748	ILE
2	I	765	ILE
2	I	773	LEU
2	I	781	ASP
2	I	782	VAL
2	I	788	SER
2	I	815	SER
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	895	LEU
2	I	974	ARG
2	I	990	ASP
2	I	992	LEU
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	1155	VAL
2	I	1156	ARG
2	I	1161	LEU
2	I	1198	LEU
2	I	1204	LEU
2	I	1210	ILE
2	I	1233	LEU
2	I	1237	HIS
2	I	1240	ASP
2	I	1248	THR
2	I	1264	GLN
2	I	1265	PHE
2	I	1310	ASP
2	I	1313	HIS

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Mol	Chain	Res	Type
2	I	1326	LEU
2	I	1327	LEU
2	I	1342	GLU
3	J	18	ASP
3	J	20	ILE
3	J	46	TYR
3	J	79	LYS
3	J	92	VAL
3	J	95	THR
3	J	97	VAL
3	J	117	LEU
3	J	119	SER
3	J	120	LEU
3	J	169	LEU
3	J	175	GLU
3	J	176	PHE
3	J	217	LEU
3	J	248	ASP
3	J	252	LEU
3	J	255	LEU
3	J	256	ASP
3	J	264	ASP
3	J	311	ARG
3	J	324	LEU
3	J	356	THR
3	J	364	HIS
3	J	374	LEU
3	J	430	HIS
3	J	474	LEU
3	J	506	VAL
3	J	513	MET
3	J	545	HIS
3	J	547	ARG
3	J	568	SER
3	J	593	ASN
3	J	594	GLN
3	J	641	ILE
3	J	660	GLU
3	J	678	ARG
3	J	697	MET
3	J	698	MET
3	J	701	LEU

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Mol	Chain	Res	Type
3	J	707	ILE
3	J	708	ASN
3	J	710	ASP
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	757	THR
3	J	764	ARG
3	J	767	LEU
3	J	772	TYR
3	J	810	THR
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	918	ILE
3	J	928	THR
3	J	931	THR
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	1115	ILE
3	J	1155	ILE
3	J	1163	VAL
3	J	1167	LYS
3	J	1173	ARG
3	J	1177	ILE
3	J	1186	TYR
3	J	1199	PHE

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Mol	Chain	Res	Type
3	J	1202	GLU
3	J	1208	ASP
3	J	1209	VAL
3	J	1215	GLU
3	J	1244	GLN
3	J	1274	PHE
3	J	1275	LEU
3	J	1281	GLU
3	J	1284	ARG
3	J	1289	ASN
3	J	1293	GLU
3	J	1327	GLU
3	J	1333	THR
4	K	18	ASP
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	154	GLU
5	L	305	LEU
5	L	306	PHE
5	L	341	LEU
5	L	395	THR
5	L	417	ASP
5	L	421	TYR
5	L	429	THR
5	L	445	ASP
5	L	449	THR
5	L	479	THR
5	L	486	ARG
5	L	488	LEU
5	L	491	GLU

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Mol	Chain	Res	Type
5	L	496	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	573	LEU
5	L	580	PHE
5	L	583	THR
5	L	600	HIS
5	L	606	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	128	HIS
1	A	283	GLN
1	A	320	ASN
2	C	343	HIS
2	C	1111	GLN
2	C	1116	HIS
2	C	1257	GLN
2	C	1288	GLN
2	C	1314	GLN
3	D	364	HIS
3	D	419	HIS
3	D	450	HIS
3	D	477	GLN
3	D	560	ASN
3	D	777	HIS
3	D	897	HIS
3	D	1367	GLN
5	F	345	GLN
5	F	406	GLN
5	F	472	GLN
1	G	128	HIS
2	I	343	HIS
2	I	1116	HIS
2	I	1257	GLN
2	I	1314	GLN

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Mol	Chain	Res	Type
3	J	419	HIS
3	J	560	ASN
3	J	777	HIS
3	J	1367	GLN
5	L	406	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 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	4OE	C	2001	-	24,25,25	4.18	6 (25%)	30,37,37	1.39	5 (16%)
6	4OE	I	2001	-	24,25,25	4.16	6 (25%)	30,37,37	1.39	5 (16%)

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	4OE	C	2001	-	-	0/14/14/14	0/3/3/3
6	4OE	I	2001	-	-	0/14/14/14	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	2001	4OE	CAR-CAV	-14.35	1.33	1.49
6	I	2001	4OE	CAR-CAV	-14.25	1.33	1.49
6	C	2001	4OE	CAT-CAS	-9.61	1.33	1.49
6	I	2001	4OE	CAT-CAS	-9.55	1.33	1.49
6	C	2001	4OE	NAN-NAO	-6.73	1.23	1.37
6	I	2001	4OE	NAN-NAO	-6.71	1.23	1.37
6	I	2001	4OE	CAT-CAV	-6.00	1.32	1.40
6	C	2001	4OE	CAT-CAV	-5.97	1.32	1.40
6	I	2001	4OE	CAW-CAU	-5.06	1.40	1.50
6	C	2001	4OE	CAW-CAU	-5.02	1.40	1.50
6	I	2001	4OE	FAA-CAP	-2.07	1.31	1.36
6	C	2001	4OE	FAA-CAP	-2.06	1.31	1.36

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	2001	4OE	CAW-CAU-CAQ	-2.39	117.29	121.98
6	I	2001	4OE	CAW-CAU-CAQ	-2.38	117.30	121.98
6	I	2001	4OE	FAD-CAW-CAU	-2.36	108.65	112.67
6	C	2001	4OE	FAD-CAW-CAU	-2.35	108.67	112.67
6	C	2001	4OE	CAH-CAQ-CAU	-2.22	120.75	123.80
6	I	2001	4OE	CAH-CAQ-CAU	-2.20	120.78	123.80
6	I	2001	4OE	CAR-CAV-NAO	2.71	124.29	120.58
6	C	2001	4OE	CAR-CAV-NAO	2.74	124.35	120.58
6	C	2001	4OE	CAM-CAU-CAW	2.93	123.20	116.67
6	I	2001	4OE	CAM-CAU-CAW	2.96	123.28	116.67

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	2001	4OE	5	0
6	I	2001	4OE	4	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

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%)	0.38	25 (8%) 14 10	29, 105, 230, 394	0
1	B	216/335 (64%)	0.49	19 (8%) 12 9	42, 129, 228, 299	0
1	G	224/335 (66%)	0.26	16 (7%) 19 13	57, 116, 198, 279	0
1	H	216/335 (64%)	0.72	36 (16%) 2 3	57, 136, 228, 269	0
2	C	1340/1342 (99%)	0.42	120 (8%) 12 8	13, 89, 219, 379	0
2	I	1340/1342 (99%)	0.54	164 (12%) 5 5	14, 112, 225, 339	0
3	D	1151/1407 (81%)	0.15	40 (3%) 48 37	15, 70, 173, 283	0
3	J	1319/1407 (93%)	0.60	149 (11%) 7 6	19, 94, 230, 319	0
4	E	89/91 (97%)	0.10	1 (1%) 82 75	27, 78, 123, 186	0
4	K	79/91 (86%)	0.44	3 (3%) 44 34	60, 124, 203, 243	0
5	F	542/613 (88%)	0.78	90 (16%) 2 3	27, 158, 265, 368	0
5	L	539/613 (87%)	0.69	86 (15%) 3 3	41, 153, 254, 312	0
All	All	7357/8246 (89%)	0.48	749 (10%) 9 7	13, 105, 230, 394	0

All (749) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	J	1054	THR	15.9
5	F	70	ASN	13.7
5	F	167	ASP	13.1
5	F	259	PHE	13.0
5	F	89	SER	12.1
2	C	251	ALA	10.1
5	F	75	ASP	9.9
2	C	311	CYS	9.8
2	I	999	GLU	9.4
5	F	88	GLU	9.1
2	I	982	GLY	8.8

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Mol	Chain	Res	Type	RSRZ
3	J	1109	LEU	8.6
3	J	987	GLU	8.5
2	C	322	LEU	8.0
2	C	205	PRO	8.0
2	I	979	LEU	8.0
5	F	319	ALA	7.8
5	F	318	ALA	7.7
5	L	7	SER	7.7
2	I	998	LEU	7.7
5	F	165	PHE	7.6
2	I	978	VAL	7.5
2	C	323	ALA	7.4
2	I	1005	GLU	7.4
2	I	1010	GLN	7.4
5	F	137	TYR	7.4
3	J	1030	GLU	7.2
5	L	89	SER	7.2
3	J	1053	LEU	7.2
5	L	314	THR	7.2
2	I	981	ALA	7.1
5	L	312	SER	7.0
3	J	985	ILE	7.0
2	I	1004	ASP	6.9
5	L	290	LEU	6.9
3	J	682	VAL	6.8
5	F	317	ASN	6.7
3	J	1078	LEU	6.7
2	C	292	ILE	6.6
5	L	315	TRP	6.6
5	F	162	ILE	6.5
5	L	167	ASP	6.5
2	C	265	LYS	6.5
5	F	287	ILE	6.4
3	J	1088	VAL	6.4
2	C	305	SER	6.4
2	I	230	PHE	6.4
1	H	172	LEU	6.4
5	F	314	THR	6.4
5	F	34	ASP	6.3
3	J	955	LYS	6.2
2	C	333	ILE	6.2
2	C	317	LEU	6.2

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Mol	Chain	Res	Type	RSRZ
5	F	312	SER	6.1
2	I	882	ILE	6.0
3	J	857	LEU	5.9
3	J	217	LEU	5.8
5	L	490	PRO	5.8
2	C	264	GLU	5.8
3	J	1123	ARG	5.8
3	D	1165	PHE	5.8
3	J	1055	GLY	5.8
5	F	74	GLU	5.7
5	F	76	ALA	5.7
3	D	1200	GLU	5.7
5	F	258	GLN	5.7
3	J	1080	ILE	5.6
3	J	1108	GLN	5.6
2	I	1006	GLU	5.6
5	F	313	ASP	5.5
3	J	542	ALA	5.5
3	J	686	TRP	5.4
2	C	291	TYR	5.4
5	L	305	LEU	5.4
3	J	1056	LEU	5.4
5	F	283	GLN	5.4
1	A	318	LEU	5.3
2	C	301	TYR	5.3
3	J	1198	VAL	5.3
1	B	55	ALA	5.3
3	J	1051	ASP	5.3
5	F	579	GLN	5.2
2	C	68	LEU	5.2
3	J	993	GLU	5.2
2	I	234	ASP	5.2
2	I	231	GLU	5.2
3	J	1029	THR	5.2
3	J	1070	GLY	5.1
5	L	308	GLY	5.1
2	I	254	ASP	5.1
5	L	318	ALA	5.1
3	J	1028	ILE	5.1
5	L	287	ILE	5.1
1	A	262	LEU	5.0
3	J	1161	GLY	5.0

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Mol	Chain	Res	Type	RSRZ
1	H	56	VAL	5.0
2	I	479	LEU	5.0
3	J	1077	ALA	5.0
2	C	269	ILE	4.9
3	D	1175	LEU	4.9
3	J	1101	LEU	4.9
1	H	147	GLN	4.9
2	C	992	LEU	4.9
2	C	207	THR	4.9
5	L	165	PHE	4.9
2	I	1003	THR	4.9
3	J	989	GLY	4.9
3	J	974	VAL	4.9
2	C	102	LEU	4.8
5	F	288	MET	4.8
5	L	137	TYR	4.8
5	F	71	THR	4.8
2	C	326	SER	4.8
2	I	165	HIS	4.8
3	J	1215	GLU	4.8
1	H	52	PRO	4.8
5	L	8	GLN	4.8
2	I	333	ILE	4.7
5	F	256	PHE	4.7
2	I	1002	LEU	4.7
2	C	304	GLU	4.7
1	B	65	LEU	4.7
2	I	492	MET	4.6
5	L	45	ILE	4.6
3	J	1013	GLY	4.6
3	J	991	THR	4.6
5	F	87	VAL	4.5
2	I	475	VAL	4.5
1	H	55	ALA	4.5
5	F	584	ARG	4.5
2	I	420	LEU	4.5
3	D	1296	GLY	4.5
5	F	321	ALA	4.5
1	H	51	MET	4.5
3	J	1069	ALA	4.5
1	B	91	ARG	4.5
2	C	288	PRO	4.5

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Mol	Chain	Res	Type	RSRZ
2	I	1020	GLU	4.4
2	C	270	THR	4.4
1	B	90	VAL	4.4
3	J	1032	SER	4.4
2	I	1024	GLU	4.4
3	J	546	ALA	4.4
1	H	67	GLU	4.4
2	C	206	ALA	4.4
3	J	1102	PRO	4.4
5	L	309	ASN	4.4
2	I	1011	LEU	4.4
3	J	547	ARG	4.3
2	I	997	TRP	4.3
5	L	291	CYS	4.3
2	C	300	ASP	4.3
2	I	1007	LYS	4.3
3	J	988	PHE	4.3
2	C	252	SER	4.3
1	H	146	VAL	4.3
3	J	1125	PRO	4.3
2	C	601	ASP	4.3
1	H	152	TYR	4.3
2	I	263	VAL	4.3
2	I	973	SER	4.3
2	C	645	PHE	4.3
2	I	255	ILE	4.3
3	J	517	CYS	4.2
2	C	188	PHE	4.2
5	L	313	ASP	4.2
3	D	1203	ARG	4.2
2	I	725	GLN	4.2
2	I	493	ILE	4.2
1	H	173	VAL	4.2
5	L	489	MET	4.2
3	J	518	VAL	4.2
2	I	1014	LEU	4.1
2	I	258	ASN	4.1
2	C	230	PHE	4.1
2	I	203	LYS	4.1
3	J	663	GLU	4.1
3	J	975	ILE	4.1
3	D	1198	VAL	4.1

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Mol	Chain	Res	Type	RSRZ
2	I	264	GLU	4.1
3	J	204	GLU	4.1
3	J	1375	ALA	4.1
3	J	1103	GLY	4.1
2	C	312	ALA	4.0
2	C	56	VAL	4.0
2	I	269	ILE	4.0
3	J	976	THR	4.0
4	K	58	LEU	4.0
5	F	338	HIS	4.0
2	C	298	ALA	4.0
3	J	543	SER	4.0
2	I	867	GLU	4.0
3	D	1201	GLY	4.0
1	A	320	ASN	4.0
3	J	1007	ASP	3.9
2	I	969	ALA	3.9
5	F	575	GLU	3.9
5	F	315	TRP	3.9
3	D	682	VAL	3.9
5	L	140	ALA	3.9
5	L	337	VAL	3.9
2	C	53	PHE	3.9
2	C	59	ILE	3.9
5	F	93	ARG	3.9
3	J	712	GLN	3.9
3	D	830	ASP	3.9
2	I	1008	GLN	3.9
1	A	140	ILE	3.9
2	C	263	VAL	3.9
1	A	303	ILE	3.9
5	F	158	LEU	3.8
2	C	1000	LEU	3.8
2	I	928	VAL	3.8
2	I	975	ILE	3.8
4	K	75	GLN	3.8
5	L	225	ARG	3.8
1	H	123	ILE	3.8
3	J	1068	THR	3.8
2	C	321	LEU	3.8
2	I	246	LEU	3.8
3	J	850	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
2	C	104	ILE	3.7
5	F	291	CYS	3.7
5	L	304	THR	3.7
1	H	57	THR	3.7
1	A	281	LEU	3.7
5	F	161	LEU	3.7
5	L	316	PHE	3.7
3	J	1000	GLY	3.6
5	F	466	ILE	3.6
3	D	1204	VAL	3.6
5	L	487	MET	3.6
2	I	233	ARG	3.6
3	J	1099	TYR	3.6
2	I	262	TYR	3.6
1	G	205	MET	3.6
3	J	756	GLU	3.6
2	I	224	PHE	3.6
2	I	976	ARG	3.6
3	J	990	ARG	3.6
1	H	194	GLN	3.6
3	J	1010	GLN	3.6
1	H	99	ILE	3.6
2	C	319	LEU	3.6
5	L	307	THR	3.6
3	J	994	SER	3.6
3	J	1036	ARG	3.6
2	C	253	PHE	3.6
2	I	980	VAL	3.6
3	J	1190	ILE	3.6
2	C	314	ASN	3.5
2	I	485	ASP	3.5
5	F	86	SER	3.5
2	C	486	THR	3.5
5	L	317	ASN	3.5
3	J	522	GLY	3.5
5	L	20	GLY	3.5
5	L	326	TRP	3.5
2	C	318	SER	3.5
2	C	347	ILE	3.5
3	J	956	GLY	3.5
5	F	72	ALA	3.5
5	L	283	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
2	I	273	HIS	3.5
3	J	743	MET	3.5
1	H	158	ARG	3.4
2	C	250	THR	3.4
2	C	66	SER	3.4
3	J	965	SER	3.4
5	F	301	ASN	3.4
2	I	983	GLY	3.4
3	J	512	TYR	3.4
2	C	196	VAL	3.4
2	I	634	VAL	3.4
5	L	610	PHE	3.4
2	I	937	ASP	3.4
5	F	35	ILE	3.4
5	L	48	ILE	3.4
3	D	826	ILE	3.4
2	I	232	ILE	3.4
5	L	18	GLU	3.4
1	H	148	ARG	3.4
2	I	282	VAL	3.4
2	I	972	PHE	3.4
5	F	290	LEU	3.4
5	F	306	PHE	3.4
5	F	284	GLU	3.4
1	A	284	ARG	3.4
2	C	338	THR	3.3
1	G	90	VAL	3.3
2	I	733	VAL	3.3
3	J	986	ASP	3.3
5	L	259	PHE	3.3
2	C	492	MET	3.3
1	B	98	VAL	3.3
5	F	334	SER	3.3
2	C	464	PHE	3.3
1	B	121	VAL	3.3
5	F	305	LEU	3.3
1	B	147	GLN	3.3
2	I	989	LEU	3.3
3	J	1091	PRO	3.3
3	J	1097	ALA	3.3
2	I	1000	LEU	3.3
1	H	233	ASP	3.2

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Mol	Chain	Res	Type	RSRZ
3	J	957	SER	3.2
3	J	1188	GLU	3.2
1	B	66	HIS	3.2
5	L	70	ASN	3.2
3	J	1203	ARG	3.2
5	F	32	PRO	3.2
3	J	685	ILE	3.2
2	I	102	LEU	3.2
3	J	1001	ALA	3.2
3	J	1089	LEU	3.2
3	J	1049	GLN	3.2
2	C	287	VAL	3.2
5	F	323	ASN	3.2
2	I	478	ARG	3.2
5	F	136	GLU	3.2
1	H	100	LEU	3.2
3	D	756	GLU	3.2
2	I	696	ASP	3.2
3	J	1017	VAL	3.2
2	I	1021	LEU	3.2
2	C	600	THR	3.1
2	I	389	PHE	3.1
1	A	205	MET	3.1
2	C	273	HIS	3.1
1	B	227	GLN	3.1
2	I	67	GLU	3.1
1	B	130	ILE	3.1
2	I	468	LEU	3.1
5	L	49	ASN	3.1
2	C	332	ARG	3.1
2	I	251	ALA	3.1
2	I	236	LYS	3.1
3	J	1071	GLY	3.1
5	L	221	PHE	3.1
3	D	1202	GLU	3.1
5	F	463	LEU	3.1
3	D	1199	PHE	3.1
3	J	1121	LEU	3.1
2	I	743	PRO	3.1
3	J	1052	GLU	3.1
2	I	257	ALA	3.1
2	I	235	ASN	3.1

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Mol	Chain	Res	Type	RSRZ
3	J	747	MET	3.1
3	D	879	ALA	3.0
3	J	1168	GLU	3.0
5	L	273	MET	3.0
1	G	201	LEU	3.0
2	C	194	LEU	3.0
1	H	231	PHE	3.0
5	F	141	ILE	3.0
2	C	100	LEU	3.0
2	C	696	ASP	3.0
2	I	855	PRO	3.0
2	I	277	LEU	3.0
2	C	235	ASN	3.0
2	C	330	HIS	3.0
1	G	95	LYS	3.0
2	I	169	LYS	3.0
2	I	931	VAL	3.0
5	L	328	GLU	3.0
2	C	267	ARG	3.0
2	I	915	ASP	3.0
1	H	144	ILE	3.0
3	J	1106	ILE	3.0
1	G	39	LEU	3.0
3	J	1047	THR	3.0
2	C	255	ILE	3.0
1	A	9	LEU	3.0
1	A	266	SER	3.0
3	D	596	LEU	3.0
2	I	987	GLU	3.0
3	D	743	MET	3.0
5	F	73	ASP	3.0
2	C	997	TRP	3.0
2	I	629	PHE	3.0
2	I	970	GLY	3.0
5	F	337	VAL	3.0
2	I	745	GLU	2.9
2	C	331	LYS	2.9
5	L	55	VAL	2.9
1	H	188	GLU	2.9
2	C	713	GLY	2.9
3	J	984	LEU	2.9
2	I	1013	GLN	2.9

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Mol	Chain	Res	Type	RSRZ
1	G	35	PHE	2.9
2	C	483	ASP	2.9
2	I	1052	VAL	2.9
5	L	134	VAL	2.9
4	K	38	LEU	2.9
3	J	516	ASP	2.9
3	J	1031	VAL	2.9
2	C	231	GLU	2.9
3	J	548	VAL	2.9
2	I	971	LEU	2.9
5	L	294	GLN	2.9
3	J	744	ARG	2.9
2	C	237	LEU	2.9
3	J	203	GLU	2.9
3	J	1204	VAL	2.9
5	F	578	LYS	2.9
5	L	29	ASP	2.9
3	J	715	LYS	2.9
1	H	97	GLU	2.9
5	F	322	MET	2.9
2	I	256	GLU	2.9
2	I	68	LEU	2.9
3	J	1087	ASP	2.9
3	D	1180	VAL	2.8
5	F	289	LYS	2.8
1	A	322	PRO	2.8
5	F	285	ARG	2.8
1	G	227	GLN	2.8
2	I	1050	VAL	2.8
5	L	497	VAL	2.8
2	I	974	ARG	2.8
2	I	253	PHE	2.8
5	F	261	LEU	2.8
5	F	320	ILE	2.8
2	I	990	ASP	2.8
2	C	644	LEU	2.8
3	J	1082	ASP	2.8
3	D	155	GLU	2.8
3	D	1190	ILE	2.8
3	D	1173	ARG	2.8
2	I	938	GLY	2.8
2	C	57	PHE	2.8

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Mol	Chain	Res	Type	RSRZ
2	C	179	TYR	2.8
2	I	11	ILE	2.8
5	L	88	GLU	2.8
2	C	172	TYR	2.8
5	L	40	GLN	2.8
5	L	325	PRO	2.8
3	D	1152	GLU	2.8
2	C	236	LYS	2.8
1	G	92	VAL	2.7
3	J	998	PRO	2.7
5	L	43	ASP	2.7
2	C	996	ARG	2.7
2	C	336	LEU	2.7
2	I	120	GLN	2.7
2	C	1001	GLY	2.7
5	F	446	GLN	2.7
2	I	883	LEU	2.7
2	C	315	MET	2.7
4	E	35	LYS	2.7
1	H	59	VAL	2.7
2	I	1012	GLU	2.7
1	G	160	HIS	2.7
3	J	707	ILE	2.7
5	F	294	GLN	2.7
5	F	92	GLY	2.7
2	I	207	THR	2.7
5	F	587	ILE	2.7
2	I	330	HIS	2.7
1	H	186	ASN	2.7
5	F	85	SER	2.7
2	C	621	SER	2.7
3	J	571	ASP	2.7
5	F	336	GLU	2.7
5	F	222	ALA	2.7
3	J	1196	LEU	2.7
3	J	1044	GLN	2.7
1	H	72	GLU	2.6
5	L	34	ASP	2.6
5	F	138	PRO	2.6
1	G	203	ILE	2.6
3	J	76	LYS	2.6
1	A	295	LEU	2.6

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Mol	Chain	Res	Type	RSRZ
1	G	231	PHE	2.6
1	A	193	GLU	2.6
2	I	332	ARG	2.6
3	J	830	ASP	2.6
3	D	880	VAL	2.6
3	J	1210	ILE	2.6
3	J	858	VAL	2.6
3	J	1180	VAL	2.6
2	C	268	ARG	2.6
5	L	311	THR	2.6
3	J	689	ALA	2.6
3	J	1195	GLN	2.6
5	L	319	ALA	2.6
5	L	17	LYS	2.6
1	G	202	VAL	2.6
5	L	453	PRO	2.6
1	B	123	ILE	2.6
1	H	193	GLU	2.6
5	L	338	HIS	2.6
2	I	221	LEU	2.6
3	J	1115	ILE	2.6
5	L	421	TYR	2.6
2	I	100	LEU	2.6
1	A	321	TRP	2.6
3	J	1058	SER	2.6
5	L	344	LEU	2.6
5	L	333	VAL	2.6
5	L	162	ILE	2.5
3	J	966	VAL	2.5
2	C	629	PHE	2.5
3	D	754	ILE	2.5
2	I	429	MET	2.5
3	J	1162	ILE	2.5
2	I	472	GLU	2.5
3	J	1163	VAL	2.5
2	C	299	LYS	2.5
5	L	16	GLY	2.5
2	C	208	ILE	2.5
2	I	304	GLU	2.5
3	J	521	LYS	2.5
5	F	140	ALA	2.5
5	L	321	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
3	J	545	HIS	2.5
5	L	330	LEU	2.5
1	H	98	VAL	2.5
5	L	492	ASP	2.5
1	B	122	GLU	2.5
2	I	1001	GLY	2.5
5	L	264	LYS	2.5
3	J	1090	ILE	2.5
5	F	134	VAL	2.5
2	I	9	LYS	2.5
3	J	714	GLU	2.5
5	L	19	GLN	2.5
2	C	248	GLY	2.5
2	I	292	ILE	2.5
3	J	574	VAL	2.5
5	F	280	VAL	2.5
5	L	150	ARG	2.5
3	J	208	THR	2.5
5	L	143	TYR	2.5
1	H	150	ARG	2.5
2	I	322	LEU	2.4
3	J	1175	LEU	2.4
2	C	272	ARG	2.4
2	I	875	ALA	2.4
2	I	1015	ALA	2.4
2	C	261	VAL	2.4
5	L	488	LEU	2.4
3	D	1163	VAL	2.4
1	A	55	ALA	2.4
3	J	1120	THR	2.4
2	C	634	VAL	2.4
3	D	1215	GLU	2.4
5	F	310	GLU	2.4
5	L	86	SER	2.4
5	L	279	ARG	2.4
2	I	854	ILE	2.4
2	I	489	PRO	2.4
5	F	307	THR	2.4
5	F	309	ASN	2.4
1	H	53	GLY	2.4
2	C	266	GLY	2.4
2	I	186	PHE	2.4

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Mol	Chain	Res	Type	RSRZ
2	C	246	LEU	2.4
5	F	163	THR	2.4
2	I	732	ILE	2.4
2	C	60	GLN	2.4
2	C	941	LYS	2.4
2	C	310	ILE	2.4
3	D	1161	GLY	2.4
1	A	264	VAL	2.4
2	C	204	LEU	2.4
3	J	1074	LEU	2.4
3	J	1081	VAL	2.4
3	J	662	ALA	2.4
2	I	494	ASN	2.4
3	D	857	LEU	2.4
5	F	330	LEU	2.4
3	J	1084	GLN	2.4
1	G	28	LEU	2.4
5	L	155	GLU	2.3
1	A	270	LEU	2.3
2	I	69	GLN	2.3
3	J	978	ARG	2.3
3	D	1156	LEU	2.3
2	I	237	LEU	2.3
2	I	261	VAL	2.3
3	J	1012	ALA	2.3
2	I	1018	TYR	2.3
2	I	317	LEU	2.3
5	F	164	GLY	2.3
2	C	52	ALA	2.3
2	I	245	ARG	2.3
2	C	979	LEU	2.3
1	B	72	GLU	2.3
5	F	166	VAL	2.3
5	L	286	LEU	2.3
5	L	493	LYS	2.3
2	C	1173	ALA	2.3
1	A	317	ARG	2.3
2	I	584	TYR	2.3
3	J	681	LYS	2.3
3	J	952	VAL	2.3
2	I	1009	ASN	2.3
5	F	333	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	90	VAL	2.3
2	C	241	LEU	2.3
2	I	204	LEU	2.3
2	I	428	VAL	2.3
2	I	919	ARG	2.3
5	F	135	ALA	2.3
2	I	347	ILE	2.3
5	F	255	VAL	2.3
5	F	7	SER	2.3
2	I	209	ILE	2.3
2	C	224	PHE	2.3
2	C	259	GLY	2.3
1	B	24	ALA	2.3
2	C	1018	TYR	2.3
5	F	588	ARG	2.3
5	L	256	PHE	2.3
5	L	276	MET	2.3
3	D	41	PRO	2.2
1	B	56	VAL	2.2
3	J	1073	ASP	2.2
3	J	1199	PHE	2.2
5	F	477	GLU	2.2
2	I	388	LEU	2.2
5	F	33	GLU	2.2
3	J	324	LEU	2.2
3	J	525	MET	2.2
5	L	44	ILE	2.2
2	I	1017	GLN	2.2
1	H	121	VAL	2.2
2	I	103	VAL	2.2
3	J	1095	MET	2.2
1	A	299	SER	2.2
5	F	15	ARG	2.2
2	C	320	ASP	2.2
2	I	645	PHE	2.2
3	J	670	SER	2.2
1	H	96	ASP	2.2
2	I	124	MET	2.2
2	I	194	LEU	2.2
3	J	89	GLY	2.2
2	I	977	ALA	2.2
1	B	97	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
2	I	176	ILE	2.2
3	J	1156	LEU	2.2
2	I	861	ALA	2.2
2	C	47	TYR	2.2
2	I	190	PRO	2.2
1	A	289	LEU	2.2
2	I	385	PHE	2.2
2	I	1104	PRO	2.2
3	D	824	PRO	2.2
2	I	593	LYS	2.2
2	I	31	GLN	2.2
5	L	21	TYR	2.2
5	L	228	TYR	2.2
2	C	101	ARG	2.2
2	C	493	ILE	2.2
5	F	451	ARG	2.2
2	C	999	GLU	2.2
2	I	289	VAL	2.2
1	H	228	LEU	2.2
1	A	292	THR	2.2
3	J	774	ILE	2.2
2	I	252	SER	2.2
3	J	176	PHE	2.2
1	B	148	ARG	2.2
1	H	90	VAL	2.2
3	J	1065	ALA	2.2
2	C	21	VAL	2.2
3	J	1202	GLU	2.2
5	L	46	GLN	2.2
5	L	446	GLN	2.2
2	I	172	TYR	2.1
1	H	54	CYS	2.1
2	I	713	GLY	2.1
2	I	155	VAL	2.1
2	I	241	LEU	2.1
3	D	1151	LYS	2.1
3	J	708	ASN	2.1
2	I	239	MET	2.1
3	J	178	ALA	2.1
3	J	541	LEU	2.1
5	F	6	GLN	2.1
2	C	260	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
2	C	313	ALA	2.1
3	D	877	VAL	2.1
5	L	306	PHE	2.1
1	A	263	THR	2.1
1	H	197	ASP	2.1
2	I	884	VAL	2.1
2	C	487	LEU	2.1
2	I	284	LEU	2.1
3	J	312	ARG	2.1
2	C	603	ILE	2.1
2	C	602	GLU	2.1
2	C	1169	VAL	2.1
2	I	821	ARG	2.1
2	I	986	ALA	2.1
2	I	425	ILE	2.1
5	F	5	PRO	2.1
5	L	480	PRO	2.1
3	D	68	TYR	2.1
2	I	871	VAL	2.1
5	F	326	TRP	2.1
3	D	878	ASP	2.1
3	J	1026	PRO	2.1
1	B	172	LEU	2.1
2	C	573	ASN	2.1
3	J	1110	GLU	2.1
3	D	481	ARG	2.1
1	H	149	GLY	2.1
2	C	184	LEU	2.1
2	I	168	GLY	2.1
3	D	889	ASP	2.1
3	D	1376	GLY	2.1
3	J	1096	PRO	2.1
2	C	186	PHE	2.1
1	B	144	ILE	2.1
5	F	228	TYR	2.1
2	C	468	LEU	2.1
2	C	904	ALA	2.1
3	J	269	TYR	2.1
5	L	598	LEU	2.1
2	I	206	ALA	2.1
1	G	217	ILE	2.1
2	C	433	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
5	L	39	ASP	2.1
5	L	548	LEU	2.1
2	I	561	ILE	2.0
2	C	103	VAL	2.0
2	I	644	LEU	2.0
3	D	1291	GLU	2.0
1	G	213	PRO	2.0
2	C	69	GLN	2.0
3	J	1295	ASN	2.0
3	D	1214	PRO	2.0
2	C	789	THR	2.0
2	I	1149	TYR	2.0
1	G	193	GLU	2.0
2	I	192	ASP	2.0
1	A	278	ILE	2.0
5	F	221	PHE	2.0
2	I	471	VAL	2.0
5	L	296	LYS	2.0
2	C	67	GLU	2.0
3	J	460	ASP	2.0
2	I	771	VAL	2.0
1	A	323	PRO	2.0
2	I	188	PHE	2.0
2	I	621	SER	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 carbohydrates in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
6	4OE	I	2001	23/23	0.73	0.96	4.70	100,113,125,126	0
6	4OE	C	2001	23/23	0.91	0.67	2.94	48,74,93,102	0
8	ZN	J	1503	1/1	0.98	0.25	-0.01	54,54,54,54	0
8	ZN	D	1503	1/1	0.99	0.23	-0.61	33,33,33,33	0
8	ZN	D	1502	1/1	0.96	0.12	-0.76	84,84,84,84	0
8	ZN	J	1502	1/1	0.91	0.16	-0.82	94,94,94,94	0
7	MG	J	1501	1/1	0.83	0.71	-	69,69,69,69	0
7	MG	D	1501	1/1	0.80	0.53	-	28,28,28,28	0

6.5 Other polymers [i](#)

There are no such residues in this entry.