



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:26 PM GMT

PDB ID : 1K5G
Title : Crystal structure of Ran-GDP-AlFx-RanBP1-RanGAP complex
Authors : Seewald, M.J.; Koerner, C.; Wittinghofer, A.; Vetter, I.R.
Deposited on : 2001-10-10
Resolution : 3.10 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 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
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) : trunk26865

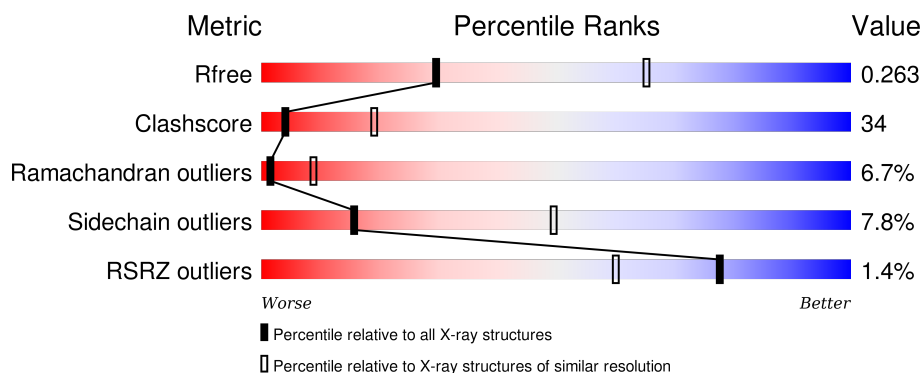
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.10 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	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	216	<div> <div>2%</div> <div>38% 49% 8% 5%</div> </div>
1	D	216	<div> <div>4%</div> <div>34% 52% 9% 5%</div> </div>
1	G	216	<div> <div>%</div> <div>35% 51% 8% 5%</div> </div>
1	J	216	<div> <div>%</div> <div>34% 51% 9% 5%</div> </div>
2	B	201	<div> <div>2%</div> <div>24% 40% 8% 27%</div> </div>

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Mol	Chain	Length	Quality of chain
2	E	201	
2	H	201	
2	K	201	
3	C	386	
3	F	386	
3	I	386	
3	L	386	

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
4	MG	A	1251	-	-	-	X
4	MG	D	2251	-	-	-	X
4	MG	G	3251	-	-	-	X
4	MG	J	4251	-	-	-	X
6	AF3	D	2252	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 22396 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 GTP-binding nuclear protein RAN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	206	Total	C	N	O	S	0	0	0
			1652	1067	284	295	6			
1	D	206	Total	C	N	O	S	0	0	0
			1652	1067	284	295	6			
1	G	206	Total	C	N	O	S	0	0	0
			1652	1067	284	295	6			
1	J	206	Total	C	N	O	S	0	0	0
			1652	1067	284	295	6			

- Molecule 2 is a protein called Ran-specific GTPase-activating protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	146	Total	C	N	O	S	0	0	0
			1216	769	214	226	7			
2	E	146	Total	C	N	O	S	0	0	0
			1216	769	214	226	7			
2	H	146	Total	C	N	O	S	0	0	0
			1216	769	214	226	7			
2	K	146	Total	C	N	O	S	0	0	0
			1216	769	214	226	7			

- Molecule 3 is a protein called Ran GTPase activating protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	344	Total	C	N	O	S	0	0	0
			2698	1699	469	522	8			
3	F	344	Total	C	N	O	S	0	0	0
			2698	1699	469	522	8			
3	I	344	Total	C	N	O	S	0	0	0
			2698	1699	469	522	8			
3	L	344	Total	C	N	O	S	0	0	0
			2698	1699	469	522	8			

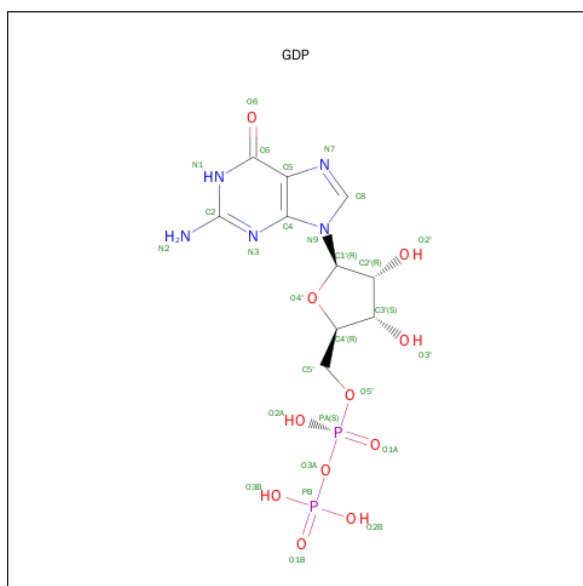
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2	ALA	SER	SEE REMARK 999	UNP P41391
F	2	ALA	SER	SEE REMARK 999	UNP P41391
I	2	ALA	SER	SEE REMARK 999	UNP P41391
L	2	ALA	SER	SEE REMARK 999	UNP P41391

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	G	1	Total Mg 1 1	0	0
4	J	1	Total Mg 1 1	0	0
4	A	1	Total Mg 1 1	0	0
4	D	1	Total Mg 1 1	0	0

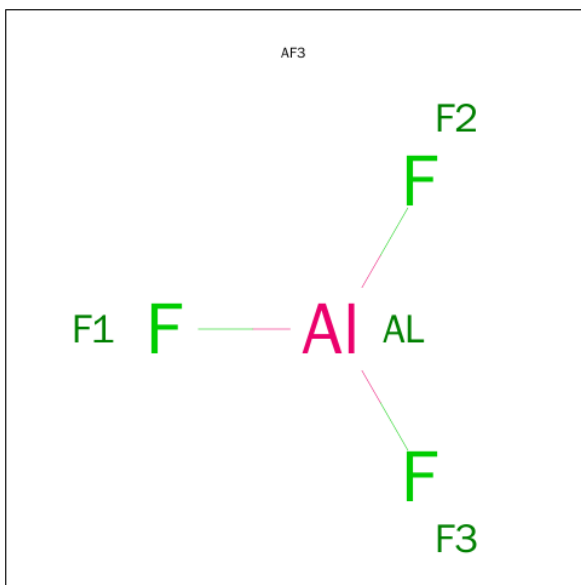
- Molecule 5 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: C₁₀H₁₅N₅O₁₁P₂).



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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	G	1	Total	C	N	O	P	0	0
			28	10	5	11	2		
5	J	1	Total	C	N	O	P	0	0
			28	10	5	11	2		

- Molecule 6 is ALUMINUM FLUORIDE (three-letter code: AF3) (formula: AlF_3).

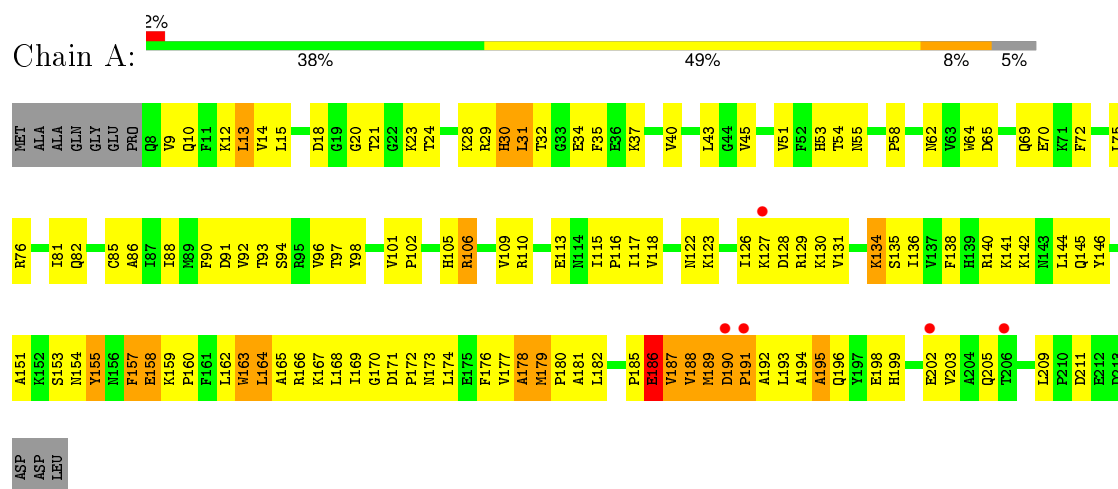


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	Al	F	0	0
			4	1	3		
6	D	1	Total	Al	F	0	0
			4	1	3		
6	G	1	Total	Al	F	0	0
			4	1	3		
6	J	1	Total	Al	F	0	0
			4	1	3		

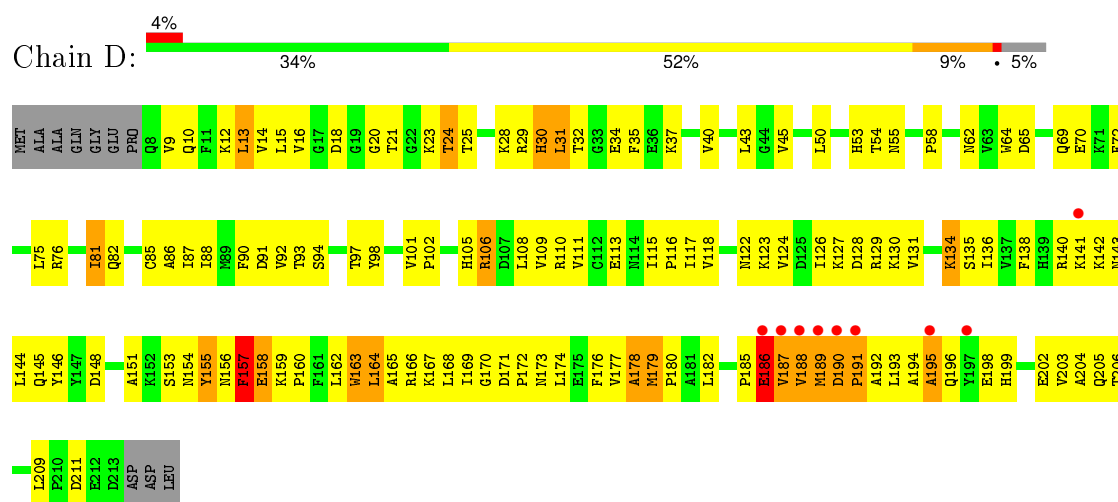
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

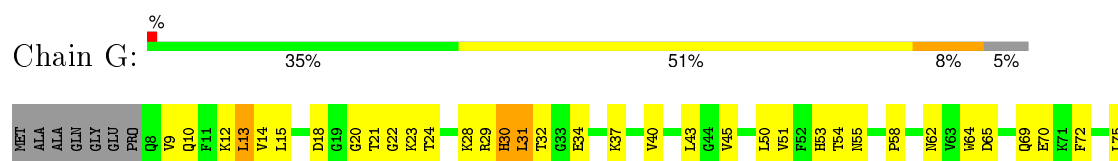
• Molecule 1: GTP-binding nuclear protein RAN

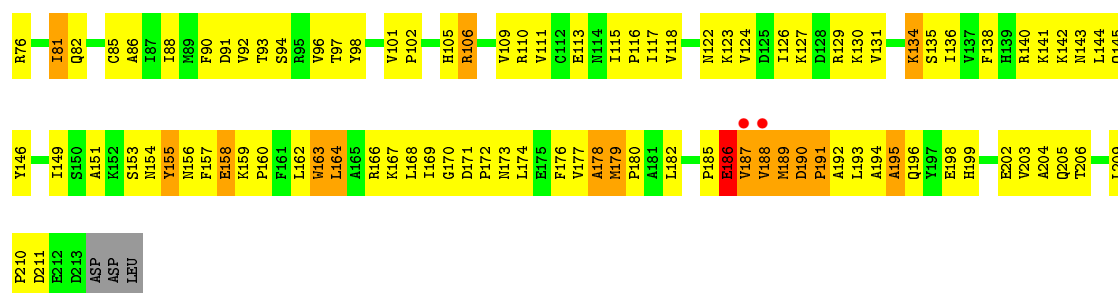


• Molecule 1: GTP-binding nuclear protein RAN

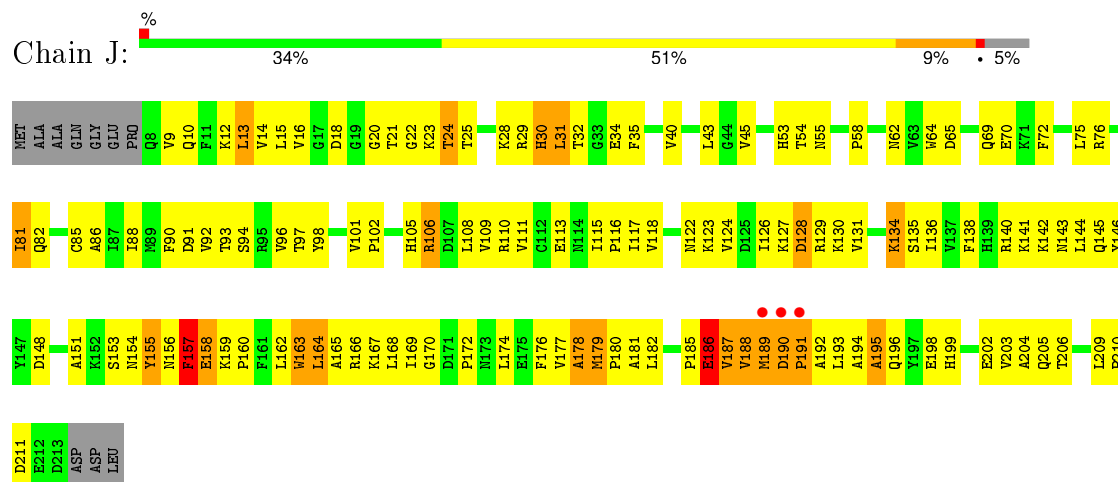


• Molecule 1: GTP-binding nuclear protein RAN

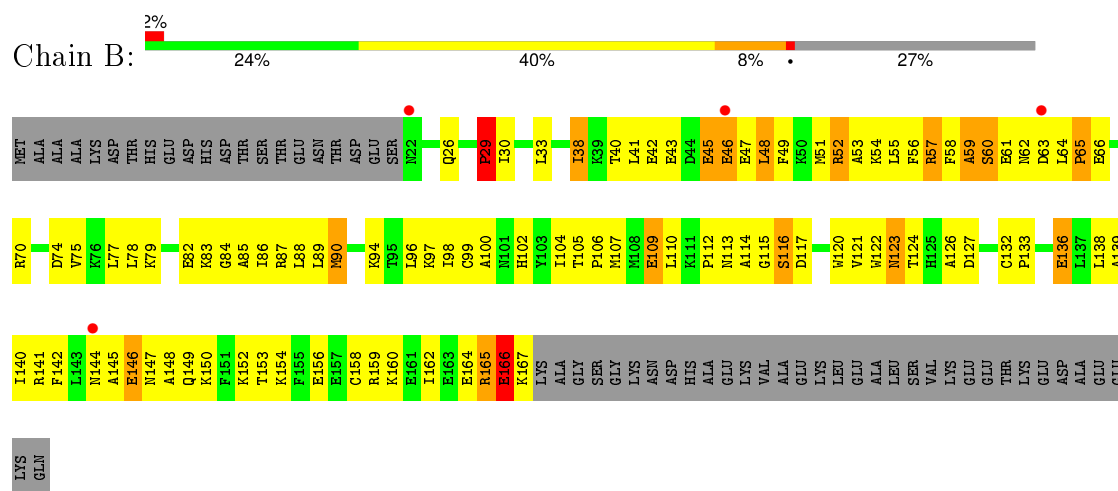




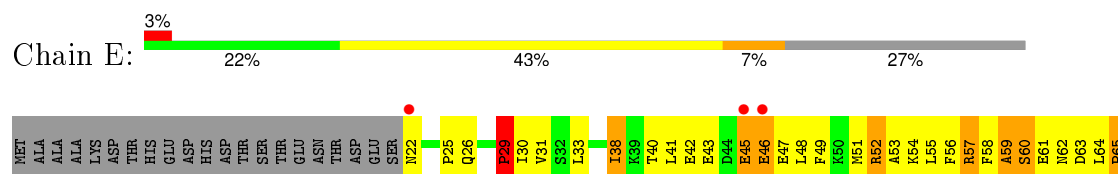
- Molecule 1: GTP-binding nuclear protein RAN

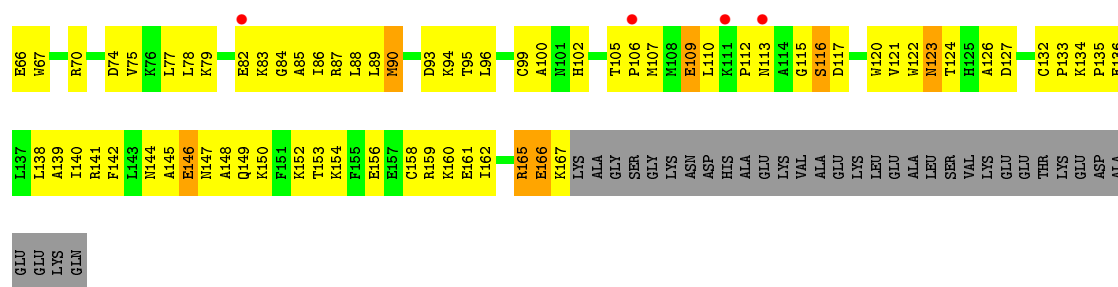


- Molecule 2: Ran-specific GTPase-activating protein

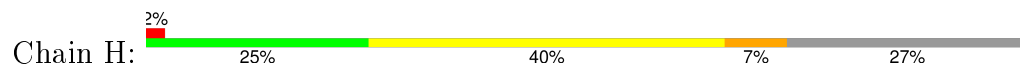


- Molecule 2: Ran-specific GTPase-activating protein

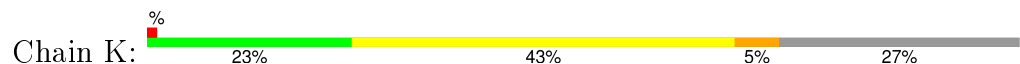




• Molecule 2: Ran-specific GTPase-activating protein

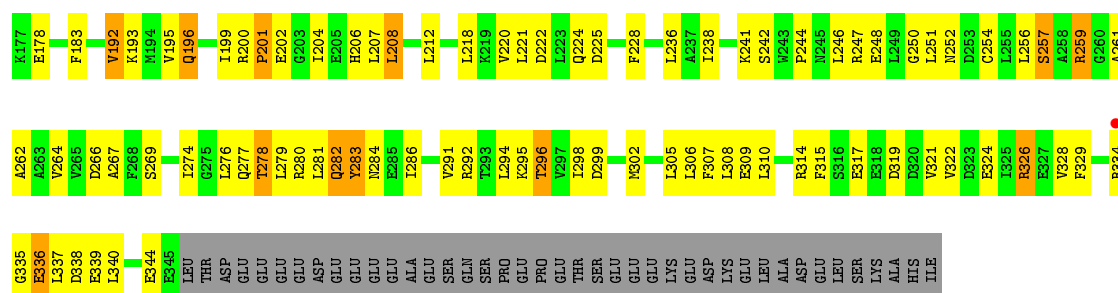


• Molecule 2: Ran-specific GTPase-activating protein

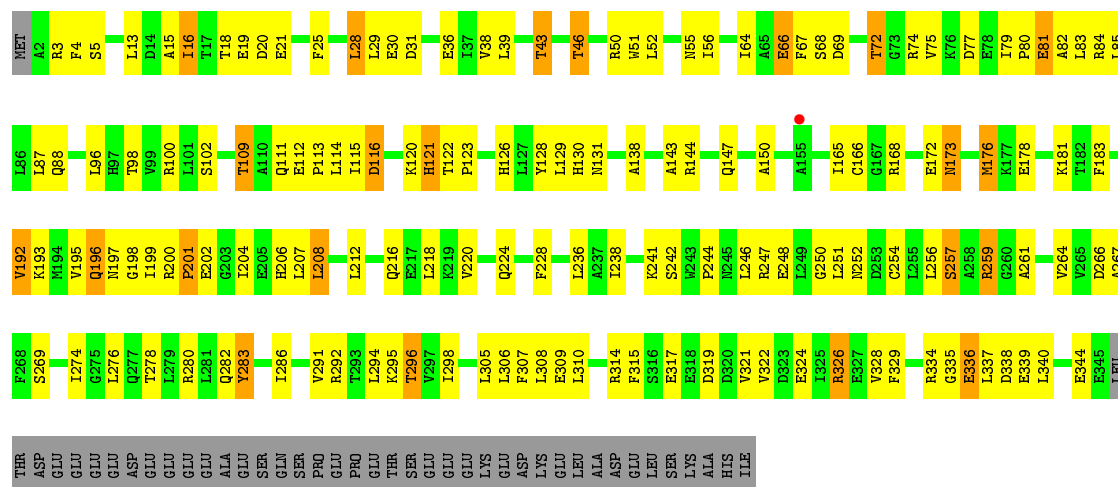


• Molecule 3: Ran GTPase activating protein 1

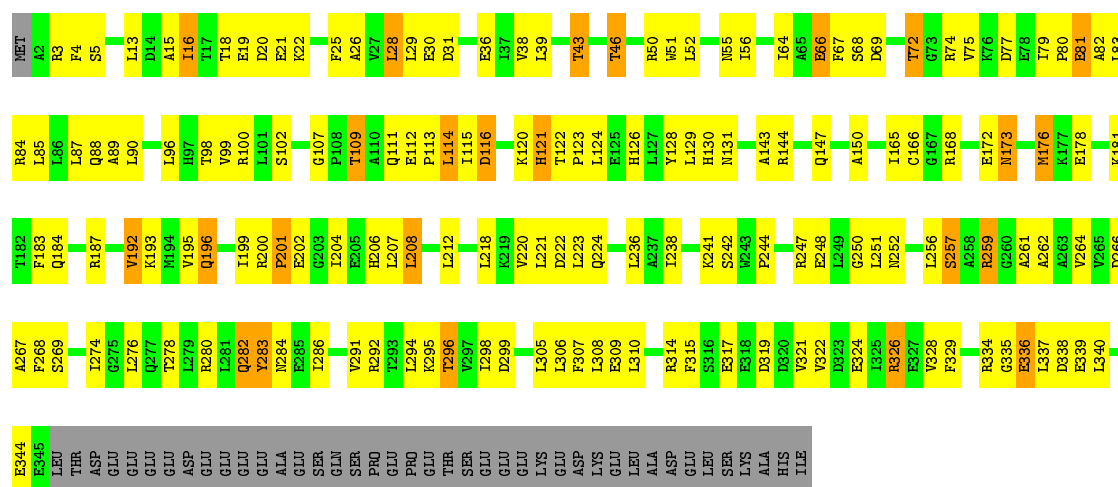




- Molecule 3: Ran GTPase activating protein 1



- Molecule 3: Ran GTPase activating protein 1



- Molecule 3: Ran GTPase activating protein 1



E324	L255	K177	R84
L325	L256	E178	L85
R326	S257	F183	L86
E327	A258	H186	L87
V328	R259		Q88
F329	G260		
	A261		L96
R334	A262	V192	R97
G335	A263	K193	T98
E336	V264	M194	V99
L337	V265	V195	R100
D338	D266	Q196	L101
E339	A267	N197	S102
L340	F268	G198	
	S269	I199	T109
E344	K270	R200	A110
E345		P201	Q111
LEU	I274	E202	E112
THR	G275	G203	P113
ASP	L276	L204	L114
GLU	D277	E205	I115
GLU	T278	H206	D116
GLU	L279	L207	F117
GLU	R280	L208	L118
ASP	L281		S119
GLU	Q282	L212	K120
GLU	Y283	A213	H121
GLU	N284		T122
GLU	E285	Q216	P123
ALA	L286	E217	
GLU		L218	H126
SER	V291	K219	L127
GLN	R292	V220	Y128
SER	T293	L221	L129
PRO	L294	D222	L129
GLU	K295	L223	M131
PRO	T296	Q224	N131
GLU	V297	D225	
THR	L298		A138
SER	D299		L56
GLU		F228	
GLU	M302		A143
GLU	L305	S234	R144
LVS	L306	A235	A145
ASP	F307	L236	L146
LVS	L308	A237	Q147
GLU	E309	L238	E148
LEU	L310		L149
ALA		R241	A150
ASP	R314	S242	V151
GLU	F315	V243	
LEU	S316	P244	L161
SER	E317		
LVS	E318	R247	L165
ALA	D319	E248	C166
HIS	D320	L249	R168
TLE	V321	G250	
	V322	L251	E172
	D323	N252	M173
		C254	M176

4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	99.93Å 102.57Å 118.85Å 71.67° 79.09° 67.81°	Depositor
Resolution (Å)	31.00 – 3.10 31.22 – 2.88	Depositor EDS
% Data completeness (in resolution range)	96.2 (31.00-3.10) 86.6 (31.22-2.88)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.23 (at 2.90Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.250 , 0.269 0.224 , 0.263	Depositor DCC
R_{free} test set	7166 reflections (11.03%)	DCC
Wilson B-factor (Å ²)	63.8	Xtriage
Anisotropy	0.113	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 59.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Outliers	0 of 88616 reflections	Xtriage
F_o, F_c correlation	0.90	EDS
Total number of atoms	22396	wwPDB-VP
Average B, all atoms (Å ²)	65.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.43% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, MG, AF3

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	0.42	0/1693	0.67	0/2296
1	D	0.45	0/1693	0.68	0/2296
1	G	0.43	0/1693	0.67	0/2296
1	J	0.46	0/1693	0.69	0/2296
2	B	0.37	0/1242	0.63	0/1666
2	E	0.36	0/1242	0.62	0/1666
2	H	0.38	0/1242	0.62	0/1666
2	K	0.38	0/1242	0.63	0/1666
3	C	0.41	0/2737	0.68	0/3697
3	F	0.41	0/2737	0.68	0/3697
3	I	0.41	0/2737	0.67	0/3697
3	L	0.42	0/2737	0.69	0/3697
All	All	0.41	0/22688	0.67	0/30636

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1652	0	1660	129	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	1652	0	1659	141	0
1	G	1652	0	1659	140	0
1	J	1652	0	1660	145	0
2	B	1216	0	1208	117	0
2	E	1216	0	1208	118	0
2	H	1216	0	1208	107	0
2	K	1216	0	1208	110	0
3	C	2698	0	2733	166	0
3	F	2698	0	2733	143	0
3	I	2698	0	2733	162	0
3	L	2698	0	2733	164	0
4	A	1	0	0	0	0
4	D	1	0	0	0	0
4	G	1	0	0	0	0
4	J	1	0	0	0	0
5	A	28	0	12	5	0
5	D	28	0	12	5	0
5	G	28	0	12	5	0
5	J	28	0	12	4	0
6	A	4	0	0	0	0
6	D	4	0	0	0	0
6	G	4	0	0	0	0
6	J	4	0	0	0	0
All	All	22396	0	22450	1526	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 34.

All (1526) 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:I:259:ARG:NH1	3:I:259:ARG:HB3	1.68	1.07
3:F:259:ARG:HB3	3:F:259:ARG:NH1	1.69	1.06
3:L:259:ARG:NH1	3:L:259:ARG:HB3	1.71	1.04
3:C:259:ARG:HB3	3:C:259:ARG:NH1	1.73	1.04
3:I:259:ARG:HH11	3:I:259:ARG:HB3	1.20	1.03
3:L:259:ARG:HB3	3:L:259:ARG:HH11	1.25	1.00
3:F:259:ARG:HB3	3:F:259:ARG:HH11	1.22	1.00
3:C:259:ARG:HH11	3:C:259:ARG:HB3	1.26	0.99
1:J:91:ASP:H	1:J:97:THR:HG21	1.32	0.94
3:F:173:ASN:HD21	3:F:200:ARG:H	1.14	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:91:ASP:H	1:A:97:THR:HG21	1.34	0.92
1:G:91:ASP:H	1:G:97:THR:HG21	1.36	0.91
2:H:154:LYS:O	2:H:158:CYS:HB2	1.70	0.90
3:I:173:ASN:HD21	3:I:200:ARG:H	1.17	0.90
1:G:158:GLU:HG2	2:H:94:LYS:HB3	1.55	0.89
1:J:158:GLU:HG2	2:K:94:LYS:HB3	1.54	0.89
1:D:91:ASP:H	1:D:97:THR:HG21	1.37	0.89
1:J:185:PRO:HG2	2:K:133:PRO:HG3	1.54	0.89
3:L:173:ASN:HD21	3:L:200:ARG:H	1.21	0.88
1:D:85:CYS:HB2	1:D:164:LEU:HD22	1.54	0.87
1:D:158:GLU:HG2	2:E:94:LYS:HB3	1.55	0.87
1:G:85:CYS:HB2	1:G:164:LEU:HD22	1.55	0.87
1:D:123:LYS:HB3	1:D:126:ILE:HD13	1.57	0.87
1:A:123:LYS:HB3	1:A:126:ILE:HD13	1.56	0.87
3:C:173:ASN:HD21	3:C:200:ARG:H	1.20	0.86
1:A:85:CYS:HB2	1:A:164:LEU:HD22	1.56	0.86
1:J:85:CYS:HB2	1:J:164:LEU:HD22	1.57	0.86
1:A:168:LEU:HD22	2:B:30:ILE:HD12	1.56	0.86
1:J:123:LYS:HB3	1:J:126:ILE:HD13	1.60	0.84
3:I:204:ILE:HG23	3:I:208:LEU:HD23	1.58	0.83
1:J:209:LEU:HD23	2:K:113:ASN:ND2	1.93	0.83
2:B:122:TRP:HZ3	2:B:140:ILE:HG22	1.42	0.83
2:K:122:TRP:HZ3	2:K:140:ILE:HG22	1.43	0.82
1:G:123:LYS:HB3	1:G:126:ILE:HD13	1.58	0.82
3:F:204:ILE:HG23	3:F:208:LEU:HD23	1.60	0.82
2:E:122:TRP:HZ3	2:E:140:ILE:HG22	1.43	0.82
1:J:30:HIS:HE1	1:J:157:PHE:O	1.63	0.82
3:F:173:ASN:HD22	3:F:173:ASN:N	1.75	0.82
3:L:204:ILE:HG23	3:L:208:LEU:HD23	1.59	0.81
1:A:30:HIS:HE1	1:A:157:PHE:O	1.64	0.81
1:G:168:LEU:HD22	2:H:30:ILE:HD12	1.62	0.81
3:C:204:ILE:HG23	3:C:208:LEU:HD23	1.60	0.81
1:A:158:GLU:HG2	2:B:94:LYS:HB3	1.61	0.81
1:G:30:HIS:HE1	1:G:157:PHE:O	1.63	0.80
3:I:173:ASN:N	3:I:173:ASN:HD22	1.78	0.80
3:F:176:MET:HE2	3:F:207:LEU:HD13	1.63	0.80
3:C:204:ILE:HG23	3:C:208:LEU:CD2	2.11	0.80
1:D:28:LYS:O	1:D:31:LEU:HD12	1.82	0.80
1:D:168:LEU:HD22	2:E:30:ILE:HD12	1.64	0.80
3:L:204:ILE:HG23	3:L:208:LEU:CD2	2.12	0.79
2:H:122:TRP:HZ3	2:H:140:ILE:HG22	1.47	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:91:ASP:N	1:G:97:THR:HG21	1.98	0.79
3:C:173:ASN:N	3:C:173:ASN:HD22	1.81	0.79
3:I:204:ILE:HG23	3:I:208:LEU:CD2	2.13	0.79
1:J:168:LEU:HD22	2:K:30:ILE:HD12	1.65	0.79
1:D:30:HIS:HE1	1:D:157:PHE:O	1.66	0.79
1:D:94:SER:O	1:D:97:THR:HG22	1.81	0.78
3:L:173:ASN:HD22	3:L:173:ASN:N	1.77	0.78
2:B:154:LYS:O	2:B:158:CYS:HB2	1.84	0.77
1:D:13:LEU:HD12	1:D:13:LEU:C	2.05	0.77
1:A:28:LYS:O	1:A:31:LEU:HD12	1.83	0.77
2:K:86:ILE:HG21	2:K:158:CYS:SG	2.24	0.77
1:J:90:PHE:HB2	1:J:97:THR:HG23	1.67	0.77
1:A:90:PHE:HB2	1:A:97:THR:HG23	1.67	0.76
1:G:94:SER:O	1:G:97:THR:HG22	1.84	0.76
1:G:28:LYS:O	1:G:31:LEU:HD12	1.85	0.76
1:A:94:SER:O	1:A:97:THR:HG22	1.85	0.76
2:K:59:ALA:O	2:K:60:SER:HB3	1.85	0.76
1:A:186:GLU:CD	1:A:187:VAL:H	1.89	0.76
2:H:59:ALA:O	2:H:60:SER:HB3	1.85	0.76
1:J:94:SER:O	1:J:97:THR:HG22	1.85	0.76
3:C:324:GLU:O	3:C:328:VAL:HG23	1.86	0.76
2:K:57:ARG:HD3	2:K:136:GLU:OE2	1.86	0.76
1:J:91:ASP:N	1:J:97:THR:HG21	1.99	0.75
1:A:91:ASP:N	1:A:97:THR:HG21	2.00	0.75
3:L:176:MET:HE2	3:L:207:LEU:HD13	1.67	0.75
2:B:59:ALA:O	2:B:60:SER:HB3	1.86	0.75
1:D:186:GLU:CD	1:D:187:VAL:H	1.90	0.75
3:L:200:ARG:HB3	3:L:201:PRO:HD2	1.66	0.75
3:I:176:MET:HE2	3:I:207:LEU:HD13	1.68	0.75
3:F:204:ILE:HG23	3:F:208:LEU:CD2	2.16	0.75
1:D:92:VAL:CG1	1:D:129:ARG:HG3	2.17	0.75
1:J:186:GLU:CD	1:J:187:VAL:H	1.90	0.74
2:E:154:LYS:O	2:E:158:CYS:HB2	1.87	0.74
1:D:10:GLN:HE21	1:D:62:ASN:HD21	1.35	0.74
1:G:186:GLU:CD	1:G:187:VAL:H	1.91	0.74
1:A:13:LEU:C	1:A:13:LEU:HD12	2.06	0.74
2:H:57:ARG:HD3	2:H:136:GLU:OE2	1.88	0.74
1:D:90:PHE:HB2	1:D:97:THR:HG23	1.68	0.74
1:G:126:ILE:HD11	5:G:3250:GDP:N2	2.03	0.74
3:L:324:GLU:O	3:L:328:VAL:HG23	1.87	0.74
1:A:55:ASN:OD1	1:A:174:LEU:HD12	1.88	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:117:ASP:OD2	2:E:145:ALA:HB1	1.88	0.74
1:J:13:LEU:HD12	1:J:13:LEU:C	2.08	0.74
3:I:317:GLU:HG2	3:I:340:LEU:HB2	1.70	0.74
2:E:57:ARG:HD3	2:E:136:GLU:OE2	1.88	0.73
1:D:91:ASP:N	1:D:97:THR:HG21	2.04	0.73
2:B:57:ARG:HD3	2:B:136:GLU:OE2	1.88	0.73
3:F:200:ARG:HB3	3:F:201:PRO:HD2	1.71	0.73
3:I:200:ARG:HB3	3:I:201:PRO:HD2	1.70	0.73
2:E:59:ALA:O	2:E:60:SER:HB3	1.87	0.73
3:I:324:GLU:O	3:I:328:VAL:HG23	1.89	0.73
1:D:13:LEU:HD12	1:D:14:VAL:N	2.03	0.72
1:A:185:PRO:HG2	2:B:133:PRO:HG3	1.70	0.72
2:K:86:ILE:HD13	2:K:158:CYS:SG	2.29	0.72
3:F:176:MET:HE1	3:F:207:LEU:HD22	1.71	0.72
1:G:13:LEU:C	1:G:13:LEU:HD12	2.09	0.72
3:L:176:MET:HE1	3:L:207:LEU:HD22	1.72	0.72
2:B:117:ASP:OD2	2:B:145:ALA:HB1	1.90	0.72
1:G:55:ASN:OD1	1:G:174:LEU:HD12	1.90	0.71
3:C:200:ARG:HB3	3:C:201:PRO:HD2	1.71	0.71
1:G:178:ALA:N	2:H:96:LEU:HD23	2.04	0.71
2:H:49:PHE:HB3	2:H:77:LEU:HD12	1.72	0.71
2:B:59:ALA:HB2	2:B:66:GLU:H	1.56	0.71
3:F:324:GLU:O	3:F:328:VAL:HG23	1.89	0.71
1:G:90:PHE:HB2	1:G:97:THR:HG23	1.71	0.71
2:H:78:LEU:O	2:H:86:ILE:HA	1.90	0.71
1:J:28:LYS:O	1:J:31:LEU:HD12	1.89	0.71
1:G:10:GLN:HE21	1:G:62:ASN:HD21	1.38	0.71
1:D:189:MET:HB2	1:D:193:LEU:HD22	1.73	0.71
2:H:86:ILE:HG21	2:H:158:CYS:SG	2.31	0.71
1:A:209:LEU:HD23	2:B:113:ASN:ND2	2.06	0.71
2:B:86:ILE:HG21	2:B:158:CYS:SG	2.31	0.70
1:D:185:PRO:HG2	2:E:133:PRO:HG3	1.73	0.70
2:E:59:ALA:HB2	2:E:66:GLU:H	1.56	0.70
1:G:32:THR:HB	1:G:34:GLU:HG2	1.71	0.70
3:F:199:ILE:CG2	3:F:204:ILE:HD12	2.21	0.70
2:H:117:ASP:OD2	2:H:145:ALA:HB1	1.91	0.70
3:C:192:VAL:HG12	3:C:218:LEU:HD11	1.74	0.70
3:F:192:VAL:HG12	3:F:218:LEU:HD11	1.74	0.70
3:C:317:GLU:HG2	3:C:340:LEU:HB2	1.73	0.70
3:F:317:GLU:HG2	3:F:340:LEU:HB2	1.72	0.70
1:A:178:ALA:N	2:B:96:LEU:HD23	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:9:VAL:HG21	2:H:33:LEU:HD11	1.74	0.70
3:I:247:ARG:HG3	3:I:247:ARG:HH11	1.57	0.70
3:C:247:ARG:HG3	3:C:247:ARG:HH11	1.56	0.70
2:H:59:ALA:HB2	2:H:66:GLU:H	1.56	0.70
3:I:176:MET:HE1	3:I:207:LEU:HD22	1.73	0.70
1:G:189:MET:HB2	1:G:193:LEU:HD22	1.74	0.70
3:C:176:MET:HE2	3:C:207:LEU:HD13	1.71	0.69
1:J:10:GLN:HE21	1:J:62:ASN:HD21	1.39	0.69
1:J:189:MET:HB2	1:J:193:LEU:HD22	1.73	0.69
3:L:317:GLU:HG2	3:L:340:LEU:HB2	1.74	0.69
3:I:4:PHE:CD2	3:I:28:LEU:HD23	2.27	0.69
2:B:49:PHE:HB3	2:B:77:LEU:HD12	1.73	0.69
2:B:122:TRP:CZ3	2:B:140:ILE:HG22	2.26	0.69
1:D:10:GLN:NE2	1:D:62:ASN:HD21	1.90	0.69
2:K:117:ASP:OD2	2:K:145:ALA:HB1	1.93	0.69
2:H:86:ILE:HB	2:H:162:ILE:HD11	1.73	0.69
2:H:57:ARG:HG3	2:H:70:ARG:HD3	1.74	0.69
3:C:266:ASP:O	3:C:269:SER:HB3	1.91	0.69
1:J:32:THR:HB	1:J:34:GLU:HG2	1.75	0.69
1:G:13:LEU:HD12	1:G:14:VAL:N	2.08	0.69
1:D:126:ILE:HD11	5:D:2250:GDP:N2	2.07	0.69
2:K:90:MET:HB3	2:K:99:CYS:SG	2.32	0.69
2:B:78:LEU:O	2:B:86:ILE:HA	1.92	0.69
2:K:59:ALA:HB2	2:K:66:GLU:H	1.56	0.68
2:K:122:TRP:CZ3	2:K:140:ILE:HG22	2.27	0.68
2:E:110:LEU:HD12	2:E:152:LYS:HA	1.76	0.68
1:J:55:ASN:OD1	1:J:174:LEU:HD12	1.92	0.68
3:F:247:ARG:HH11	3:F:247:ARG:HG3	1.57	0.68
3:I:128:TYR:CE2	3:I:165:ILE:HG13	2.29	0.68
1:G:10:GLN:NE2	1:G:62:ASN:HD21	1.92	0.68
1:A:32:THR:HB	1:A:34:GLU:HG2	1.76	0.68
3:I:192:VAL:HG12	3:I:218:LEU:HD11	1.76	0.68
2:E:49:PHE:HB3	2:E:77:LEU:HD12	1.74	0.68
3:L:247:ARG:HG3	3:L:247:ARG:HH11	1.58	0.68
1:G:13:LEU:HB2	1:G:85:CYS:SG	2.33	0.68
2:E:86:ILE:HB	2:E:162:ILE:HD11	1.76	0.68
1:A:189:MET:HB2	1:A:193:LEU:HD22	1.75	0.68
1:G:13:LEU:HD13	1:G:86:ALA:HA	1.76	0.68
1:A:13:LEU:HD12	1:A:14:VAL:N	2.09	0.68
3:I:75:VAL:HG23	3:I:77:ASP:HB3	1.76	0.68
3:I:112:GLU:HB2	3:I:113:PRO:HD3	1.75	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:43:THR:CG2	3:L:72:THR:O	2.42	0.68
3:L:192:VAL:HG12	3:L:218:LEU:HD11	1.75	0.68
3:C:75:VAL:HG23	3:C:77:ASP:HB3	1.75	0.68
1:A:10:GLN:HE21	1:A:62:ASN:HD21	1.39	0.68
3:F:112:GLU:HB2	3:F:113:PRO:HD3	1.75	0.68
2:K:110:LEU:HD12	2:K:152:LYS:HA	1.76	0.68
3:I:266:ASP:O	3:I:269:SER:HB3	1.94	0.67
1:A:169:ILE:HD12	2:B:33:LEU:HD12	1.76	0.67
2:K:62:ASN:O	2:K:64:LEU:HD13	1.94	0.67
1:D:55:ASN:OD1	1:D:174:LEU:HD12	1.94	0.67
2:K:42:GLU:O	2:K:45:GLU:HB3	1.94	0.67
1:A:10:GLN:NE2	1:A:62:ASN:HD21	1.91	0.67
1:D:13:LEU:HD13	1:D:86:ALA:HA	1.75	0.67
1:G:122:ASN:ND2	1:G:123:LYS:HG3	2.09	0.67
3:C:4:PHE:CD2	3:C:28:LEU:HD23	2.30	0.67
3:L:112:GLU:HB2	3:L:113:PRO:HD3	1.76	0.67
3:L:75:VAL:HG23	3:L:77:ASP:HB3	1.75	0.67
1:A:101:VAL:HB	1:A:102:PRO:HD3	1.77	0.67
2:K:49:PHE:HB3	2:K:77:LEU:HD12	1.77	0.67
3:L:128:TYR:CE2	3:L:165:ILE:HG13	2.30	0.67
1:G:32:THR:CG2	1:G:34:GLU:HG2	2.25	0.66
1:D:101:VAL:HB	1:D:102:PRO:HD3	1.77	0.66
2:H:42:GLU:O	2:H:45:GLU:HB3	1.95	0.66
3:I:199:ILE:CG2	3:I:204:ILE:HD12	2.25	0.66
1:J:101:VAL:HB	1:J:102:PRO:HD3	1.76	0.66
3:L:96:LEU:O	3:L:121:HIS:HE1	1.78	0.66
2:B:110:LEU:HD12	2:B:152:LYS:HA	1.77	0.66
1:D:32:THR:HB	1:D:34:GLU:HG2	1.76	0.66
2:E:78:LEU:O	2:E:86:ILE:HA	1.94	0.66
1:A:92:VAL:CG1	1:A:129:ARG:HG3	2.26	0.66
1:A:126:ILE:HD11	5:A:1250:GDP:N2	2.10	0.66
3:L:199:ILE:CG2	3:L:204:ILE:HD12	2.25	0.66
3:I:96:LEU:O	3:I:121:HIS:HE1	1.78	0.66
2:K:78:LEU:O	2:K:86:ILE:HA	1.96	0.66
3:F:128:TYR:CE2	3:F:165:ILE:HG13	2.30	0.66
1:J:92:VAL:CG1	1:J:129:ARG:HG3	2.26	0.66
2:B:42:GLU:O	2:B:45:GLU:HB3	1.95	0.66
1:J:13:LEU:HD12	1:J:14:VAL:N	2.12	0.65
3:C:96:LEU:O	3:C:121:HIS:HE1	1.79	0.65
3:I:36:GLU:HG3	3:I:64:ILE:HB	1.78	0.65
3:C:128:TYR:CE2	3:C:165:ILE:HG13	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:62:ASN:O	2:H:64:LEU:HD13	1.96	0.65
3:F:266:ASP:O	3:F:269:SER:HB3	1.95	0.65
3:L:176:MET:CE	3:L:207:LEU:HD22	2.27	0.65
3:C:112:GLU:HB2	3:C:113:PRO:HD3	1.79	0.65
3:I:144:ARG:HA	3:I:147:GLN:NE2	2.10	0.65
2:H:110:LEU:HD12	2:H:152:LYS:HA	1.77	0.65
1:D:178:ALA:N	2:E:96:LEU:HD23	2.12	0.65
3:C:84:ARG:HH11	3:C:88:GLN:NE2	1.95	0.65
2:E:122:TRP:CZ3	2:E:140:ILE:HG22	2.28	0.65
2:E:90:MET:HB3	2:E:99:CYS:SG	2.36	0.65
3:C:308:LEU:HD21	3:C:310:LEU:HD11	1.77	0.65
3:C:144:ARG:HA	3:C:147:GLN:NE2	2.11	0.65
3:C:46:THR:HG21	3:C:81:GLU:HB3	1.77	0.65
3:F:84:ARG:HH11	3:F:88:GLN:NE2	1.95	0.65
1:J:13:LEU:HD13	1:J:86:ALA:HA	1.79	0.65
3:C:46:THR:CG2	3:C:81:GLU:HB3	2.26	0.65
1:J:209:LEU:HD23	2:K:113:ASN:CG	2.17	0.65
1:A:32:THR:CG2	1:A:34:GLU:HG2	2.26	0.65
3:C:43:THR:CG2	3:C:72:THR:O	2.45	0.65
2:E:86:ILE:HD13	2:E:158:CYS:SG	2.37	0.64
3:C:252:ASN:ND2	3:C:280:ARG:HB3	2.12	0.64
1:G:92:VAL:CG1	1:G:129:ARG:HG3	2.27	0.64
3:I:308:LEU:HD21	3:I:310:LEU:HD11	1.78	0.64
3:I:20:ASP:O	3:I:21:GLU:HB2	1.97	0.64
1:G:101:VAL:HB	1:G:102:PRO:HD3	1.78	0.64
2:B:86:ILE:HD13	2:B:158:CYS:SG	2.37	0.64
1:J:10:GLN:NE2	1:J:62:ASN:HD21	1.95	0.64
3:C:84:ARG:HH11	3:C:88:GLN:HE22	1.45	0.64
3:F:75:VAL:HG23	3:F:77:ASP:HB3	1.79	0.64
3:L:84:ARG:HH11	3:L:88:GLN:NE2	1.95	0.64
1:G:209:LEU:HD23	2:H:113:ASN:ND2	2.12	0.64
2:B:57:ARG:HG3	2:B:70:ARG:HD3	1.80	0.64
1:J:126:ILE:HD11	5:J:4250:GDP:N2	2.12	0.64
3:F:96:LEU:O	3:F:121:HIS:HE1	1.81	0.64
2:B:62:ASN:O	2:B:64:LEU:HD13	1.98	0.64
1:J:211:ASP:HA	2:K:141:ARG:HH12	1.62	0.64
3:I:252:ASN:ND2	3:I:280:ARG:HB3	2.12	0.64
1:D:13:LEU:HB2	1:D:85:CYS:SG	2.37	0.64
2:K:154:LYS:O	2:K:158:CYS:HB2	1.98	0.64
3:I:46:THR:HG21	3:I:81:GLU:HB3	1.79	0.64
3:F:195:VAL:HG22	3:F:224:GLN:HB3	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:GLY:N	5:A:1250:GDP:O3B	2.30	0.64
1:J:122:ASN:ND2	1:J:123:LYS:HG3	2.12	0.64
1:D:92:VAL:HG13	1:D:129:ARG:HG3	1.79	0.64
3:F:4:PHE:CD2	3:F:28:LEU:HD23	2.33	0.64
3:F:39:LEU:HD12	3:F:67:PHE:CE2	2.32	0.64
2:E:62:ASN:O	2:E:64:LEU:HD13	1.97	0.64
2:E:42:GLU:O	2:E:45:GLU:HB3	1.98	0.64
2:K:146:GLU:OE1	2:K:147:ASN:N	2.31	0.63
2:K:59:ALA:O	2:K:60:SER:CB	2.46	0.63
3:I:176:MET:HG3	3:I:207:LEU:HB2	1.79	0.63
1:A:141:LYS:O	1:A:142:LYS:HD2	1.99	0.63
2:H:153:THR:HG23	2:H:154:LYS:N	2.13	0.63
3:L:84:ARG:HH11	3:L:88:GLN:HE22	1.44	0.63
1:D:189:MET:CB	1:D:193:LEU:HD22	2.29	0.63
2:B:153:THR:HG23	2:B:154:LYS:N	2.14	0.63
2:E:57:ARG:HG3	2:E:70:ARG:HD3	1.79	0.63
3:F:252:ASN:ND2	3:F:280:ARG:HB3	2.13	0.63
3:I:46:THR:CG2	3:I:81:GLU:HB3	2.29	0.63
2:E:62:ASN:C	2:E:64:LEU:H	2.02	0.63
2:B:90:MET:HB3	2:B:99:CYS:SG	2.39	0.63
3:I:176:MET:CE	3:I:207:LEU:HD22	2.28	0.63
3:C:183:PHE:HE1	3:C:207:LEU:HD11	1.64	0.63
1:D:9:VAL:HG21	2:E:33:LEU:HD11	1.80	0.63
3:L:20:ASP:O	3:L:21:GLU:HB2	1.98	0.63
3:L:200:ARG:HB3	3:L:201:PRO:CD	2.27	0.63
3:C:176:MET:HE1	3:C:207:LEU:HD22	1.79	0.63
3:I:294:LEU:O	3:I:298:ILE:HG13	1.99	0.63
1:A:122:ASN:ND2	1:A:123:LYS:HG3	2.14	0.63
1:G:169:ILE:HD12	2:H:33:LEU:HD12	1.81	0.63
3:L:195:VAL:HG22	3:L:224:GLN:HB3	1.79	0.63
1:G:141:LYS:O	1:G:142:LYS:HD2	1.99	0.63
1:J:178:ALA:N	2:K:96:LEU:HD23	2.14	0.62
3:C:199:ILE:CG2	3:C:204:ILE:HD12	2.29	0.62
2:H:122:TRP:CZ3	2:H:140:ILE:HG22	2.33	0.62
3:C:176:MET:CE	3:C:207:LEU:HD22	2.29	0.62
3:C:176:MET:HG3	3:C:207:LEU:HB2	1.81	0.62
3:F:176:MET:CE	3:F:207:LEU:HD22	2.30	0.62
3:L:4:PHE:CD2	3:L:28:LEU:HD23	2.34	0.62
3:L:46:THR:CG2	3:L:81:GLU:HB3	2.29	0.62
3:F:46:THR:CG2	3:F:81:GLU:HB3	2.29	0.62
2:K:57:ARG:HG3	2:K:70:ARG:HD3	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:252:ASN:ND2	3:L:282:GLN:H	1.98	0.62
3:C:36:GLU:HG3	3:C:64:ILE:HB	1.80	0.62
3:F:183:PHE:HE1	3:F:207:LEU:HD11	1.64	0.62
2:H:59:ALA:O	2:H:60:SER:CB	2.46	0.62
3:L:46:THR:HG21	3:L:81:GLU:HB3	1.81	0.62
3:L:252:ASN:ND2	3:L:280:ARG:HB3	2.13	0.62
1:J:189:MET:CB	1:J:193:LEU:HD22	2.30	0.62
2:K:62:ASN:C	2:K:64:LEU:H	2.03	0.62
1:J:91:ASP:H	1:J:97:THR:CG2	2.08	0.62
2:H:146:GLU:OE1	2:H:147:ASN:N	2.33	0.62
3:F:252:ASN:ND2	3:F:282:GLN:H	1.97	0.62
1:J:13:LEU:HB2	1:J:85:CYS:SG	2.40	0.62
2:H:90:MET:HB3	2:H:99:CYS:SG	2.40	0.62
3:I:200:ARG:HB3	3:I:201:PRO:CD	2.29	0.62
3:F:129:LEU:O	3:F:166:CYS:HA	2.00	0.62
2:E:153:THR:HG23	2:E:154:LYS:N	2.13	0.61
1:D:209:LEU:HD23	2:E:113:ASN:ND2	2.15	0.61
3:F:46:THR:HG21	3:F:81:GLU:HB3	1.80	0.61
3:C:329:PHE:CG	3:C:335:GLY:HA3	2.35	0.61
1:G:91:ASP:H	1:G:97:THR:CG2	2.10	0.61
2:B:59:ALA:O	2:B:60:SER:CB	2.47	0.61
3:I:43:THR:CG2	3:I:72:THR:O	2.48	0.61
3:F:199:ILE:HG22	3:F:204:ILE:HD12	1.82	0.61
2:B:146:GLU:OE1	2:B:147:ASN:N	2.34	0.61
3:L:18:THR:HG23	3:L:20:ASP:O	2.01	0.61
3:L:308:LEU:HD21	3:L:310:LEU:HD11	1.81	0.61
1:D:122:ASN:ND2	1:D:123:LYS:HG3	2.14	0.61
2:E:59:ALA:O	2:E:60:SER:CB	2.48	0.61
1:G:105:HIS:CD2	1:G:144:LEU:HD21	2.36	0.61
3:F:144:ARG:HA	3:F:147:GLN:NE2	2.16	0.61
3:F:84:ARG:HH11	3:F:88:GLN:HE22	1.47	0.61
3:L:266:ASP:O	3:L:269:SER:HB3	2.01	0.61
3:F:176:MET:HG3	3:F:207:LEU:HB2	1.83	0.61
1:A:178:ALA:H	2:B:96:LEU:HD23	1.65	0.61
2:K:153:THR:HG23	2:K:154:LYS:N	2.14	0.61
2:H:62:ASN:C	2:H:64:LEU:H	2.03	0.61
3:I:18:THR:HG23	3:I:20:ASP:O	2.00	0.61
1:J:170:GLY:HA3	2:K:29:PRO:HG3	1.82	0.61
1:A:13:LEU:HD13	1:A:86:ALA:HA	1.81	0.61
1:G:178:ALA:H	2:H:96:LEU:HD23	1.64	0.61
1:G:93:THR:O	1:G:130:LYS:HD2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:115:ILE:O	1:J:117:ILE:HG13	1.99	0.61
3:C:20:ASP:O	3:C:21:GLU:HB2	1.99	0.61
2:E:146:GLU:OE1	2:E:147:ASN:N	2.34	0.60
3:F:264:VAL:O	3:F:267:ALA:HB3	2.01	0.60
1:A:92:VAL:HG13	1:A:129:ARG:HG3	1.82	0.60
2:K:86:ILE:HB	2:K:162:ILE:HD11	1.84	0.60
1:G:189:MET:CB	1:G:193:LEU:HD22	2.31	0.60
3:L:43:THR:HG23	3:L:72:THR:O	2.01	0.60
3:I:84:ARG:HH11	3:I:88:GLN:NE2	1.99	0.60
2:B:53:ALA:HB3	2:B:140:ILE:HD11	1.83	0.60
1:A:194:ALA:O	1:A:195:ALA:HB3	2.02	0.60
2:B:62:ASN:C	2:B:64:LEU:H	2.03	0.60
3:F:20:ASP:O	3:F:21:GLU:HB2	2.00	0.60
3:F:36:GLU:HG3	3:F:64:ILE:HB	1.82	0.60
2:E:79:LYS:HG3	2:E:84:GLY:O	2.01	0.60
3:I:184:GLN:HE22	3:L:270:LYS:NZ	2.00	0.60
1:J:177:VAL:HG21	2:K:38:ILE:HG12	1.82	0.60
1:A:13:LEU:HB2	1:A:85:CYS:SG	2.42	0.60
1:J:32:THR:CG2	1:J:34:GLU:HG2	2.31	0.60
1:J:158:GLU:HG2	2:K:94:LYS:CB	2.29	0.60
2:E:53:ALA:HB3	2:E:140:ILE:HD11	1.84	0.60
1:J:194:ALA:O	1:J:195:ALA:HB3	2.01	0.60
1:D:32:THR:CG2	1:D:34:GLU:HG2	2.32	0.60
1:G:32:THR:CB	1:G:34:GLU:HG2	2.31	0.60
2:H:162:ILE:O	2:H:165:ARG:HB3	2.02	0.60
1:G:20:GLY:N	5:G:3250:GDP:O3B	2.35	0.60
3:I:183:PHE:HE1	3:I:207:LEU:HD11	1.67	0.60
3:F:43:THR:CG2	3:F:72:THR:O	2.49	0.60
3:L:36:GLU:HG3	3:L:64:ILE:HB	1.82	0.60
3:F:309:GLU:HA	3:F:338:ASP:OD1	2.02	0.60
3:C:195:VAL:HG22	3:C:224:GLN:HB3	1.83	0.59
1:G:122:ASN:HD22	1:G:123:LYS:HG3	1.66	0.59
3:L:176:MET:HG3	3:L:207:LEU:HB2	1.84	0.59
3:L:183:PHE:HE1	3:L:207:LEU:HD11	1.67	0.59
3:F:200:ARG:HB3	3:F:201:PRO:CD	2.31	0.59
2:B:79:LYS:HG3	2:B:84:GLY:O	2.02	0.59
3:C:309:GLU:HA	3:C:338:ASP:OD1	2.02	0.59
3:I:84:ARG:HH11	3:I:88:GLN:HE22	1.50	0.59
3:I:187:ARG:NH2	3:L:270:LYS:O	2.20	0.59
3:F:308:LEU:HD21	3:F:310:LEU:HD11	1.85	0.59
1:J:92:VAL:HG13	1:J:129:ARG:HG3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:38:VAL:HG22	3:C:66:GLU:HB2	1.84	0.59
3:L:30:GLU:HG3	3:L:31:ASP:N	2.17	0.59
1:D:141:LYS:O	1:D:142:LYS:HD2	2.02	0.59
1:D:105:HIS:CD2	1:D:144:LEU:HD21	2.37	0.59
3:C:200:ARG:HB3	3:C:201:PRO:CD	2.32	0.59
2:K:75:VAL:HG21	2:K:140:ILE:HD11	1.85	0.59
2:E:75:VAL:HG21	2:E:140:ILE:HD11	1.84	0.59
1:A:189:MET:CB	1:A:193:LEU:HD22	2.31	0.59
3:C:147:GLN:O	3:C:150:ALA:HB3	2.03	0.59
3:C:30:GLU:HG3	3:C:31:ASP:N	2.17	0.59
1:A:105:HIS:CD2	1:A:144:LEU:HD21	2.37	0.59
1:D:209:LEU:HD23	2:E:113:ASN:CG	2.22	0.59
3:I:309:GLU:HA	3:I:338:ASP:OD1	2.03	0.59
3:I:298:ILE:HG23	3:I:305:LEU:HD23	1.85	0.59
3:L:309:GLU:HA	3:L:338:ASP:OD1	2.01	0.59
1:J:20:GLY:N	5:J:4250:GDP:O3B	2.33	0.58
1:G:92:VAL:HG13	1:G:129:ARG:HG3	1.84	0.58
1:D:115:ILE:O	1:D:117:ILE:HG13	2.02	0.58
1:D:211:ASP:HA	2:E:141:ARG:HH12	1.68	0.58
3:L:199:ILE:HG22	3:L:204:ILE:HD12	1.84	0.58
2:H:57:ARG:HH22	2:H:60:SER:HB2	1.68	0.58
3:I:291:VAL:HG21	3:I:315:PHE:CD2	2.38	0.58
1:G:180:PRO:HB3	2:H:41:LEU:HD13	1.85	0.58
3:I:195:VAL:HG22	3:I:224:GLN:HB3	1.85	0.58
3:L:144:ARG:HA	3:L:147:GLN:NE2	2.17	0.58
1:G:194:ALA:O	1:G:195:ALA:HB3	2.03	0.58
3:L:39:LEU:HD12	3:L:67:PHE:CE2	2.39	0.58
3:I:30:GLU:HG3	3:I:31:ASP:N	2.18	0.58
3:C:129:LEU:O	3:C:166:CYS:HA	2.04	0.58
1:A:91:ASP:H	1:A:97:THR:CG2	2.10	0.58
1:J:122:ASN:HD22	1:J:123:LYS:HG3	1.69	0.58
1:D:194:ALA:O	1:D:195:ALA:HB3	2.03	0.58
3:C:111:GLN:O	3:C:115:ILE:HG13	2.03	0.58
1:D:91:ASP:H	1:D:97:THR:CG2	2.13	0.58
1:J:106:ARG:HA	1:J:109:VAL:HG22	1.85	0.58
3:I:173:ASN:ND2	3:I:173:ASN:N	2.50	0.58
3:F:30:GLU:HG3	3:F:31:ASP:N	2.18	0.58
2:H:79:LYS:HG3	2:H:84:GLY:O	2.04	0.58
3:L:173:ASN:ND2	3:L:173:ASN:N	2.50	0.58
3:I:252:ASN:ND2	3:I:282:GLN:H	2.02	0.58
1:J:141:LYS:O	1:J:142:LYS:HD2	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:98:THR:OG1	3:L:126:HIS:HB2	2.03	0.58
3:F:329:PHE:CG	3:F:335:GLY:HA3	2.39	0.58
3:C:264:VAL:O	3:C:267:ALA:HB3	2.04	0.58
1:A:93:THR:O	1:A:130:LYS:HD2	2.04	0.57
1:J:54:THR:HB	1:J:174:LEU:HD11	1.86	0.57
3:F:18:THR:HG23	3:F:20:ASP:O	2.04	0.57
3:C:242:SER:O	3:C:244:PRO:HD3	2.04	0.57
3:L:116:ASP:OD2	3:L:120:LYS:HE2	2.04	0.57
3:I:43:THR:HG23	3:I:72:THR:O	2.04	0.57
1:G:106:ARG:HA	1:G:109:VAL:HG22	1.86	0.57
1:J:169:ILE:HD12	2:K:33:LEU:HD12	1.85	0.57
2:H:124:THR:HG22	2:H:126:ALA:H	1.69	0.57
1:D:122:ASN:HD22	1:D:123:LYS:HG3	1.68	0.57
2:H:75:VAL:HG21	2:H:140:ILE:HD11	1.87	0.57
1:D:12:LYS:HE3	1:D:64:TRP:CE2	2.39	0.57
2:E:112:PRO:HG3	2:E:120:TRP:CZ3	2.40	0.57
2:B:86:ILE:HB	2:B:162:ILE:HD11	1.86	0.57
1:A:188:VAL:O	1:A:189:MET:HG2	2.04	0.57
3:C:294:LEU:O	3:C:298:ILE:HG13	2.04	0.57
1:J:117:ILE:HB	1:J:144:LEU:HD22	1.85	0.57
3:F:51:TRP:CZ3	3:F:52:LEU:HD23	2.40	0.57
1:A:180:PRO:HB3	2:B:41:LEU:HD13	1.86	0.57
1:A:193:LEU:H	1:A:193:LEU:HD12	1.70	0.57
3:F:111:GLN:O	3:F:115:ILE:HG13	2.05	0.57
1:A:185:PRO:O	1:A:187:VAL:HG23	2.04	0.57
1:D:190:ASP:O	1:D:194:ALA:HB3	2.05	0.57
3:C:280:ARG:HG3	3:C:280:ARG:HH11	1.68	0.57
3:F:51:TRP:CE3	3:F:52:LEU:HD23	2.40	0.57
1:J:40:VAL:HG12	1:J:40:VAL:O	2.02	0.57
1:A:32:THR:CB	1:A:34:GLU:HG2	2.35	0.57
1:D:93:THR:O	1:D:130:LYS:HD2	2.04	0.57
1:G:185:PRO:HG2	2:H:133:PRO:HG3	1.86	0.57
1:G:177:VAL:HG21	2:H:38:ILE:HG12	1.87	0.57
1:J:188:VAL:O	1:J:189:MET:HG2	2.05	0.57
3:L:129:LEU:O	3:L:166:CYS:HA	2.05	0.57
3:I:259:ARG:CB	3:I:259:ARG:HH11	2.06	0.56
3:C:173:ASN:N	3:C:173:ASN:ND2	2.53	0.56
1:A:177:VAL:HG21	2:B:38:ILE:HG12	1.87	0.56
3:I:144:ARG:HA	3:I:147:GLN:HE21	1.69	0.56
3:C:252:ASN:ND2	3:C:282:GLN:H	2.03	0.56
2:K:53:ALA:HB3	2:K:140:ILE:HD11	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:70:ARG:HH11	2:K:70:ARG:HG2	1.71	0.56
2:B:57:ARG:HH22	2:B:60:SER:HB2	1.71	0.56
3:L:51:TRP:CE3	3:L:52:LEU:HD23	2.39	0.56
3:L:79:ILE:HB	3:L:80:PRO:HD3	1.87	0.56
2:B:75:VAL:HG21	2:B:140:ILE:HD11	1.88	0.56
3:C:51:TRP:CE3	3:C:52:LEU:HD23	2.41	0.56
2:H:144:ASN:HB2	2:H:146:GLU:OE1	2.06	0.56
2:K:38:ILE:H	2:K:38:ILE:HD12	1.70	0.56
3:C:43:THR:HG23	3:C:72:THR:O	2.05	0.56
1:A:115:ILE:O	1:A:117:ILE:HG13	2.05	0.56
3:L:51:TRP:CZ3	3:L:52:LEU:HD23	2.40	0.56
3:C:51:TRP:CZ3	3:C:52:LEU:HD23	2.41	0.56
3:F:259:ARG:CB	3:F:259:ARG:HH11	2.09	0.56
1:G:193:LEU:H	1:G:193:LEU:HD12	1.70	0.56
2:H:45:GLU:O	2:H:46:GLU:HG2	2.06	0.56
3:L:294:LEU:O	3:L:298:ILE:HG13	2.06	0.56
2:H:55:LEU:CD2	2:H:100:ALA:HB2	2.36	0.56
3:I:51:TRP:CE3	3:I:52:LEU:HD23	2.40	0.56
3:L:280:ARG:HG3	3:L:280:ARG:HH11	1.71	0.56
3:C:18:THR:HG23	3:C:20:ASP:O	2.05	0.56
3:L:298:ILE:HG23	3:L:305:LEU:HD23	1.88	0.56
3:I:51:TRP:CZ3	3:I:52:LEU:HD23	2.41	0.56
3:C:39:LEU:HD12	3:C:67:PHE:CE2	2.40	0.56
1:G:158:GLU:HG2	2:H:94:LYS:CB	2.32	0.56
1:J:163:TRP:O	1:J:166:ARG:N	2.38	0.56
2:K:57:ARG:HH22	2:K:60:SER:HB2	1.70	0.56
3:I:280:ARG:HG3	3:I:280:ARG:HH11	1.70	0.56
1:J:190:ASP:O	1:J:194:ALA:HB3	2.06	0.56
3:F:43:THR:HG23	3:F:72:THR:O	2.06	0.56
2:K:79:LYS:HG3	2:K:84:GLY:O	2.05	0.56
3:F:298:ILE:HG23	3:F:305:LEU:HD23	1.88	0.56
3:F:122:THR:N	3:F:123:PRO:CD	2.69	0.56
3:L:242:SER:O	3:L:244:PRO:HD3	2.06	0.56
2:E:75:VAL:HG21	2:E:140:ILE:CD1	2.36	0.55
2:K:144:ASN:HB2	2:K:146:GLU:OE1	2.06	0.55
1:J:193:LEU:HD12	1:J:193:LEU:H	1.70	0.55
1:A:190:ASP:O	1:A:194:ALA:HB3	2.06	0.55
3:C:144:ARG:HA	3:C:147:GLN:HE21	1.71	0.55
2:E:45:GLU:O	2:E:46:GLU:HG2	2.06	0.55
3:F:147:GLN:O	3:F:150:ALA:HB3	2.07	0.55
3:L:264:VAL:O	3:L:267:ALA:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:188:VAL:O	1:G:189:MET:HG2	2.05	0.55
2:K:124:THR:HG22	2:K:126:ALA:H	1.70	0.55
1:J:189:MET:O	1:J:190:ASP:HB2	2.05	0.55
1:A:45:VAL:HG23	1:A:65:ASP:O	2.06	0.55
3:F:79:ILE:HB	3:F:80:PRO:HD3	1.87	0.55
1:D:188:VAL:O	1:D:189:MET:HG2	2.06	0.55
3:C:250:GLY:HA2	3:C:280:ARG:HB2	1.89	0.55
1:D:40:VAL:O	1:D:40:VAL:HG12	2.07	0.55
1:D:54:THR:HB	1:D:174:LEU:HD11	1.89	0.55
2:E:167:LYS:N	2:E:167:LYS:HD2	2.21	0.55
1:D:178:ALA:H	2:E:96:LEU:HD23	1.71	0.55
1:G:209:LEU:HD23	2:H:113:ASN:CG	2.25	0.55
1:D:106:ARG:HA	1:D:109:VAL:HG22	1.87	0.55
2:E:38:ILE:HD12	2:E:38:ILE:H	1.72	0.55
2:E:55:LEU:CD2	2:E:100:ALA:HB2	2.35	0.55
3:I:264:VAL:O	3:I:267:ALA:HB3	2.06	0.55
1:A:106:ARG:HA	1:A:109:VAL:HG22	1.87	0.55
3:L:173:ASN:ND2	3:L:200:ARG:H	2.00	0.55
3:C:165:ILE:HD12	3:C:193:LYS:HD2	1.89	0.55
3:I:202:GLU:CD	3:I:202:GLU:H	2.10	0.55
1:J:185:PRO:O	1:J:187:VAL:HG23	2.07	0.55
1:D:123:LYS:HB3	1:D:126:ILE:CD1	2.34	0.55
2:K:75:VAL:HG21	2:K:140:ILE:CD1	2.37	0.55
2:B:144:ASN:HB2	2:B:146:GLU:OE1	2.07	0.55
3:F:66:GLU:HG2	3:F:100:ARG:HH11	1.72	0.55
2:E:86:ILE:HG21	2:E:158:CYS:SG	2.47	0.55
1:G:185:PRO:O	1:G:187:VAL:HG23	2.06	0.55
3:I:250:GLY:HA2	3:I:280:ARG:HB2	1.88	0.55
2:E:102:HIS:HB3	2:E:127:ASP:HA	1.89	0.55
3:L:329:PHE:CG	3:L:335:GLY:HA3	2.41	0.55
1:D:189:MET:O	1:D:190:ASP:HB2	2.07	0.54
2:H:156:GLU:OE2	2:H:159:ARG:HD3	2.08	0.54
2:B:124:THR:HG22	2:B:126:ALA:H	1.71	0.54
3:I:199:ILE:HG22	3:I:204:ILE:HD12	1.89	0.54
2:H:53:ALA:HB3	2:H:140:ILE:HD11	1.89	0.54
1:D:193:LEU:H	1:D:193:LEU:HD12	1.72	0.54
1:J:32:THR:CB	1:J:34:GLU:HG2	2.37	0.54
3:I:38:VAL:HG22	3:I:66:GLU:HB2	1.90	0.54
1:A:189:MET:O	1:A:190:ASP:HB2	2.07	0.54
2:K:45:GLU:O	2:K:46:GLU:HG2	2.07	0.54
3:I:43:THR:HB	3:I:74:ARG:HH21	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:295:LYS:HE2	3:F:296:THR:HG22	1.89	0.54
3:F:173:ASN:ND2	3:F:200:ARG:H	1.96	0.54
1:A:122:ASN:HD22	1:A:123:LYS:HG3	1.72	0.54
1:G:15:LEU:HG	1:G:23:LYS:HG2	1.88	0.54
1:G:190:ASP:O	1:G:194:ALA:HB3	2.07	0.54
1:J:45:VAL:HG23	1:J:65:ASP:O	2.08	0.54
3:C:321:VAL:HG23	3:C:322:VAL:N	2.21	0.54
3:C:220:VAL:HG13	3:C:248:GLU:HB3	1.89	0.54
2:H:70:ARG:HG2	2:H:70:ARG:HH11	1.72	0.54
1:G:189:MET:O	1:G:190:ASP:HB2	2.07	0.54
3:I:66:GLU:HG2	3:I:100:ARG:HH11	1.73	0.54
2:B:45:GLU:O	2:B:46:GLU:HG2	2.07	0.54
3:C:66:GLU:HG2	3:C:100:ARG:HH11	1.72	0.54
3:C:329:PHE:HB3	3:C:335:GLY:HA3	1.89	0.54
2:K:102:HIS:HB3	2:K:127:ASP:HA	1.90	0.54
3:C:291:VAL:HG21	3:C:315:PHE:CD2	2.42	0.54
3:I:39:LEU:HD12	3:I:67:PHE:CE2	2.42	0.54
3:L:250:GLY:HA2	3:L:280:ARG:HB2	1.90	0.54
1:G:115:ILE:O	1:G:117:ILE:HG13	2.08	0.54
3:I:184:GLN:HE22	3:L:270:LYS:HZ1	1.55	0.54
3:C:79:ILE:HB	3:C:80:PRO:HD3	1.90	0.54
2:E:57:ARG:HH22	2:E:60:SER:HB2	1.72	0.54
3:L:38:VAL:HG22	3:L:66:GLU:HB2	1.90	0.54
1:A:199:HIS:O	1:A:203:VAL:HG23	2.08	0.54
3:L:122:THR:N	3:L:123:PRO:CD	2.71	0.54
2:B:53:ALA:HB2	2:B:142:PHE:CD1	2.42	0.54
2:B:55:LEU:CD2	2:B:100:ALA:HB2	2.37	0.54
1:D:177:VAL:HG21	2:E:38:ILE:HG12	1.89	0.54
2:E:112:PRO:HG3	2:E:120:TRP:HZ3	1.73	0.54
3:L:43:THR:HB	3:L:74:ARG:HH21	1.73	0.54
1:A:123:LYS:HB3	1:A:126:ILE:CD1	2.35	0.54
1:J:105:HIS:CD2	1:J:144:LEU:HD21	2.41	0.54
3:I:30:GLU:HG3	3:I:31:ASP:H	1.73	0.54
1:G:54:THR:HB	1:G:174:LEU:HD11	1.89	0.54
1:A:163:TRP:O	1:A:166:ARG:N	2.41	0.54
1:A:54:THR:HB	1:A:174:LEU:HD11	1.89	0.54
3:C:98:THR:OG1	3:C:126:HIS:HB2	2.08	0.54
1:A:117:ILE:HB	1:A:144:LEU:HD22	1.90	0.53
1:J:202:GLU:HA	1:J:205:GLN:HG2	1.91	0.53
3:I:329:PHE:CG	3:I:335:GLY:HA3	2.42	0.53
1:D:199:HIS:O	1:D:203:VAL:HG23	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:15:LEU:HG	1:A:23:LYS:HG2	1.89	0.53
3:C:122:THR:N	3:C:123:PRO:CD	2.72	0.53
1:G:69:GLN:HG3	3:I:131:ASN:ND2	2.24	0.53
1:A:182:LEU:N	1:A:182:LEU:HD12	2.22	0.53
1:D:45:VAL:HG23	1:D:65:ASP:O	2.08	0.53
3:L:259:ARG:CB	3:L:259:ARG:HH11	2.11	0.53
1:A:145:GLN:NE2	1:A:146:TYR:H	2.07	0.53
1:J:93:THR:O	1:J:130:LYS:HD2	2.08	0.53
2:E:144:ASN:HB2	2:E:146:GLU:OE1	2.08	0.53
1:D:32:THR:CB	1:D:34:GLU:HG2	2.38	0.53
1:A:170:GLY:HA3	2:B:29:PRO:HG3	1.90	0.53
1:D:185:PRO:O	1:D:187:VAL:HG23	2.09	0.53
2:E:70:ARG:HG2	2:E:70:ARG:HH11	1.74	0.53
1:A:209:LEU:HD23	2:B:113:ASN:CG	2.29	0.53
3:L:66:GLU:HG2	3:L:100:ARG:HH11	1.74	0.53
2:B:123:ASN:HD22	2:B:124:THR:H	1.57	0.53
3:F:291:VAL:HG21	3:F:315:PHE:CD2	2.43	0.53
2:B:38:ILE:H	2:B:38:ILE:HD12	1.74	0.53
2:K:112:PRO:HG3	2:K:120:TRP:CZ3	2.43	0.53
3:C:298:ILE:HG23	3:C:305:LEU:HD23	1.89	0.53
2:K:55:LEU:CD2	2:K:100:ALA:HB2	2.39	0.53
3:I:129:LEU:O	3:I:166:CYS:HA	2.09	0.53
3:F:116:ASP:OD2	3:F:120:LYS:HE2	2.09	0.53
2:B:167:LYS:HD2	2:B:167:LYS:H	1.72	0.53
1:D:20:GLY:N	5:D:2250:GDP:O3B	2.36	0.53
2:E:159:ARG:C	2:E:159:ARG:HD3	2.29	0.53
1:D:117:ILE:HB	1:D:144:LEU:HD22	1.90	0.53
3:L:144:ARG:HA	3:L:147:GLN:HE21	1.73	0.53
3:I:111:GLN:O	3:I:115:ILE:HG13	2.08	0.53
1:D:145:GLN:NE2	1:D:146:TYR:H	2.07	0.53
1:A:186:GLU:O	1:A:187:VAL:HB	2.09	0.53
3:I:321:VAL:HG23	3:I:322:VAL:N	2.24	0.53
2:B:48:LEU:HD12	2:B:158:CYS:SG	2.48	0.53
1:G:202:GLU:HA	1:G:205:GLN:HG2	1.91	0.53
3:C:295:LYS:HE2	3:C:296:THR:HG22	1.90	0.53
1:D:15:LEU:HG	1:D:23:LYS:HG2	1.90	0.53
2:E:146:GLU:O	2:E:150:LYS:HG3	2.09	0.53
1:D:188:VAL:C	1:D:189:MET:HG2	2.30	0.53
1:G:188:VAL:C	1:G:189:MET:HG2	2.29	0.53
1:J:70:GLU:CB	3:L:72:THR:HG22	2.39	0.53
3:I:29:LEU:HD23	3:I:55:ASN:OD1	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:GLU:HA	1:A:205:GLN:HG2	1.91	0.53
3:L:321:VAL:HG23	3:L:322:VAL:N	2.23	0.53
1:J:182:LEU:HD12	1:J:182:LEU:N	2.24	0.53
1:G:193:LEU:N	1:G:193:LEU:HD12	2.24	0.52
3:F:259:ARG:HB3	3:F:259:ARG:CZ	2.37	0.52
1:J:178:ALA:H	2:K:96:LEU:HD23	1.74	0.52
1:A:123:LYS:HG2	5:A:1250:GDP:C6	2.44	0.52
1:A:193:LEU:N	1:A:193:LEU:HD12	2.24	0.52
2:B:102:HIS:HB3	2:B:127:ASP:HA	1.91	0.52
2:H:102:HIS:HB3	2:H:127:ASP:HA	1.90	0.52
3:L:259:ARG:HB3	3:L:259:ARG:CZ	2.38	0.52
2:H:38:ILE:H	2:H:38:ILE:HD12	1.74	0.52
3:F:280:ARG:HG3	3:F:280:ARG:HH11	1.74	0.52
1:A:182:LEU:H	1:A:182:LEU:HD12	1.73	0.52
1:G:12:LYS:HE3	1:G:64:TRP:CE2	2.44	0.52
1:G:117:ILE:HB	1:G:144:LEU:HD22	1.90	0.52
3:F:298:ILE:CG2	3:F:305:LEU:HD23	2.40	0.52
3:I:122:THR:N	3:I:123:PRO:CD	2.73	0.52
1:J:199:HIS:O	1:J:203:VAL:HG23	2.10	0.52
1:D:170:GLY:HA3	2:E:29:PRO:HG3	1.91	0.52
1:A:168:LEU:CD2	2:B:30:ILE:HD12	2.32	0.52
1:J:188:VAL:C	1:J:189:MET:HG2	2.30	0.52
1:G:70:GLU:CB	3:I:72:THR:HG22	2.39	0.52
3:F:43:THR:HB	3:F:74:ARG:HH21	1.74	0.52
2:E:55:LEU:HD21	2:E:100:ALA:HB2	1.90	0.52
3:I:79:ILE:HB	3:I:80:PRO:HD3	1.92	0.52
3:I:116:ASP:OD2	3:I:120:LYS:HE2	2.09	0.52
3:I:261:ALA:HB2	3:I:286:ILE:HG12	1.90	0.52
1:D:202:GLU:HA	1:D:205:GLN:HG2	1.92	0.52
3:F:321:VAL:HG23	3:F:322:VAL:N	2.25	0.52
2:E:124:THR:HG22	2:E:126:ALA:H	1.75	0.52
3:L:111:GLN:O	3:L:115:ILE:HG13	2.10	0.52
2:B:70:ARG:HH11	2:B:70:ARG:HG2	1.74	0.52
3:C:52:LEU:O	3:C:56:ILE:HG13	2.10	0.52
1:A:205:GLN:O	2:B:114:ALA:HB2	2.10	0.52
3:C:199:ILE:HG22	3:C:204:ILE:HD12	1.91	0.52
1:J:70:GLU:HG2	3:L:72:THR:HA	1.91	0.52
3:L:30:GLU:HG3	3:L:31:ASP:H	1.74	0.52
2:B:55:LEU:HD21	2:B:100:ALA:HB2	1.92	0.52
3:F:202:GLU:H	3:F:202:GLU:CD	2.12	0.52
1:J:160:PRO:O	1:J:164:LEU:HD12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:282:GLN:HB3	3:F:283:TYR:HD1	1.75	0.52
3:C:274:ILE:HG22	3:C:276:LEU:H	1.75	0.52
3:F:250:GLY:HA2	3:F:280:ARG:HB2	1.90	0.52
3:F:98:THR:OG1	3:F:126:HIS:HB2	2.09	0.52
1:D:75:LEU:HD13	3:F:72:THR:OG1	2.09	0.51
2:B:121:VAL:O	2:B:122:TRP:HB3	2.09	0.51
1:A:158:GLU:HG2	2:B:94:LYS:CB	2.37	0.51
1:A:211:ASP:HA	2:B:141:ARG:HH12	1.73	0.51
2:B:52:ARG:HA	2:B:74:ASP:HA	1.93	0.51
2:H:112:PRO:HG3	2:H:120:TRP:CZ3	2.45	0.51
2:H:121:VAL:O	2:H:122:TRP:HB3	2.10	0.51
3:C:116:ASP:OD2	3:C:120:LYS:HE2	2.10	0.51
2:B:160:LYS:O	2:B:164:GLU:HG3	2.09	0.51
1:G:123:LYS:HB3	1:G:126:ILE:CD1	2.38	0.51
2:B:153:THR:HG23	2:B:154:LYS:H	1.75	0.51
1:A:188:VAL:C	1:A:189:MET:HG2	2.30	0.51
3:L:192:VAL:HG21	3:L:212:LEU:HD11	1.93	0.51
3:F:165:ILE:HD12	3:F:193:LYS:HD2	1.93	0.51
3:F:39:LEU:HD12	3:F:67:PHE:CD2	2.46	0.51
2:H:123:ASN:ND2	2:H:124:THR:H	2.09	0.51
2:K:55:LEU:HD21	2:K:100:ALA:HB2	1.92	0.51
2:E:53:ALA:HB2	2:E:142:PHE:CD1	2.46	0.51
2:B:43:GLU:C	2:B:45:GLU:H	2.14	0.51
3:C:43:THR:HB	3:C:74:ARG:HH21	1.75	0.51
3:I:282:GLN:HB3	3:I:283:TYR:HD1	1.76	0.51
3:L:282:GLN:HB3	3:L:283:TYR:HD1	1.75	0.51
3:I:242:SER:O	3:I:244:PRO:HD3	2.11	0.51
1:A:53:HIS:CD2	1:A:58:PRO:HB3	2.44	0.51
2:B:112:PRO:HG3	2:B:120:TRP:CZ3	2.46	0.51
3:F:329:PHE:HB3	3:F:335:GLY:HA3	1.93	0.51
2:H:123:ASN:HD22	2:H:124:THR:H	1.57	0.51
2:H:55:LEU:HD21	2:H:100:ALA:HB2	1.92	0.51
3:C:202:GLU:H	3:C:202:GLU:CD	2.13	0.51
3:I:295:LYS:HE2	3:I:296:THR:HG22	1.92	0.51
1:D:163:TRP:O	1:D:166:ARG:N	2.43	0.51
1:J:123:LYS:HG2	5:J:4250:GDP:C6	2.45	0.51
3:C:282:GLN:HB3	3:C:283:TYR:HD1	1.74	0.51
3:F:30:GLU:HG3	3:F:31:ASP:H	1.74	0.51
1:J:145:GLN:NE2	1:J:146:TYR:H	2.08	0.51
1:D:186:GLU:O	1:D:187:VAL:HB	2.10	0.51
1:G:186:GLU:O	1:G:187:VAL:HB	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:170:GLY:HA3	2:K:29:PRO:CG	2.41	0.51
2:B:123:ASN:ND2	2:B:124:THR:H	2.09	0.51
2:K:52:ARG:HA	2:K:74:ASP:HA	1.92	0.51
1:G:199:HIS:O	1:G:203:VAL:HG23	2.11	0.51
3:L:50:ARG:HA	3:L:85:LEU:HD13	1.93	0.51
2:K:121:VAL:O	2:K:122:TRP:HB3	2.10	0.51
2:K:120:TRP:HH2	2:K:149:GLN:NE2	2.09	0.51
1:A:98:TYR:O	1:A:101:VAL:HG23	2.11	0.51
3:C:100:ARG:HG2	3:C:128:TYR:HB2	1.93	0.51
3:F:144:ARG:HA	3:F:147:GLN:HE21	1.75	0.51
3:F:122:THR:N	3:F:123:PRO:HD3	2.26	0.51
1:J:143:ASN:HA	2:K:22:ASN:HB2	1.93	0.51
3:C:29:LEU:HD23	3:C:55:ASN:OD1	2.11	0.51
3:F:176:MET:SD	3:F:199:ILE:HD13	2.51	0.51
2:K:112:PRO:HG3	2:K:120:TRP:HZ3	1.76	0.51
3:C:247:ARG:HG3	3:C:247:ARG:NH1	2.24	0.51
3:C:183:PHE:CE1	3:C:207:LEU:HD11	2.45	0.51
3:L:165:ILE:HD12	3:L:193:LYS:HD2	1.92	0.51
2:K:53:ALA:HB2	2:K:142:PHE:CD1	2.46	0.50
2:E:121:VAL:O	2:E:122:TRP:HB3	2.10	0.50
2:H:53:ALA:HB2	2:H:142:PHE:CD1	2.45	0.50
1:J:54:THR:CB	1:J:174:LEU:HD11	2.41	0.50
1:J:205:GLN:O	2:K:114:ALA:HB2	2.11	0.50
2:K:167:LYS:N	2:K:167:LYS:HD2	2.27	0.50
1:A:13:LEU:C	1:A:13:LEU:CD1	2.78	0.50
3:L:247:ARG:HG3	3:L:247:ARG:NH1	2.26	0.50
3:C:84:ARG:NH1	3:C:88:GLN:HE22	2.08	0.50
3:F:173:ASN:ND2	3:F:173:ASN:N	2.48	0.50
2:H:153:THR:HG23	2:H:154:LYS:H	1.77	0.50
1:J:21:THR:O	1:J:123:LYS:HE3	2.11	0.50
1:G:21:THR:O	1:G:123:LYS:HE3	2.11	0.50
2:E:75:VAL:HA	2:E:90:MET:HG3	1.92	0.50
3:F:212:LEU:HD22	3:F:212:LEU:H	1.76	0.50
1:G:188:VAL:HG12	1:G:189:MET:N	2.27	0.50
1:J:193:LEU:HD12	1:J:193:LEU:N	2.25	0.50
1:D:70:GLU:HG2	3:F:72:THR:HA	1.91	0.50
3:C:30:GLU:HG3	3:C:31:ASP:H	1.75	0.50
2:E:123:ASN:HD22	2:E:124:THR:H	1.60	0.50
1:J:209:LEU:HB3	2:K:141:ARG:NH2	2.26	0.50
2:B:162:ILE:O	2:B:165:ARG:HB3	2.11	0.50
3:I:247:ARG:HG3	3:I:247:ARG:NH1	2.25	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:147:GLN:O	3:I:150:ALA:HB3	2.11	0.50
3:F:29:LEU:HD23	3:F:55:ASN:OD1	2.11	0.50
3:C:236:LEU:HD21	3:C:251:LEU:HD11	1.93	0.50
2:B:60:SER:OG	2:B:61:GLU:N	2.44	0.50
3:F:38:VAL:HG22	3:F:66:GLU:HB2	1.92	0.50
2:E:52:ARG:HA	2:E:74:ASP:HA	1.93	0.50
3:L:261:ALA:HB2	3:L:286:ILE:HG12	1.93	0.50
1:D:124:VAL:HG11	1:D:148:ASP:HB3	1.94	0.50
2:H:75:VAL:HA	2:H:90:MET:HG3	1.94	0.50
2:B:120:TRP:HH2	2:B:149:GLN:NE2	2.10	0.50
2:E:60:SER:OG	2:E:61:GLU:N	2.44	0.50
3:L:84:ARG:NH1	3:L:88:GLN:HE22	2.07	0.50
3:L:291:VAL:HG21	3:L:315:PHE:CD2	2.46	0.50
2:H:146:GLU:O	2:H:150:LYS:HG3	2.12	0.50
1:G:163:TRP:O	1:G:166:ARG:N	2.44	0.50
3:L:298:ILE:CG2	3:L:305:LEU:HD23	2.42	0.50
3:I:52:LEU:O	3:I:56:ILE:HG13	2.11	0.50
1:A:198:GLU:O	1:A:202:GLU:HG3	2.12	0.50
2:B:75:VAL:HG21	2:B:140:ILE:CD1	2.41	0.50
3:L:147:GLN:O	3:L:150:ALA:HB3	2.11	0.50
1:J:198:GLU:O	1:J:202:GLU:HG3	2.12	0.50
1:D:198:GLU:O	1:D:202:GLU:HG3	2.12	0.50
1:J:186:GLU:O	1:J:187:VAL:HB	2.11	0.50
1:G:163:TRP:CZ2	1:G:167:LYS:HE3	2.47	0.50
1:G:116:PRO:HB2	1:G:164:LEU:HD23	1.94	0.50
2:H:43:GLU:C	2:H:45:GLU:H	2.14	0.50
3:F:314:ARG:NH1	3:F:344:GLU:OE1	2.45	0.50
1:A:131:VAL:CG1	1:A:136:ILE:HD11	2.42	0.50
3:L:204:ILE:CG2	3:L:208:LEU:HD23	2.37	0.49
2:K:60:SER:OG	2:K:61:GLU:N	2.44	0.49
3:I:165:ILE:HD12	3:I:193:LYS:HD2	1.94	0.49
3:C:298:ILE:CG2	3:C:305:LEU:HD23	2.41	0.49
2:E:54:LYS:HG2	2:E:56:PHE:CE1	2.47	0.49
3:I:335:GLY:O	3:I:336:GLU:HB2	2.12	0.49
3:C:122:THR:N	3:C:123:PRO:HD3	2.27	0.49
3:I:259:ARG:HB3	3:I:259:ARG:CZ	2.39	0.49
3:C:259:ARG:CZ	3:C:259:ARG:HB3	2.41	0.49
2:H:57:ARG:NH2	2:H:60:SER:HB2	2.26	0.49
1:J:12:LYS:HE3	1:J:64:TRP:CE2	2.47	0.49
1:D:180:PRO:HB3	2:E:41:LEU:HD13	1.94	0.49
3:L:220:VAL:HG13	3:L:248:GLU:HB3	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:200:ARG:NH1	3:I:200:ARG:HB3	2.28	0.49
2:E:120:TRP:HH2	2:E:149:GLN:NE2	2.10	0.49
3:C:192:VAL:HG21	3:C:212:LEU:HD11	1.94	0.49
3:L:274:ILE:HG22	3:L:276:LEU:H	1.76	0.49
1:G:182:LEU:N	1:G:182:LEU:HD12	2.27	0.49
1:D:160:PRO:O	1:D:164:LEU:HD12	2.13	0.49
1:J:163:TRP:CZ2	1:J:167:LYS:HE3	2.47	0.49
1:G:145:GLN:NE2	1:G:146:TYR:H	2.11	0.49
3:I:173:ASN:ND2	3:I:200:ARG:H	1.97	0.49
3:L:5:SER:OG	3:L:38:VAL:HB	2.12	0.49
3:F:5:SER:OG	3:F:38:VAL:HB	2.13	0.49
3:F:84:ARG:NH1	3:F:88:GLN:HE22	2.09	0.49
1:G:211:ASP:HA	2:H:141:ARG:HH12	1.77	0.49
3:L:200:ARG:NH1	3:L:200:ARG:HB3	2.28	0.49
2:B:57:ARG:NH2	2:B:60:SER:HB2	2.27	0.49
2:B:49:PHE:CB	2:B:77:LEU:HD12	2.42	0.49
1:A:70:GLU:HG2	3:C:72:THR:HA	1.94	0.49
3:I:308:LEU:CD2	3:I:310:LEU:HD11	2.43	0.49
3:C:221:LEU:HD12	3:C:222:ASP:N	2.28	0.49
1:A:93:THR:HG21	1:A:126:ILE:HG21	1.95	0.49
2:H:75:VAL:HG21	2:H:140:ILE:CD1	2.42	0.49
2:K:57:ARG:HD3	2:K:136:GLU:CD	2.32	0.49
1:D:193:LEU:N	1:D:193:LEU:HD12	2.27	0.49
3:I:18:THR:HG23	3:I:21:GLU:HB2	1.94	0.49
1:D:169:ILE:HD12	2:E:33:LEU:HD12	1.94	0.49
1:J:170:GLY:CA	2:K:29:PRO:HG3	2.43	0.49
3:I:326:ARG:HH11	3:I:326:ARG:HG3	1.78	0.49
1:G:40:VAL:O	1:G:40:VAL:HG12	2.12	0.49
2:B:54:LYS:HG2	2:B:56:PHE:CE1	2.48	0.49
3:L:13:LEU:HD13	3:L:25:PHE:HZ	1.77	0.49
2:B:57:ARG:HD3	2:B:136:GLU:CD	2.33	0.49
3:I:298:ILE:CG2	3:I:305:LEU:HD23	2.42	0.49
3:L:256:LEU:O	3:L:257:SER:CB	2.61	0.49
3:L:202:GLU:CD	3:L:202:GLU:H	2.16	0.49
1:D:158:GLU:HG2	2:E:94:LYS:CB	2.34	0.49
1:G:13:LEU:C	1:G:13:LEU:CD1	2.80	0.49
1:G:122:ASN:CG	1:G:123:LYS:N	2.66	0.49
3:C:335:GLY:O	3:C:336:GLU:HB2	2.13	0.49
3:I:292:ARG:HG2	3:I:321:VAL:HG11	1.95	0.49
1:G:198:GLU:O	1:G:202:GLU:HG3	2.12	0.49
3:C:261:ALA:HB2	3:C:286:ILE:HG12	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:204:ILE:CG2	3:I:208:LEU:HD23	2.38	0.48
2:E:84:GLY:H	2:E:165:ARG:NH2	2.10	0.48
2:H:60:SER:OG	2:H:61:GLU:N	2.45	0.48
2:E:57:ARG:NH2	2:E:60:SER:HB2	2.28	0.48
3:F:52:LEU:O	3:F:56:ILE:HG13	2.13	0.48
1:A:53:HIS:O	1:A:176:PHE:HA	2.13	0.48
2:K:115:GLY:O	2:K:116:SER:HB3	2.13	0.48
3:L:335:GLY:O	3:L:336:GLU:HB2	2.12	0.48
2:E:123:ASN:ND2	2:E:124:THR:H	2.11	0.48
3:L:295:LYS:HE2	3:L:296:THR:HG22	1.95	0.48
1:G:93:THR:HG21	1:G:126:ILE:HG21	1.94	0.48
2:K:57:ARG:NH2	2:K:60:SER:HB2	2.27	0.48
2:K:123:ASN:ND2	2:K:124:THR:H	2.11	0.48
1:G:153:SER:O	1:G:154:ASN:HB2	2.14	0.48
1:D:153:SER:O	1:D:154:ASN:HB2	2.13	0.48
1:J:15:LEU:HG	1:J:23:LYS:HG2	1.96	0.48
2:H:153:THR:CG2	2:H:154:LYS:N	2.76	0.48
2:K:75:VAL:HA	2:K:90:MET:HG3	1.95	0.48
1:J:182:LEU:H	1:J:182:LEU:HD12	1.78	0.48
3:F:292:ARG:HG2	3:F:321:VAL:HG11	1.95	0.48
1:D:182:LEU:HD12	1:D:182:LEU:N	2.28	0.48
1:D:13:LEU:CD1	1:D:13:LEU:C	2.77	0.48
2:B:104:ILE:HB	2:B:162:ILE:CD1	2.44	0.48
1:J:188:VAL:HG12	1:J:189:MET:N	2.29	0.48
3:L:100:ARG:HG2	3:L:128:TYR:HB2	1.95	0.48
3:I:13:LEU:HD13	3:I:25:PHE:HZ	1.78	0.48
2:K:123:ASN:HD22	2:K:124:THR:H	1.61	0.48
1:A:70:GLU:CB	3:C:72:THR:HG22	2.44	0.48
3:I:18:THR:CG2	3:I:21:GLU:HB2	2.43	0.48
1:G:168:LEU:CD2	2:H:30:ILE:HD12	2.39	0.48
2:B:75:VAL:HA	2:B:90:MET:HG3	1.96	0.48
3:I:83:LEU:HD21	3:I:114:LEU:HD13	1.95	0.48
3:I:261:ALA:CB	3:I:286:ILE:HG12	2.44	0.48
1:G:45:VAL:HG23	1:G:65:ASP:O	2.13	0.48
3:L:18:THR:HG23	3:L:21:GLU:HB2	1.96	0.48
1:J:93:THR:HG21	1:J:126:ILE:HG21	1.96	0.48
2:K:43:GLU:C	2:K:45:GLU:H	2.15	0.48
3:C:15:ALA:O	3:C:16:ILE:HB	2.13	0.48
3:L:111:GLN:NE2	3:L:138:ALA:HB2	2.29	0.48
3:L:334:ARG:HG2	3:L:334:ARG:HH11	1.78	0.48
2:H:109:GLU:CD	2:H:109:GLU:N	2.67	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:LYS:HA	5:A:1250:GDP:O2'	2.13	0.48
2:K:61:GLU:O	2:K:61:GLU:HG3	2.14	0.48
3:F:340:LEU:HD23	3:F:340:LEU:N	2.28	0.48
3:F:335:GLY:O	3:F:336:GLU:HB2	2.13	0.48
2:H:108:MET:O	2:H:159:ARG:HD2	2.14	0.48
3:I:329:PHE:HB3	3:I:335:GLY:HA3	1.96	0.48
1:J:53:HIS:CD2	1:J:58:PRO:HB3	2.49	0.48
3:F:274:ILE:HG22	3:F:276:LEU:H	1.77	0.48
1:J:128:ASP:OD1	3:L:200:ARG:NH2	2.47	0.47
1:G:160:PRO:O	1:G:164:LEU:HD12	2.14	0.47
2:E:153:THR:CG2	2:E:154:LYS:N	2.76	0.47
3:C:212:LEU:HD22	3:C:212:LEU:H	1.79	0.47
3:F:192:VAL:HG21	3:F:212:LEU:HD11	1.95	0.47
1:A:9:VAL:HG21	2:B:33:LEU:HD11	1.95	0.47
2:B:62:ASN:C	2:B:64:LEU:N	2.67	0.47
3:C:130:HIS:CE1	3:C:168:ARG:HD3	2.48	0.47
3:C:334:ARG:HG2	3:C:334:ARG:HH11	1.79	0.47
2:B:146:GLU:O	2:B:150:LYS:HG3	2.14	0.47
2:K:153:THR:CG2	2:K:154:LYS:N	2.77	0.47
1:D:188:VAL:HG12	1:D:189:MET:N	2.29	0.47
2:K:62:ASN:C	2:K:64:LEU:N	2.67	0.47
3:I:84:ARG:NH1	3:I:88:GLN:HE22	2.12	0.47
1:D:70:GLU:CB	3:F:72:THR:HG22	2.44	0.47
2:H:41:LEU:N	2:H:41:LEU:HD12	2.29	0.47
3:L:122:THR:N	3:L:123:PRO:HD3	2.30	0.47
3:I:122:THR:N	3:I:123:PRO:HD3	2.29	0.47
1:D:143:ASN:ND2	2:E:25:PRO:HB3	2.29	0.47
2:E:57:ARG:HD3	2:E:136:GLU:CD	2.34	0.47
1:A:209:LEU:HD23	2:B:113:ASN:HD21	1.79	0.47
2:B:167:LYS:N	2:B:167:LYS:HD2	2.29	0.47
1:A:29:ARG:NH2	1:A:35:PHE:HB2	2.29	0.47
3:F:326:ARG:HG3	3:F:326:ARG:HH11	1.78	0.47
1:D:13:LEU:HD21	1:D:87:ILE:HD11	1.96	0.47
3:C:111:GLN:NE2	3:C:138:ALA:HB2	2.30	0.47
1:G:53:HIS:CD2	1:G:58:PRO:HB3	2.50	0.47
3:I:98:THR:OG1	3:I:126:HIS:HB2	2.14	0.47
2:H:52:ARG:HA	2:H:74:ASP:HA	1.96	0.47
3:I:259:ARG:O	3:I:262:ALA:HB3	2.13	0.47
3:C:204:ILE:CG2	3:C:208:LEU:HD23	2.39	0.47
3:C:308:LEU:CD2	3:C:310:LEU:HD11	2.42	0.47
3:C:195:VAL:HG12	3:C:196:GLN:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:295:LYS:CE	3:I:296:THR:HG22	2.45	0.47
1:G:29:ARG:NH1	1:G:151:ALA:O	2.46	0.47
2:H:115:GLY:O	2:H:116:SER:HB3	2.15	0.47
1:J:164:LEU:O	1:J:168:LEU:HG	2.14	0.47
1:D:28:LYS:HA	1:D:31:LEU:HD11	1.97	0.47
1:A:54:THR:CB	1:A:174:LEU:HD11	2.45	0.47
1:D:209:LEU:HD23	2:E:113:ASN:OD1	2.15	0.47
3:I:314:ARG:NH1	3:I:344:GLU:OE1	2.47	0.47
2:H:120:TRP:CZ2	2:H:148:ALA:HB1	2.49	0.47
2:H:120:TRP:HH2	2:H:149:GLN:NE2	2.13	0.47
1:D:116:PRO:HB2	1:D:164:LEU:HD23	1.97	0.47
1:G:122:ASN:CG	1:G:123:LYS:H	2.18	0.47
1:G:123:LYS:HG2	5:G:3250:GDP:C6	2.50	0.47
2:B:112:PRO:HG3	2:B:120:TRP:HZ3	1.80	0.47
2:B:153:THR:CG2	2:B:154:LYS:N	2.77	0.47
2:H:59:ALA:HB2	2:H:66:GLU:N	2.28	0.47
3:C:83:LEU:HD21	3:C:114:LEU:HD13	1.97	0.47
1:A:75:LEU:HD13	3:C:72:THR:OG1	2.15	0.47
1:G:96:VAL:CG2	3:I:224:GLN:HE21	2.27	0.47
3:C:20:ASP:O	3:C:22:LYS:N	2.44	0.47
3:F:18:THR:HG23	3:F:21:GLU:HB2	1.96	0.47
1:A:153:SER:O	1:A:154:ASN:HB2	2.15	0.47
3:I:306:LEU:HB2	3:I:307:PHE:CD1	2.50	0.47
1:J:96:VAL:HG23	3:L:225:ASP:OD2	2.14	0.47
3:F:15:ALA:O	3:F:16:ILE:HB	2.14	0.47
3:F:261:ALA:HB2	3:F:286:ILE:HG12	1.96	0.47
3:I:236:LEU:HD21	3:I:251:LEU:HD11	1.95	0.47
3:I:15:ALA:O	3:I:16:ILE:HB	2.14	0.47
3:C:259:ARG:CB	3:C:259:ARG:HH11	2.12	0.47
1:D:159:LYS:HB2	1:D:160:PRO:HD3	1.97	0.47
1:D:122:ASN:CG	1:D:123:LYS:N	2.68	0.47
1:A:188:VAL:HG12	1:A:189:MET:N	2.30	0.47
3:F:294:LEU:O	3:F:298:ILE:HG13	2.14	0.47
3:I:200:ARG:NH1	3:I:201:PRO:HD2	2.30	0.47
1:A:21:THR:O	1:A:123:LYS:HE3	2.15	0.47
3:C:143:ALA:O	3:C:147:GLN:HG3	2.15	0.47
1:D:115:ILE:O	1:D:115:ILE:HG13	2.14	0.47
3:C:306:LEU:HB2	3:C:307:PHE:CD1	2.50	0.47
3:I:130:HIS:CE1	3:I:168:ARG:HD3	2.50	0.47
3:L:29:LEU:HD23	3:L:55:ASN:OD1	2.15	0.47
3:F:228:PHE:CD1	3:F:254:CYS:HB3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:334:ARG:HH11	3:I:334:ARG:HG2	1.80	0.47
2:H:57:ARG:HD3	2:H:136:GLU:CD	2.34	0.47
2:B:61:GLU:HG3	2:B:61:GLU:O	2.15	0.47
2:K:49:PHE:CB	2:K:77:LEU:HD12	2.45	0.47
2:K:54:LYS:HG2	2:K:56:PHE:CE1	2.49	0.47
1:A:181:ALA:HA	2:B:98:ILE:HD11	1.96	0.47
1:G:131:VAL:CG1	1:G:136:ILE:HD11	2.45	0.47
1:J:192:ALA:C	1:J:194:ALA:H	2.19	0.46
3:F:13:LEU:HD13	3:F:25:PHE:HZ	1.80	0.46
1:J:53:HIS:O	1:J:176:PHE:HA	2.15	0.46
3:L:279:LEU:HD21	3:L:281:LEU:HD11	1.96	0.46
3:L:221:LEU:HD11	3:L:223:LEU:HG	1.97	0.46
1:D:123:LYS:HG2	5:D:2250:GDP:C6	2.50	0.46
1:G:190:ASP:O	1:G:191:PRO:O	2.34	0.46
3:F:247:ARG:NH1	3:F:247:ARG:HG3	2.25	0.46
2:E:43:GLU:C	2:E:45:GLU:H	2.17	0.46
3:L:308:LEU:CD2	3:L:310:LEU:HD11	2.45	0.46
1:A:40:VAL:O	1:A:40:VAL:HG12	2.14	0.46
2:K:146:GLU:O	2:K:150:LYS:HG3	2.15	0.46
1:D:98:TYR:O	1:D:101:VAL:HG23	2.15	0.46
3:I:144:ARG:HG2	3:I:178:GLU:HG2	1.98	0.46
3:C:18:THR:HG23	3:C:21:GLU:HB2	1.95	0.46
3:I:50:ARG:HA	3:I:85:LEU:HD13	1.96	0.46
3:F:334:ARG:HG2	3:F:334:ARG:HH11	1.80	0.46
1:D:163:TRP:O	1:D:164:LEU:C	2.54	0.46
2:B:59:ALA:HB2	2:B:66:GLU:N	2.28	0.46
3:I:5:SER:OG	3:I:38:VAL:HB	2.15	0.46
3:L:18:THR:CG2	3:L:21:GLU:HB2	2.44	0.46
3:C:18:THR:CG2	3:C:21:GLU:HB2	2.45	0.46
3:L:15:ALA:O	3:L:16:ILE:HB	2.15	0.46
3:C:314:ARG:NH1	3:C:344:GLU:OE1	2.47	0.46
3:I:299:ASP:OD1	3:I:328:VAL:HG13	2.16	0.46
3:F:87:LEU:HD12	3:F:113:PRO:CB	2.46	0.46
1:D:43:LEU:HD23	3:F:79:ILE:HB	1.95	0.46
2:B:87:ARG:HB2	2:B:102:HIS:O	2.14	0.46
1:G:182:LEU:H	1:G:182:LEU:HD12	1.81	0.46
3:C:306:LEU:HB2	3:C:307:PHE:HD1	1.81	0.46
2:K:41:LEU:N	2:K:41:LEU:HD12	2.31	0.46
3:F:50:ARG:HA	3:F:85:LEU:HD13	1.97	0.46
1:G:143:ASN:ND2	2:H:25:PRO:HB3	2.30	0.46
3:I:87:LEU:HD12	3:I:113:PRO:CB	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:143:ALA:O	3:L:147:GLN:HG3	2.16	0.46
3:L:329:PHE:HB3	3:L:335:GLY:HA3	1.98	0.46
2:E:41:LEU:N	2:E:41:LEU:HD12	2.30	0.46
1:J:131:VAL:CG1	1:J:136:ILE:HD11	2.45	0.46
2:H:144:ASN:O	2:H:147:ASN:HB2	2.16	0.46
1:D:93:THR:HG21	1:D:126:ILE:HG21	1.98	0.46
3:F:199:ILE:HG21	3:F:204:ILE:HD12	1.98	0.46
2:H:62:ASN:C	2:H:64:LEU:N	2.68	0.46
3:L:306:LEU:HB2	3:L:307:PHE:CD1	2.50	0.46
2:B:38:ILE:H	2:B:38:ILE:CD1	2.28	0.46
3:F:100:ARG:HG2	3:F:128:TYR:HB2	1.98	0.46
3:L:39:LEU:HD12	3:L:67:PHE:CD2	2.51	0.46
3:C:295:LYS:CE	3:C:296:THR:HG22	2.45	0.46
3:L:183:PHE:CE1	3:L:207:LEU:HD11	2.48	0.46
3:I:224:GLN:HG3	3:I:252:ASN:O	2.16	0.46
3:F:143:ALA:O	3:F:147:GLN:HG3	2.15	0.46
3:C:321:VAL:CG2	3:C:322:VAL:N	2.79	0.46
1:J:29:ARG:NH2	1:J:35:PHE:HB2	2.31	0.46
3:F:200:ARG:NH1	3:F:200:ARG:HB3	2.31	0.46
2:K:70:ARG:HA	2:K:70:ARG:HD2	1.72	0.46
2:E:61:GLU:O	2:E:61:GLU:HG3	2.15	0.46
1:A:192:ALA:C	1:A:194:ALA:H	2.19	0.46
3:F:295:LYS:CE	3:F:296:THR:HG22	2.46	0.46
2:K:87:ARG:HB2	2:K:102:HIS:O	2.14	0.46
3:I:306:LEU:HB2	3:I:307:PHE:HD1	1.81	0.46
1:G:134:LYS:O	1:G:136:ILE:N	2.49	0.46
1:J:181:ALA:HA	2:K:98:ILE:HD11	1.98	0.46
3:L:200:ARG:NH1	3:L:201:PRO:HD2	2.31	0.45
3:C:200:ARG:NH1	3:C:200:ARG:HB3	2.31	0.45
1:J:122:ASN:CG	1:J:123:LYS:N	2.69	0.45
2:K:75:VAL:HG13	2:K:88:LEU:HD21	1.96	0.45
3:F:183:PHE:CE1	3:F:207:LEU:HD11	2.47	0.45
2:E:120:TRP:O	2:E:139:ALA:HA	2.16	0.45
2:K:149:GLN:O	2:K:153:THR:HG22	2.17	0.45
1:D:190:ASP:O	1:D:191:PRO:O	2.34	0.45
3:F:144:ARG:HG2	3:F:178:GLU:HG2	1.98	0.45
3:F:18:THR:CG2	3:F:21:GLU:HB2	2.46	0.45
3:L:292:ARG:HG2	3:L:321:VAL:HG11	1.98	0.45
3:I:220:VAL:HG13	3:I:248:GLU:HB3	1.98	0.45
1:G:51:VAL:HG23	2:H:97:LYS:NZ	2.31	0.45
2:E:134:LYS:HA	2:E:135:PRO:HD3	1.83	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:L:314:ARG:NH1	3:L:344:GLU:OE1	2.49	0.45
2:E:109:GLU:CD	2:E:109:GLU:N	2.69	0.45
2:H:149:GLN:O	2:H:153:THR:HG22	2.16	0.45
1:J:177:VAL:O	1:J:178:ALA:C	2.54	0.45
1:D:163:TRP:O	1:D:165:ALA:N	2.49	0.45
1:J:159:LYS:HB2	1:J:160:PRO:HD3	1.97	0.45
2:K:153:THR:HG23	2:K:154:LYS:H	1.79	0.45
3:I:212:LEU:HD22	3:I:212:LEU:H	1.82	0.45
3:C:329:PHE:CB	3:C:335:GLY:HA3	2.47	0.45
3:F:242:SER:O	3:F:244:PRO:HD3	2.16	0.45
1:G:124:VAL:HG22	1:G:149:ILE:O	2.16	0.45
1:J:209:LEU:HD23	2:K:113:ASN:HD21	1.76	0.45
2:E:156:GLU:C	2:E:158:CYS:N	2.69	0.45
2:K:120:TRP:CZ2	2:K:148:ALA:HB1	2.51	0.45
3:L:87:LEU:HD12	3:L:113:PRO:CB	2.46	0.45
3:C:13:LEU:HD13	3:C:25:PHE:HZ	1.81	0.45
3:I:183:PHE:CE1	3:I:207:LEU:HD11	2.49	0.45
2:E:62:ASN:C	2:E:64:LEU:N	2.67	0.45
3:L:306:LEU:HB2	3:L:307:PHE:HD1	1.81	0.45
1:D:178:ALA:O	1:D:179:MET:HB2	2.16	0.45
1:A:126:ILE:HD12	1:A:126:ILE:N	2.32	0.45
2:E:153:THR:HG23	2:E:154:LYS:H	1.79	0.45
2:H:61:GLU:HG3	2:H:61:GLU:O	2.16	0.45
2:E:59:ALA:HB2	2:E:66:GLU:N	2.29	0.45
1:G:178:ALA:O	1:G:179:MET:HB2	2.17	0.45
1:J:190:ASP:O	1:J:191:PRO:O	2.34	0.45
3:I:143:ALA:O	3:I:147:GLN:HG3	2.16	0.45
3:L:46:THR:HG22	3:L:82:ALA:N	2.32	0.45
1:D:143:ASN:HA	2:E:22:ASN:HB2	1.99	0.45
2:B:109:GLU:CD	2:B:109:GLU:N	2.69	0.45
3:I:339:GLU:OE1	3:I:339:GLU:HA	2.17	0.45
1:A:96:VAL:HG23	3:C:225:ASP:OD2	2.17	0.45
2:K:59:ALA:HB2	2:K:66:GLU:N	2.27	0.45
1:A:194:ALA:O	1:A:195:ALA:CB	2.64	0.45
1:A:51:VAL:HG23	2:B:97:LYS:NZ	2.31	0.45
1:A:69:GLN:HG3	3:C:131:ASN:ND2	2.31	0.45
1:J:155:TYR:CD2	1:J:155:TYR:C	2.90	0.45
1:D:155:TYR:CD2	1:D:155:TYR:C	2.89	0.45
1:A:110:ARG:HG2	1:A:110:ARG:O	2.16	0.45
1:G:54:THR:CB	1:G:174:LEU:HD11	2.46	0.45
1:D:37:LYS:HA	5:D:2250:GDP:O2'	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:98:TYR:O	1:J:101:VAL:HG23	2.16	0.45
1:J:29:ARG:HD3	1:J:154:ASN:OD1	2.16	0.45
3:F:236:LEU:HD21	3:F:251:LEU:HD11	1.99	0.45
1:D:69:GLN:HG3	3:F:131:ASN:ND2	2.32	0.45
2:H:112:PRO:HG3	2:H:120:TRP:HZ3	1.79	0.45
2:K:75:VAL:CG1	2:K:88:LEU:HD21	2.46	0.45
2:H:38:ILE:H	2:H:38:ILE:CD1	2.29	0.45
2:E:49:PHE:CB	2:E:77:LEU:HD12	2.43	0.45
1:J:115:ILE:HG13	1:J:115:ILE:O	2.16	0.45
3:L:221:LEU:HD12	3:L:222:ASP:N	2.31	0.45
1:J:153:SER:O	1:J:154:ASN:HB2	2.16	0.45
3:L:277:GLN:C	3:L:278:THR:HG22	2.38	0.45
1:G:171:ASP:O	1:G:173:ASN:N	2.50	0.45
3:F:130:HIS:CE1	3:F:168:ARG:HD3	2.52	0.45
1:D:54:THR:CB	1:D:174:LEU:HD11	2.46	0.45
1:G:37:LYS:HA	5:G:3250:GDP:O2'	2.17	0.45
2:K:47:GLU:HA	2:K:78:LEU:HD23	1.98	0.45
3:F:310:LEU:HD12	3:F:337:LEU:HD11	1.99	0.45
2:E:160:LYS:C	2:E:162:ILE:N	2.68	0.45
2:B:120:TRP:CZ2	2:B:148:ALA:HB1	2.51	0.45
1:A:190:ASP:O	1:A:191:PRO:O	2.34	0.45
3:I:20:ASP:O	3:I:22:LYS:N	2.45	0.45
3:L:321:VAL:CG2	3:L:322:VAL:N	2.79	0.45
1:D:182:LEU:H	1:D:182:LEU:HD12	1.82	0.45
2:B:115:GLY:O	2:B:116:SER:HB3	2.17	0.45
1:J:13:LEU:CD1	1:J:13:LEU:C	2.79	0.44
2:K:88:LEU:HD23	2:K:89:LEU:N	2.32	0.44
2:E:47:GLU:HA	2:E:78:LEU:HD23	1.98	0.44
2:E:84:GLY:N	2:E:165:ARG:NH2	2.66	0.44
3:C:144:ARG:HG2	3:C:178:GLU:HG2	1.99	0.44
3:I:46:THR:HG22	3:I:82:ALA:N	2.32	0.44
1:A:170:GLY:HA3	2:B:29:PRO:CG	2.46	0.44
2:B:160:LYS:HE3	2:B:164:GLU:OE2	2.18	0.44
1:D:131:VAL:CG1	1:D:136:ILE:HD11	2.47	0.44
3:L:68:SER:HA	3:L:102:SER:O	2.17	0.44
1:G:155:TYR:C	1:G:155:TYR:CD2	2.90	0.44
2:H:79:LYS:HB2	2:H:86:ILE:HG12	1.99	0.44
1:D:164:LEU:O	1:D:168:LEU:HG	2.18	0.44
1:D:122:ASN:CG	1:D:123:LYS:H	2.20	0.44
2:E:120:TRP:CZ2	2:E:148:ALA:HB1	2.53	0.44
3:I:100:ARG:HG2	3:I:128:TYR:HB2	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:43:THR:HG21	3:C:72:THR:O	2.17	0.44
3:L:195:VAL:HG12	3:L:196:GLN:HB2	1.98	0.44
3:F:178:GLU:O	3:F:181:LYS:HB2	2.17	0.44
1:A:170:GLY:CA	2:B:29:PRO:HG3	2.47	0.44
1:D:162:LEU:HB2	1:D:176:PHE:CE2	2.52	0.44
3:F:220:VAL:HG13	3:F:248:GLU:HB3	1.99	0.44
1:J:110:ARG:HG2	1:J:110:ARG:O	2.18	0.44
2:K:109:GLU:CD	2:K:109:GLU:N	2.70	0.44
3:L:234:SER:O	3:L:238:ILE:HG13	2.17	0.44
2:H:47:GLU:HA	2:H:78:LEU:HD23	2.00	0.44
1:D:177:VAL:O	1:D:178:ALA:C	2.56	0.44
2:E:75:VAL:CG1	2:E:88:LEU:HD21	2.47	0.44
2:H:75:VAL:HG13	2:H:88:LEU:HD21	1.98	0.44
3:I:192:VAL:HG21	3:I:212:LEU:HD11	1.99	0.44
3:C:310:LEU:HD12	3:C:337:LEU:HD11	2.00	0.44
1:J:43:LEU:HD23	3:L:79:ILE:HD12	1.99	0.44
1:A:162:LEU:HB2	1:A:176:PHE:CE2	2.53	0.44
1:D:29:ARG:NH2	1:D:35:PHE:HB2	2.32	0.44
2:E:93:ASP:O	2:E:95:THR:N	2.50	0.44
1:J:143:ASN:ND2	2:K:25:PRO:HB3	2.33	0.44
3:L:236:LEU:HD21	3:L:251:LEU:HD11	1.99	0.44
1:A:145:GLN:HB2	1:A:163:TRP:CZ2	2.53	0.44
2:E:150:LYS:C	2:E:153:THR:HG22	2.37	0.44
2:E:75:VAL:HG13	2:E:88:LEU:HD21	1.99	0.44
1:D:194:ALA:O	1:D:195:ALA:CB	2.66	0.44
3:L:43:THR:HG21	3:L:72:THR:O	2.15	0.44
1:A:29:ARG:HD3	1:A:154:ASN:OD1	2.17	0.44
1:D:53:HIS:CD2	1:D:58:PRO:HB3	2.53	0.44
1:D:53:HIS:O	1:D:176:PHE:HA	2.18	0.44
1:A:159:LYS:HB2	1:A:160:PRO:HD3	1.99	0.44
2:E:160:LYS:C	2:E:162:ILE:H	2.21	0.44
2:K:58:PHE:O	2:K:60:SER:N	2.51	0.44
1:G:192:ALA:C	1:G:194:ALA:H	2.20	0.44
3:C:38:VAL:HG22	3:C:66:GLU:CB	2.48	0.44
1:J:43:LEU:HD23	3:L:79:ILE:HB	2.00	0.44
2:B:55:LEU:HD12	2:B:56:PHE:H	1.81	0.44
3:I:321:VAL:CG2	3:I:322:VAL:N	2.81	0.44
1:D:204:ALA:C	1:D:206:THR:H	2.21	0.44
3:C:256:LEU:O	3:C:257:SER:CB	2.65	0.44
2:H:54:LYS:HG2	2:H:56:PHE:CE1	2.53	0.44
1:A:23:LYS:HB2	5:A:1250:GDP:O1B	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:160:PRO:O	1:A:164:LEU:HD12	2.17	0.44
1:J:163:TRP:O	1:J:165:ALA:N	2.51	0.44
1:A:177:VAL:O	1:A:178:ALA:C	2.55	0.44
2:B:104:ILE:O	2:B:162:ILE:HD13	2.17	0.44
3:C:66:GLU:OE1	3:C:100:ARG:HB2	2.17	0.44
3:L:16:ILE:O	3:L:16:ILE:HG22	2.17	0.44
3:L:161:LEU:HB3	3:L:186:HIS:CD2	2.53	0.44
3:L:299:ASP:OD1	3:L:328:VAL:HG13	2.18	0.44
1:J:194:ALA:O	1:J:195:ALA:CB	2.63	0.44
2:K:110:LEU:CD1	2:K:152:LYS:HA	2.47	0.44
3:I:195:VAL:HG12	3:I:196:GLN:HB2	1.98	0.44
3:F:224:GLN:HG3	3:F:252:ASN:O	2.18	0.44
2:B:41:LEU:HD12	2:B:41:LEU:N	2.33	0.44
1:J:162:LEU:HB2	1:J:176:PHE:CE2	2.53	0.44
3:C:50:ARG:HA	3:C:85:LEU:HD13	1.99	0.44
3:L:130:HIS:CE1	3:L:168:ARG:HD3	2.53	0.44
3:L:167:GLY:O	3:L:168:ARG:HB2	2.18	0.44
1:J:122:ASN:CG	1:J:123:LYS:H	2.21	0.44
2:B:88:LEU:HD23	2:B:89:LEU:N	2.33	0.44
2:B:153:THR:CG2	2:B:154:LYS:H	2.31	0.44
1:A:182:LEU:H	1:A:182:LEU:CD1	2.31	0.44
3:C:238:ILE:O	3:C:241:LYS:HG2	2.18	0.44
1:D:21:THR:O	1:D:123:LYS:HE3	2.17	0.43
3:C:173:ASN:ND2	3:C:200:ARG:H	2.00	0.43
2:H:75:VAL:CG1	2:H:88:LEU:HD21	2.47	0.43
3:I:206:HIS:O	3:I:207:LEU:C	2.56	0.43
2:H:49:PHE:CB	2:H:77:LEU:HD12	2.43	0.43
1:G:70:GLU:HG2	3:I:72:THR:HA	2.00	0.43
2:B:123:ASN:ND2	2:B:124:THR:N	2.66	0.43
2:H:87:ARG:HB2	2:H:102:HIS:O	2.18	0.43
3:F:306:LEU:CD2	3:F:334:ARG:HD2	2.48	0.43
2:B:166:GLU:O	2:B:166:GLU:CG	2.65	0.43
2:H:120:TRP:O	2:H:139:ALA:HA	2.19	0.43
2:H:57:ARG:CG	2:H:70:ARG:HD3	2.46	0.43
1:D:209:LEU:HD22	2:E:67:TRP:NE1	2.33	0.43
1:D:192:ALA:C	1:D:194:ALA:H	2.20	0.43
1:J:70:GLU:HG2	3:L:72:THR:HG22	2.00	0.43
3:C:111:GLN:HE21	3:C:138:ALA:HB2	1.83	0.43
3:C:292:ARG:HG2	3:C:321:VAL:HG11	2.00	0.43
1:J:69:GLN:HG3	3:L:131:ASN:ND2	2.34	0.43
1:A:163:TRP:CZ2	1:A:167:LYS:HE3	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:177:VAL:O	1:G:178:ALA:C	2.56	0.43
2:H:40:THR:HG21	2:H:42:GLU:OE2	2.18	0.43
3:C:308:LEU:HD12	3:C:308:LEU:HA	1.79	0.43
1:G:29:ARG:HD3	1:G:154:ASN:OD1	2.18	0.43
1:A:12:LYS:HE3	1:A:64:TRP:CE2	2.52	0.43
1:J:75:LEU:HD23	1:J:75:LEU:HA	1.84	0.43
2:E:149:GLN:O	2:E:153:THR:HG22	2.18	0.43
2:H:70:ARG:HD2	2:H:70:ARG:HA	1.74	0.43
3:L:52:LEU:O	3:L:56:ILE:HG13	2.18	0.43
1:A:43:LEU:HD23	3:C:79:ILE:HB	2.00	0.43
3:F:306:LEU:HB2	3:F:307:PHE:CD1	2.54	0.43
3:F:238:ILE:O	3:F:241:LYS:HG2	2.19	0.43
2:E:166:GLU:HG2	2:E:166:GLU:O	2.19	0.43
1:G:110:ARG:O	1:G:110:ARG:HG2	2.18	0.43
1:A:163:TRP:O	1:A:164:LEU:C	2.57	0.43
3:C:206:HIS:O	3:C:207:LEU:C	2.57	0.43
2:B:40:THR:HG21	2:B:42:GLU:OE2	2.18	0.43
3:F:308:LEU:CD2	3:F:310:LEU:HD11	2.48	0.43
3:F:321:VAL:CG2	3:F:322:VAL:N	2.81	0.43
3:L:111:GLN:HE21	3:L:138:ALA:HB2	1.82	0.43
1:G:170:GLY:HA3	2:H:29:PRO:HG3	2.01	0.43
3:C:151:VAL:HG12	3:C:152:ASN:N	2.34	0.43
3:C:326:ARG:HH11	3:C:326:ARG:HG3	1.83	0.43
2:K:95:THR:O	2:K:96:LEU:HB2	2.18	0.43
1:A:164:LEU:O	1:A:168:LEU:HG	2.19	0.43
3:L:197:ASN:O	3:L:199:ILE:N	2.52	0.43
2:K:144:ASN:O	2:K:147:ASN:HB2	2.18	0.43
1:G:188:VAL:HG12	1:G:189:MET:H	1.83	0.43
3:F:66:GLU:OE1	3:F:100:ARG:HB2	2.19	0.43
2:E:87:ARG:HB2	2:E:102:HIS:O	2.18	0.43
2:B:58:PHE:O	2:B:60:SER:N	2.52	0.43
2:E:70:ARG:HA	2:E:70:ARG:HD2	1.73	0.43
3:I:178:GLU:O	3:I:181:LYS:HB2	2.18	0.43
1:G:209:LEU:HD22	2:H:67:TRP:NE1	2.34	0.43
3:F:111:GLN:NE2	3:F:138:ALA:HB2	2.33	0.43
1:D:204:ALA:C	1:D:206:THR:N	2.71	0.43
1:D:29:ARG:HD3	1:D:154:ASN:OD1	2.19	0.43
1:A:29:ARG:NH1	1:A:151:ALA:O	2.52	0.43
3:C:228:PHE:CD1	3:C:254:CYS:HB3	2.54	0.43
1:G:23:LYS:HB2	5:G:3250:GDP:O1B	2.17	0.43
2:E:88:LEU:HD23	2:E:89:LEU:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:K:159:ARG:C	2:K:159:ARG:HD3	2.38	0.43
2:H:153:THR:CG2	2:H:154:LYS:H	2.32	0.43
2:B:149:GLN:O	2:B:153:THR:HG22	2.19	0.43
2:K:150:LYS:C	2:K:153:THR:HG22	2.39	0.43
3:C:252:ASN:HD21	3:C:280:ARG:HB3	1.82	0.43
1:G:70:GLU:HB3	3:I:72:THR:HG22	2.00	0.43
2:H:123:ASN:ND2	2:H:124:THR:N	2.67	0.43
3:I:326:ARG:NH1	3:I:326:ARG:HG3	2.34	0.43
2:K:156:GLU:OE2	2:K:159:ARG:HD2	2.18	0.43
3:L:326:ARG:HG3	3:L:326:ARG:HH11	1.83	0.43
3:L:148:GLU:O	3:L:151:VAL:N	2.52	0.43
3:I:68:SER:HA	3:I:102:SER:O	2.18	0.43
3:L:228:PHE:CD1	3:L:254:CYS:HB3	2.53	0.43
1:D:190:ASP:N	1:D:191:PRO:CD	2.82	0.43
3:C:83:LEU:HG	3:C:87:LEU:HD12	2.01	0.43
3:L:308:LEU:HD12	3:L:308:LEU:HA	1.78	0.43
1:A:134:LYS:O	1:A:136:ILE:N	2.52	0.43
1:G:162:LEU:HB2	1:G:176:PHE:CE2	2.53	0.43
3:C:279:LEU:HD21	3:C:281:LEU:HD11	2.00	0.43
2:K:134:LYS:HA	2:K:135:PRO:HD3	1.85	0.43
1:D:159:LYS:N	1:D:160:PRO:CD	2.81	0.42
1:G:159:LYS:N	1:G:160:PRO:CD	2.82	0.42
3:F:197:ASN:O	3:F:199:ILE:N	2.52	0.42
2:E:144:ASN:O	2:E:147:ASN:HB2	2.18	0.42
1:A:190:ASP:N	1:A:191:PRO:CD	2.82	0.42
1:G:115:ILE:O	1:G:115:ILE:HG13	2.19	0.42
1:J:204:ALA:C	1:J:206:THR:N	2.72	0.42
3:C:261:ALA:CB	3:C:286:ILE:HG12	2.49	0.42
1:A:155:TYR:CD2	1:A:155:TYR:C	2.93	0.42
2:E:95:THR:O	2:E:96:LEU:HB2	2.18	0.42
1:G:166:ARG:HG2	1:G:174:LEU:HB3	2.00	0.42
1:J:123:LYS:HG2	5:J:4250:GDP:C5	2.54	0.42
3:C:224:GLN:HG3	3:C:252:ASN:O	2.19	0.42
3:I:291:VAL:HG13	3:I:310:LEU:HD22	2.01	0.42
3:I:310:LEU:HD12	3:I:337:LEU:HD11	2.01	0.42
1:G:209:LEU:HD23	2:H:113:ASN:OD1	2.18	0.42
1:J:204:ALA:C	1:J:206:THR:H	2.22	0.42
3:L:256:LEU:HB2	3:L:284:ASN:HB3	2.00	0.42
2:K:105:THR:HB	2:K:106:PRO:CD	2.49	0.42
3:C:339:GLU:HA	3:C:339:GLU:OE1	2.19	0.42
3:C:200:ARG:NH1	3:C:201:PRO:HD2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:163:TRP:O	1:J:164:LEU:C	2.57	0.42
1:A:178:ALA:O	1:A:179:MET:HB2	2.19	0.42
2:B:79:LYS:HB2	2:B:86:ILE:HG12	2.01	0.42
3:F:83:LEU:HG	3:F:87:LEU:HD12	2.00	0.42
3:I:308:LEU:HD12	3:I:308:LEU:HA	1.80	0.42
1:D:12:LYS:HE3	1:D:64:TRP:CD2	2.54	0.42
1:G:43:LEU:HD23	3:I:79:ILE:HB	2.01	0.42
3:C:118:LEU:HB3	3:C:146:LEU:HD12	2.01	0.42
3:C:259:ARG:O	3:C:262:ALA:HB3	2.19	0.42
2:H:158:CYS:O	2:H:162:ILE:HG13	2.19	0.42
1:D:163:TRP:CZ2	1:D:167:LYS:HE3	2.54	0.42
1:G:164:LEU:O	1:G:168:LEU:HG	2.20	0.42
1:A:163:TRP:O	1:A:165:ALA:N	2.53	0.42
1:J:159:LYS:N	1:J:160:PRO:CD	2.82	0.42
2:B:144:ASN:O	2:B:147:ASN:HB2	2.19	0.42
2:H:58:PHE:O	2:H:60:SER:N	2.52	0.42
2:H:33:LEU:HA	2:H:34:PRO:HD3	1.80	0.42
3:I:112:GLU:OE1	3:I:112:GLU:HA	2.19	0.42
3:L:238:ILE:O	3:L:241:LYS:HG2	2.19	0.42
3:F:339:GLU:OE1	3:F:339:GLU:HA	2.19	0.42
3:L:259:ARG:O	3:L:262:ALA:HB3	2.18	0.42
1:A:186:GLU:O	1:A:187:VAL:CB	2.66	0.42
1:J:190:ASP:N	1:J:191:PRO:CD	2.82	0.42
3:C:87:LEU:HD12	3:C:113:PRO:CB	2.49	0.42
1:D:88:ILE:CD1	1:D:105:HIS:HB2	2.50	0.42
1:A:88:ILE:CD1	1:A:105:HIS:HB2	2.48	0.42
1:D:202:GLU:O	1:D:206:THR:HG23	2.20	0.42
2:B:105:THR:HB	2:B:106:PRO:CD	2.49	0.42
2:E:105:THR:HB	2:E:106:PRO:CD	2.50	0.42
1:J:124:VAL:HG11	1:J:148:ASP:HB3	2.01	0.42
3:I:268:PHE:CE2	3:I:276:LEU:HD22	2.54	0.42
2:E:153:THR:CG2	2:E:154:LYS:H	2.32	0.42
2:E:79:LYS:HB2	2:E:86:ILE:HG12	2.01	0.42
2:B:47:GLU:HA	2:B:78:LEU:HD23	2.00	0.42
1:G:75:LEU:HD13	3:I:72:THR:OG1	2.19	0.42
3:F:326:ARG:HG3	3:F:326:ARG:NH1	2.34	0.42
2:H:104:ILE:HB	2:H:162:ILE:HD12	2.00	0.42
3:C:299:ASP:OD1	3:C:328:VAL:HG13	2.19	0.42
1:G:194:ALA:O	1:G:195:ALA:CB	2.65	0.42
3:I:75:VAL:CG2	3:I:77:ASP:HB3	2.47	0.42
1:A:101:VAL:N	1:A:102:PRO:CD	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:71:PHE:O	3:C:74:ARG:HG2	2.19	0.42
1:J:106:ARG:C	1:J:108:LEU:N	2.73	0.42
1:J:202:GLU:O	1:J:206:THR:HG23	2.20	0.42
1:G:43:LEU:HD23	3:I:79:ILE:HD12	2.01	0.42
1:J:180:PRO:HB3	2:K:41:LEU:HD13	2.00	0.42
1:D:155:TYR:C	1:D:155:TYR:HD2	2.22	0.42
1:D:24:THR:O	1:D:25:THR:C	2.57	0.42
3:I:89:ALA:O	3:I:90:LEU:C	2.57	0.42
1:D:156:ASN:ND2	1:D:159:LYS:NZ	2.68	0.42
1:A:122:ASN:CG	1:A:123:LYS:N	2.72	0.42
3:C:46:THR:HG22	3:C:82:ALA:N	2.35	0.42
3:F:195:VAL:HG12	3:F:196:GLN:HB2	2.01	0.42
1:J:9:VAL:HG21	2:K:33:LEU:HD11	2.02	0.42
2:H:150:LYS:C	2:H:153:THR:HG22	2.40	0.42
3:I:208:LEU:HA	3:I:208:LEU:HD13	1.88	0.42
2:E:115:GLY:O	2:E:116:SER:HB3	2.19	0.42
3:C:192:VAL:CG1	3:C:218:LEU:HD11	2.47	0.42
1:G:190:ASP:N	1:G:191:PRO:CD	2.83	0.42
3:L:66:GLU:OE1	3:L:100:ARG:HB2	2.20	0.42
3:I:252:ASN:HD21	3:I:280:ARG:HB3	1.83	0.42
3:I:282:GLN:HG3	3:I:309:GLU:HB3	2.01	0.42
3:C:39:LEU:HD12	3:C:67:PHE:CD2	2.54	0.42
1:G:53:HIS:O	1:G:176:PHE:HA	2.20	0.42
3:F:256:LEU:O	3:F:257:SER:CB	2.68	0.42
1:G:204:ALA:C	1:G:206:THR:H	2.23	0.42
3:C:277:GLN:C	3:C:278:THR:HG22	2.39	0.42
2:H:110:LEU:HB3	2:H:120:TRP:HB3	2.02	0.42
3:I:200:ARG:HH11	3:I:200:ARG:HB3	1.85	0.42
1:D:145:GLN:HB2	1:D:163:TRP:CZ2	2.55	0.42
1:A:167:LYS:HD3	1:A:167:LYS:HA	1.80	0.42
3:L:75:VAL:CG2	3:L:77:ASP:HB3	2.46	0.42
3:F:25:PHE:CD2	3:F:52:LEU:HD21	2.55	0.42
3:L:261:ALA:CB	3:L:286:ILE:HG12	2.50	0.42
3:C:148:GLU:O	3:C:151:VAL:N	2.52	0.42
2:H:134:LYS:HA	2:H:135:PRO:HD3	1.84	0.42
1:J:178:ALA:O	1:J:179:MET:HB2	2.20	0.41
1:D:23:LYS:HB2	5:D:2250:GDP:O1B	2.19	0.41
2:E:156:GLU:OE2	2:E:159:ARG:HD2	2.20	0.41
3:L:212:LEU:H	3:L:212:LEU:HD22	1.84	0.41
3:C:118:LEU:HD23	3:C:118:LEU:HA	1.83	0.41
3:C:118:LEU:HD13	3:C:146:LEU:HD11	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:171:ASP:O	1:A:173:ASN:N	2.53	0.41
2:K:164:GLU:O	2:K:165:ARG:C	2.58	0.41
2:B:63:ASP:O	2:B:65:PRO:HD3	2.20	0.41
1:D:110:ARG:HG2	1:D:110:ARG:O	2.19	0.41
1:J:24:THR:O	1:J:25:THR:C	2.58	0.41
1:D:166:ARG:HG2	1:D:174:LEU:HB3	2.02	0.41
2:E:58:PHE:O	2:E:60:SER:N	2.53	0.41
3:I:192:VAL:CG1	3:I:218:LEU:HD11	2.48	0.41
1:J:102:PRO:O	1:J:105:HIS:O	2.37	0.41
3:C:5:SER:OG	3:C:38:VAL:HB	2.20	0.41
1:G:98:TYR:O	1:G:101:VAL:HG23	2.20	0.41
1:G:88:ILE:CD1	1:G:105:HIS:HB2	2.50	0.41
3:C:16:ILE:HG21	3:C:51:TRP:CD2	2.54	0.41
3:I:39:LEU:HD12	3:I:67:PHE:CD2	2.55	0.41
2:K:22:ASN:HB3	2:K:25:PRO:HG3	2.02	0.41
1:J:181:ALA:HA	2:K:98:ILE:CD1	2.50	0.41
1:J:155:TYR:HD2	1:J:155:TYR:C	2.24	0.41
2:B:166:GLU:HG2	2:B:166:GLU:O	2.20	0.41
3:I:274:ILE:HG22	3:I:276:LEU:H	1.84	0.41
1:J:116:PRO:HB2	1:J:164:LEU:HD23	2.02	0.41
3:F:206:HIS:O	3:F:207:LEU:C	2.57	0.41
1:J:30:HIS:CE1	1:J:157:PHE:O	2.55	0.41
2:B:150:LYS:C	2:B:153:THR:HG22	2.40	0.41
2:B:48:LEU:CD1	2:B:158:CYS:SG	3.08	0.41
1:J:88:ILE:CD1	1:J:105:HIS:HB2	2.50	0.41
2:E:40:THR:HG21	2:E:42:GLU:OE2	2.20	0.41
3:L:46:THR:HG22	3:L:81:GLU:HB3	2.01	0.41
3:C:246:LEU:HA	3:C:246:LEU:HD12	1.84	0.41
2:H:120:TRP:CE2	2:H:148:ALA:HB1	2.55	0.41
2:H:79:LYS:CB	2:H:86:ILE:HG12	2.50	0.41
2:K:30:ILE:HG22	2:K:31:VAL:HG13	2.02	0.41
2:B:75:VAL:HG13	2:B:88:LEU:HD21	2.01	0.41
1:G:30:HIS:CE1	1:G:157:PHE:O	2.55	0.41
3:L:339:GLU:OE1	3:L:339:GLU:HA	2.20	0.41
3:F:246:LEU:HD12	3:F:246:LEU:HA	1.84	0.41
1:G:91:ASP:N	1:G:97:THR:CG2	2.75	0.41
1:G:156:ASN:ND2	1:G:159:LYS:NZ	2.69	0.41
1:J:126:ILE:N	1:J:126:ILE:HD12	2.36	0.41
2:K:51:MET:HE3	2:K:142:PHE:CD1	2.56	0.41
2:E:79:LYS:CB	2:E:86:ILE:HG12	2.51	0.41
2:B:150:LYS:NZ	2:B:150:LYS:HB3	2.36	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:28:LYS:HA	1:G:31:LEU:HD11	2.02	0.41
3:I:83:LEU:HG	3:I:87:LEU:HD12	2.01	0.41
3:C:283:TYR:CD1	3:C:283:TYR:N	2.88	0.41
1:D:70:GLU:HA	3:F:72:THR:HG22	2.02	0.41
3:I:221:LEU:HD11	3:I:223:LEU:HG	2.03	0.41
2:E:63:ASP:O	2:E:65:PRO:HD3	2.21	0.41
3:L:118:LEU:HB3	3:L:146:LEU:HD12	2.03	0.41
3:L:42:ASN:O	3:L:70:ILE:HA	2.21	0.41
2:K:94:LYS:O	2:K:96:LEU:HD13	2.20	0.41
1:D:158:GLU:CD	2:E:94:LYS:HG2	2.40	0.41
1:J:209:LEU:HA	1:J:210:PRO:HD3	1.91	0.41
1:G:30:HIS:HB3	1:G:50:LEU:HD13	2.03	0.41
3:F:192:VAL:HG12	3:F:218:LEU:CD1	2.46	0.41
3:I:99:VAL:HG12	3:I:124:LEU:HD13	2.02	0.41
2:H:167:LYS:HD2	2:H:167:LYS:N	2.35	0.41
1:A:116:PRO:HB2	1:A:164:LEU:HD23	2.03	0.41
2:E:120:TRP:CE2	2:E:148:ALA:HB1	2.56	0.41
3:L:176:MET:SD	3:L:199:ILE:HD13	2.60	0.41
2:B:94:LYS:O	2:B:96:LEU:HD13	2.21	0.41
3:I:26:ALA:C	3:I:28:LEU:N	2.74	0.41
2:B:49:PHE:HZ	2:B:51:MET:HE1	1.86	0.41
3:I:112:GLU:CB	3:I:113:PRO:HD3	2.48	0.41
3:C:329:PHE:CD1	3:C:336:GLU:N	2.88	0.41
2:E:55:LEU:HD11	2:E:138:LEU:HB3	2.02	0.41
1:D:29:ARG:NH1	1:D:151:ALA:O	2.54	0.41
1:G:204:ALA:C	1:G:206:THR:N	2.73	0.41
1:G:159:LYS:HB2	1:G:160:PRO:HD3	2.01	0.41
2:E:160:LYS:O	2:E:162:ILE:N	2.53	0.41
1:D:186:GLU:O	1:D:187:VAL:CB	2.68	0.41
3:F:39:LEU:CD1	3:F:67:PHE:CE2	3.02	0.41
3:C:16:ILE:HG22	3:C:16:ILE:O	2.21	0.41
2:E:55:LEU:HD12	2:E:56:PHE:H	1.85	0.41
2:K:55:LEU:HD11	2:K:138:LEU:HB3	2.02	0.41
3:L:268:PHE:HE2	3:L:276:LEU:HD22	1.86	0.41
1:D:134:LYS:O	1:D:136:ILE:N	2.53	0.41
1:G:155:TYR:HD2	1:G:155:TYR:C	2.23	0.41
3:I:256:LEU:O	3:I:257:SER:CB	2.68	0.41
2:H:105:THR:HB	2:H:106:PRO:CD	2.50	0.41
1:J:158:GLU:CD	2:K:94:LYS:HG2	2.41	0.41
1:D:13:LEU:HD21	1:D:87:ILE:CD1	2.50	0.41
1:G:163:TRP:O	1:G:164:LEU:C	2.58	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:13:LEU:CD1	1:G:86:ALA:HA	2.48	0.41
1:J:156:ASN:ND2	1:J:159:LYS:NZ	2.69	0.41
1:G:22:GLY:O	1:G:23:LYS:C	2.58	0.41
3:L:206:HIS:O	3:L:207:LEU:C	2.59	0.41
2:E:58:PHE:HD2	2:E:67:TRP:CE2	2.39	0.41
1:D:188:VAL:O	1:D:189:MET:O	2.39	0.41
3:C:176:MET:HE2	3:C:207:LEU:HD22	2.02	0.41
1:J:188:VAL:HG12	1:J:189:MET:H	1.86	0.41
2:E:110:LEU:CD1	2:E:152:LYS:HA	2.46	0.41
3:I:66:GLU:OE1	3:I:100:ARG:HB2	2.21	0.41
3:L:192:VAL:HG12	3:L:218:LEU:CD1	2.48	0.41
1:J:70:GLU:HB3	3:L:72:THR:HG22	2.03	0.41
3:L:96:LEU:HB3	3:L:121:HIS:CE1	2.56	0.41
3:C:282:GLN:HG3	3:C:309:GLU:HB3	2.01	0.41
3:C:298:ILE:HA	3:C:302:MET:HB2	2.02	0.41
3:L:298:ILE:HA	3:L:302:MET:HB2	2.03	0.41
3:I:25:PHE:CD2	3:I:52:LEU:HD21	2.55	0.41
1:A:203:VAL:O	1:A:203:VAL:HG12	2.21	0.41
2:B:55:LEU:HD11	2:B:138:LEU:HB3	2.01	0.41
2:K:55:LEU:HD12	2:K:56:PHE:H	1.86	0.41
3:L:306:LEU:CD2	3:L:334:ARG:HD2	2.51	0.41
1:J:29:ARG:NH1	1:J:151:ALA:O	2.54	0.41
3:I:268:PHE:HE2	3:I:276:LEU:HD22	1.86	0.41
3:L:118:LEU:HA	3:L:118:LEU:HD23	1.88	0.41
3:I:256:LEU:HB2	3:I:284:ASN:HB3	2.03	0.41
3:L:83:LEU:HD21	3:L:114:LEU:HD13	2.03	0.41
3:C:68:SER:HA	3:C:102:SER:O	2.21	0.41
1:J:186:GLU:O	1:J:187:VAL:CB	2.69	0.41
1:D:85:CYS:HB2	1:D:164:LEU:CD2	2.38	0.41
2:E:94:LYS:O	2:E:96:LEU:HD13	2.21	0.41
2:E:121:VAL:HA	2:E:139:ALA:HA	2.03	0.41
3:L:329:PHE:CD1	3:L:336:GLU:N	2.89	0.41
3:F:306:LEU:HB2	3:F:307:PHE:HD1	1.86	0.41
1:D:171:ASP:O	1:D:173:ASN:N	2.54	0.41
3:I:238:ILE:O	3:I:241:LYS:HG2	2.21	0.41
3:F:68:SER:HA	3:F:102:SER:O	2.21	0.41
2:E:30:ILE:HG22	2:E:31:VAL:HG13	2.03	0.40
1:G:126:ILE:HD12	1:G:126:ILE:N	2.36	0.40
1:A:177:VAL:O	1:A:177:VAL:HG23	2.21	0.40
1:A:28:LYS:HA	1:A:31:LEU:HD11	2.03	0.40
2:K:120:TRP:O	2:K:139:ALA:HA	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:186:GLU:O	1:G:187:VAL:CB	2.68	0.40
1:G:210:PRO:CD	2:H:67:TRP:HB2	2.51	0.40
3:F:329:PHE:CB	3:F:335:GLY:HA3	2.51	0.40
2:H:104:ILE:HB	2:H:162:ILE:CD1	2.51	0.40
1:G:188:VAL:O	1:G:189:MET:O	2.38	0.40
2:K:40:THR:HG21	2:K:42:GLU:OE2	2.21	0.40
3:F:46:THR:HG22	3:F:82:ALA:N	2.36	0.40
3:L:144:ARG:HG2	3:L:178:GLU:HG2	2.02	0.40
1:D:106:ARG:C	1:D:108:LEU:N	2.72	0.40
3:I:221:LEU:HD12	3:I:222:ASP:N	2.36	0.40
1:J:145:GLN:HB2	1:J:163:TRP:CZ2	2.56	0.40
3:I:199:ILE:HG21	3:I:204:ILE:HD12	2.00	0.40
2:B:120:TRP:O	2:B:139:ALA:HA	2.22	0.40
2:B:79:LYS:CB	2:B:86:ILE:HG12	2.51	0.40
1:D:92:VAL:CG1	1:D:92:VAL:O	2.69	0.40
1:J:188:VAL:O	1:J:189:MET:O	2.39	0.40
3:C:71:PHE:O	3:C:72:THR:C	2.57	0.40
3:F:43:THR:HG21	3:F:72:THR:O	2.22	0.40
1:G:12:LYS:HE3	1:G:64:TRP:CD2	2.55	0.40
1:J:134:LYS:O	1:J:136:ILE:N	2.55	0.40
3:C:256:LEU:HB2	3:C:284:ASN:HB3	2.02	0.40
2:B:75:VAL:CG1	2:B:88:LEU:HD21	2.51	0.40
1:D:30:HIS:HB3	1:D:50:LEU:HD13	2.04	0.40
2:K:153:THR:CG2	2:K:154:LYS:H	2.34	0.40
2:E:113:ASN:O	2:E:115:GLY:O	2.40	0.40
1:G:177:VAL:O	1:G:177:VAL:HG23	2.22	0.40
1:D:188:VAL:HG12	1:D:189:MET:H	1.86	0.40
3:C:96:LEU:HB3	3:C:121:HIS:CE1	2.57	0.40
3:I:43:THR:HG21	3:I:72:THR:O	2.21	0.40
1:J:22:GLY:O	1:J:23:LYS:C	2.59	0.40
2:B:105:THR:HB	2:B:106:PRO:HD2	2.04	0.40
2:B:156:GLU:C	2:B:158:CYS:H	2.24	0.40
2:E:49:PHE:HZ	2:E:51:MET:HE1	1.86	0.40
3:F:87:LEU:HD12	3:F:113:PRO:HB2	2.03	0.40
3:L:283:TYR:CD1	3:L:283:TYR:N	2.90	0.40
3:C:18:THR:O	3:C:20:ASP:O	2.40	0.40
3:C:120:LYS:O	3:C:122:THR:N	2.54	0.40
1:J:203:VAL:O	1:J:203:VAL:HG12	2.21	0.40
2:B:106:PRO:O	2:B:159:ARG:NE	2.46	0.40
3:C:99:VAL:HG12	3:C:124:LEU:HD13	2.03	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	204/216 (94%)	156 (76%)	27 (13%)	21 (10%)	1	4
1	D	204/216 (94%)	153 (75%)	29 (14%)	22 (11%)	0	3
1	G	204/216 (94%)	156 (76%)	28 (14%)	20 (10%)	1	4
1	J	204/216 (94%)	154 (76%)	28 (14%)	22 (11%)	0	3
2	B	144/201 (72%)	118 (82%)	14 (10%)	12 (8%)	1	6
2	E	144/201 (72%)	117 (81%)	15 (10%)	12 (8%)	1	6
2	H	144/201 (72%)	119 (83%)	14 (10%)	11 (8%)	1	7
2	K	144/201 (72%)	117 (81%)	18 (12%)	9 (6%)	2	10
3	C	342/386 (89%)	275 (80%)	54 (16%)	13 (4%)	4	22
3	F	342/386 (89%)	280 (82%)	48 (14%)	14 (4%)	3	20
3	I	342/386 (89%)	278 (81%)	50 (15%)	14 (4%)	3	20
3	L	342/386 (89%)	278 (81%)	50 (15%)	14 (4%)	3	20
All	All	2760/3212 (86%)	2201 (80%)	375 (14%)	184 (7%)	1	9

All (184) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	GLN
1	A	106	ARG
1	A	135	SER
1	A	179	MET
1	A	186	GLU
1	A	189	MET
1	A	190	ASP
1	A	191	PRO
2	B	45	GLU
2	B	46	GLU
2	B	59	ALA
2	B	60	SER

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Mol	Chain	Res	Type
2	B	165	ARG
3	C	121	HIS
1	D	82	GLN
1	D	106	ARG
1	D	135	SER
1	D	179	MET
1	D	186	GLU
1	D	189	MET
1	D	190	ASP
1	D	191	PRO
2	E	45	GLU
2	E	46	GLU
2	E	59	ALA
2	E	60	SER
3	F	121	HIS
1	G	82	GLN
1	G	106	ARG
1	G	135	SER
1	G	179	MET
1	G	186	GLU
1	G	189	MET
1	G	190	ASP
1	G	191	PRO
2	H	45	GLU
2	H	46	GLU
2	H	59	ALA
2	H	60	SER
2	H	165	ARG
3	I	121	HIS
1	J	82	GLN
1	J	106	ARG
1	J	135	SER
1	J	179	MET
1	J	186	GLU
1	J	189	MET
1	J	190	ASP
1	J	191	PRO
2	K	45	GLU
2	K	46	GLU
2	K	59	ALA
2	K	60	SER
3	L	121	HIS

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Mol	Chain	Res	Type
1	A	113	GLU
1	A	127	LYS
1	A	134	LYS
1	A	187	VAL
2	B	85	ALA
3	C	172	GLU
3	C	319	ASP
1	D	113	GLU
1	D	134	LYS
1	D	138	PHE
1	D	187	VAL
2	E	85	ALA
2	E	165	ARG
3	F	172	GLU
3	F	319	ASP
1	G	113	GLU
1	G	134	LYS
1	G	187	VAL
2	H	85	ALA
3	I	109	THR
3	I	319	ASP
1	J	113	GLU
1	J	134	LYS
1	J	163	TRP
1	J	187	VAL
2	K	85	ALA
3	L	172	GLU
3	L	319	ASP
1	A	138	PHE
1	A	163	TRP
1	A	164	LEU
1	A	178	ALA
1	A	188	VAL
2	B	29	PRO
3	C	109	THR
3	C	116	ASP
3	C	283	TYR
3	C	336	GLU
1	D	127	LYS
1	D	163	TRP
1	D	164	LEU
1	D	178	ALA

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Mol	Chain	Res	Type
1	D	188	VAL
3	F	109	THR
3	F	216	GLN
3	F	336	GLU
1	G	127	LYS
1	G	138	PHE
1	G	163	TRP
1	G	164	LEU
1	G	178	ALA
1	G	188	VAL
3	I	172	GLU
3	I	283	TYR
3	I	336	GLU
1	J	127	LYS
1	J	138	PHE
1	J	157	PHE
1	J	164	LEU
1	J	178	ALA
1	J	188	VAL
2	K	29	PRO
3	L	109	THR
3	L	283	TYR
3	L	336	GLU
1	A	157	PHE
2	B	65	PRO
2	B	166	GLU
3	C	69	ASP
1	D	157	PHE
2	E	29	PRO
2	E	65	PRO
2	E	82	GLU
2	E	83	LYS
3	F	69	ASP
3	F	198	GLY
3	F	283	TYR
2	H	29	PRO
2	H	65	PRO
2	H	82	GLU
2	H	83	LYS
3	I	69	ASP
3	I	116	ASP
1	J	128	ASP

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Mol	Chain	Res	Type
1	J	195	ALA
2	K	65	PRO
2	K	83	LYS
3	L	69	ASP
3	L	116	ASP
3	L	257	SER
1	A	128	ASP
1	A	195	ALA
2	B	82	GLU
2	B	83	LYS
3	C	72	THR
3	C	257	SER
1	D	128	ASP
1	D	195	ALA
3	F	72	THR
3	F	116	ASP
3	F	257	SER
1	G	172	PRO
1	G	195	ALA
3	I	257	SER
2	K	82	GLU
3	L	213	ALA
3	L	282	GLN
1	A	172	PRO
2	B	116	SER
3	C	282	GLN
1	D	172	PRO
2	E	116	SER
2	E	161	GLU
2	H	116	SER
3	I	72	THR
3	I	282	GLN
3	L	201	PRO
3	L	216	GLN
3	C	16	ILE
3	C	201	PRO
3	F	16	ILE
3	I	16	ILE
1	J	172	PRO
3	L	16	ILE
1	D	81	ILE
3	I	201	PRO

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Mol	Chain	Res	Type
3	F	201	PRO
3	I	107	GLY
1	J	81	ILE
1	G	81	ILE

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	178/185 (96%)	164 (92%)	14 (8%)	15	49
1	D	178/185 (96%)	161 (90%)	17 (10%)	10	37
1	G	178/185 (96%)	163 (92%)	15 (8%)	14	46
1	J	178/185 (96%)	161 (90%)	17 (10%)	10	37
2	B	131/176 (74%)	117 (89%)	14 (11%)	8	31
2	E	131/176 (74%)	118 (90%)	13 (10%)	10	34
2	H	131/176 (74%)	117 (89%)	14 (11%)	8	31
2	K	131/176 (74%)	119 (91%)	12 (9%)	11	40
3	C	295/334 (88%)	277 (94%)	18 (6%)	23	59
3	F	295/334 (88%)	277 (94%)	18 (6%)	23	59
3	I	295/334 (88%)	277 (94%)	18 (6%)	23	59
3	L	295/334 (88%)	277 (94%)	18 (6%)	23	59
All	All	2416/2780 (87%)	2228 (92%)	188 (8%)	16	49

All (188) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	18	ASP
1	A	24	THR
1	A	30	HIS
1	A	31	LEU
1	A	72	PHE

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Mol	Chain	Res	Type
1	A	76	ARG
1	A	81	ILE
1	A	118	VAL
1	A	140	ARG
1	A	155	TYR
1	A	158	GLU
1	A	186	GLU
1	A	196	GLN
2	B	26	GLN
2	B	29	PRO
2	B	38	ILE
2	B	48	LEU
2	B	52	ARG
2	B	57	ARG
2	B	90	MET
2	B	107	MET
2	B	109	GLU
2	B	123	ASN
2	B	132	CYS
2	B	136	GLU
2	B	146	GLU
2	B	166	GLU
3	C	3	ARG
3	C	19	GLU
3	C	28	LEU
3	C	43	THR
3	C	46	THR
3	C	66	GLU
3	C	81	GLU
3	C	109	THR
3	C	114	LEU
3	C	173	ASN
3	C	176	MET
3	C	192	VAL
3	C	196	GLN
3	C	208	LEU
3	C	259	ARG
3	C	278	THR
3	C	296	THR
3	C	326	ARG
1	D	13	LEU
1	D	16	VAL

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Mol	Chain	Res	Type
1	D	18	ASP
1	D	24	THR
1	D	30	HIS
1	D	31	LEU
1	D	72	PHE
1	D	76	ARG
1	D	81	ILE
1	D	111	VAL
1	D	118	VAL
1	D	140	ARG
1	D	155	TYR
1	D	157	PHE
1	D	158	GLU
1	D	186	GLU
1	D	196	GLN
2	E	26	GLN
2	E	29	PRO
2	E	38	ILE
2	E	48	LEU
2	E	52	ARG
2	E	57	ARG
2	E	90	MET
2	E	107	MET
2	E	109	GLU
2	E	123	ASN
2	E	132	CYS
2	E	146	GLU
2	E	166	GLU
3	F	3	ARG
3	F	19	GLU
3	F	28	LEU
3	F	43	THR
3	F	46	THR
3	F	66	GLU
3	F	81	GLU
3	F	109	THR
3	F	114	LEU
3	F	173	ASN
3	F	176	MET
3	F	192	VAL
3	F	196	GLN
3	F	208	LEU

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Mol	Chain	Res	Type
3	F	259	ARG
3	F	278	THR
3	F	296	THR
3	F	326	ARG
1	G	13	LEU
1	G	18	ASP
1	G	24	THR
1	G	30	HIS
1	G	31	LEU
1	G	72	PHE
1	G	76	ARG
1	G	81	ILE
1	G	111	VAL
1	G	118	VAL
1	G	140	ARG
1	G	155	TYR
1	G	158	GLU
1	G	186	GLU
1	G	196	GLN
2	H	26	GLN
2	H	29	PRO
2	H	38	ILE
2	H	48	LEU
2	H	52	ARG
2	H	57	ARG
2	H	90	MET
2	H	107	MET
2	H	109	GLU
2	H	123	ASN
2	H	132	CYS
2	H	136	GLU
2	H	146	GLU
2	H	166	GLU
3	I	3	ARG
3	I	19	GLU
3	I	28	LEU
3	I	43	THR
3	I	46	THR
3	I	66	GLU
3	I	81	GLU
3	I	109	THR
3	I	114	LEU

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Mol	Chain	Res	Type
3	I	173	ASN
3	I	176	MET
3	I	192	VAL
3	I	196	GLN
3	I	208	LEU
3	I	259	ARG
3	I	278	THR
3	I	296	THR
3	I	326	ARG
1	J	13	LEU
1	J	16	VAL
1	J	18	ASP
1	J	24	THR
1	J	30	HIS
1	J	31	LEU
1	J	72	PHE
1	J	76	ARG
1	J	81	ILE
1	J	111	VAL
1	J	118	VAL
1	J	140	ARG
1	J	155	TYR
1	J	157	PHE
1	J	158	GLU
1	J	186	GLU
1	J	196	GLN
2	K	26	GLN
2	K	29	PRO
2	K	38	ILE
2	K	48	LEU
2	K	52	ARG
2	K	57	ARG
2	K	90	MET
2	K	107	MET
2	K	109	GLU
2	K	123	ASN
2	K	132	CYS
2	K	146	GLU
3	L	3	ARG
3	L	19	GLU
3	L	28	LEU
3	L	43	THR

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Mol	Chain	Res	Type
3	L	46	THR
3	L	66	GLU
3	L	81	GLU
3	L	109	THR
3	L	114	LEU
3	L	131	ASN
3	L	173	ASN
3	L	176	MET
3	L	192	VAL
3	L	196	GLN
3	L	208	LEU
3	L	259	ARG
3	L	278	THR
3	L	296	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (69) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	GLN
1	A	30	HIS
1	A	145	GLN
1	A	156	ASN
2	B	113	ASN
2	B	123	ASN
2	B	149	GLN
3	C	88	GLN
3	C	121	HIS
3	C	130	HIS
3	C	131	ASN
3	C	147	GLN
3	C	173	ASN
3	C	186	HIS
3	C	206	HIS
3	C	224	GLN
3	C	252	ASN
1	D	10	GLN
1	D	30	HIS
1	D	145	GLN
1	D	156	ASN
2	E	113	ASN
2	E	123	ASN
2	E	149	GLN

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Mol	Chain	Res	Type
3	F	88	GLN
3	F	121	HIS
3	F	130	HIS
3	F	131	ASN
3	F	147	GLN
3	F	173	ASN
3	F	206	HIS
3	F	224	GLN
3	F	252	ASN
1	G	10	GLN
1	G	30	HIS
1	G	145	GLN
1	G	156	ASN
2	H	113	ASN
2	H	123	ASN
2	H	149	GLN
3	I	88	GLN
3	I	121	HIS
3	I	130	HIS
3	I	131	ASN
3	I	147	GLN
3	I	173	ASN
3	I	184	GLN
3	I	186	HIS
3	I	206	HIS
3	I	224	GLN
3	I	252	ASN
1	J	10	GLN
1	J	30	HIS
1	J	53	HIS
1	J	145	GLN
1	J	156	ASN
2	K	113	ASN
2	K	123	ASN
2	K	149	GLN
3	L	88	GLN
3	L	121	HIS
3	L	130	HIS
3	L	131	ASN
3	L	147	GLN
3	L	173	ASN
3	L	186	HIS

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Mol	Chain	Res	Type
3	L	206	HIS
3	L	224	GLN
3	L	252	ASN

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 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	GDP	A	1250	4,6	23,30,30	1.62	3 (13%)	30,47,47	2.42	5 (16%)
6	AF3	A	1252	5,4	0,3,3	0.00	-	0,3,3	0.00	-
5	GDP	D	2250	4,6	23,30,30	1.69	5 (21%)	30,47,47	2.39	5 (16%)
6	AF3	D	2252	5,4	0,3,3	0.00	-	0,3,3	0.00	-
5	GDP	G	3250	4,6	23,30,30	1.63	4 (17%)	30,47,47	2.46	6 (20%)
6	AF3	G	3252	5,4	0,3,3	0.00	-	0,3,3	0.00	-
5	GDP	J	4250	4,6	23,30,30	1.64	3 (13%)	30,47,47	2.48	7 (23%)
6	AF3	J	4252	5,4	0,3,3	0.00	-	0,3,3	0.00	-

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

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	GDP	A	1250	4,6	-	0/12/32/32	0/3/3/3
6	AF3	A	1252	5,4	-	0/0/0/0	0/0/0/0
5	GDP	D	2250	4,6	-	0/12/32/32	0/3/3/3
6	AF3	D	2252	5,4	-	0/0/0/0	0/0/0/0
5	GDP	G	3250	4,6	-	0/12/32/32	0/3/3/3
6	AF3	G	3252	5,4	-	0/0/0/0	0/0/0/0
5	GDP	J	4250	4,6	-	0/12/32/32	0/3/3/3
6	AF3	J	4252	5,4	-	0/0/0/0	0/0/0/0

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	J	4250	GDP	C8-N7	-3.02	1.28	1.34
5	A	1250	GDP	C8-N7	-2.80	1.29	1.34
5	G	3250	GDP	C8-N7	-2.78	1.29	1.34
5	D	2250	GDP	C8-N7	-2.67	1.29	1.34
5	D	2250	GDP	PA-O2A	-2.41	1.44	1.54
5	G	3250	GDP	PA-O2A	-2.14	1.45	1.54
5	D	2250	GDP	C2-N1	2.11	1.39	1.35
5	G	3250	GDP	C6-C5	2.85	1.47	1.41
5	A	1250	GDP	C6-C5	2.95	1.47	1.41
5	J	4250	GDP	C6-C5	3.36	1.48	1.41
5	D	2250	GDP	C6-C5	3.57	1.48	1.41
5	D	2250	GDP	C6-N1	4.24	1.41	1.33
5	J	4250	GDP	C6-N1	4.39	1.41	1.33
5	G	3250	GDP	C6-N1	4.67	1.41	1.33
5	A	1250	GDP	C6-N1	4.75	1.41	1.33

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	G	3250	GDP	C5-C6-N1	-8.63	111.79	123.59
5	D	2250	GDP	C5-C6-N1	-8.51	111.95	123.59
5	J	4250	GDP	C5-C6-N1	-8.42	112.08	123.59
5	A	1250	GDP	C5-C6-N1	-8.40	112.10	123.59
5	J	4250	GDP	N3-C2-N1	-3.67	121.85	127.44
5	J	4250	GDP	PA-O3A-PB	-3.61	120.56	132.67
5	G	3250	GDP	PA-O3A-PB	-3.39	121.30	132.67
5	A	1250	GDP	PA-O3A-PB	-3.37	121.36	132.67

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
5	A	1250	GDP	N3-C2-N1	-3.37	122.31	127.44
5	G	3250	GDP	N3-C2-N1	-3.37	122.32	127.44
5	D	2250	GDP	PA-O3A-PB	-3.26	121.73	132.67
5	D	2250	GDP	N3-C2-N1	-3.11	122.71	127.44
5	J	4250	GDP	O3'-C3'-C4'	-2.31	104.12	111.05
5	G	3250	GDP	O3'-C3'-C4'	-2.20	104.46	111.05
5	J	4250	GDP	O3B-PB-O3A	-2.14	95.38	105.09
5	G	3250	GDP	O3B-PB-O3A	-2.11	95.50	105.09
5	D	2250	GDP	C4'-O4'-C1'	2.05	111.97	109.72
5	J	4250	GDP	C4'-O4'-C1'	2.20	112.13	109.72
5	A	1250	GDP	C4'-O4'-C1'	2.20	112.14	109.72
5	D	2250	GDP	C6-N1-C2	6.45	124.89	115.94
5	A	1250	GDP	C6-N1-C2	6.55	125.03	115.94
5	G	3250	GDP	C6-N1-C2	6.75	125.31	115.94
5	J	4250	GDP	C6-N1-C2	6.77	125.34	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1250	GDP	5	0
5	D	2250	GDP	5	0
5	G	3250	GDP	5	0
5	J	4250	GDP	4	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	206/216 (95%)	-0.47	5 (2%) 62 39	21, 57, 156, 186	0
1	D	206/216 (95%)	-0.49	9 (4%) 38 17	13, 46, 161, 199	0
1	G	206/216 (95%)	-0.55	2 (0%) 84 69	14, 50, 159, 198	0
1	J	206/216 (95%)	-0.62	3 (1%) 76 58	11, 47, 148, 199	0
2	B	146/201 (72%)	-0.25	4 (2%) 58 34	43, 88, 148, 200	0
2	E	146/201 (72%)	0.05	7 (4%) 34 15	43, 100, 162, 195	0
2	H	146/201 (72%)	-0.22	5 (3%) 49 24	32, 80, 158, 187	0
2	K	146/201 (72%)	-0.29	2 (1%) 78 60	44, 80, 145, 188	0
3	C	344/386 (89%)	-0.72	1 (0%) 94 88	18, 48, 107, 144	0
3	F	344/386 (89%)	-0.82	1 (0%) 94 88	11, 47, 93, 143	0
3	I	344/386 (89%)	-0.74	0 100 100	15, 50, 100, 148	0
3	L	344/386 (89%)	-0.79	0 100 100	8, 43, 97, 150	0
All	All	2784/3212 (86%)	-0.57	39 (1%) 78 60	8, 55, 139, 200	0

All (39) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	191	PRO	7.2
2	H	63	ASP	5.2
1	D	188	VAL	3.8
1	D	195	ALA	3.8
1	A	206	THR	3.6
1	D	190	ASP	3.4
2	E	82	GLU	3.4
2	K	63	ASP	3.3
2	E	113	ASN	3.2
1	A	191	PRO	3.0
2	H	117	ASP	2.9

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Mol	Chain	Res	Type	RSRZ
1	J	189	MET	2.8
2	E	22	ASN	2.8
2	H	65	PRO	2.8
1	D	187	VAL	2.7
2	E	106	PRO	2.7
1	G	188	VAL	2.7
2	H	22	ASN	2.7
1	D	189	MET	2.6
2	B	63	ASP	2.5
1	A	190	ASP	2.5
3	F	155	ALA	2.5
2	E	46	GLU	2.4
1	D	141	LYS	2.4
2	E	45	GLU	2.4
1	A	127	LYS	2.3
3	C	334	ARG	2.3
1	J	190	ASP	2.2
1	D	186	GLU	2.2
2	H	116	SER	2.1
1	D	197	TYR	2.1
1	J	191	PRO	2.1
2	B	144	ASN	2.1
2	E	111	LYS	2.1
2	B	22	ASN	2.1
1	G	187	VAL	2.1
2	B	46	GLU	2.1
2	K	22	ASN	2.1
1	A	202	GLU	2.1

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

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

6.3 Carbohydrates [i](#)

There are no 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(Å ²)	Q<0.9
4	MG	J	4251	1/1	0.89	0.40	13.55	33,33,33,33	0
4	MG	D	2251	1/1	0.63	0.30	9.39	45,45,45,45	0
4	MG	A	1251	1/1	0.91	0.39	8.23	31,31,31,31	0
4	MG	G	3251	1/1	0.86	0.37	8.01	44,44,44,44	0
6	AF3	D	2252	4/4	0.97	0.26	4.12	57,57,57,57	0
6	AF3	J	4252	4/4	0.98	0.24	1.54	57,57,57,57	0
6	AF3	A	1252	4/4	0.95	0.26	1.13	57,57,57,57	0
6	AF3	G	3252	4/4	0.97	0.19	0.42	57,57,57,57	0
5	GDP	A	1250	28/28	0.95	0.15	-0.51	43,43,43,43	0
5	GDP	G	3250	28/28	0.96	0.13	-0.64	35,35,35,35	0
5	GDP	J	4250	28/28	0.97	0.13	-0.72	29,29,29,29	0
5	GDP	D	2250	28/28	0.97	0.12	-0.78	31,31,31,31	0

6.5 Other polymers ⓘ

There are no such residues in this entry.