Full wwPDB X-ray Structure Validation Report (i)

Jun 15, 2024 – 11:37 AM EDT

PDB ID	:	2EHO
Title	:	Crystal structure of human GINS complex
Authors	:	Choi, J.M.; Lim, H.S.; Kim, J.J.; Song, O.K.; Cho, Y.
Deposited on	:	2007-03-07
Resolution	:	3.00 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

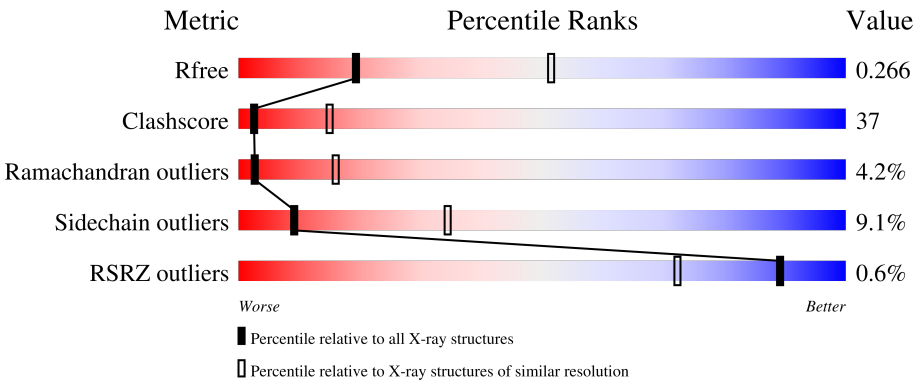
MolProbity	:	4.02b-467
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	1.20.1
EDS	:	2.37.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.37.1

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	203	% 27% 47% 5% 21%
1	E	203	43% 45% 5% 6%
1	I	203	41% 45% 6% • 5%
2	B	152	% 41% 45% 9% • 5%
2	F	152	49% 42% 5% •

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Mol	Chain	Length	Quality of chain
2	J	152	50% 38% 7% 5%
3	C	186	% 26% 57% 6% • 10%
3	G	186	% 35% 53% 7% 5%
3	K	186	40% 47% 8% 6%
4	D	216	% 31% 44% 9% 16%
4	H	216	41% 35% 8% 15%
4	L	216	37% 38% 8% • 16%

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
5	SO4	B	1016	-	-	X	-
5	SO4	F	1010	-	-	X	-
5	SO4	K	1007	-	-	-	X

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 16937 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 GINS complex subunit 4.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	161	1340	857	227	246	2	8	0	0	0
1	E	190	1583	1005	269	299	2	8	0	0	0
1	I	192	1604	1016	278	300	2	8	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	MSE	MET	MODIFIED RESIDUE	UNP Q9BRT9
A	55	MSE	MET	MODIFIED RESIDUE	UNP Q9BRT9
A	61	MSE	MET	MODIFIED RESIDUE	UNP Q9BRT9
A	80	MSE	MET	MODIFIED RESIDUE	UNP Q9BRT9
A	82	MSE	MET	MODIFIED RESIDUE	UNP Q9BRT9
A	98	MSE	MET	MODIFIED RESIDUE	UNP Q9BRT9
A	134	MSE	MET	MODIFIED RESIDUE	UNP Q9BRT9
A	149	MSE	MET	MODIFIED RESIDUE	UNP Q9BRT9
E	35	MSE	MET	MODIFIED RESIDUE	UNP Q9BRT9
E	55	MSE	MET	MODIFIED RESIDUE	UNP Q9BRT9
E	61	MSE	MET	MODIFIED RESIDUE	UNP Q9BRT9
E	80	MSE	MET	MODIFIED RESIDUE	UNP Q9BRT9
E	82	MSE	MET	MODIFIED RESIDUE	UNP Q9BRT9
E	98	MSE	MET	MODIFIED RESIDUE	UNP Q9BRT9
E	134	MSE	MET	MODIFIED RESIDUE	UNP Q9BRT9
E	149	MSE	MET	MODIFIED RESIDUE	UNP Q9BRT9
I	35	MSE	MET	MODIFIED RESIDUE	UNP Q9BRT9
I	55	MSE	MET	MODIFIED RESIDUE	UNP Q9BRT9
I	61	MSE	MET	MODIFIED RESIDUE	UNP Q9BRT9
I	80	MSE	MET	MODIFIED RESIDUE	UNP Q9BRT9
I	82	MSE	MET	MODIFIED RESIDUE	UNP Q9BRT9
I	98	MSE	MET	MODIFIED RESIDUE	UNP Q9BRT9
I	134	MSE	MET	MODIFIED RESIDUE	UNP Q9BRT9

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Chain	Residue	Modelled	Actual	Comment	Reference
I	149	MSE	MET	MODIFIED RESIDUE	UNP Q9BRT9

- Molecule 2 is a protein called DNA replication complex GINS protein PSF1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
2	B	145	1188	744	217	217	3	7	0	0	0
2	F	146	1196	749	218	218	3	8	0	0	0
2	J	145	1188	744	217	217	3	7	0	0	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	0	MSE	-	CLONING ARTIFACT	UNP Q14691
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q14691
B	7	MSE	MET	MODIFIED RESIDUE	UNP Q14691
B	36	MSE	MET	MODIFIED RESIDUE	UNP Q14691
B	97	ILE	VAL	SEE REMARK 999	UNP Q14691
B	106	MSE	MET	MODIFIED RESIDUE	UNP Q14691
B	111	MSE	MET	MODIFIED RESIDUE	UNP Q14691
B	125	MSE	MET	MODIFIED RESIDUE	UNP Q14691
B	140	MSE	MET	MODIFIED RESIDUE	UNP Q14691
F	0	MSE	-	CLONING ARTIFACT	UNP Q14691
F	1	MSE	MET	MODIFIED RESIDUE	UNP Q14691
F	7	MSE	MET	MODIFIED RESIDUE	UNP Q14691
F	36	MSE	MET	MODIFIED RESIDUE	UNP Q14691
F	97	ILE	VAL	SEE REMARK 999	UNP Q14691
F	106	MSE	MET	MODIFIED RESIDUE	UNP Q14691
F	111	MSE	MET	MODIFIED RESIDUE	UNP Q14691
F	125	MSE	MET	MODIFIED RESIDUE	UNP Q14691
F	140	MSE	MET	MODIFIED RESIDUE	UNP Q14691
J	0	MSE	-	CLONING ARTIFACT	UNP Q14691
J	1	MSE	MET	MODIFIED RESIDUE	UNP Q14691
J	7	MSE	MET	MODIFIED RESIDUE	UNP Q14691
J	36	MSE	MET	MODIFIED RESIDUE	UNP Q14691
J	97	ILE	VAL	SEE REMARK 999	UNP Q14691
J	106	MSE	MET	MODIFIED RESIDUE	UNP Q14691
J	111	MSE	MET	MODIFIED RESIDUE	UNP Q14691
J	125	MSE	MET	MODIFIED RESIDUE	UNP Q14691
J	140	MSE	MET	MODIFIED RESIDUE	UNP Q14691

- Molecule 3 is a protein called DNA replication complex GINS protein PSF2.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
3	C	168	1369	876	230	253	1	9	0	0	0
			Total	C	N	O	S	Se			
3	G	176	1432	916	242	264	1	9	0	0	0
			Total	C	N	O	S	Se			
3	K	175	1423	911	240	262	1	9	0	0	0

There are 27 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	0	MSE	-	CLONING ARTIFACT	UNP Q9Y248
C	1	MSE	MET	MODIFIED RESIDUE	UNP Q9Y248
C	66	MSE	MET	MODIFIED RESIDUE	UNP Q9Y248
C	74	MSE	MET	MODIFIED RESIDUE	UNP Q9Y248
C	87	MSE	MET	MODIFIED RESIDUE	UNP Q9Y248
C	93	MSE	MET	MODIFIED RESIDUE	UNP Q9Y248
C	120	MSE	MET	MODIFIED RESIDUE	UNP Q9Y248
C	151	MSE	MET	MODIFIED RESIDUE	UNP Q9Y248
C	167	MSE	MET	MODIFIED RESIDUE	UNP Q9Y248
G	0	MSE	-	CLONING ARTIFACT	UNP Q9Y248
G	1	MSE	MET	MODIFIED RESIDUE	UNP Q9Y248
G	66	MSE	MET	MODIFIED RESIDUE	UNP Q9Y248
G	74	MSE	MET	MODIFIED RESIDUE	UNP Q9Y248
G	87	MSE	MET	MODIFIED RESIDUE	UNP Q9Y248
G	93	MSE	MET	MODIFIED RESIDUE	UNP Q9Y248
G	120	MSE	MET	MODIFIED RESIDUE	UNP Q9Y248
G	151	MSE	MET	MODIFIED RESIDUE	UNP Q9Y248
G	167	MSE	MET	MODIFIED RESIDUE	UNP Q9Y248
K	0	MSE	-	CLONING ARTIFACT	UNP Q9Y248
K	1	MSE	MET	MODIFIED RESIDUE	UNP Q9Y248
K	66	MSE	MET	MODIFIED RESIDUE	UNP Q9Y248
K	74	MSE	MET	MODIFIED RESIDUE	UNP Q9Y248
K	87	MSE	MET	MODIFIED RESIDUE	UNP Q9Y248
K	93	MSE	MET	MODIFIED RESIDUE	UNP Q9Y248
K	120	MSE	MET	MODIFIED RESIDUE	UNP Q9Y248
K	151	MSE	MET	MODIFIED RESIDUE	UNP Q9Y248
K	167	MSE	MET	MODIFIED RESIDUE	UNP Q9Y248

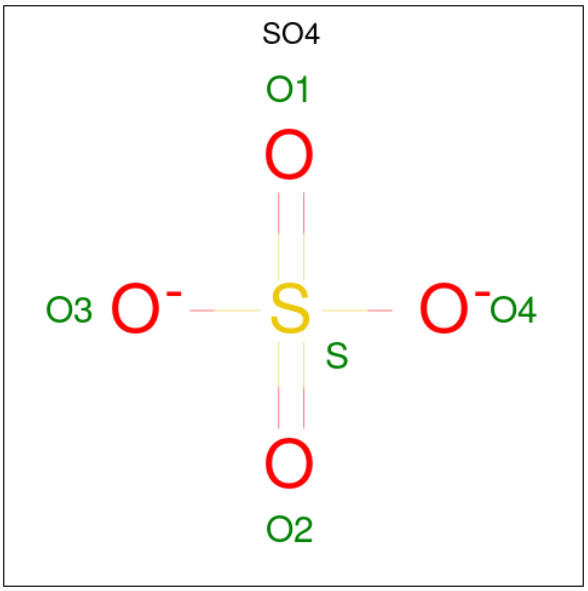
- Molecule 4 is a protein called GINS complex subunit 3.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
4	D	182	1462	931	251	274	1	5	0	0	0
4	H	183	1470	935	253	276	1	5	0	0	0
4	L	182	1462	931	252	273	1	5	0	0	0

There are 18 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MSE	MET	MODIFIED RESIDUE	UNP Q9BRX5
D	27	MSE	MET	MODIFIED RESIDUE	UNP Q9BRX5
D	40	MSE	MET	MODIFIED RESIDUE	UNP Q9BRX5
D	112	MSE	MET	MODIFIED RESIDUE	UNP Q9BRX5
D	150	MSE	MET	MODIFIED RESIDUE	UNP Q9BRX5
D	171	MSE	MET	MODIFIED RESIDUE	UNP Q9BRX5
H	1	MSE	MET	MODIFIED RESIDUE	UNP Q9BRX5
H	27	MSE	MET	MODIFIED RESIDUE	UNP Q9BRX5
H	40	MSE	MET	MODIFIED RESIDUE	UNP Q9BRX5
H	112	MSE	MET	MODIFIED RESIDUE	UNP Q9BRX5
H	150	MSE	MET	MODIFIED RESIDUE	UNP Q9BRX5
H	171	MSE	MET	MODIFIED RESIDUE	UNP Q9BRX5
L	1	MSE	MET	MODIFIED RESIDUE	UNP Q9BRX5
L	27	MSE	MET	MODIFIED RESIDUE	UNP Q9BRX5
L	40	MSE	MET	MODIFIED RESIDUE	UNP Q9BRX5
L	112	MSE	MET	MODIFIED RESIDUE	UNP Q9BRX5
L	150	MSE	MET	MODIFIED RESIDUE	UNP Q9BRX5
L	171	MSE	MET	MODIFIED RESIDUE	UNP Q9BRX5

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	O	S			
5	A	1	5	4	1		0	0
5	B	1	5	4	1		0	0
5	E	1	5	4	1		0	0
5	E	1	5	4	1		0	0
5	E	1	5	4	1		0	0
5	E	1	5	4	1		0	0
5	F	1	5	4	1		0	0
5	F	1	5	4	1		0	0
5	F	1	5	4	1		0	0
5	F	1	5	4	1		0	0
5	I	1	5	4	1		0	0
5	I	1	5	4	1		0	0
5	I	1	5	4	1		0	0
5	J	1	5	4	1		0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	O	S		
5	K	1	5	4	1	0	0
			Total	O	S		
5	L	1	5	4	1	0	0
			Total	O	S		
5	L	1	5	4	1	0	0

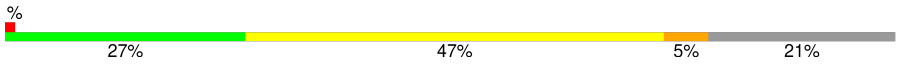
- Molecule 6 is water.

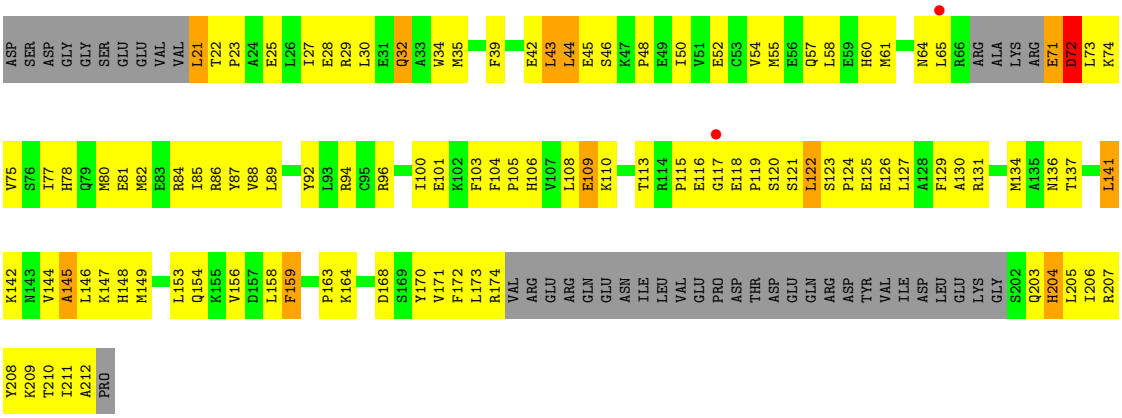
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
6	A	8	8	8	0	0
			Total	O		
6	B	5	5	5	0	0
			Total	O		
6	C	2	2	2	0	0
			Total	O		
6	D	1	1	1	0	0
			Total	O		
6	E	22	22	22	0	0
			Total	O		
6	F	11	11	11	0	0
			Total	O		
6	G	6	6	6	0	0
			Total	O		
6	H	7	7	7	0	0
			Total	O		
6	I	18	18	18	0	0
			Total	O		
6	J	23	23	23	0	0
			Total	O		
6	K	13	13	13	0	0
			Total	O		
6	L	19	19	19	0	0

3 Residue-property plots (i)

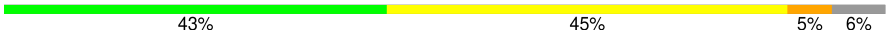
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

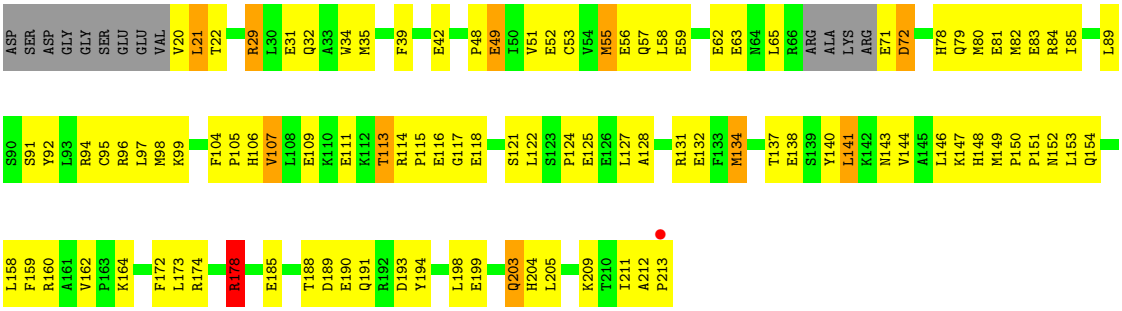
• Molecule 1: GINS complex subunit 4

Chain A: 

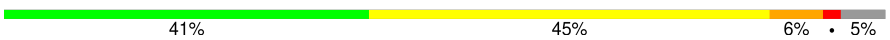


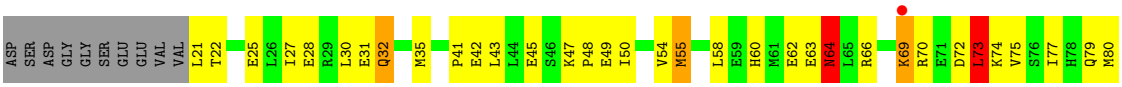
• Molecule 1: GINS complex subunit 4

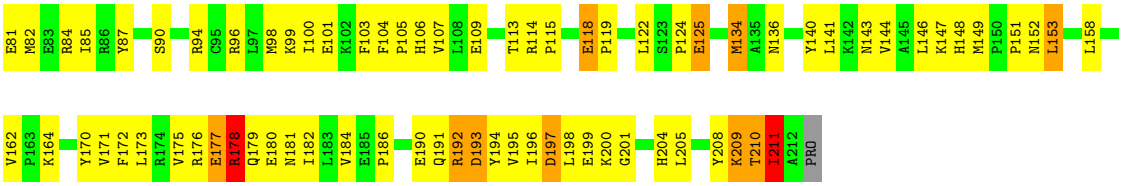
Chain E: 



• Molecule 1: GINS complex subunit 4

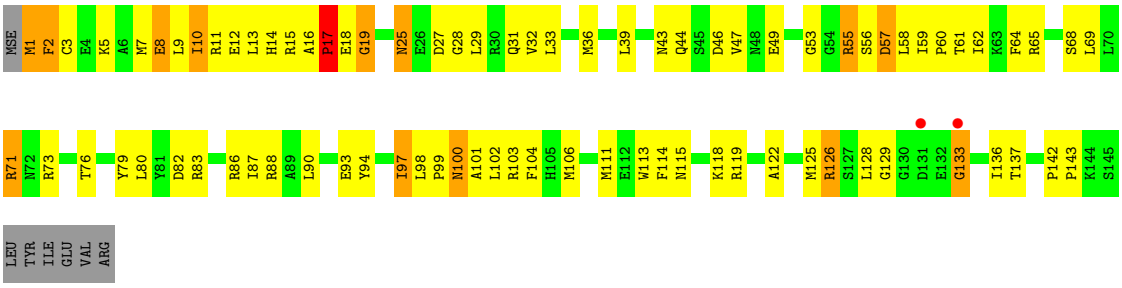
Chain I: 





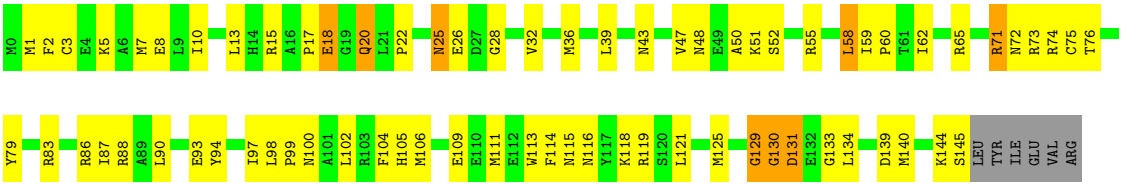
• Molecule 2: DNA replication complex GINS protein PSF1

Chain B:



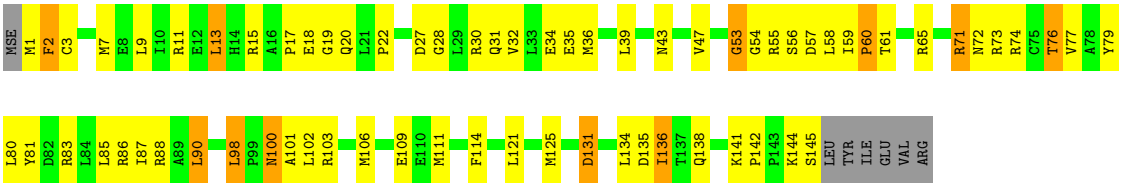
• Molecule 2: DNA replication complex GINS protein PSF1

Chain F:



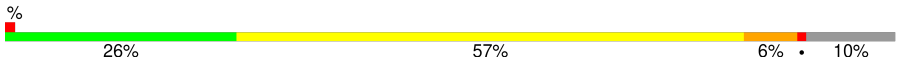
• Molecule 2: DNA replication complex GINS protein PSF1

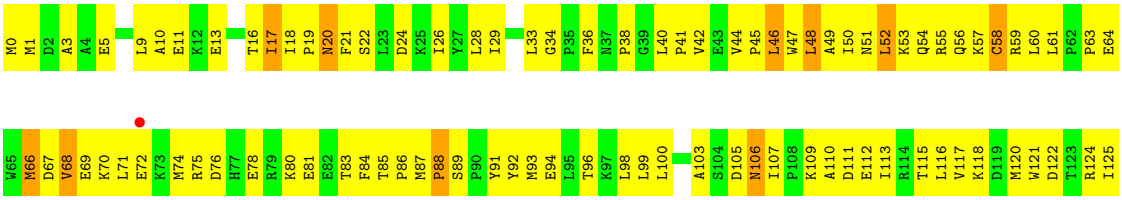
Chain J:



• Molecule 3: DNA replication complex GINS protein PSF2

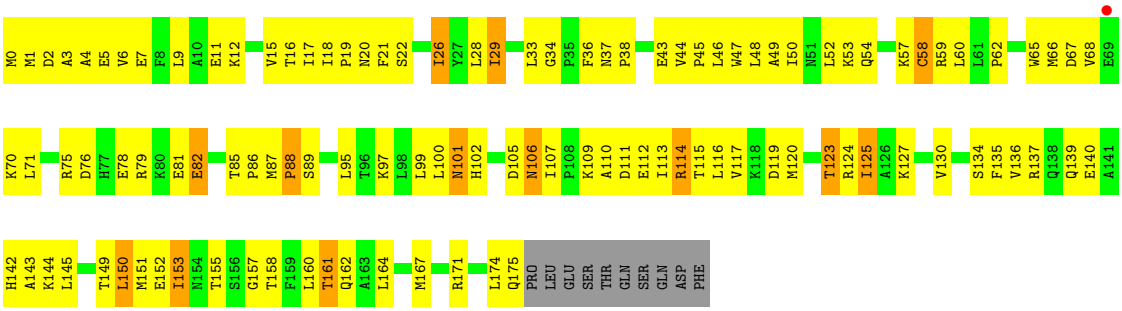
Chain C:





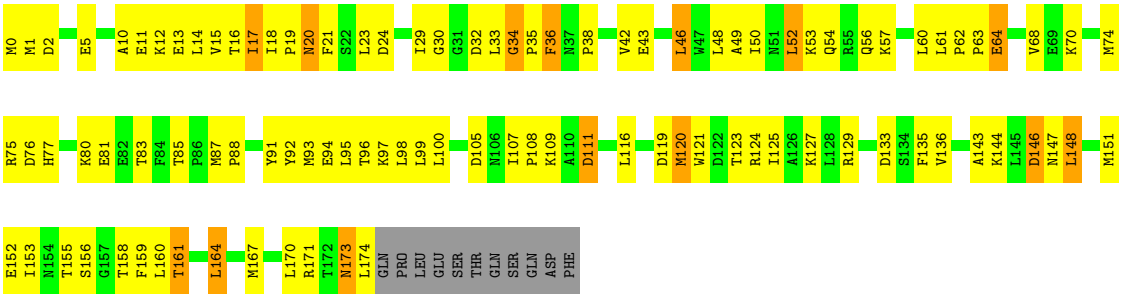
• Molecule 3: DNA replication complex GINS protein PSF2

Chain G:



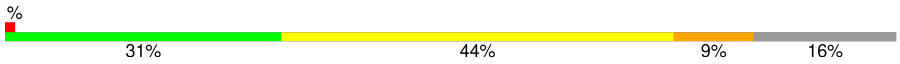
• Molecule 3: DNA replication complex GINS protein PSF2

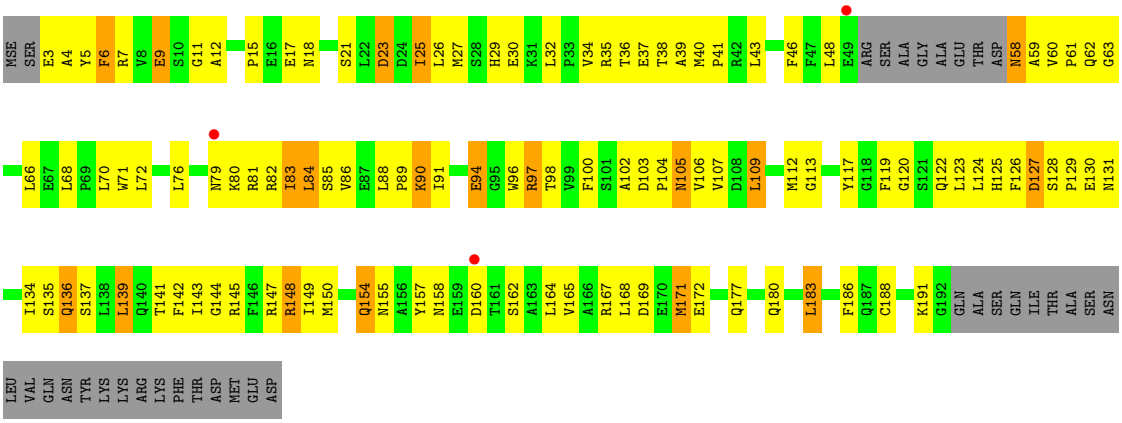
Chain K:



• Molecule 4: GINS complex subunit 3

Chain D:





• Molecule 4: GINS complex subunit 3

Chain H:

MSE SER E3 A4 Y5 S10 L13 F19 L20 S21 D24 I25 L26 M27 S28 H29 E30 K31 L32 P33 V34 R35 T36 E37 T38 P41 R42 L43 G44 A45 F46 F47 L48 GLU ARG SER ALA GLY ALA GLU THR D57 N58 A59 V60 P61 Q62 G63 S64 K65 L66 E67 L68 P69 L70

W71 L72 L76 F77 R81 L84 S85 V86 E87 L88 I91 G95 V99 D103 V106 V107 D108 L109 M112 L124 S128 P129 E130 N131 I134 S135 Q136 S137 L138 L139 Q140 T141 F142 I143 G144 R145 F146 R147 R148 I149 M150 D151 S152 S153 Q154 N158 E159

D160 T161 S162 A163 L164 V165 A166 R167 L168 D169 E170 M171 E172 R173 G174 L175 T178 L183 N184 D185 F186 Q187 C188 W189 E190 K191 G192 Q193 ALA SER GLN ILE THR ALA SER ASN LEU VAL GLN ASN TYR LYS LYS ARG LYS PHE THR ASP MET GLU ASP

- Molecule 4: GINS complex subunit 3

Chain L: 37% 38% 8% • 16%

MSE SER E3 A4 Y5 F6 L13 G14 P15 E16 E17 N18 I25 L26 M27 L32 P33 V34 T38 A39 M40 P41 R42 L43 G44 A45 F46 F47 L48 GLU ARG SER ALA GLY ALA GLU THR ASP N58 A59 V60 P61 Q62 G63 L66 E67 L68 P69 L70 W71 F77 D78 N79 K80

R81 L84 S85 V86 E87 L88 P89 K90 I91 Y92 Q93 E94 G95 F100 S101 A102 D103 P104 N105 V106 V107 D108 L109 H110 K111 M112 G113 F119 G120 S121 Q122 L123 L124 H125 F126 E130 I134 S135 Q136 S137 L138 L139 Q140 T141 F142 I143 G144 R145 F146 R147 R148 I149 M150 D151 S152

S153 Q154 N155 N158 E159 D160 T161 L164 R167 L168 D169 E170 M171 L175 L183 N184 D185 F186 W189 E190 K191 G192 Q193 ALA SER GLN ILE THR ALA SER ASN LEU VAL GLN ASN TYR LYS LYS ARG LYS PHE THR ASP MET GLU ASP

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	164.94Å 177.00Å 126.51Å 90.00° 105.91° 90.00°	Depositor
Resolution (Å)	29.90 – 3.00 50.08 – 2.81	Depositor EDS
% Data completeness (in resolution range)	91.9 (29.90-3.00) 96.0 (50.08-2.81)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.01	Depositor
$< I/\sigma(I) >$ [1]	2.58 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.221 , 0.274 0.216 , 0.266	Depositor DCC
R_{free} test set	4073 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å^2)	52.9	Xtriage
Anisotropy	0.240	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 66.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	16937	wwPDB-VP
Average B, all atoms (Å^2)	58.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.95% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: SO4

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	0.34	0/1359	0.56	1/1814 (0.1%)
1	E	0.42	0/1606	0.67	1/2150 (0.0%)
1	I	0.43	0/1627	0.85	9/2177 (0.4%)
2	B	0.37	0/1205	0.60	0/1608
2	F	0.42	0/1212	0.62	0/1615
2	J	0.44	0/1205	0.64	0/1608
3	C	0.32	0/1389	0.58	0/1866
3	G	0.37	0/1454	0.59	0/1955
3	K	0.42	0/1445	0.64	0/1943
4	D	0.35	0/1491	0.59	0/2003
4	H	0.46	0/1499	0.70	0/2014
4	L	0.76	4/1491 (0.3%)	1.04	12/2003 (0.6%)
All	All	0.44	4/16983 (0.0%)	0.69	23/22756 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
4	L	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	L	58	ASN	C-O	18.93	1.59	1.23
4	L	60	VAL	C-O	10.76	1.43	1.23
4	L	41	PRO	N-CD	8.00	1.59	1.47
4	L	38	THR	C-O	-6.51	1.10	1.23

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	L	38	THR	O-C-N	-15.98	97.13	122.70
4	L	60	VAL	O-C-N	13.99	147.68	121.10
4	L	60	VAL	CA-C-O	-12.51	93.82	120.10
1	I	211	ILE	CB-CA-C	-12.32	86.97	111.60
4	L	38	THR	CA-C-O	11.87	145.02	120.10
4	L	58	ASN	O-C-N	-11.66	104.05	122.70
1	I	192	ARG	N-CA-C	-8.76	87.35	111.00
1	I	211	ILE	N-CA-CB	-8.69	90.82	110.80
1	I	193	ASP	N-CA-CB	8.46	125.83	110.60
1	I	179	GLN	N-CA-CB	7.85	124.74	110.60
4	L	40	MSE	CB-CA-C	7.64	125.68	110.40
4	L	39	ALA	N-CA-C	-7.50	90.75	111.00
1	I	193	ASP	N-CA-C	-7.33	91.22	111.00
1	I	178	ARG	CB-CA-C	7.17	124.75	110.40
4	L	38	THR	N-CA-C	-7.00	92.11	111.00
4	L	38	THR	CB-CA-C	6.37	128.81	111.60
1	I	209	LYS	N-CA-C	-6.19	94.29	111.00
4	L	113	GLY	N-CA-C	-5.81	98.57	113.10
1	A	122	LEU	CA-CB-CG	5.54	128.05	115.30
1	E	117	GLY	N-CA-C	-5.44	99.51	113.10
4	L	61	PRO	N-CA-C	5.41	126.16	112.10
4	L	40	MSE	C-N-CD	-5.39	108.74	120.60
1	I	73	LEU	CA-CB-CG	5.07	126.95	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
4	L	58	ASN	Mainchain

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	1340	0	1353	130	0
1	E	1583	0	1587	118	0
1	I	1604	0	1616	134	0
2	B	1188	0	1180	110	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	1196	0	1189	83	0
2	J	1188	0	1180	81	0
3	C	1369	0	1391	153	0
3	G	1432	0	1458	112	0
3	K	1423	0	1450	117	0
4	D	1462	0	1418	126	0
4	H	1470	0	1424	115	0
4	L	1462	0	1420	115	0
5	A	5	0	0	0	0
5	B	5	0	0	5	0
5	E	20	0	0	0	0
5	F	20	0	0	5	0
5	I	15	0	0	1	0
5	J	5	0	0	0	0
5	K	5	0	0	0	0
5	L	10	0	0	0	0
6	A	8	0	0	2	0
6	B	5	0	0	3	0
6	C	2	0	0	0	0
6	D	1	0	0	0	0
6	E	22	0	0	5	0
6	F	11	0	0	1	0
6	G	6	0	0	0	0
6	H	7	0	0	0	0
6	I	18	0	0	6	0
6	J	23	0	0	1	0
6	K	13	0	0	2	0
6	L	19	0	0	5	0
All	All	16937	0	16666	1234	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 37.

All (1234) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:211:ILE:CG2	1:I:211:ILE:O	1.92	1.18
1:I:144:VAL:HG22	2:J:109:GLU:HG3	1.29	1.13
4:L:13:LEU:HD21	4:L:171:MSE:HE2	1.27	1.11
1:I:149:MSE:HE3	2:J:36:MSE:HE1	1.15	1.10
4:L:90:LYS:HE3	4:L:90:LYS:H	1.12	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:16:THR:HG22	3:G:43:GLU:HG2	1.37	1.07
4:D:80:LYS:HG2	4:D:82:ARG:HE	1.21	1.04
1:E:35:MSE:HG2	6:E:1028:HOH:O	1.61	1.01
1:I:211:ILE:O	1:I:211:ILE:HG22	1.55	1.00
3:K:93:MSE:HE1	3:K:121:TRP:HB2	1.43	1.00
3:K:87:MSE:HE2	3:K:124:ARG:HD2	1.40	1.00
1:I:80:MSE:HE3	2:J:145:SER:HB2	1.40	1.00
4:D:90:LYS:HE3	4:D:90:LYS:H	1.24	1.00
1:I:101:GLU:OE2	2:J:88:ARG:HD3	1.62	0.99
1:A:171:VAL:HG12	1:A:172:PHE:H	1.25	0.99
1:E:144:VAL:HG22	2:F:109:GLU:HG3	1.44	0.99
3:G:66:MSE:HE1	3:G:100:LEU:HD11	1.44	0.99
1:I:186:PRO:HD2	1:I:192:ARG:O	1.61	0.98
4:L:38:THR:O	4:L:62:GLN:HA	1.61	0.98
3:K:75:ARG:NH2	3:K:119:ASP:HB3	1.80	0.97
3:G:44:VAL:HG21	3:G:48:LEU:HD22	1.43	0.97
3:K:57:LYS:HA	3:K:57:LYS:HE2	1.44	0.97
2:J:17:PRO:HB2	2:J:20:GLN:HG3	1.44	0.96
4:D:35:ARG:HB3	4:D:85:SER:HB2	1.47	0.95
3:K:75:ARG:HH22	3:K:119:ASP:HB3	1.28	0.95
3:K:87:MSE:HE3	3:K:92:TYR:CZ	2.01	0.95
4:H:91:ILE:HD13	4:H:112:MSE:HE2	1.48	0.93
1:I:27:ILE:HD13	3:K:29:ILE:HD11	1.50	0.91
2:B:12:GLU:HG3	2:F:17:PRO:HG3	1.54	0.90
4:H:88:LEU:HD12	4:H:88:LEU:H	1.35	0.90
4:H:34:VAL:HG21	4:H:84:LEU:HD12	1.55	0.89
4:H:109:LEU:HD22	4:H:145:ARG:NH2	1.88	0.89
2:B:98:LEU:HD21	2:B:114:PHE:CE2	2.08	0.88
1:I:211:ILE:O	1:I:211:ILE:HG23	1.74	0.88
2:J:98:LEU:HD23	2:J:106:MSE:HE1	1.54	0.88
3:G:1:MSE:HE3	3:G:6:VAL:HG22	1.56	0.88
3:C:66:MSE:HE1	3:C:99:LEU:HD12	1.56	0.87
1:A:149:MSE:HE1	2:B:73:ARG:HG3	1.55	0.86
1:I:149:MSE:HE2	1:I:153:LEU:O	1.75	0.86
1:E:212:ALA:HB3	1:E:213:PRO:HD3	1.57	0.86
3:K:93:MSE:CE	3:K:121:TRP:HB2	2.06	0.85
1:E:149:MSE:HE3	2:F:36:MSE:HE1	1.58	0.85
3:K:87:MSE:HE3	3:K:92:TYR:CE1	2.11	0.85
1:E:209:LYS:O	1:E:213:PRO:HD2	1.76	0.85
1:A:23:PRO:HG3	1:A:57:GLN:NE2	1.90	0.85
3:C:75:ARG:HH11	3:C:75:ARG:HB3	1.42	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:20:ASN:C	3:K:20:ASN:HD22	1.80	0.85
3:K:17:ILE:HG22	3:K:60:LEU:HD13	1.60	0.84
4:L:41:PRO:O	4:L:42:ARG:HG2	1.77	0.83
1:E:109:GLU:HG3	1:E:159:PHE:CE1	2.13	0.83
2:J:17:PRO:HB2	2:J:20:GLN:CG	2.09	0.83
2:B:28:GLY:O	2:B:32:VAL:HG23	1.77	0.83
2:J:121:LEU:HG	2:J:125:MSE:HE2	1.60	0.83
3:G:18:ILE:HG23	3:G:59:ARG:HB3	1.59	0.83
3:K:133:ASP:OD2	4:L:147:ARG:HG2	1.79	0.82
3:C:71:LEU:HD12	3:C:113:ILE:HD11	1.61	0.82
2:J:71:ARG:HG3	2:J:71:ARG:HH11	1.45	0.82
3:G:1:MSE:HE1	3:G:150:LEU:HD13	1.61	0.81
4:L:90:LYS:HE3	4:L:90:LYS:N	1.94	0.81
1:A:163:PRO:HB3	4:D:18:ASN:HD21	1.46	0.81
4:D:90:LYS:H	4:D:90:LYS:CE	1.92	0.81
3:K:92:TYR:CE2	3:K:93:MSE:HE2	2.15	0.81
3:C:75:ARG:HB3	3:C:75:ARG:NH1	1.97	0.80
3:G:136:VAL:HG12	4:H:143:ILE:HG23	1.62	0.80
3:K:87:MSE:CE	3:K:124:ARG:HD2	2.10	0.80
1:I:104:PHE:CG	1:I:105:PRO:HD3	2.17	0.80
1:I:32:GLN:HE21	1:I:176:ARG:HE	1.31	0.80
4:L:91:ILE:HD12	4:L:112:MSE:HB3	1.64	0.80
1:I:80:MSE:HE3	2:J:145:SER:CB	2.12	0.79
4:H:34:VAL:HG11	4:H:68:LEU:HG	1.62	0.79
2:J:73:ARG:O	2:J:77:VAL:HG23	1.82	0.79
3:C:139:GLN:NE2	3:C:171:ARG:HD3	1.98	0.79
1:I:73:LEU:HD12	1:I:74:LYS:N	1.98	0.79
1:E:55:MSE:HE3	1:E:89:LEU:HD23	1.65	0.78
4:L:105:ASN:HD21	4:L:145:ARG:HA	1.48	0.78
4:H:109:LEU:HD22	4:H:145:ARG:HH21	1.46	0.77
1:A:27:ILE:HD12	1:A:85:ILE:HD12	1.65	0.77
2:B:98:LEU:HD21	2:B:114:PHE:HE2	1.48	0.77
2:J:30:ARG:O	2:J:34:GLU:HG2	1.83	0.77
4:H:193:GLN:HE21	4:H:193:GLN:HA	1.49	0.77
4:D:34:VAL:CG2	4:D:84:LEU:HG	2.15	0.77
4:D:34:VAL:HG21	4:D:84:LEU:HG	1.66	0.77
2:J:72:ASN:O	2:J:76:THR:HG23	1.83	0.77
4:L:90:LYS:H	4:L:90:LYS:CE	1.95	0.77
1:E:134:MSE:HE3	1:E:158:LEU:HD12	1.67	0.77
1:E:173:LEU:HD22	1:E:211:ILE:HD13	1.66	0.77
2:J:88:ARG:HH22	4:L:6:PHE:HZ	1.32	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:49:ALA:HB1	3:C:60:LEU:HD21	1.67	0.76
2:J:43:ASN:O	2:J:47:VAL:HG23	1.84	0.76
2:F:59:ILE:HB	2:F:60:PRO:HD3	1.67	0.76
3:G:123:THR:O	3:G:127:LYS:HG3	1.86	0.76
3:K:87:MSE:HE2	3:K:124:ARG:CD	2.14	0.76
1:E:149:MSE:HE1	2:F:73:ARG:CD	2.16	0.76
1:A:149:MSE:HE1	2:B:73:ARG:CG	2.15	0.75
1:I:204:HIS:HE1	3:K:144:LYS:HE3	1.51	0.75
1:A:35:MSE:HE3	3:C:1:MSE:SE	2.36	0.75
3:C:106:ASN:N	3:C:106:ASN:HD22	1.85	0.75
2:J:71:ARG:HH11	2:J:71:ARG:CG	2.00	0.75
3:K:93:MSE:HE3	3:K:121:TRP:CE3	2.21	0.75
1:E:134:MSE:CE	1:E:158:LEU:HD12	2.17	0.75
2:J:59:ILE:HB	2:J:60:PRO:HD3	1.68	0.75
3:G:66:MSE:HE3	3:G:113:ILE:HG21	1.69	0.75
1:I:81:GLU:OE2	3:K:29:ILE:HG13	1.87	0.74
4:D:94:GLU:HB3	4:D:97:ARG:HH21	1.50	0.74
4:H:38:THR:HA	4:H:62:GLN:HG3	1.69	0.74
1:I:180:GLU:O	1:I:197:ASP:HA	1.87	0.74
3:K:93:MSE:HE3	3:K:121:TRP:HE3	1.51	0.74
3:G:60:LEU:O	3:G:62:PRO:HD3	1.87	0.74
1:A:118:GLU:HB2	1:A:119:PRO:HD2	1.69	0.74
3:C:160:LEU:O	3:C:164:LEU:HD23	1.88	0.74
2:B:61:THR:HG23	4:D:43:LEU:HD13	1.70	0.73
3:G:44:VAL:HG22	3:G:45:PRO:HD2	1.68	0.73
3:C:48:LEU:HD22	3:C:52:LEU:HD22	1.70	0.73
4:H:158:ASN:C	4:H:158:ASN:HD22	1.92	0.73
2:B:99:PRO:HB2	2:B:102:LEU:HD23	1.69	0.73
4:D:141:THR:O	4:D:145:ARG:HG3	1.87	0.73
3:C:20:ASN:C	3:C:20:ASN:HD22	1.92	0.72
3:C:67:ASP:HB3	3:C:70:LYS:HB2	1.70	0.72
1:I:73:LEU:O	1:I:77:ILE:HG12	1.88	0.72
1:A:163:PRO:HB3	4:D:18:ASN:ND2	2.02	0.72
1:I:124:PRO:HG2	1:I:125:GLU:OE1	1.88	0.72
1:A:108:LEU:HD11	1:A:130:ALA:O	1.89	0.72
1:A:122:LEU:HD11	1:A:127:LEU:HA	1.70	0.72
2:F:1:MSE:HB2	5:F:1004:SO4:S	2.30	0.72
3:G:97:LYS:O	3:G:101:ASN:HB2	1.90	0.72
1:I:200:LYS:HD3	1:I:200:LYS:C	2.09	0.72
3:K:29:ILE:HD12	3:K:29:ILE:C	2.10	0.72
2:B:8:GLU:HG3	6:F:1015:HOH:O	1.89	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:22:PRO:O	2:J:83:ARG:NH2	2.22	0.72
3:C:72:GLU:HA	3:C:116:LEU:HD11	1.70	0.71
1:I:172:PHE:HB3	3:K:0:MSE:HE1	1.72	0.71
4:D:27:MSE:HE1	4:D:122:GLN:HG3	1.72	0.71
1:E:128:ALA:O	1:E:132:GLU:HG3	1.89	0.71
2:F:7:MSE:HE3	2:F:71:ARG:NH1	2.05	0.71
3:G:100:LEU:HD23	3:G:114:ARG:HB2	1.72	0.71
1:E:71:GLU:O	1:E:72:ASP:HB2	1.90	0.71
1:E:149:MSE:HE2	1:E:153:LEU:HB3	1.73	0.71
1:E:124:PRO:HG2	1:E:125:GLU:OE2	1.90	0.71
1:I:204:HIS:CE1	3:K:144:LYS:HE3	2.24	0.71
2:F:74:ARG:CZ	4:H:25:ILE:HG22	2.20	0.71
1:I:149:MSE:CE	2:J:36:MSE:HE1	2.09	0.71
1:A:81:GLU:O	1:A:85:ILE:HG12	1.91	0.71
1:E:211:ILE:HG13	1:E:212:ALA:N	2.06	0.71
2:J:55:ARG:HG2	2:J:57:ASP:OD2	1.91	0.71
4:D:157:TYR:HE2	4:D:162:SER:HB2	1.56	0.70
4:D:79:ASN:HA	4:D:81:ARG:NH1	2.06	0.70
1:I:109:GLU:O	1:I:113:THR:HG22	1.91	0.70
1:I:80:MSE:CE	2:J:145:SER:HB2	2.17	0.70
1:E:55:MSE:HE2	1:E:55:MSE:HA	1.72	0.70
1:I:77:ILE:HA	6:I:1009:HOH:O	1.91	0.70
1:I:74:LYS:HD2	3:K:23:LEU:HD11	1.71	0.70
3:G:71:LEU:HB2	3:G:116:LEU:HD23	1.74	0.70
3:C:93:MSE:HG3	3:C:121:TRP:CE3	2.26	0.70
1:I:177:GLU:O	1:I:178:ARG:HB2	1.92	0.70
4:L:91:ILE:CD1	4:L:112:MSE:HB3	2.22	0.70
3:K:70:LYS:O	3:K:74:MSE:HG3	1.91	0.69
2:J:55:ARG:NH2	4:L:42:ARG:HH21	1.90	0.69
4:L:38:THR:O	4:L:62:GLN:CA	2.37	0.69
1:A:106:HIS:ND1	1:A:164:LYS:HB3	2.07	0.69
4:D:128:SER:HB3	4:D:131:ASN:ND2	2.07	0.69
1:E:188:THR:HG22	1:E:189:ASP:H	1.58	0.69
3:C:120:MSE:O	3:C:124:ARG:HB2	1.92	0.69
3:K:18:ILE:CD1	3:K:61:LEU:HD13	2.23	0.69
3:K:48:LEU:HD22	3:K:52:LEU:HD22	1.75	0.69
4:D:37:GLU:HG3	4:D:81:ARG:O	1.93	0.69
1:I:35:MSE:HG2	3:K:1:MSE:HE1	1.75	0.69
2:F:71:ARG:NH2	4:H:28:SER:HB3	2.07	0.69
2:J:103:ARG:HA	2:J:106:MSE:HE3	1.74	0.68
3:K:68:VAL:HG13	3:K:116:LEU:HD11	1.73	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:158:ASN:HD22	4:H:159:GLU:N	1.91	0.68
1:I:77:ILE:HD13	6:I:1009:HOH:O	1.92	0.68
1:A:108:LEU:HD21	1:A:131:ARG:N	2.09	0.68
2:F:115:ASN:HA	2:F:118:LYS:HG2	1.74	0.68
1:I:90:SER:HB3	1:I:94:ARG:HH21	1.58	0.68
4:H:148:ARG:HG3	4:H:148:ARG:HH11	1.59	0.68
4:D:94:GLU:HA	4:D:97:ARG:HE	1.58	0.68
1:E:91:SER:HA	1:E:94:ARG:NH1	2.09	0.68
1:A:171:VAL:HG12	1:A:172:PHE:N	2.05	0.68
4:H:34:VAL:HG23	4:H:85:SER:O	1.93	0.68
4:H:175:LEU:O	4:H:178:THR:HG23	1.93	0.67
1:A:210:THR:HG21	6:A:1022:HOH:O	1.94	0.67
1:E:115:PRO:O	1:E:118:GLU:HB3	1.95	0.67
3:G:33:LEU:HD21	3:G:45:PRO:HD3	1.76	0.67
4:H:88:LEU:H	4:H:88:LEU:CD1	2.07	0.67
4:H:145:ARG:O	4:H:149:ILE:HG12	1.95	0.67
4:H:149:ILE:CD1	4:H:168:LEU:HD11	2.25	0.67
3:C:68:VAL:HG11	3:C:112:GLU:OE2	1.93	0.67
2:F:88:ARG:NH2	5:F:1010:SO4:O4	2.24	0.67
4:H:68:LEU:HD13	4:H:72:LEU:HD12	1.77	0.67
1:I:32:GLN:HE21	1:I:176:ARG:NE	1.93	0.67
1:A:105:PRO:HG2	1:A:106:HIS:CD2	2.29	0.67
1:E:21:LEU:N	1:E:21:LEU:HD23	2.10	0.67
1:E:143:ASN:HA	1:E:147:LYS:HE2	1.76	0.67
1:E:198:LEU:HD22	1:E:204:HIS:CD2	2.29	0.67
1:A:106:HIS:CE1	1:A:164:LYS:HB3	2.30	0.67
2:B:118:LYS:HG3	2:B:119:ARG:N	2.10	0.67
4:H:41:PRO:HA	4:H:59:ALA:HB2	1.77	0.67
4:D:94:GLU:HA	4:D:97:ARG:HB3	1.75	0.66
3:C:78:GLU:OE1	3:C:85:THR:HB	1.96	0.66
3:K:74:MSE:SE	3:K:88:PRO:HG3	2.45	0.66
2:J:27:ASP:O	2:J:31:GLN:HG3	1.95	0.66
2:B:8:GLU:HB3	6:B:1021:HOH:O	1.96	0.66
3:G:19:PRO:O	3:G:38:PRO:HA	1.95	0.66
2:F:39:LEU:HD23	2:F:65:ARG:HD3	1.75	0.66
2:J:19:GLY:HA2	4:L:5:TYR:CD2	2.31	0.66
1:A:149:MSE:CE	2:B:73:ARG:HG3	2.25	0.66
1:I:209:LYS:HE3	5:I:1001:SO4:O3	1.96	0.66
2:B:83:ARG:O	2:B:87:ILE:HG13	1.96	0.66
4:D:58:ASN:N	4:D:58:ASN:HD22	1.94	0.65
1:E:134:MSE:O	1:E:138:GLU:HB2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:91:ILE:CD1	4:H:112:MSE:HE2	2.26	0.65
4:L:41:PRO:O	4:L:42:ARG:CG	2.45	0.65
4:L:148:ARG:HH11	4:L:148:ARG:HG3	1.61	0.65
1:I:27:ILE:O	1:I:31:GLU:HG3	1.96	0.65
2:B:10:ILE:HG13	4:D:25:ILE:HD11	1.78	0.65
4:D:80:LYS:CG	4:D:82:ARG:HE	2.03	0.65
3:C:44:VAL:HG22	3:C:45:PRO:HD2	1.79	0.65
3:G:21:PHE:O	3:G:38:PRO:HD3	1.97	0.65
4:L:3:GLU:HG3	4:L:5:TYR:H	1.62	0.65
4:L:58:ASN:ND2	4:L:59:ALA:H	1.95	0.65
1:E:140:TYR:CE1	1:E:144:VAL:HG21	2.31	0.65
1:E:173:LEU:HD22	1:E:211:ILE:CD1	2.26	0.65
1:I:31:GLU:OE2	3:K:12:LYS:HE3	1.96	0.65
1:A:104:PHE:CD1	1:A:105:PRO:HD3	2.32	0.65
2:B:17:PRO:HG2	2:F:94:TYR:OH	1.97	0.65
3:C:75:ARG:HH11	3:C:75:ARG:CB	2.10	0.65
4:D:38:THR:HA	4:D:62:GLN:NE2	2.11	0.65
3:C:33:LEU:HD22	3:C:44:VAL:HG23	1.79	0.65
3:C:151:MSE:HE3	4:D:186:PHE:HD2	1.62	0.65
1:E:134:MSE:HE2	1:E:138:GLU:CD	2.17	0.65
3:K:18:ILE:HD13	3:K:61:LEU:HD13	1.77	0.64
1:A:23:PRO:HG3	1:A:57:GLN:HE22	1.63	0.64
3:C:18:ILE:HG13	3:C:18:ILE:O	1.97	0.64
1:E:21:LEU:HD23	1:E:21:LEU:H	1.61	0.64
1:I:149:MSE:HE1	2:J:73:ARG:HD2	1.79	0.64
3:C:137:ARG:HH11	3:C:137:ARG:HB2	1.62	0.64
6:E:1028:HOH:O	3:G:1:MSE:SE	2.64	0.64
3:G:119:ASP:O	3:G:123:THR:HG23	1.97	0.64
4:H:21:SER:HB3	4:H:24:ASP:HB2	1.79	0.64
4:H:68:LEU:HD13	4:H:72:LEU:CD1	2.28	0.64
3:K:20:ASN:C	3:K:20:ASN:ND2	2.51	0.64
1:A:29:ARG:HG2	1:A:50:ILE:CD1	2.27	0.64
2:B:98:LEU:N	2:B:98:LEU:HD22	2.12	0.64
1:E:85:ILE:HG13	3:G:29:ILE:HD11	1.79	0.64
3:G:44:VAL:CG2	3:G:48:LEU:HD22	2.21	0.64
1:I:180:GLU:HG2	1:I:181:ASN:H	1.60	0.64
4:L:109:LEU:HD22	4:L:145:ARG:CZ	2.27	0.64
4:D:43:LEU:O	4:D:60:VAL:HG13	1.98	0.64
1:E:172:PHE:CD2	3:G:0:MSE:HE1	2.33	0.64
4:H:21:SER:O	4:H:25:ILE:HG23	1.98	0.64
4:H:193:GLN:HA	4:H:193:GLN:NE2	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:61:MSE:HE2	1:A:61:MSE:HA	1.80	0.64
4:D:105:ASN:HB3	4:D:148:ARG:HD2	1.79	0.64
3:G:26:ILE:HG13	3:G:33:LEU:HB2	1.80	0.64
2:B:7:MSE:O	2:B:10:ILE:HD13	1.98	0.63
3:C:74:MSE:HE1	3:C:88:PRO:HG3	1.80	0.63
1:E:56:GLU:O	1:E:59:GLU:HG2	1.97	0.63
4:D:90:LYS:HE3	4:D:90:LYS:N	2.06	0.63
1:E:48:PRO:O	1:E:52:GLU:HG2	1.98	0.63
3:G:67:ASP:HB3	3:G:70:LYS:HD3	1.79	0.63
1:I:45:GLU:OE2	1:I:119:PRO:HB2	1.98	0.63
6:I:1015:HOH:O	2:J:88:ARG:HD2	1.98	0.63
1:A:77:ILE:HD12	3:C:48:LEU:HD21	1.80	0.63
1:E:149:MSE:HE1	2:F:73:ARG:HD3	1.81	0.63
4:H:41:PRO:HA	4:H:59:ALA:CB	2.29	0.63
4:H:88:LEU:HD12	4:H:88:LEU:N	2.12	0.63
2:B:43:ASN:O	2:B:47:VAL:HG23	1.98	0.63
3:C:153:ILE:HG13	3:C:154:ASN:ND2	2.13	0.63
3:K:173:ASN:HD22	3:K:174:LEU:N	1.97	0.63
1:I:149:MSE:HE1	2:J:73:ARG:CG	2.29	0.63
1:I:196:ILE:HG22	1:I:197:ASP:N	2.14	0.63
1:A:48:PRO:O	1:A:52:GLU:HG2	1.98	0.62
2:J:144:LYS:C	2:J:144:LYS:HD3	2.19	0.62
2:B:64:PHE:CE1	4:D:72:LEU:HD21	2.34	0.62
4:D:36:THR:HB	4:D:63:GLY:H	1.64	0.62
3:C:18:ILE:CG1	3:C:59:ARG:HB3	2.29	0.62
1:E:104:PHE:CG	1:E:105:PRO:HD3	2.34	0.62
3:G:109:LYS:HB3	3:G:112:GLU:HB3	1.81	0.62
2:F:74:ARG:NH2	4:H:25:ILE:HG22	2.15	0.62
1:I:58:LEU:O	1:I:62:GLU:HB2	1.98	0.62
1:I:96:ARG:O	1:I:100:ILE:HG13	1.99	0.62
1:I:140:TYR:CE1	1:I:144:VAL:HG21	2.35	0.62
1:A:96:ARG:NH1	1:A:126:GLU:OE1	2.33	0.62
2:F:144:LYS:O	2:F:145:SER:HB3	1.99	0.62
2:F:28:GLY:O	2:F:32:VAL:HG23	2.00	0.62
4:H:61:PRO:HG2	4:H:64:SER:OG	2.00	0.62
3:K:2:ASP:HB3	3:K:5:GLU:HG3	1.81	0.62
4:L:137:SER:O	4:L:141:THR:HG22	1.99	0.62
4:L:183:LEU:C	4:L:183:LEU:HD13	2.20	0.62
1:A:106:HIS:O	1:A:110:LYS:HB2	2.00	0.62
3:C:50:ILE:O	3:C:54:GLN:HG2	2.00	0.62
3:C:64:GLU:OE1	3:C:70:LYS:HE2	2.00	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:106:ASN:N	3:C:106:ASN:ND2	2.46	0.62
1:I:134:MSE:HE1	1:I:158:LEU:HB2	1.81	0.61
3:C:10:ALA:O	3:C:13:GLU:HB2	2.00	0.61
2:J:87:ILE:O	2:J:90:LEU:HB2	1.99	0.61
3:K:151:MSE:HE3	3:K:155:THR:OG1	2.00	0.61
3:C:0:MSE:HE3	3:C:158:THR:N	2.16	0.61
1:E:53:CYS:O	1:E:57:GLN:HG2	2.00	0.61
2:F:102:LEU:HD12	2:F:102:LEU:H	1.63	0.61
1:E:118:GLU:O	1:E:118:GLU:HG3	2.00	0.61
2:J:61:THR:HG23	4:L:43:LEU:HD21	1.82	0.61
1:A:123:SER:HB2	1:A:124:PRO:HD2	1.83	0.61
3:C:153:ILE:C	3:C:154:ASN:HD22	2.03	0.61
1:E:137:THR:CG2	2:F:113:TRP:HE1	2.14	0.61
4:H:168:LEU:HG	4:H:172:GLU:HB3	1.83	0.61
4:L:191:LYS:HD2	4:L:191:LYS:O	2.01	0.61
1:E:149:MSE:CE	1:E:153:LEU:HB3	2.30	0.61
3:G:120:MSE:O	3:G:124:ARG:HG3	2.01	0.60
4:H:3:GLU:HG3	4:H:5:TYR:HB3	1.82	0.60
4:L:34:VAL:HG11	4:L:68:LEU:HD12	1.82	0.60
4:D:100:PHE:HB3	4:D:141:THR:HG22	1.81	0.60
3:G:88:PRO:HG2	3:G:89:SER:H	1.66	0.60
3:G:134:SER:HA	3:G:137:ARG:HH21	1.65	0.60
1:A:110:LYS:HA	1:A:113:THR:HG22	1.82	0.60
1:A:149:MSE:HE1	2:B:73:ARG:CD	2.31	0.60
4:D:167:ARG:HG3	4:D:167:ARG:HH11	1.66	0.60
3:G:75:ARG:HD2	3:G:119:ASP:OD2	2.02	0.60
3:G:162:GLN:OE1	4:H:178:THR:HG21	2.01	0.60
1:A:30:LEU:HD22	1:A:54:VAL:HG11	1.83	0.60
4:D:180:GLN:HG2	2:F:100:ASN:HD21	1.66	0.60
2:B:73:ARG:HA	2:B:76:THR:HG22	1.82	0.60
4:L:34:VAL:HG21	4:L:84:LEU:HG	1.83	0.60
1:A:149:MSE:HE3	2:B:36:MSE:HE1	1.83	0.60
3:C:139:GLN:HB3	3:C:171:ARG:NH2	2.17	0.60
3:C:173:ASN:ND2	4:D:135:SER:HB3	2.16	0.60
3:G:144:LYS:O	3:G:145:LEU:HD23	2.02	0.60
3:G:174:LEU:H	3:G:174:LEU:HD23	1.67	0.60
1:E:52:GLU:HA	1:E:55:MSE:HB2	1.84	0.59
1:E:55:MSE:HE3	1:E:89:LEU:CD2	2.31	0.59
3:G:49:ALA:HB1	3:G:60:LEU:HD11	1.83	0.59
1:I:209:LYS:O	1:I:210:THR:CB	2.48	0.59
4:L:122:GLN:HG3	6:L:1020:HOH:O	2.01	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:GLN:O	2:B:47:VAL:HB	2.03	0.59
4:L:41:PRO:O	4:L:42:ARG:CB	2.49	0.59
4:L:137:SER:O	4:L:141:THR:CG2	2.49	0.59
3:C:19:PRO:O	3:C:38:PRO:HA	2.03	0.59
4:H:34:VAL:CG1	4:H:68:LEU:HG	2.31	0.59
1:I:104:PHE:HE1	1:I:134:MSE:HE3	1.66	0.59
2:J:11:ARG:HB3	2:J:15:ARG:NH2	2.17	0.59
2:B:16:ALA:HB3	2:B:86:ARG:HH12	1.67	0.59
2:F:7:MSE:HE3	2:F:71:ARG:HH11	1.68	0.59
2:B:61:THR:HG22	2:B:65:ARG:NH1	2.18	0.59
2:F:10:ILE:HG13	4:H:25:ILE:HD11	1.83	0.59
4:L:34:VAL:CG2	4:L:84:LEU:HG	2.33	0.59
3:C:54:GLN:C	3:C:56:GLN:H	2.05	0.59
3:C:129:ARG:HH11	3:C:129:ARG:HB2	1.68	0.59
3:G:46:LEU:O	3:G:50:ILE:HG12	2.03	0.59
1:I:170:TYR:CD1	3:K:164:LEU:HB3	2.38	0.59
2:J:88:ARG:NH2	4:L:6:PHE:CZ	2.71	0.59
3:G:66:MSE:CE	3:G:113:ILE:HG21	2.33	0.59
1:I:196:ILE:HG22	1:I:197:ASP:H	1.68	0.59
3:C:20:ASN:C	3:C:20:ASN:ND2	2.56	0.59
4:D:39:ALA:H	4:D:62:GLN:HE21	1.49	0.59
4:D:39:ALA:N	4:D:62:GLN:HG2	2.17	0.58
4:D:25:ILE:C	4:D:25:ILE:HD12	2.23	0.58
3:C:33:LEU:HD21	3:C:45:PRO:HD3	1.85	0.58
4:D:103:ASP:O	4:D:106:VAL:HG12	2.03	0.58
4:D:117:TYR:CE1	4:D:142:PHE:HB2	2.37	0.58
4:L:38:THR:HA	4:L:62:GLN:HE21	1.68	0.58
3:K:50:ILE:O	3:K:54:GLN:HG3	2.03	0.58
3:K:119:ASP:O	3:K:123:THR:HG23	2.03	0.58
4:L:183:LEU:HD13	4:L:183:LEU:O	2.03	0.58
4:D:68:LEU:HD22	4:D:72:LEU:HD23	1.85	0.58
3:G:17:ILE:O	3:G:17:ILE:HD12	2.04	0.58
1:A:203:GLN:O	3:C:146:ASP:HB3	2.04	0.58
3:C:22:SER:HA	3:C:36:PHE:O	2.02	0.58
3:C:129:ARG:HH11	3:C:129:ARG:CB	2.16	0.58
4:D:88:LEU:HD22	4:D:130:GLU:OE1	2.03	0.58
4:H:13:LEU:HD11	4:H:171:MSE:HG3	1.86	0.58
2:J:61:THR:HG23	4:L:43:LEU:CD2	2.34	0.58
1:A:205:LEU:HD12	1:A:205:LEU:O	2.03	0.58
1:E:194:TYR:OH	3:G:142:HIS:HD2	1.87	0.58
1:A:122:LEU:HD11	1:A:127:LEU:CA	2.33	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:107:VAL:HG13	1:E:122:LEU:HD11	1.86	0.57
4:H:158:ASN:C	4:H:158:ASN:ND2	2.57	0.57
1:E:20:VAL:HG12	1:E:21:LEU:N	2.19	0.57
1:E:172:PHE:HD2	3:G:0:MSE:HE1	1.68	0.57
2:F:10:ILE:CD1	4:H:25:ILE:HD11	2.33	0.57
3:G:22:SER:HA	3:G:36:PHE:O	2.04	0.57
1:A:43:LEU:HD22	1:A:100:ILE:HG22	1.86	0.57
3:C:84:PHE:CE1	3:C:148:LEU:HD11	2.40	0.57
1:E:188:THR:HG22	6:E:1037:HOH:O	2.03	0.57
3:C:137:ARG:HB2	3:C:137:ARG:NH1	2.19	0.57
2:F:55:ARG:NH1	4:H:57:ASP:OD2	2.29	0.57
2:F:102:LEU:O	2:F:106:MSE:HG3	2.05	0.57
1:A:29:ARG:HG2	1:A:50:ILE:HD13	1.85	0.57
3:K:57:LYS:HE2	3:K:57:LYS:CA	2.27	0.57
3:K:124:ARG:HD3	3:K:152:GLU:OE2	2.04	0.57
4:D:48:LEU:H	4:D:48:LEU:HD22	1.69	0.57
4:D:125:HIS:C	4:D:127:ASP:H	2.07	0.57
1:E:106:HIS:CD2	1:E:164:LYS:HG2	2.40	0.57
1:I:125:GLU:OE1	1:I:125:GLU:N	2.38	0.57
1:A:64:ASN:N	1:A:64:ASN:HD22	2.02	0.57
2:B:3:CYS:SG	2:B:71:ARG:HB3	2.45	0.57
3:C:71:LEU:HD12	3:C:113:ILE:CD1	2.34	0.57
3:G:151:MSE:O	3:G:155:THR:HG23	2.05	0.57
2:F:99:PRO:HD2	2:F:102:LEU:HD13	1.86	0.57
2:F:129:GLY:O	2:F:131:ASP:N	2.38	0.57
1:I:143:ASN:HA	1:I:147:LYS:HE3	1.85	0.57
4:L:153:SER:O	4:L:155:ASN:N	2.37	0.57
2:B:87:ILE:HD13	2:B:106:MSE:HE3	1.87	0.56
1:E:35:MSE:O	1:E:39:PHE:HD1	1.88	0.56
1:E:137:THR:HG22	2:F:113:TRP:NE1	2.19	0.56
1:A:65:LEU:HG	1:A:75:VAL:HG13	1.87	0.56
6:B:1020:HOH:O	2:F:15:ARG:HD2	2.04	0.56
1:I:22:THR:OG1	1:I:25:GLU:HG3	2.05	0.56
1:I:94:ARG:O	1:I:98:MSE:HG2	2.05	0.56
3:C:86:PRO:HB3	3:C:147:ASN:HD21	1.70	0.56
3:C:94:GLU:OE1	3:C:94:GLU:N	2.38	0.56
2:F:7:MSE:HE1	4:H:25:ILE:HG13	1.87	0.56
2:F:71:ARG:HG3	4:H:71:TRP:CD2	2.40	0.56
2:F:71:ARG:HG3	4:H:71:TRP:CE2	2.40	0.56
3:G:11:GLU:HB3	3:G:47:TRP:HB3	1.87	0.56
3:G:87:MSE:HE2	3:G:87:MSE:HA	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:106:HIS:HE1	1:I:162:VAL:O	1.89	0.56
2:J:100:ASN:HD22	2:J:101:ALA:N	2.03	0.56
3:K:18:ILE:HD12	3:K:18:ILE:N	2.20	0.56
2:B:100:ASN:H	4:H:191:LYS:HZ3	1.52	0.56
1:E:144:VAL:CG2	2:F:109:GLU:HG3	2.27	0.56
4:H:109:LEU:HB2	4:H:145:ARG:HH22	1.69	0.56
1:I:144:VAL:HG22	2:J:109:GLU:CG	2.18	0.56
3:K:158:THR:HB	6:K:1020:HOH:O	2.05	0.56
3:C:92:TYR:CE1	3:C:93:MSE:HG2	2.41	0.56
1:E:211:ILE:HG13	1:E:212:ALA:H	1.70	0.56
1:A:146:LEU:HD12	1:A:149:MSE:SE	2.56	0.56
2:B:58:LEU:HD23	4:D:41:PRO:HG3	1.87	0.56
1:I:149:MSE:HE1	2:J:73:ARG:HG3	1.86	0.56
3:K:20:ASN:HD22	3:K:21:PHE:N	2.03	0.56
1:E:137:THR:HG22	2:F:113:TRP:HE1	1.69	0.56
4:H:158:ASN:ND2	4:H:160:ASP:N	2.54	0.56
3:G:174:LEU:HD22	4:H:135:SER:OG	2.06	0.56
4:H:108:ASP:OD2	4:H:108:ASP:C	2.45	0.56
2:J:136:ILE:HG12	2:J:136:ILE:O	2.06	0.56
1:E:127:LEU:O	1:E:131:ARG:HG3	2.06	0.56
2:F:48:ASN:HA	2:F:51:LYS:HE2	1.86	0.56
3:G:67:ASP:OD2	3:G:70:LYS:HG3	2.06	0.56
1:A:106:HIS:CD2	1:A:106:HIS:N	2.74	0.55
3:G:2:ASP:HB3	3:G:5:GLU:HG3	1.88	0.55
3:G:44:VAL:HG22	3:G:45:PRO:CD	2.34	0.55
3:G:71:LEU:HD22	3:G:120:MSE:HE1	1.88	0.55
1:I:62:GLU:O	1:I:66:ARG:NE	2.39	0.55
1:I:30:LEU:HD22	1:I:54:VAL:HG21	1.87	0.55
1:I:104:PHE:CD1	1:I:105:PRO:HD3	2.41	0.55
3:C:63:PRO:HD2	3:C:66:MSE:HE3	1.87	0.55
1:I:181:ASN:N	1:I:181:ASN:HD22	2.04	0.55
3:K:160:LEU:O	3:K:164:LEU:HD22	2.06	0.55
4:L:27:MSE:HE1	4:L:122:GLN:HG2	1.87	0.55
4:L:167:ARG:HG2	4:L:167:ARG:HH11	1.71	0.55
2:B:15:ARG:HD3	2:F:22:PRO:HA	1.87	0.55
2:B:14:HIS:NE2	5:B:1016:SO4:S	2.80	0.55
2:B:18:GLU:CD	2:B:19:GLY:N	2.59	0.55
2:B:55:ARG:HG2	2:B:57:ASP:OD2	2.06	0.55
2:B:115:ASN:HA	2:B:118:LYS:HG2	1.87	0.55
4:H:167:ARG:HH11	4:H:167:ARG:HG2	1.71	0.55
1:I:70:ARG:NH2	3:K:24:ASP:OD2	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:110:LYS:O	1:A:110:LYS:HD3	2.07	0.55
2:B:122:ALA:O	2:B:126:ARG:HG3	2.07	0.55
3:C:136:VAL:HG22	3:C:167:MSE:HE3	1.88	0.55
3:C:67:ASP:HB3	3:C:70:LYS:HD2	1.89	0.55
4:D:91:ILE:HD12	4:D:112:MSE:HE3	1.88	0.55
4:D:149:ILE:HG12	4:D:168:LEU:HD21	1.88	0.55
3:G:85:THR:HG23	3:G:86:PRO:HD2	1.87	0.55
4:L:34:VAL:HG11	4:L:68:LEU:CD1	2.37	0.55
2:B:14:HIS:NE2	5:B:1016:SO4:O2	2.35	0.55
3:C:136:VAL:HG13	3:C:167:MSE:CE	2.36	0.55
1:I:104:PHE:CD2	1:I:105:PRO:HD3	2.41	0.55
2:B:9:LEU:HG	2:B:79:TYR:CD1	2.42	0.55
1:E:56:GLU:HA	1:E:59:GLU:HG2	1.88	0.55
4:H:183:LEU:O	4:H:187:GLN:HG3	2.06	0.55
1:A:57:GLN:O	1:A:60:HIS:HB3	2.07	0.55
2:F:73:ARG:O	2:F:76:THR:HG22	2.07	0.55
3:G:157:GLY:O	3:G:161:THR:HB	2.07	0.55
3:C:115:THR:HG23	3:C:116:LEU:N	2.23	0.54
3:K:29:ILE:HD12	3:K:30:GLY:N	2.22	0.54
1:E:63:GLU:C	1:E:65:LEU:H	2.10	0.54
4:L:16:GLU:CD	6:L:1013:HOH:O	2.46	0.54
1:A:74:LYS:HZ2	3:C:26:ILE:HG22	1.73	0.54
4:D:38:THR:HA	4:D:62:GLN:HE21	1.72	0.54
1:A:30:LEU:HD13	1:A:50:ILE:HG22	1.89	0.54
3:C:87:MSE:HA	3:C:87:MSE:HE2	1.89	0.54
4:D:135:SER:C	4:D:137:SER:H	2.11	0.54
4:D:183:LEU:HD13	4:D:183:LEU:O	2.06	0.54
4:H:106:VAL:O	4:H:167:ARG:NH2	2.40	0.54
1:A:110:LYS:HA	1:A:113:THR:CG2	2.37	0.54
4:D:70:LEU:HD22	4:D:119:PHE:CE1	2.41	0.54
1:I:177:GLU:CD	1:I:178:ARG:H	2.11	0.54
3:K:94:GLU:N	3:K:94:GLU:OE1	2.40	0.54
4:L:89:PRO:HD2	4:L:123:LEU:HD21	1.89	0.54
2:B:98:LEU:HD11	2:B:114:PHE:CZ	2.43	0.54
4:D:94:GLU:CB	4:D:97:ARG:HH21	2.21	0.54
3:G:15:VAL:HG13	3:G:15:VAL:O	2.08	0.54
3:G:158:THR:O	3:G:162:GLN:HG3	2.07	0.54
1:I:106:HIS:CD2	1:I:164:LYS:HG2	2.41	0.54
2:J:56:SER:C	2:J:58:LEU:H	2.11	0.54
2:B:87:ILE:CG2	2:B:106:MSE:HE3	2.37	0.54
2:F:25:ASN:H	2:F:25:ASN:HD22	1.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:103:ASP:O	4:H:106:VAL:HG12	2.08	0.54
2:J:1:MSE:HE3	2:J:39:LEU:HD21	1.90	0.54
1:A:173:LEU:C	1:A:173:LEU:HD23	2.29	0.54
1:E:104:PHE:CE1	1:E:105:PRO:HG3	2.43	0.54
2:J:1:MSE:C	2:J:3:CYS:H	2.12	0.54
3:G:109:LYS:HB3	3:G:112:GLU:CB	2.38	0.54
4:D:105:ASN:HD22	4:D:148:ARG:HD2	1.73	0.54
2:F:144:LYS:O	2:F:145:SER:CB	2.56	0.54
1:A:23:PRO:HG3	1:A:57:GLN:HE21	1.70	0.53
2:B:9:LEU:HG	2:B:79:TYR:CE1	2.44	0.53
4:D:112:MSE:O	4:D:113:GLY:C	2.46	0.53
4:D:164:LEU:HD13	4:D:164:LEU:C	2.29	0.53
1:E:92:TYR:O	1:E:96:ARG:HG3	2.08	0.53
3:G:19:PRO:HA	3:G:58:CYS:HA	1.90	0.53
1:I:170:TYR:O	3:K:161:THR:CG2	2.56	0.53
2:J:28:GLY:O	2:J:32:VAL:HG23	2.08	0.53
1:A:39:PHE:CE2	1:A:172:PHE:HD2	2.24	0.53
3:C:50:ILE:HD11	3:C:98:LEU:HB3	1.91	0.53
1:E:147:LYS:HG3	1:E:148:HIS:CD2	2.42	0.53
3:G:134:SER:CA	3:G:137:ARG:HH21	2.21	0.53
1:A:100:ILE:HG13	1:A:101:GLU:N	2.22	0.53
3:C:113:ILE:O	3:C:117:VAL:HG23	2.09	0.53
4:H:158:ASN:ND2	4:H:161:THR:H	2.07	0.53
2:B:100:ASN:HB3	4:H:188:CYS:SG	2.48	0.53
3:C:17:ILE:HD13	3:C:42:VAL:O	2.09	0.53
1:A:42:GLU:O	1:A:44:LEU:HD13	2.09	0.53
1:I:180:GLU:HG2	1:I:181:ASN:ND2	2.24	0.53
2:B:87:ILE:O	2:B:90:LEU:HB2	2.09	0.53
3:C:139:GLN:HE22	3:C:171:ARG:HD3	1.72	0.53
1:I:85:ILE:HD11	3:K:29:ILE:HG12	1.90	0.53
3:K:75:ARG:HG3	3:K:76:ASP:N	2.24	0.53
4:L:90:LYS:O	4:L:93:GLN:HB2	2.09	0.53
1:A:22:THR:HG23	1:A:25:GLU:OE1	2.09	0.53
4:D:21:SER:O	4:D:25:ILE:HG23	2.09	0.53
1:A:168:ASP:OD1	1:A:209:LYS:HD2	2.09	0.53
2:B:9:LEU:HD11	2:B:25:ASN:HB3	1.91	0.53
2:B:99:PRO:O	2:B:101:ALA:N	2.42	0.53
4:D:80:LYS:HG2	4:D:82:ARG:NE	2.05	0.53
1:A:100:ILE:O	1:A:104:PHE:N	2.42	0.53
2:B:33:LEU:O	2:B:36:MSE:N	2.41	0.53
3:C:103:ALA:O	3:C:107:ILE:HD13	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:82:ASP:O	2:B:86:ARG:HG3	2.09	0.53
3:C:85:THR:O	3:C:87:MSE:HE3	2.08	0.53
1:I:184:VAL:O	1:I:186:PRO:HD3	2.09	0.53
2:J:74:ARG:CZ	4:L:25:ILE:HD13	2.39	0.53
4:L:105:ASN:HD21	4:L:145:ARG:CA	2.21	0.53
1:A:145:ALA:HB2	2:B:29:LEU:HD21	1.92	0.52
3:C:170:LEU:O	4:D:139:LEU:HD21	2.08	0.52
4:D:3:GLU:HG3	4:D:5:TYR:H	1.74	0.52
1:I:107:VAL:HG12	1:I:122:LEU:HD11	1.90	0.52
3:K:77:HIS:O	3:K:80:LYS:HB3	2.09	0.52
2:B:5:LYS:HE3	2:B:31:GLN:OE1	2.09	0.52
2:B:99:PRO:C	2:B:101:ALA:H	2.11	0.52
4:H:3:GLU:CG	4:H:5:TYR:HB3	2.39	0.52
3:C:139:GLN:CD	3:C:171:ARG:HH21	2.12	0.52
2:F:25:ASN:HD22	2:F:25:ASN:N	2.07	0.52
3:G:99:LEU:C	3:G:100:LEU:HD12	2.30	0.52
4:H:137:SER:O	4:H:141:THR:CG2	2.57	0.52
1:E:109:GLU:HG3	1:E:159:PHE:CD1	2.43	0.52
1:I:98:MSE:HE3	4:L:4:ALA:HB1	1.90	0.52
1:I:149:MSE:HE1	2:J:73:ARG:CD	2.38	0.52
2:J:20:GLN:O	2:J:86:ARG:HD3	2.09	0.52
3:C:139:GLN:CD	3:C:171:ARG:HD3	2.29	0.52
2:F:22:PRO:O	2:F:83:ARG:NH2	2.43	0.52
3:K:92:TYR:CE2	3:K:93:MSE:CE	2.91	0.52
1:A:22:THR:OG1	1:A:25:GLU:HG3	2.09	0.52
2:B:58:LEU:O	2:B:62:ILE:HG12	2.10	0.52
4:D:34:VAL:HG13	4:D:66:LEU:HB2	1.91	0.52
4:D:100:PHE:HB3	4:D:141:THR:CG2	2.39	0.52
1:E:49:GLU:HB2	6:E:1032:HOH:O	2.10	0.52
2:F:13:LEU:HD22	2:F:79:TYR:CD1	2.44	0.52
2:F:86:ARG:O	2:F:90:LEU:HD13	2.10	0.52
3:C:153:ILE:HG13	3:C:154:ASN:HD22	1.74	0.52
3:G:171:ARG:O	3:G:171:ARG:HG2	2.10	0.52
1:I:176:ARG:HG3	1:I:176:ARG:HH11	1.74	0.52
1:A:149:MSE:HE1	2:B:73:ARG:HD3	1.91	0.52
1:A:206:ILE:CG2	1:A:211:ILE:HD11	2.40	0.52
1:E:204:HIS:ND1	3:G:142:HIS:HE1	2.08	0.52
4:H:36:THR:HG23	4:H:66:LEU:CD2	2.40	0.52
2:J:144:LYS:HD3	2:J:145:SER:N	2.24	0.52
1:A:32:GLN:NE2	6:A:1023:HOH:O	2.42	0.52
4:D:89:PRO:HD2	4:D:123:LEU:HD21	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:146:LEU:HB3	1:E:154:GLN:O	2.09	0.52
4:L:122:GLN:NE2	4:L:125:HIS:NE2	2.58	0.52
2:B:2:PHE:HB2	4:D:46:PHE:CE2	2.44	0.52
1:E:199:GLU:OE1	1:E:199:GLU:HA	2.10	0.52
3:G:16:THR:HA	3:G:43:GLU:HA	1.91	0.52
4:H:103:ASP:OD2	4:H:106:VAL:HB	2.09	0.52
1:I:180:GLU:HG2	1:I:181:ASN:N	2.25	0.52
2:B:32:VAL:O	2:B:36:MSE:HG3	2.10	0.51
3:C:110:ALA:HA	3:C:113:ILE:HG22	1.91	0.51
3:C:125:ILE:O	3:C:128:LEU:N	2.41	0.51
4:D:40:MSE:HE3	4:D:60:VAL:HG21	1.92	0.51
2:J:98:LEU:HD11	2:J:114:PHE:CZ	2.45	0.51
4:L:41:PRO:C	4:L:42:ARG:HG2	2.30	0.51
1:A:149:MSE:HE3	2:B:36:MSE:CE	2.40	0.51
2:B:56:SER:C	2:B:58:LEU:H	2.12	0.51
4:H:148:ARG:HG3	4:H:148:ARG:NH1	2.25	0.51
1:A:146:LEU:HD21	1:A:156:VAL:HG23	1.93	0.51
3:C:78:GLU:C	3:C:80:LYS:H	2.13	0.51
4:D:17:GLU:HG3	4:D:122:GLN:NE2	2.24	0.51
1:E:149:MSE:HE3	2:F:36:MSE:CE	2.37	0.51
1:I:103:PHE:O	1:I:107:VAL:HG23	2.10	0.51
1:I:175:VAL:HG21	1:I:198:LEU:HB3	1.91	0.51
3:K:75:ARG:CZ	3:K:119:ASP:HB3	2.39	0.51
1:A:74:LYS:NZ	3:C:26:ILE:HG22	2.25	0.51
1:A:115:PRO:O	1:A:117:GLY:N	2.43	0.51
1:A:55:MSE:HE2	2:B:128:LEU:O	2.11	0.51
1:A:148:HIS:HB2	2:B:33:LEU:HD13	1.92	0.51
1:I:177:GLU:O	1:I:178:ARG:CB	2.58	0.51
3:K:36:PHE:N	3:K:36:PHE:CD2	2.78	0.51
1:I:42:GLU:C	1:I:99:LYS:HD3	2.31	0.51
1:I:190:GLU:N	1:I:190:GLU:OE1	2.44	0.51
3:K:48:LEU:CD2	3:K:52:LEU:HD22	2.40	0.51
4:D:109:LEU:HD22	4:D:145:ARG:NH2	2.25	0.51
4:H:147:ARG:HG3	4:H:147:ARG:HH11	1.75	0.51
1:E:20:VAL:CG1	1:E:21:LEU:N	2.74	0.51
1:E:34:TRP:HZ3	3:G:9:LEU:HD11	1.75	0.51
1:E:48:PRO:HG2	1:E:49:GLU:H	1.75	0.51
3:G:53:LYS:HD2	3:G:60:LEU:HD23	1.93	0.51
4:H:32:LEU:HD21	4:H:86:VAL:HG11	1.93	0.51
1:I:147:LYS:HD2	1:I:148:HIS:NE2	2.26	0.51
1:I:209:LYS:O	1:I:210:THR:HB	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:17:PRO:O	2:J:20:GLN:HG2	2.10	0.51
2:J:111:MSE:HE3	2:J:111:MSE:O	2.11	0.51
1:A:21:LEU:HD23	1:A:21:LEU:N	2.25	0.51
1:A:89:LEU:O	1:A:92:TYR:HB3	2.11	0.51
2:B:103:ARG:HH11	2:B:111:MSE:HE3	1.76	0.51
2:B:129:GLY:N	2:B:133:GLY:HA2	2.26	0.51
4:D:100:PHE:CD1	4:D:141:THR:HG21	2.46	0.51
3:G:89:SER:OG	3:G:95:LEU:HD12	2.11	0.51
1:A:147:LYS:HG2	1:A:148:HIS:HD2	1.76	0.50
3:C:18:ILE:HG13	3:C:59:ARG:HB3	1.94	0.50
4:D:40:MSE:CE	4:D:60:VAL:HG21	2.41	0.50
2:F:47:VAL:HG22	2:F:62:ILE:HD13	1.93	0.50
4:H:31:LYS:HE3	4:H:69:PRO:HG3	1.91	0.50
1:I:27:ILE:HG21	3:K:29:ILE:CD1	2.41	0.50
3:C:84:PHE:CD1	3:C:148:LEU:HD21	2.46	0.50
1:E:78:HIS:O	1:E:82:MSE:HB2	2.11	0.50
2:F:17:PRO:HG2	2:F:20:GLN:HG3	1.93	0.50
4:L:108:ASP:O	4:L:112:MSE:HG2	2.11	0.50
1:E:56:GLU:HA	1:E:59:GLU:CG	2.41	0.50
1:I:22:THR:O	1:I:25:GLU:HB2	2.11	0.50
1:A:77:ILE:CD1	3:C:48:LEU:HD21	2.42	0.50
1:A:86:ARG:HG3	1:A:86:ARG:HH11	1.77	0.50
2:B:18:GLU:CG	2:B:19:GLY:H	2.24	0.50
3:G:87:MSE:HB3	3:G:88:PRO:HD2	1.92	0.50
1:I:85:ILE:CD1	3:K:29:ILE:HG12	2.41	0.50
3:K:10:ALA:O	3:K:13:GLU:HB2	2.11	0.50
3:C:129:ARG:HB3	4:D:150:MSE:HE3	1.94	0.50
1:I:63:GLU:O	1:I:64:ASN:C	2.50	0.50
3:K:170:LEU:HD21	4:L:13:LEU:HG	1.93	0.50
4:L:167:ARG:HG2	4:L:167:ARG:NH1	2.25	0.50
2:J:81:TYR:O	2:J:85:LEU:HG	2.11	0.50
2:J:100:ASN:HD22	2:J:101:ALA:H	1.58	0.50
1:A:74:LYS:HG3	3:C:26:ILE:HG22	1.93	0.50
3:C:44:VAL:HG22	3:C:45:PRO:CD	2.42	0.50
4:D:37:GLU:O	4:D:62:GLN:HB3	2.11	0.50
1:E:140:TYR:O	1:E:144:VAL:HG23	2.11	0.50
2:B:71:ARG:HH11	2:B:71:ARG:HG2	1.77	0.50
2:F:93:GLU:HG2	2:F:94:TYR:CD1	2.46	0.50
2:F:129:GLY:O	2:F:130:GLY:C	2.50	0.50
4:H:108:ASP:HB2	4:H:167:ARG:NH1	2.27	0.50
4:H:174:GLY:O	4:H:178:THR:HG22	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:147:LYS:HD2	1:I:148:HIS:CD2	2.47	0.50
5:B:1016:SO4:S	2:F:105:HIS:NE2	2.84	0.50
3:K:53:LYS:HB2	3:K:60:LEU:HD21	1.94	0.50
3:C:136:VAL:HG13	3:C:167:MSE:HE3	1.94	0.49
1:E:80:MSE:C	1:E:82:MSE:H	2.15	0.49
1:E:114:ARG:HH12	1:E:121:SER:H	1.59	0.49
1:E:114:ARG:HH12	1:E:121:SER:N	2.09	0.49
1:E:134:MSE:HE1	1:E:158:LEU:HD12	1.94	0.49
2:B:125:MSE:SE	2:B:137:THR:HG23	2.62	0.49
1:E:149:MSE:HE1	2:F:73:ARG:CG	2.41	0.49
2:B:1:MSE:SE	2:B:64:PHE:HE2	2.45	0.49
2:F:47:VAL:O	2:F:50:ALA:HB3	2.11	0.49
4:H:103:ASP:HB2	3:K:64:GLU:HB2	1.94	0.49
3:K:159:PHE:CE2	4:L:175:LEU:HG	2.47	0.49
1:A:103:PHE:C	1:A:105:PRO:HD2	2.32	0.49
2:B:8:GLU:CB	6:B:1021:HOH:O	2.58	0.49
3:C:57:LYS:O	3:C:58:CYS:HB3	2.12	0.49
3:C:67:ASP:HB3	3:C:70:LYS:CB	2.42	0.49
1:E:146:LEU:N	1:E:146:LEU:HD12	2.27	0.49
1:E:172:PHE:CE1	1:E:205:LEU:HD13	2.47	0.49
2:F:111:MSE:HE1	2:F:114:PHE:HD2	1.75	0.49
4:H:137:SER:O	4:H:141:THR:HG22	2.11	0.49
3:K:136:VAL:HG12	4:L:143:ILE:HG23	1.94	0.49
1:A:120:SER:C	1:A:122:LEU:H	2.15	0.49
1:A:124:PRO:HG2	1:A:125:GLU:OE2	2.13	0.49
4:D:129:PRO:HG2	4:D:130:GLU:H	1.77	0.49
2:F:10:ILE:CG1	4:H:25:ILE:HD11	2.42	0.49
3:G:52:LEU:HB2	3:G:58:CYS:SG	2.53	0.49
3:G:109:LYS:HB3	3:G:109:LYS:HZ2	1.77	0.49
3:K:74:MSE:HE1	3:K:88:PRO:HG3	1.93	0.49
3:C:173:ASN:HD21	4:D:135:SER:HB3	1.76	0.49
1:E:212:ALA:HB3	1:E:213:PRO:CD	2.37	0.49
2:B:1:MSE:HE3	2:B:65:ARG:HG2	1.95	0.49
2:B:59:ILE:HB	2:B:60:PRO:HD3	1.94	0.49
3:C:17:ILE:HD12	3:C:44:VAL:HG12	1.93	0.49
3:C:71:LEU:HD23	3:C:74:MSE:SE	2.63	0.49
4:D:40:MSE:HB2	4:D:60:VAL:CG2	2.43	0.49
1:E:81:GLU:CD	3:G:28:LEU:HB3	2.33	0.49
1:E:149:MSE:SE	2:F:73:ARG:HG3	2.62	0.49
4:H:186:PHE:O	4:H:190:GLU:HG2	2.11	0.49
2:J:1:MSE:C	2:J:3:CYS:N	2.66	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:K:133:ASP:OD2	4:L:147:ARG:CG	2.54	0.49
1:E:63:GLU:C	1:E:65:LEU:N	2.65	0.49
2:F:5:LYS:O	2:F:8:GLU:HG2	2.13	0.49
3:G:70:LYS:NZ	3:G:70:LYS:HB3	2.27	0.49
4:H:41:PRO:O	4:H:42:ARG:HB2	2.12	0.49
1:I:41:PRO:HD2	1:I:208:TYR:CD2	2.48	0.49
4:L:70:LEU:HD23	4:L:70:LEU:O	2.12	0.49
6:I:1015:HOH:O	2:J:88:ARG:CD	2.58	0.49
3:K:144:LYS:HG2	3:K:146:ASP:OD1	2.13	0.49
4:L:158:ASN:H	4:L:161:THR:HG23	1.78	0.49
2:B:104:PHE:CE2	4:H:184:ASN:HB2	2.47	0.48
2:J:9:LEU:HG	2:J:79:TYR:CD1	2.47	0.48
2:B:99:PRO:C	2:B:101:ALA:N	2.65	0.48
3:C:154:ASN:HD22	3:C:154:ASN:N	2.11	0.48
4:D:12:ALA:HB1	4:D:27:MSE:HE2	1.94	0.48
1:E:79:GLN:O	1:E:83:GLU:HG3	2.12	0.48
3:K:91:TYR:O	3:K:95:LEU:HD23	2.13	0.48
4:L:42:ARG:N	4:L:58:ASN:O	2.43	0.48
4:L:58:ASN:CG	4:L:59:ALA:H	2.16	0.48
1:E:174:ARG:HG2	1:E:174:ARG:HH11	1.78	0.48
3:K:19:PRO:O	3:K:38:PRO:HA	2.13	0.48
4:L:40:MSE:O	4:L:59:ALA:HB1	2.13	0.48
2:B:58:LEU:HD23	4:D:41:PRO:CG	2.43	0.48
2:B:98:LEU:N	2:B:98:LEU:CD2	2.75	0.48
2:B:100:ASN:H	4:H:191:LYS:NZ	2.10	0.48
4:D:136:GLN:O	4:D:136:GLN:HG2	2.14	0.48
3:G:130:VAL:HG22	4:H:147:ARG:HH22	1.77	0.48
1:I:173:LEU:HD22	1:I:211:ILE:HD11	1.96	0.48
1:I:177:GLU:O	1:I:200:LYS:HB2	2.12	0.48
2:B:18:GLU:CG	2:B:19:GLY:N	2.77	0.48
1:E:98:MSE:HB2	5:F:1010:SO4:O1	2.12	0.48
6:E:1030:HOH:O	3:G:0:MSE:HE2	2.13	0.48
3:G:17:ILE:HD12	3:G:17:ILE:C	2.34	0.48
3:G:142:HIS:CG	3:G:143:ALA:N	2.81	0.48
3:K:64:GLU:CD	3:K:64:GLU:C	2.70	0.48
2:F:79:TYR:O	2:F:83:ARG:HG3	2.13	0.48
2:F:88:ARG:NH2	5:F:1010:SO4:O2	2.47	0.48
1:A:108:LEU:HD11	1:A:131:ARG:HA	1.95	0.48
1:A:137:THR:O	1:A:141:LEU:HD22	2.14	0.48
3:C:51:ASN:HD21	3:C:55:ARG:NE	2.12	0.48
4:H:149:ILE:HD13	4:H:168:LEU:HD11	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:H:169:ASP:OD1	4:H:169:ASP:C	2.51	0.48
2:J:111:MSE:HE1	2:J:114:PHE:HD2	1.78	0.48
2:J:125:MSE:SE	2:J:136:ILE:HD13	2.64	0.48
1:A:73:LEU:O	1:A:77:ILE:HG12	2.14	0.48
1:A:94:ARG:HD3	2:B:136:ILE:O	2.14	0.48
3:C:146:ASP:O	3:C:147:ASN:HB2	2.14	0.48
1:E:134:MSE:HE2	1:E:138:GLU:OE1	2.13	0.48
4:H:160:ASP:O	4:H:163:ALA:HB3	2.13	0.48
4:L:34:VAL:HG12	4:L:66:LEU:O	2.14	0.48
3:C:136:VAL:HG13	3:C:167:MSE:SE	2.64	0.48
3:G:113:ILE:C	3:G:115:THR:H	2.16	0.48
3:G:149:THR:OG1	3:G:152:GLU:HG3	2.14	0.48
4:H:91:ILE:HB	4:H:112:MSE:HE2	1.95	0.48
2:J:111:MSE:HG2	6:J:1029:HOH:O	2.14	0.48
2:J:121:LEU:O	2:J:125:MSE:HG3	2.14	0.48
3:K:87:MSE:SE	3:K:120:MSE:HE3	2.64	0.48
4:D:76:LEU:CB	4:D:84:LEU:HD22	2.44	0.47
4:D:109:LEU:HB2	4:D:145:ARG:HH22	1.79	0.47
1:E:185:GLU:HG2	1:E:193:ASP:OD2	2.14	0.47
1:E:188:THR:HG22	1:E:190:GLU:OE2	2.14	0.47
2:F:7:MSE:HG3	4:H:29:HIS:CE1	2.49	0.47
2:F:32:VAL:O	2:F:36:MSE:HG3	2.13	0.47
4:H:169:ASP:OD1	4:H:171:MSE:N	2.47	0.47
2:J:1:MSE:HE3	2:J:39:LEU:CD2	2.44	0.47
3:K:17:ILE:HG22	3:K:60:LEU:CD1	2.38	0.47
3:K:21:PHE:HE2	3:K:23:LEU:HB2	1.79	0.47
4:L:32:LEU:HD12	4:L:33:PRO:CD	2.44	0.47
1:A:81:GLU:O	1:A:81:GLU:HG2	2.15	0.47
2:B:88:ARG:NH1	4:D:6:PHE:HE1	2.11	0.47
1:E:56:GLU:HA	1:E:59:GLU:CD	2.34	0.47
2:F:97:ILE:HG23	2:F:97:ILE:O	2.14	0.47
3:G:70:LYS:HB3	3:G:70:LYS:HZ3	1.78	0.47
3:K:91:TYR:HD1	3:K:94:GLU:OE2	1.96	0.47
3:K:167:MSE:HE2	3:K:171:ARG:NH1	2.29	0.47
4:L:89:PRO:CD	4:L:123:LEU:HD21	2.44	0.47
2:B:102:LEU:N	2:B:102:LEU:HD22	2.29	0.47
3:C:44:VAL:HG21	3:C:48:LEU:HD13	1.96	0.47
4:D:9:GLU:CD	4:D:9:GLU:H	2.18	0.47
3:G:85:THR:O	3:G:124:ARG:NH1	2.47	0.47
2:J:87:ILE:HA	2:J:90:LEU:HD22	1.96	0.47
1:E:71:GLU:O	1:E:72:ASP:CB	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:139:GLN:NE2	3:G:171:ARG:HH21	2.13	0.47
3:G:150:LEU:O	3:G:151:MSE:C	2.52	0.47
1:A:108:LEU:HD21	1:A:131:ARG:CA	2.44	0.47
3:C:121:TRP:CZ3	3:C:152:GLU:HG2	2.50	0.47
1:E:80:MSE:O	1:E:84:ARG:HG3	2.14	0.47
1:I:90:SER:CB	1:I:94:ARG:HH21	2.24	0.47
3:G:99:LEU:HB3	3:G:107:ILE:HD11	1.97	0.47
2:J:56:SER:C	2:J:58:LEU:N	2.68	0.47
3:K:148:LEU:HD12	3:K:148:LEU:HA	1.76	0.47
4:L:158:ASN:H	4:L:161:THR:CG2	2.28	0.47
2:B:39:LEU:HD13	2:B:68:SER:HB3	1.96	0.47
2:B:88:ARG:NH1	4:D:4:ALA:O	2.47	0.47
3:C:18:ILE:HG12	3:C:59:ARG:HB3	1.96	0.47
3:C:89:SER:C	3:C:91:TYR:H	2.18	0.47
3:C:110:ALA:HA	3:C:113:ILE:CG2	2.43	0.47
3:C:137:ARG:HA	4:D:143:ILE:CG2	2.44	0.47
1:I:80:MSE:O	1:I:84:ARG:HG3	2.15	0.47
1:I:178:ARG:O	1:I:198:LEU:O	2.32	0.47
2:J:53:GLY:C	2:J:55:ARG:H	2.18	0.47
1:A:78:HIS:CE1	3:C:28:LEU:HD23	2.50	0.47
1:A:146:LEU:HG	1:A:154:GLN:O	2.15	0.47
2:B:10:ILE:HD13	2:B:11:ARG:N	2.29	0.47
3:C:146:ASP:O	3:C:147:ASN:CB	2.62	0.47
4:D:76:LEU:O	4:D:83:ILE:HG21	2.15	0.47
1:I:75:VAL:O	1:I:79:GLN:HG3	2.15	0.47
1:I:81:GLU:CD	3:K:29:ILE:HG13	2.34	0.47
4:L:152:SER:CB	4:L:164:LEU:HD23	2.45	0.47
1:A:58:LEU:HD21	1:A:85:ILE:HB	1.96	0.47
4:D:125:HIS:O	4:D:127:ASP:N	2.48	0.47
3:G:2:ASP:OD1	3:G:3:ALA:N	2.48	0.47
4:H:34:VAL:HG11	4:H:68:LEU:CG	2.38	0.47
1:A:208:TYR:CE1	1:A:212:ALA:HB2	2.50	0.46
1:E:178:ARG:HE	1:E:178:ARG:HB3	1.54	0.46
1:A:173:LEU:HD23	1:A:174:ARG:N	2.29	0.46
4:D:29:HIS:O	4:D:29:HIS:ND1	2.48	0.46
4:D:145:ARG:NH2	4:D:172:GLU:OE2	2.48	0.46
2:F:121:LEU:O	2:F:125:MSE:HG3	2.15	0.46
1:I:54:VAL:O	1:I:58:LEU:HD23	2.16	0.46
4:L:100:PHE:CE1	4:L:107:VAL:HG21	2.50	0.46
1:A:27:ILE:CD1	1:A:85:ILE:HD12	2.42	0.46
4:D:70:LEU:HD22	4:D:119:PHE:CD1	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:31:GLU:OE2	3:G:12:LYS:HE2	2.15	0.46
2:J:111:MSE:HE1	2:J:114:PHE:CD2	2.51	0.46
3:K:151:MSE:HE3	3:K:155:THR:HG1	1.80	0.46
3:K:167:MSE:HE2	3:K:171:ARG:HH12	1.79	0.46
1:A:87:TYR:OH	3:C:5:GLU:HG2	2.15	0.46
3:C:75:ARG:N	3:C:120:MSE:HE2	2.30	0.46
4:D:96:TRP:C	4:D:98:THR:H	2.19	0.46
1:I:21:LEU:HD12	1:I:25:GLU:HB3	1.97	0.46
4:L:41:PRO:HA	4:L:59:ALA:CB	2.45	0.46
1:A:134:MSE:HE2	1:A:158:LEU:HD12	1.98	0.46
2:B:65:ARG:O	2:B:69:LEU:HD22	2.16	0.46
2:B:115:ASN:O	2:B:119:ARG:HB2	2.15	0.46
4:D:76:LEU:HB2	4:D:84:LEU:HD22	1.97	0.46
4:D:145:ARG:HH21	4:D:172:GLU:CD	2.18	0.46
4:D:158:ASN:OD1	4:D:160:ASP:HB2	2.15	0.46
1:I:49:GLU:O	1:I:50:ILE:C	2.54	0.46
3:K:85:THR:O	3:K:124:ARG:NH1	2.48	0.46
4:L:88:LEU:HD21	4:L:134:ILE:HD11	1.97	0.46
1:A:171:VAL:CG1	1:A:172:PHE:H	2.04	0.46
2:B:87:ILE:HG21	2:B:106:MSE:HE3	1.97	0.46
3:G:125:ILE:HD13	3:G:125:ILE:O	2.16	0.46
1:I:151:PRO:O	1:I:152:ASN:HB2	2.16	0.46
4:L:68:LEU:HD12	4:L:84:LEU:HD21	1.96	0.46
4:D:165:VAL:C	4:D:167:ARG:H	2.18	0.46
2:J:31:GLN:HA	2:J:34:GLU:CG	2.46	0.46
3:C:91:TYR:HD1	3:C:94:GLU:OE2	1.99	0.46
4:D:27:MSE:O	4:D:30:GLU:HG2	2.15	0.46
2:F:111:MSE:HE1	2:F:114:PHE:CD2	2.51	0.46
4:H:150:MSE:HE2	4:H:154:GLN:HE22	1.81	0.46
2:B:65:ARG:O	2:B:69:LEU:CD2	2.64	0.46
3:C:83:THR:O	3:C:127:LYS:NZ	2.32	0.46
1:E:78:HIS:CE1	3:G:28:LEU:HD23	2.50	0.46
1:I:55:MSE:HE3	2:J:134:LEU:HD12	1.97	0.46
4:L:34:VAL:HG23	4:L:86:VAL:HA	1.96	0.46
2:B:14:HIS:HE2	2:F:105:HIS:HE2	1.64	0.46
3:G:139:GLN:HE21	3:G:171:ARG:NH2	2.14	0.46
1:I:200:LYS:HD3	1:I:201:GLY:N	2.32	0.46
2:J:141:LYS:HG2	2:J:142:PRO:HD2	1.97	0.46
1:A:34:TRP:CD2	1:A:88:VAL:HG13	2.51	0.45
2:B:71:ARG:HG3	4:D:71:TRP:CE2	2.51	0.45
1:I:60:HIS:O	1:I:64:ASN:N	2.43	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:109:LEU:HD22	4:L:145:ARG:NH1	2.30	0.45
2:B:11:ARG:C	2:B:13:LEU:N	2.69	0.45
3:C:149:THR:OG1	3:C:152:GLU:HG3	2.16	0.45
3:G:1:MSE:CE	3:G:6:VAL:HG22	2.39	0.45
3:G:75:ARG:HG2	3:G:75:ARG:HH11	1.82	0.45
1:I:172:PHE:CE1	3:K:153:ILE:HD13	2.51	0.45
2:J:71:ARG:CG	2:J:71:ARG:NH1	2.68	0.45
3:K:48:LEU:HD23	3:K:48:LEU:O	2.16	0.45
3:C:3:ALA:HB2	3:C:151:MSE:HE1	1.98	0.45
4:D:143:ILE:HD12	4:D:143:ILE:H	1.82	0.45
2:F:51:LYS:HE3	2:F:51:LYS:HB2	1.82	0.45
3:G:81:GLU:O	3:G:82:GLU:HB3	2.16	0.45
3:G:135:PHE:CE2	3:G:140:GLU:HB2	2.51	0.45
4:H:145:ARG:NH2	4:H:172:GLU:OE2	2.49	0.45
4:L:139:LEU:O	4:L:143:ILE:HG12	2.14	0.45
2:B:11:ARG:HD3	2:B:15:ARG:NH2	2.31	0.45
4:D:48:LEU:HD22	4:D:48:LEU:N	2.29	0.45
3:G:50:ILE:O	3:G:54:GLN:HB2	2.16	0.45
4:L:38:THR:O	4:L:39:ALA:HB2	2.16	0.45
1:A:54:VAL:HG21	1:A:89:LEU:HD13	1.97	0.45
3:C:1:MSE:HE2	3:C:5:GLU:HB3	1.98	0.45
3:C:78:GLU:HA	3:C:85:THR:OG1	2.17	0.45
1:E:151:PRO:O	1:E:152:ASN:HB2	2.17	0.45
3:G:71:LEU:HD13	3:G:117:VAL:HG22	1.98	0.45
3:G:78:GLU:OE2	3:G:85:THR:HB	2.16	0.45
3:G:112:GLU:O	3:G:115:THR:HG22	2.15	0.45
4:H:34:VAL:HG22	4:H:35:ARG:N	2.32	0.45
1:I:182:ILE:O	1:I:195:VAL:HG23	2.16	0.45
1:A:204:HIS:N	1:A:204:HIS:CD2	2.85	0.45
3:C:50:ILE:HD13	3:C:98:LEU:HD22	1.98	0.45
3:K:15:VAL:CG1	3:K:16:THR:N	2.80	0.45
3:K:15:VAL:HG12	3:K:16:THR:N	2.32	0.45
3:K:156:SER:OG	4:L:154:GLN:NE2	2.49	0.45
3:C:46:LEU:HD22	3:C:50:ILE:CD1	2.47	0.45
4:H:88:LEU:HD23	4:H:134:ILE:HD11	1.98	0.45
3:K:109:LYS:HA	6:K:1017:HOH:O	2.17	0.45
3:K:173:ASN:HD22	3:K:173:ASN:C	2.18	0.45
4:L:17:GLU:HG3	6:L:1013:HOH:O	2.16	0.45
4:L:33:PRO:HA	4:L:67:GLU:OE1	2.17	0.45
4:L:110:HIS:CD2	6:L:1012:HOH:O	2.69	0.45
3:C:17:ILE:HD13	3:C:17:ILE:H	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:100:PHE:CD2	4:D:107:VAL:HG21	2.52	0.45
4:D:177:GLN:NE2	2:F:104:PHE:HE2	2.13	0.45
1:E:114:ARG:NH1	1:E:121:SER:H	2.15	0.45
4:L:148:ARG:HG3	4:L:148:ARG:NH1	2.31	0.45
1:A:82:MSE:HE3	1:A:86:ARG:NH1	2.32	0.45
4:H:167:ARG:HG2	4:H:167:ARG:NH1	2.32	0.45
2:J:13:LEU:HD22	2:J:79:TYR:CD1	2.52	0.45
4:L:158:ASN:HB2	4:L:160:ASP:OD1	2.16	0.45
3:C:80:LYS:O	3:C:81:GLU:C	2.55	0.45
4:D:100:PHE:HD1	4:D:141:THR:HG21	1.81	0.45
4:H:109:LEU:HB2	4:H:145:ARG:NH2	2.31	0.45
3:K:49:ALA:HB1	3:K:60:LEU:HD11	1.98	0.45
4:D:135:SER:O	4:D:139:LEU:HD23	2.17	0.44
1:E:80:MSE:C	1:E:82:MSE:N	2.70	0.44
1:I:101:GLU:HB3	2:J:88:ARG:CZ	2.47	0.44
2:J:1:MSE:O	2:J:2:PHE:HB2	2.16	0.44
4:L:94:GLU:O	4:L:95:GLY:C	2.55	0.44
2:J:1:MSE:HE1	2:J:65:ARG:HG2	1.98	0.44
4:L:153:SER:C	4:L:155:ASN:H	2.20	0.44
1:A:42:GLU:O	1:A:44:LEU:N	2.50	0.44
2:B:2:PHE:HB2	4:D:46:PHE:CZ	2.52	0.44
3:C:72:GLU:N	3:C:116:LEU:HD21	2.32	0.44
3:G:20:ASN:HD21	3:G:57:LYS:HA	1.81	0.44
3:G:151:MSE:HE1	4:H:186:PHE:HD1	1.83	0.44
4:H:158:ASN:HD22	4:H:160:ASP:N	2.15	0.44
4:H:191:LYS:HE2	4:H:193:GLN:O	2.18	0.44
1:I:173:LEU:HD22	1:I:211:ILE:CD1	2.47	0.44
4:L:6:PHE:O	4:L:6:PHE:CD2	2.70	0.44
1:A:29:ARG:O	1:A:32:GLN:HB2	2.18	0.44
1:A:147:LYS:CG	1:A:148:HIS:HD2	2.29	0.44
2:B:103:ARG:HD3	2:B:111:MSE:HE3	1.99	0.44
4:H:191:LYS:O	4:H:191:LYS:HG2	2.17	0.44
3:K:99:LEU:HB3	3:K:107:ILE:HD11	1.99	0.44
4:L:123:LEU:HD12	4:L:126:PHE:CD2	2.53	0.44
1:A:149:MSE:SE	2:B:73:ARG:HG3	2.68	0.44
2:B:36:MSE:HE3	2:B:69:LEU:O	2.17	0.44
4:D:142:PHE:C	4:D:144:GLY:N	2.70	0.44
1:E:191:GLN:NE2	1:E:193:ASP:HB2	2.32	0.44
3:G:124:ARG:NH2	3:G:152:GLU:OE1	2.50	0.44
4:H:189:TRP:C	4:H:191:LYS:H	2.20	0.44
2:J:7:MSE:HE1	4:L:26:LEU:HD12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:100:ILE:HD11	1:A:129:PHE:CD2	2.52	0.44
1:A:136:ASN:ND2	2:B:113:TRP:CD1	2.85	0.44
3:C:54:GLN:C	3:C:56:GLN:N	2.70	0.44
4:D:188:CYS:HA	4:D:191:LYS:HD3	1.98	0.44
3:G:53:LYS:HE2	3:G:106:ASN:ND2	2.32	0.44
4:H:106:VAL:HG13	4:H:107:VAL:N	2.32	0.44
2:J:135:ASP:OD2	2:J:138:GLN:HG2	2.17	0.44
3:K:53:LYS:HD3	3:K:60:LEU:CD2	2.47	0.44
3:K:121:TRP:O	3:K:125:ILE:HG12	2.18	0.44
4:L:16:GLU:HG3	4:L:17:GLU:N	2.32	0.44
4:L:86:VAL:HG12	4:L:87:GLU:N	2.32	0.44
3:C:124:ARG:NH2	3:C:152:GLU:OE1	2.51	0.44
1:E:51:VAL:O	1:E:55:MSE:HB2	2.18	0.44
3:G:53:LYS:CD	3:G:60:LEU:HD23	2.47	0.44
4:L:43:LEU:O	4:L:44:GLY:C	2.55	0.44
4:L:101:SER:HA	6:L:1027:HOH:O	2.18	0.44
4:D:41:PRO:HA	4:D:59:ALA:HB2	1.99	0.44
2:F:72:ASN:O	2:F:76:THR:HG22	2.16	0.44
3:G:36:PHE:C	3:G:37:ASN:HD22	2.21	0.44
4:H:109:LEU:CD2	4:H:145:ARG:NH2	2.72	0.44
4:H:139:LEU:O	4:H:143:ILE:HG12	2.18	0.44
1:A:106:HIS:ND1	1:A:164:LYS:CB	2.80	0.44
3:C:3:ALA:CB	3:C:151:MSE:HE1	2.47	0.44
4:H:81:ARG:HD2	4:H:81:ARG:N	2.32	0.44
3:K:87:MSE:CE	3:K:92:TYR:CZ	2.89	0.44
3:K:96:THR:O	3:K:100:LEU:HB2	2.18	0.44
1:A:25:GLU:O	1:A:28:GLU:HB3	2.17	0.43
1:E:141:LEU:O	1:E:146:LEU:HD13	2.17	0.43
2:F:87:ILE:HA	2:F:90:LEU:HD22	1.99	0.43
1:I:32:GLN:NE2	1:I:176:ARG:NE	2.65	0.43
1:A:170:TYR:CE1	1:A:207:ARG:HG2	2.53	0.43
2:B:18:GLU:HG3	2:B:19:GLY:H	1.84	0.43
2:B:18:GLU:OE2	2:B:19:GLY:N	2.51	0.43
3:C:53:LYS:NZ	3:C:106:ASN:HD21	2.16	0.43
4:D:143:ILE:HD12	4:D:143:ILE:N	2.33	0.43
1:E:58:LEU:O	1:E:62:GLU:HB2	2.18	0.43
4:L:109:LEU:HD12	4:L:109:LEU:HA	1.82	0.43
1:A:110:LYS:CA	1:A:113:THR:HG22	2.48	0.43
2:B:15:ARG:O	2:B:17:PRO:HD3	2.19	0.43
4:D:58:ASN:N	4:D:58:ASN:ND2	2.63	0.43
1:E:160:ARG:HG2	1:E:160:ARG:HH11	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:G:67:ASP:O	3:G:70:LYS:N	2.49	0.43
1:I:171:VAL:CG1	1:I:172:PHE:N	2.81	0.43
4:L:32:LEU:HD12	4:L:89:PRO:HG3	2.00	0.43
2:B:97:ILE:HD13	2:B:97:ILE:H	1.82	0.43
3:C:75:ARG:HA	3:C:120:MSE:HE2	2.00	0.43
3:C:137:ARG:HA	4:D:143:ILE:HG21	2.00	0.43
1:I:62:GLU:HG3	1:I:66:ARG:CZ	2.48	0.43
1:I:134:MSE:CE	1:I:158:LEU:HD12	2.47	0.43
1:I:146:LEU:N	1:I:146:LEU:CD1	2.81	0.43
2:J:71:ARG:HG2	4:L:71:TRP:CE2	2.53	0.43
1:A:71:GLU:O	1:A:72:ASP:C	2.57	0.43
2:B:64:PHE:HA	4:D:76:LEU:HD11	2.01	0.43
2:B:94:TYR:CD2	2:B:99:PRO:HG2	2.53	0.43
5:B:1016:SO4:O3	2:F:105:HIS:NE2	2.51	0.43
2:F:58:LEU:HD12	4:H:41:PRO:CG	2.48	0.43
4:H:145:ARG:NH2	4:H:172:GLU:OE1	2.51	0.43
3:K:83:THR:O	3:K:127:LYS:NZ	2.43	0.43
3:C:0:MSE:HG3	3:C:1:MSE:H	1.84	0.43
3:C:1:MSE:HB2	3:C:154:ASN:OD1	2.18	0.43
3:C:18:ILE:HG22	3:C:41:PRO:HG3	2.00	0.43
3:C:151:MSE:O	3:C:155:THR:HG23	2.19	0.43
4:D:157:TYR:CG	4:D:158:ASN:N	2.85	0.43
1:E:140:TYR:CZ	1:E:144:VAL:HG21	2.53	0.43
1:E:144:VAL:HG13	5:F:1014:SO4:O4	2.19	0.43
3:K:33:LEU:HD23	3:K:33:LEU:HA	1.85	0.43
3:K:74:MSE:CE	3:K:88:PRO:HG3	2.48	0.43
4:L:67:GLU:OE1	4:L:67:GLU:HA	2.18	0.43
4:L:151:ASP:O	4:L:155:ASN:HB2	2.18	0.43
1:A:34:TRP:CG	1:A:88:VAL:HG13	2.54	0.43
1:A:122:LEU:HD13	1:A:123:SER:O	2.19	0.43
1:A:173:LEU:CD1	1:A:211:ILE:HG21	2.49	0.43
2:B:142:PRO:HA	2:B:143:PRO:HD3	1.87	0.43
5:B:1016:SO4:O2	2:F:105:HIS:NE2	2.27	0.43
3:C:75:ARG:CA	3:C:120:MSE:HE2	2.48	0.43
3:C:137:ARG:NH1	3:C:137:ARG:CB	2.81	0.43
3:C:139:GLN:NE2	3:C:171:ARG:HH21	2.16	0.43
1:I:35:MSE:HE3	3:K:1:MSE:HE1	2.01	0.43
1:I:80:MSE:SE	6:I:1009:HOH:O	2.87	0.43
2:J:102:LEU:HD12	2:J:102:LEU:HA	1.87	0.43
3:K:64:GLU:HG2	3:K:70:LYS:NZ	2.33	0.43
3:K:167:MSE:CE	3:K:171:ARG:HH12	2.31	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:91:ILE:HG13	4:L:112:MSE:HE3	2.00	0.43
4:L:130:GLU:O	4:L:134:ILE:HG13	2.18	0.43
1:E:42:GLU:O	1:E:99:LYS:NZ	2.47	0.43
1:E:146:LEU:N	1:E:146:LEU:CD1	2.81	0.43
1:I:47:LYS:N	1:I:48:PRO:CD	2.82	0.43
3:K:50:ILE:HD11	3:K:98:LEU:HD13	2.01	0.43
3:C:16:THR:O	3:C:61:LEU:HB2	2.19	0.43
4:D:171:MSE:HE3	4:D:171:MSE:O	2.19	0.43
2:F:10:ILE:HD12	4:H:25:ILE:HD11	2.01	0.43
1:I:43:LEU:HA	1:I:99:LYS:HD2	2.01	0.43
1:I:79:GLN:HA	1:I:82:MSE:HE2	2.01	0.43
3:K:11:GLU:HA	3:K:46:LEU:HB3	2.00	0.43
4:L:119:PHE:O	4:L:123:LEU:N	2.51	0.43
1:A:58:LEU:HD21	1:A:85:ILE:CG2	2.49	0.43
1:A:109:GLU:HB3	1:A:159:PHE:HZ	1.84	0.43
2:B:1:MSE:CE	2:B:65:ARG:HG2	2.48	0.43
2:B:58:LEU:O	2:B:59:ILE:C	2.56	0.43
4:D:96:TRP:C	4:D:98:THR:N	2.72	0.43
4:H:95:GLY:O	4:H:99:VAL:HG23	2.18	0.43
1:I:180:GLU:CG	1:I:181:ASN:H	2.24	0.43
1:A:74:LYS:HZ2	3:C:26:ILE:HA	1.84	0.42
1:E:109:GLU:O	1:E:113:THR:HB	2.19	0.42
3:C:67:ASP:O	3:C:70:LYS:HB2	2.19	0.42
3:C:133:ASP:O	3:C:137:ARG:HD3	2.19	0.42
3:G:54:GLN:HE22	3:G:102:HIS:CE1	2.36	0.42
3:G:62:PRO:HG3	3:G:107:ILE:HG12	2.01	0.42
4:H:193:GLN:HE21	4:H:193:GLN:CA	2.18	0.42
4:L:70:LEU:HD23	4:L:70:LEU:C	2.39	0.42
4:D:157:TYR:CE2	4:D:162:SER:HB2	2.46	0.42
1:E:80:MSE:HE2	3:G:47:TRP:CE3	2.54	0.42
1:E:106:HIS:HE1	1:E:162:VAL:O	2.02	0.42
1:E:173:LEU:O	1:E:203:GLN:HA	2.20	0.42
1:I:194:TYR:C	1:I:194:TYR:CD1	2.93	0.42
4:L:42:ARG:CA	4:L:58:ASN:O	2.67	0.42
1:A:104:PHE:CE2	1:A:134:MSE:HE3	2.54	0.42
3:C:69:GLU:HA	3:C:72:GLU:HB3	2.00	0.42
3:C:105:ASP:C	3:C:106:ASN:HD22	2.22	0.42
3:C:151:MSE:HE3	4:D:186:PHE:CD2	2.50	0.42
4:D:168:LEU:HD22	4:D:172:GLU:HB3	2.00	0.42
1:E:94:ARG:NH2	2:F:140:MSE:HA	2.35	0.42
3:K:146:ASP:O	3:K:147:ASN:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:L:77:PHE:CG	4:L:78:ASP:N	2.88	0.42
1:A:80:MSE:O	1:A:84:ARG:HG3	2.19	0.42
1:E:55:MSE:HG2	1:E:89:LEU:HD21	2.00	0.42
3:G:136:VAL:HG13	3:G:167:MSE:SE	2.70	0.42
1:I:49:GLU:HB2	6:I:1014:HOH:O	2.20	0.42
3:K:33:LEU:O	3:K:34:GLY:O	2.36	0.42
3:K:135:PHE:CE2	3:K:143:ALA:HB2	2.54	0.42
1:A:64:ASN:N	1:A:64:ASN:ND2	2.67	0.42
1:A:144:VAL:CG1	2:B:80:LEU:HD13	2.50	0.42
3:C:83:THR:OG1	3:C:84:PHE:N	2.52	0.42
4:H:152:SER:CB	4:H:164:LEU:HD22	2.49	0.42
1:I:73:LEU:HD12	1:I:74:LYS:H	1.82	0.42
3:K:62:PRO:HA	3:K:63:PRO:HD3	1.98	0.42
3:C:17:ILE:HG22	3:C:60:LEU:HD23	2.00	0.42
3:C:59:ARG:HE	3:C:59:ARG:HB2	1.54	0.42
3:C:129:ARG:HD3	4:D:154:GLN:HG3	2.01	0.42
2:F:18:GLU:OE2	2:F:18:GLU:N	2.47	0.42
1:I:27:ILE:HG21	3:K:29:ILE:HD11	2.02	0.42
1:I:27:ILE:HG21	3:K:29:ILE:HD13	2.02	0.42
1:I:87:TYR:OH	2:J:142:PRO:HG3	2.19	0.42
2:J:34:GLU:O	2:J:35:GLU:C	2.57	0.42
3:G:17:ILE:HG22	3:G:60:LEU:HA	2.00	0.42
4:H:34:VAL:CG2	4:H:84:LEU:HB2	2.49	0.42
1:I:118:GLU:HA	1:I:119:PRO:HD3	1.76	0.42
4:L:16:GLU:HG3	4:L:17:GLU:H	1.84	0.42
3:G:105:ASP:O	3:G:107:ILE:N	2.53	0.42
1:I:114:ARG:HA	1:I:115:PRO:HD2	1.87	0.42
2:J:100:ASN:HD22	2:J:100:ASN:N	2.17	0.42
3:K:108:PRO:C	3:K:109:LYS:HG2	2.40	0.42
4:L:153:SER:C	4:L:155:ASN:N	2.74	0.42
4:L:183:LEU:C	4:L:183:LEU:CD1	2.88	0.42
1:A:65:LEU:HD11	1:A:78:HIS:HB2	2.02	0.42
1:A:144:VAL:HG11	2:B:80:LEU:HD13	2.01	0.42
2:B:61:THR:HG22	2:B:65:ARG:HH12	1.83	0.42
3:C:159:PHE:CD1	3:C:159:PHE:C	2.93	0.42
4:D:48:LEU:H	4:D:48:LEU:CD2	2.33	0.42
4:H:141:THR:O	4:H:145:ARG:HG3	2.20	0.42
3:K:29:ILE:C	3:K:29:ILE:CD1	2.82	0.42
4:L:103:ASP:O	4:L:106:VAL:HG12	2.20	0.42
1:A:45:GLU:OE2	1:A:119:PRO:HG3	2.20	0.41
3:C:46:LEU:CD2	3:C:50:ILE:HG13	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:F:55:ARG:HH12	4:H:57:ASP:CG	2.19	0.41
1:I:176:ARG:O	1:I:200:LYS:HG2	2.19	0.41
3:C:92:TYR:CD1	3:C:92:TYR:C	2.93	0.41
2:F:58:LEU:HD12	4:H:41:PRO:HG2	2.03	0.41
4:H:165:VAL:HA	4:H:168:LEU:HD22	2.01	0.41
4:L:137:SER:O	4:L:141:THR:HG23	2.19	0.41
1:A:147:LYS:HG2	1:A:148:HIS:CD2	2.54	0.41
3:C:74:MSE:SE	3:C:88:PRO:HG3	2.71	0.41
3:C:96:THR:O	3:C:100:LEU:HB2	2.19	0.41
4:D:7:ARG:NH1	4:D:23:ASP:OD1	2.53	0.41
4:D:120:GLY:O	4:D:124:LEU:HD13	2.19	0.41
1:E:95:CYS:O	1:E:99:LYS:HG3	2.20	0.41
2:F:13:LEU:HD12	2:F:13:LEU:HA	1.84	0.41
2:F:116:ASN:OD1	2:F:119:ARG:NH2	2.53	0.41
4:H:128:SER:OG	4:H:130:GLU:HG2	2.20	0.41
4:H:168:LEU:HD12	4:H:168:LEU:HA	1.86	0.41
2:J:141:LYS:O	2:J:142:PRO:C	2.59	0.41
4:L:120:GLY:O	4:L:124:LEU:HD13	2.20	0.41
3:C:60:LEU:N	3:C:106:ASN:OD1	2.51	0.41
4:D:39:ALA:N	4:D:62:GLN:HE21	2.17	0.41
2:F:74:ARG:HG3	4:H:19:PHE:CE1	2.55	0.41
4:H:169:ASP:O	4:H:173:ARG:HG3	2.21	0.41
4:L:100:PHE:CD1	4:L:107:VAL:HG21	2.54	0.41
1:A:46:SER:OG	1:A:48:PRO:HD3	2.21	0.41
1:A:123:SER:CB	1:A:124:PRO:HD2	2.50	0.41
2:B:56:SER:O	2:B:58:LEU:N	2.53	0.41
3:C:74:MSE:CE	3:C:88:PRO:HG3	2.49	0.41
4:D:147:ARG:O	4:D:149:ILE:N	2.54	0.41
3:G:139:GLN:NE2	3:G:171:ARG:NH2	2.68	0.41
3:K:23:LEU:HD13	3:K:24:ASP:N	2.35	0.41
4:L:123:LEU:HD12	4:L:126:PHE:HD2	1.85	0.41
3:C:48:LEU:HD22	3:C:52:LEU:CD2	2.44	0.41
3:C:110:ALA:O	3:C:113:ILE:HG22	2.21	0.41
3:C:129:ARG:HB2	3:C:129:ARG:NH1	2.33	0.41
3:C:137:ARG:C	3:C:139:GLN:H	2.24	0.41
1:E:29:ARG:HE	1:E:29:ARG:CA	2.33	0.41
2:F:25:ASN:H	2:F:25:ASN:ND2	2.17	0.41
2:F:125:MSE:HB3	2:F:134:LEU:O	2.21	0.41
1:I:54:VAL:HG12	1:I:58:LEU:HD23	2.03	0.41
3:K:97:LYS:HD3	4:L:189:TRP:CZ2	2.56	0.41
1:A:50:ILE:O	1:A:54:VAL:HG22	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:94:GLU:N	4:D:97:ARG:HH21	2.19	0.41
4:D:96:TRP:O	4:D:98:THR:N	2.53	0.41
1:E:29:ARG:HE	1:E:29:ARG:HA	1.86	0.41
3:G:68:VAL:HG11	3:G:109:LYS:HG3	2.02	0.41
1:A:209:LYS:O	1:A:212:ALA:HB3	2.20	0.41
3:G:2:ASP:OD1	3:G:4:ALA:N	2.44	0.41
3:G:82:GLU:OE1	3:G:82:GLU:C	2.59	0.41
4:H:193:GLN:NE2	4:H:193:GLN:CA	2.76	0.41
1:I:205:LEU:HD12	1:I:205:LEU:HA	1.85	0.41
4:L:41:PRO:HA	4:L:59:ALA:HB2	2.03	0.41
4:L:58:ASN:ND2	4:L:59:ALA:N	2.67	0.41
1:A:74:LYS:NZ	3:C:26:ILE:HA	2.36	0.41
1:A:173:LEU:HD12	1:A:211:ILE:HG21	2.02	0.41
2:B:39:LEU:CD1	2:B:68:SER:HB3	2.51	0.41
2:B:56:SER:C	2:B:58:LEU:N	2.73	0.41
3:C:162:GLN:O	3:C:165:ASN:N	2.53	0.41
4:D:25:ILE:HG13	4:D:26:LEU:N	2.36	0.41
4:D:104:PRO:C	4:D:106:VAL:H	2.24	0.41
1:E:55:MSE:HA	1:E:55:MSE:CE	2.45	0.41
4:H:43:LEU:O	4:H:44:GLY:C	2.59	0.41
1:I:50:ILE:HD12	1:I:50:ILE:H	1.86	0.41
1:I:73:LEU:HD11	3:K:23:LEU:CD2	2.50	0.41
1:I:176:ARG:HG3	1:I:176:ARG:NH1	2.36	0.41
1:I:181:ASN:N	1:I:181:ASN:ND2	2.68	0.41
2:J:76:THR:O	2:J:80:LEU:HG	2.20	0.41
3:K:21:PHE:CD2	3:K:21:PHE:C	2.94	0.41
3:K:21:PHE:CD1	3:K:57:LYS:HB3	2.55	0.41
4:L:18:ASN:HD22	4:L:18:ASN:HA	1.61	0.41
4:L:43:LEU:O	4:L:45:ALA:N	2.54	0.41
1:A:48:PRO:O	1:A:52:GLU:CG	2.67	0.41
1:E:55:MSE:HE2	1:E:58:LEU:HD12	2.03	0.41
2:F:87:ILE:O	2:F:90:LEU:HB2	2.21	0.41
3:G:149:THR:O	3:G:153:ILE:HG23	2.21	0.41
4:H:32:LEU:HD21	4:H:86:VAL:CG1	2.51	0.41
4:H:61:PRO:O	4:H:63:GLY:N	2.52	0.41
1:I:199:GLU:O	1:I:200:LYS:C	2.59	0.41
3:C:122:ASP:C	3:C:124:ARG:H	2.24	0.40
4:D:94:GLU:N	4:D:94:GLU:OE1	2.54	0.40
3:G:111:ASP:HA	3:G:114:ARG:HB3	2.02	0.40
1:A:100:ILE:CG1	1:A:101:GLU:N	2.84	0.40
2:B:1:MSE:HE3	2:B:39:LEU:CD2	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:43:ASN:OD1	2:B:65:ARG:HB2	2.21	0.40
1:E:97:LEU:HD23	1:E:97:LEU:HA	1.95	0.40
3:G:124:ARG:HD3	3:G:152:GLU:OE2	2.21	0.40
1:I:21:LEU:HB2	1:I:25:GLU:OE1	2.21	0.40
1:I:140:TYR:CZ	1:I:144:VAL:HG21	2.55	0.40
2:J:100:ASN:ND2	2:J:101:ALA:N	2.67	0.40
3:K:21:PHE:CE2	3:K:23:LEU:HB2	2.56	0.40
4:L:68:LEU:HA	4:L:69:PRO:HD3	1.95	0.40
4:L:141:THR:O	4:L:145:ARG:HG3	2.21	0.40
3:C:78:GLU:C	3:C:80:LYS:N	2.74	0.40
4:D:97:ARG:NH1	4:D:134:ILE:HG13	2.36	0.40
1:E:31:GLU:O	1:E:35:MSE:HG3	2.20	0.40
2:F:2:PHE:O	2:F:3:CYS:C	2.59	0.40
4:H:91:ILE:CG1	4:H:112:MSE:HE2	2.50	0.40
1:I:85:ILE:HD11	3:K:29:ILE:CG1	2.50	0.40
4:L:33:PRO:HD2	4:L:87:GLU:O	2.22	0.40
1:A:23:PRO:HB3	3:C:29:ILE:HG23	2.03	0.40
1:A:104:PHE:N	1:A:105:PRO:HD2	2.37	0.40
1:A:149:MSE:HE3	2:B:36:MSE:SE	2.72	0.40
3:C:11:GLU:O	3:C:47:TRP:HD1	2.05	0.40
3:C:33:LEU:CD1	3:C:48:LEU:HD12	2.52	0.40
3:C:51:ASN:ND2	3:C:55:ARG:CD	2.85	0.40
3:C:118:LYS:HB2	3:C:118:LYS:HE3	1.88	0.40
3:C:133:ASP:OD1	4:D:147:ARG:HB2	2.22	0.40
4:D:32:LEU:HD21	4:D:86:VAL:HG11	2.03	0.40
3:G:65:TRP:HA	3:G:70:LYS:NZ	2.37	0.40
3:G:160:LEU:O	3:G:164:LEU:HD13	2.21	0.40
4:H:77:PHE:N	4:H:84:LEU:HD21	2.36	0.40
4:H:140:GLN:HE21	4:H:140:GLN:HB2	1.66	0.40
1:I:196:ILE:CG2	1:I:197:ASP:H	2.35	0.40
3:K:129:ARG:HB3	4:L:150:MSE:HE3	2.02	0.40
3:K:151:MSE:HE2	4:L:186:PHE:HD1	1.86	0.40
4:L:147:ARG:HG3	4:L:147:ARG:HH11	1.86	0.40
1:A:172:PHE:HE1	1:A:203:GLN:HB2	1.86	0.40
2:B:39:LEU:O	2:B:43:ASN:HB2	2.21	0.40
3:C:20:ASN:ND2	3:C:21:PHE:HD1	2.20	0.40
4:D:168:LEU:HB3	4:D:172:GLU:HB2	2.04	0.40
1:E:150:PRO:HA	1:E:151:PRO:HD3	1.99	0.40
2:F:7:MSE:HE2	2:F:75:CYS:SG	2.62	0.40
4:L:47:PHE:O	4:L:48:LEU:HB2	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	155/203 (76%)	119 (77%)	28 (18%)	8 (5%)	2 12
1	E	186/203 (92%)	162 (87%)	20 (11%)	4 (2%)	6 31
1	I	190/203 (94%)	159 (84%)	25 (13%)	6 (3%)	4 22
2	B	143/152 (94%)	117 (82%)	18 (13%)	8 (6%)	2 10
2	F	144/152 (95%)	127 (88%)	10 (7%)	7 (5%)	2 13
2	J	143/152 (94%)	125 (87%)	14 (10%)	4 (3%)	5 25
3	C	164/186 (88%)	126 (77%)	30 (18%)	8 (5%)	2 13
3	G	174/186 (94%)	148 (85%)	19 (11%)	7 (4%)	3 17
3	K	173/186 (93%)	152 (88%)	17 (10%)	4 (2%)	6 30
4	D	178/216 (82%)	136 (76%)	29 (16%)	13 (7%)	1 5
4	H	179/216 (83%)	160 (89%)	14 (8%)	5 (3%)	5 25
4	L	178/216 (82%)	150 (84%)	18 (10%)	10 (6%)	2 10
All	All	2007/2271 (88%)	1681 (84%)	242 (12%)	84 (4%)	3 16

All (84) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	LEU
1	A	72	ASP
1	A	116	GLU
2	B	17	PRO
3	C	68	VAL
4	D	15	PRO
4	D	127	ASP
1	E	72	ASP
2	F	131	ASP
3	G	110	ALA
4	H	62	GLN
1	I	64	ASN

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Mol	Chain	Res	Type
4	L	62	GLN
4	L	153	SER
1	A	44	LEU
1	A	121	SER
1	A	153	LEU
2	B	53	GLY
2	B	57	ASP
2	B	133	GLY
3	C	34	GLY
4	D	105	ASN
4	D	109	LEU
4	D	126	PHE
4	D	148	ARG
1	E	116	GLU
2	F	18	GLU
2	F	130	GLY
3	G	34	GLY
3	G	106	ASN
3	G	114	ARG
1	I	210	THR
2	J	18	GLU
3	K	34	GLY
3	K	81	GLU
3	K	111	ASP
4	L	42	ARG
4	L	44	GLY
4	L	80	LYS
4	L	154	GLN
2	B	55	ARG
2	B	100	ASN
2	B	126	ARG
1	E	178	ARG
2	F	52	SER
4	H	19	PHE
4	H	47	PHE
4	H	58	ASN
1	I	178	ARG
1	I	191	GLN
4	L	63	GLY
3	C	88	PRO
3	C	109	LYS
3	C	111	ASP

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Mol	Chain	Res	Type
4	D	102	ALA
2	F	20	GLN
3	G	150	LEU
4	H	63	GLY
1	I	72	ASP
2	J	53	GLY
2	J	131	ASP
1	A	145	ALA
3	C	66	MSE
3	C	147	ASN
4	D	154	GLN
1	E	49	GLU
3	G	79	ARG
1	I	69	LYS
4	L	41	PRO
4	L	46	PHE
1	A	142	LYS
4	D	97	ARG
4	D	136	GLN
2	F	129	GLY
2	F	133	GLY
3	C	157	GLY
2	B	19	GLY
4	D	11	GLY
3	K	35	PRO
4	L	15	PRO
2	J	54	GLY
3	G	88	PRO
4	D	61	PRO
4	D	83	ILE

5.3.2 Protein sidechains (i)

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	151/181 (83%)	143 (95%)	8 (5%)	22 58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	E	179/181 (99%)	167 (93%)	12 (7%)	16	49
1	I	180/181 (99%)	164 (91%)	16 (9%)	9	35
2	B	126/125 (101%)	114 (90%)	12 (10%)	8	32
2	F	127/125 (102%)	120 (94%)	7 (6%)	21	57
2	J	126/125 (101%)	116 (92%)	10 (8%)	12	41
3	C	154/161 (96%)	140 (91%)	14 (9%)	9	34
3	G	160/161 (99%)	148 (92%)	12 (8%)	13	43
3	K	159/161 (99%)	140 (88%)	19 (12%)	5	22
4	D	157/180 (87%)	144 (92%)	13 (8%)	11	39
4	H	158/180 (88%)	134 (85%)	24 (15%)	3	14
4	L	157/180 (87%)	137 (87%)	20 (13%)	4	19
All	All	1834/1941 (94%)	1667 (91%)	167 (9%)	9	34

All (167) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	LEU
1	A	32	GLN
1	A	71	GLU
1	A	72	ASP
1	A	109	GLU
1	A	141	LEU
1	A	159	PHE
1	A	204	HIS
2	B	1	MSE
2	B	2	PHE
2	B	8	GLU
2	B	10	ILE
2	B	17	PRO
2	B	25	ASN
2	B	27	ASP
2	B	46	ASP
2	B	49	GLU
2	B	71	ARG
2	B	93	GLU
2	B	97	ILE
3	C	9	LEU
3	C	17	ILE

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Mol	Chain	Res	Type
3	C	20	ASN
3	C	24	ASP
3	C	40	LEU
3	C	46	LEU
3	C	48	LEU
3	C	52	LEU
3	C	58	CYS
3	C	76	ASP
3	C	106	ASN
3	C	129	ARG
3	C	147	ASN
3	C	154	ASN
4	D	6	PHE
4	D	9	GLU
4	D	23	ASP
4	D	25	ILE
4	D	58	ASN
4	D	84	LEU
4	D	90	LYS
4	D	94	GLU
4	D	139	LEU
4	D	155	ASN
4	D	169	ASP
4	D	171	MSE
4	D	183	LEU
1	E	21	LEU
1	E	22	THR
1	E	29	ARG
1	E	32	GLN
1	E	55	MSE
1	E	107	VAL
1	E	111	GLU
1	E	113	THR
1	E	134	MSE
1	E	141	LEU
1	E	178	ARG
1	E	203	GLN
2	F	25	ASN
2	F	26	GLU
2	F	43	ASN
2	F	58	LEU
2	F	71	ARG

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Mol	Chain	Res	Type
2	F	98	LEU
2	F	139	ASP
3	G	7	GLU
3	G	26	ILE
3	G	29	ILE
3	G	58	CYS
3	G	76	ASP
3	G	82	GLU
3	G	101	ASN
3	G	123	THR
3	G	125	ILE
3	G	153	ILE
3	G	161	THR
3	G	175	GLN
4	H	10	SER
4	H	25	ILE
4	H	26	LEU
4	H	28	SER
4	H	43	LEU
4	H	46	PHE
4	H	57	ASP
4	H	58	ASN
4	H	62	GLN
4	H	76	LEU
4	H	81	ARG
4	H	84	LEU
4	H	88	LEU
4	H	124	LEU
4	H	131	ASN
4	H	139	LEU
4	H	141	THR
4	H	147	ARG
4	H	158	ASN
4	H	168	LEU
4	H	169	ASP
4	H	170	GLU
4	H	178	THR
4	H	191	LYS
1	I	28	GLU
1	I	32	GLN
1	I	55	MSE
1	I	64	ASN

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Mol	Chain	Res	Type
1	I	69	LYS
1	I	73	LEU
1	I	118	GLU
1	I	125	GLU
1	I	134	MSE
1	I	136	ASN
1	I	141	LEU
1	I	153	LEU
1	I	177	GLU
1	I	193	ASP
1	I	197	ASP
1	I	211	ILE
2	J	2	PHE
2	J	13	LEU
2	J	60	PRO
2	J	71	ARG
2	J	76	THR
2	J	90	LEU
2	J	98	LEU
2	J	100	ASN
2	J	131	ASP
2	J	136	ILE
3	K	14	LEU
3	K	17	ILE
3	K	20	ASN
3	K	32	ASP
3	K	36	PHE
3	K	42	VAL
3	K	43	GLU
3	K	46	LEU
3	K	52	LEU
3	K	56	GLN
3	K	64	GLU
3	K	105	ASP
3	K	111	ASP
3	K	120	MSE
3	K	146	ASP
3	K	148	LEU
3	K	161	THR
3	K	164	LEU
3	K	173	ASN
4	L	18	ASN

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Mol	Chain	Res	Type
4	L	26	LEU
4	L	38	THR
4	L	41	PRO
4	L	66	LEU
4	L	81	ARG
4	L	85	SER
4	L	90	LYS
4	L	109	LEU
4	L	122	GLN
4	L	136	GLN
4	L	139	LEU
4	L	141	THR
4	L	145	ARG
4	L	147	ARG
4	L	159	GLU
4	L	169	ASP
4	L	184	ASN
4	L	191	LYS
4	L	193	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (80) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	64	ASN
1	A	78	HIS
1	A	143	ASN
1	A	148	HIS
1	A	204	HIS
2	B	25	ASN
2	B	138	GLN
3	C	20	ASN
3	C	51	ASN
3	C	101	ASN
3	C	138	GLN
3	C	139	GLN
3	C	147	ASN
3	C	154	ASN
4	D	18	ASN
4	D	62	GLN
4	D	93	GLN
4	D	122	GLN

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Mol	Chain	Res	Type
4	D	131	ASN
4	D	177	GLN
4	D	180	GLN
1	E	36	ASN
1	E	78	HIS
1	E	106	HIS
1	E	154	GLN
1	E	179	GLN
1	E	181	ASN
1	E	191	GLN
1	E	203	GLN
2	F	14	HIS
2	F	25	ASN
2	F	100	ASN
3	G	37	ASN
3	G	54	GLN
3	G	101	ASN
3	G	106	ASN
3	G	139	GLN
3	G	142	HIS
3	G	147	ASN
4	H	18	ASN
4	H	29	HIS
4	H	58	ASN
4	H	62	GLN
4	H	93	GLN
4	H	122	GLN
4	H	125	HIS
4	H	131	ASN
4	H	136	GLN
4	H	140	GLN
4	H	154	GLN
4	H	158	ASN
4	H	177	GLN
4	H	193	GLN
1	I	32	GLN
1	I	36	ASN
1	I	64	ASN
1	I	106	HIS
1	I	136	ASN
1	I	181	ASN
2	J	20	GLN

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Mol	Chain	Res	Type
2	J	31	GLN
2	J	100	ASN
3	K	20	ASN
3	K	138	GLN
3	K	139	GLN
3	K	147	ASN
3	K	173	ASN
4	L	18	ASN
4	L	58	ASN
4	L	62	GLN
4	L	105	ASN
4	L	110	HIS
4	L	122	GLN
4	L	131	ASN
4	L	140	GLN
4	L	154	GLN
4	L	180	GLN
4	L	184	ASN
4	L	187	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

17 ligands are modelled in this entry.

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	SO4	I	1003	-	4,4,4	0.39	0	6,6,6	0.11	0
5	SO4	B	1016	-	4,4,4	0.41	0	6,6,6	0.19	0
5	SO4	E	1011	-	4,4,4	0.42	0	6,6,6	0.09	0
5	SO4	A	1017	-	4,4,4	0.44	0	6,6,6	0.10	0
5	SO4	L	1009	-	4,4,4	0.42	0	6,6,6	0.13	0
5	SO4	E	1015	-	4,4,4	0.44	0	6,6,6	0.06	0
5	SO4	F	1014	-	4,4,4	0.43	0	6,6,6	0.07	0
5	SO4	F	1004	-	4,4,4	0.39	0	6,6,6	0.13	0
5	SO4	E	1013	-	4,4,4	0.43	0	6,6,6	0.12	0
5	SO4	I	1001	-	4,4,4	0.38	0	6,6,6	0.13	0
5	SO4	J	1006	-	4,4,4	0.44	0	6,6,6	0.06	0
5	SO4	I	1002	-	4,4,4	0.38	0	6,6,6	0.12	0
5	SO4	K	1007	-	4,4,4	0.45	0	6,6,6	0.19	0
5	SO4	E	1012	-	4,4,4	0.44	0	6,6,6	0.12	0
5	SO4	L	1008	-	4,4,4	0.45	0	6,6,6	0.09	0
5	SO4	F	1010	-	4,4,4	0.38	0	6,6,6	0.14	0
5	SO4	F	1005	-	4,4,4	0.40	0	6,6,6	0.06	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1016	SO4	5	0
5	F	1014	SO4	1	0
5	F	1004	SO4	1	0
5	I	1001	SO4	1	0
5	F	1010	SO4	3	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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	153/203 (75%)	-0.06	2 (1%)	77	51	48, 77, 108, 115	0
1	E	182/203 (89%)	-0.51	1 (0%)	91	75	21, 47, 79, 108	0
1	I	184/203 (90%)	-0.38	1 (0%)	91	75	21, 44, 87, 97	0
2	B	138/152 (90%)	-0.12	2 (1%)	75	49	33, 65, 92, 106	0
2	F	138/152 (90%)	-0.29	0	100	100	18, 44, 77, 98	0
2	J	138/152 (90%)	-0.42	0	100	100	19, 40, 69, 86	0
3	C	159/186 (85%)	-0.03	1 (0%)	89	72	43, 78, 115, 123	0
3	G	167/186 (89%)	-0.21	1 (0%)	89	72	22, 65, 103, 112	0
3	K	166/186 (89%)	-0.56	0	100	100	22, 41, 63, 72	0
4	D	177/216 (81%)	0.11	3 (1%)	70	41	40, 83, 104, 113	0
4	H	178/216 (82%)	-0.50	0	100	100	18, 40, 76, 88	0
4	L	177/216 (81%)	-0.41	0	100	100	19, 43, 85, 97	0
All	All	1957/2271 (86%)	-0.29	11 (0%)	89	72	18, 54, 101, 123	0

All (11) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	65	LEU	4.4
4	D	49	GLU	3.8
4	D	160	ASP	3.2
1	I	69	LYS	2.9
2	B	131	ASP	2.8
3	C	72	GLU	2.6
4	D	79	ASN	2.6
2	B	133	GLY	2.5
1	E	213	PRO	2.3
1	A	117	GLY	2.2
3	G	69	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	SO4	K	1007	5/5	0.73	0.69	114,114,115,116	0
5	SO4	A	1017	5/5	0.75	0.21	115,115,116,116	0
5	SO4	F	1004	5/5	0.76	0.31	137,138,138,138	0
5	SO4	I	1001	5/5	0.79	0.20	124,124,125,125	0
5	SO4	L	1008	5/5	0.79	0.35	118,118,118,119	0
5	SO4	E	1015	5/5	0.83	0.22	125,125,126,126	0
5	SO4	L	1009	5/5	0.83	0.35	102,102,102,103	0
5	SO4	I	1003	5/5	0.86	0.25	137,137,138,138	0
5	SO4	F	1005	5/5	0.87	0.21	111,112,112,112	0
5	SO4	E	1012	5/5	0.88	0.18	107,107,108,108	0
5	SO4	F	1014	5/5	0.89	0.18	115,116,116,116	0
5	SO4	E	1011	5/5	0.90	0.30	107,107,108,108	0
5	SO4	F	1010	5/5	0.90	0.29	106,107,107,107	0
5	SO4	B	1016	5/5	0.91	0.29	95,97,98,98	0
5	SO4	E	1013	5/5	0.91	0.25	117,118,118,118	0
5	SO4	I	1002	5/5	0.92	0.14	95,96,96,97	0
5	SO4	J	1006	5/5	0.94	0.35	96,96,96,97	0

6.5 Other polymers (i)

There are no such residues in this entry.