



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 04:49 PM UTC

PDB ID : 2E7S / pdb_00002e7s
Title : Crystal structure of the yeast Sec2p GEF domain
Authors : Fukai, S.; Sato, Y.; Nureki, O.
Deposited on : 2007-01-12
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 ⓘ symbol.

The types of validation reports are described at

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

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

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

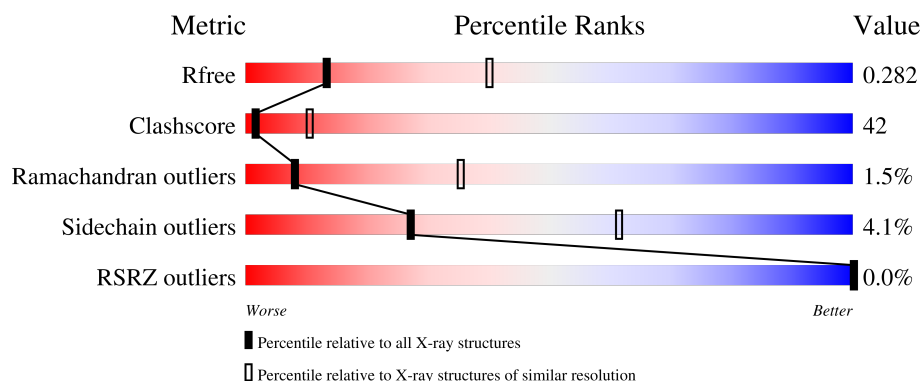
1 Overall quality at a glance

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.



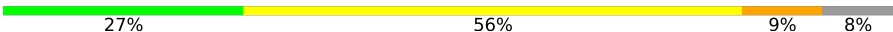
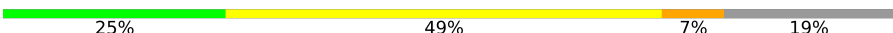
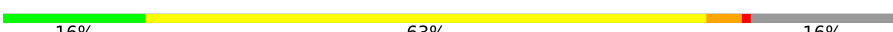
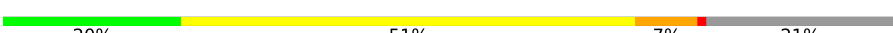
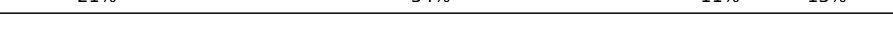
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 $\leq 5\%$. 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	135	36% 43% 6% 16%
1	B	135	30% 50% 10% 10%
1	C	135	47% 31% 10% 13%
1	D	135	% 35% 47% 10% 8%
1	E	135	43% 36% 11% 8%

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Mol	Chain	Length	Quality of chain
1	F	135	
1	G	135	
1	H	135	
1	I	135	
1	J	135	
1	K	135	
1	L	135	
1	M	135	
1	N	135	
1	O	135	
1	P	135	
1	Q	135	
1	R	135	
1	S	135	
1	T	135	

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 19270 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 Rab guanine nucleotide exchange factor SEC2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	114	Total	C	N	O	Se	0	0	0
			938	575	164	197	2			
1	B	121	Total	C	N	O	Se	0	0	0
			993	610	172	209	2			
1	C	118	Total	C	N	O	Se	0	0	0
			968	593	168	205	2			
1	D	124	Total	C	N	O	Se	0	0	0
			1018	626	177	213	2			
1	E	124	Total	C	N	O	Se	0	0	0
			1018	626	177	213	2			
1	F	124	Total	C	N	O	Se	0	0	0
			1018	626	177	213	2			
1	G	110	Total	C	N	O	Se	0	0	0
			906	554	160	191	1			
1	H	107	Total	C	N	O	Se	0	0	0
			877	537	153	186	1			
1	I	114	Total	C	N	O	Se	0	0	0
			938	575	164	197	2			
1	J	107	Total	C	N	O	Se	0	0	0
			877	537	153	186	1			
1	K	117	Total	C	N	O	Se	0	0	0
			961	589	167	203	2			
1	L	114	Total	C	N	O	Se	0	0	0
			938	575	164	197	2			
1	M	117	Total	C	N	O	Se	0	0	0
			961	589	167	203	2			
1	N	111	Total	C	N	O	Se	0	0	0
			914	558	161	194	1			
1	O	124	Total	C	N	O	Se	0	0	0
			1018	626	177	213	2			
1	P	114	Total	C	N	O	Se	0	0	0
			938	575	164	197	2			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	111	Total	C	N	O	Se	0	0	0
			914	558	161	194	1			
1	R	111	Total	C	N	O	Se	0	0	0
			914	558	161	194	1			
1	S	117	Total	C	N	O	Se	0	0	0
			961	589	167	203	2			
1	T	114	Total	C	N	O	Se	0	0	0
			938	575	164	197	2			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	26	GLY	-	expression tag	UNP P17065
A	27	PRO	-	expression tag	UNP P17065
A	28	LEU	-	expression tag	UNP P17065
A	29	GLY	-	expression tag	UNP P17065
A	30	SER	-	expression tag	UNP P17065
A	115	LEU	MET	engineered mutation	UNP P17065
B	26	GLY	-	expression tag	UNP P17065
B	27	PRO	-	expression tag	UNP P17065
B	28	LEU	-	expression tag	UNP P17065
B	29	GLY	-	expression tag	UNP P17065
B	30	SER	-	expression tag	UNP P17065
B	115	LEU	MET	engineered mutation	UNP P17065
C	26	GLY	-	expression tag	UNP P17065
C	27	PRO	-	expression tag	UNP P17065
C	28	LEU	-	expression tag	UNP P17065
C	29	GLY	-	expression tag	UNP P17065
C	30	SER	-	expression tag	UNP P17065
C	115	LEU	MET	engineered mutation	UNP P17065
D	26	GLY	-	expression tag	UNP P17065
D	27	PRO	-	expression tag	UNP P17065
D	28	LEU	-	expression tag	UNP P17065
D	29	GLY	-	expression tag	UNP P17065
D	30	SER	-	expression tag	UNP P17065
D	115	LEU	MET	engineered mutation	UNP P17065
E	26	GLY	-	expression tag	UNP P17065
E	27	PRO	-	expression tag	UNP P17065
E	28	LEU	-	expression tag	UNP P17065
E	29	GLY	-	expression tag	UNP P17065
E	30	SER	-	expression tag	UNP P17065
E	115	LEU	MET	engineered mutation	UNP P17065
F	26	GLY	-	expression tag	UNP P17065

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Chain	Residue	Modelled	Actual	Comment	Reference
F	27	PRO	-	expression tag	UNP P17065
F	28	LEU	-	expression tag	UNP P17065
F	29	GLY	-	expression tag	UNP P17065
F	30	SER	-	expression tag	UNP P17065
F	115	LEU	MET	engineered mutation	UNP P17065
G	26	GLY	-	expression tag	UNP P17065
G	27	PRO	-	expression tag	UNP P17065
G	28	LEU	-	expression tag	UNP P17065
G	29	GLY	-	expression tag	UNP P17065
G	30	SER	-	expression tag	UNP P17065
G	115	LEU	MET	engineered mutation	UNP P17065
H	26	GLY	-	expression tag	UNP P17065
H	27	PRO	-	expression tag	UNP P17065
H	28	LEU	-	expression tag	UNP P17065
H	29	GLY	-	expression tag	UNP P17065
H	30	SER	-	expression tag	UNP P17065
H	115	LEU	MET	engineered mutation	UNP P17065
I	26	GLY	-	expression tag	UNP P17065
I	27	PRO	-	expression tag	UNP P17065
I	28	LEU	-	expression tag	UNP P17065
I	29	GLY	-	expression tag	UNP P17065
I	30	SER	-	expression tag	UNP P17065
I	115	LEU	MET	engineered mutation	UNP P17065
J	26	GLY	-	expression tag	UNP P17065
J	27	PRO	-	expression tag	UNP P17065
J	28	LEU	-	expression tag	UNP P17065
J	29	GLY	-	expression tag	UNP P17065
J	30	SER	-	expression tag	UNP P17065
J	115	LEU	MET	engineered mutation	UNP P17065
K	26	GLY	-	expression tag	UNP P17065
K	27	PRO	-	expression tag	UNP P17065
K	28	LEU	-	expression tag	UNP P17065
K	29	GLY	-	expression tag	UNP P17065
K	30	SER	-	expression tag	UNP P17065
K	115	LEU	MET	engineered mutation	UNP P17065
L	26	GLY	-	expression tag	UNP P17065
L	27	PRO	-	expression tag	UNP P17065
L	28	LEU	-	expression tag	UNP P17065
L	29	GLY	-	expression tag	UNP P17065
L	30	SER	-	expression tag	UNP P17065
L	115	LEU	MET	engineered mutation	UNP P17065
M	26	GLY	-	expression tag	UNP P17065

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Chain	Residue	Modelled	Actual	Comment	Reference
M	27	PRO	-	expression tag	UNP P17065
M	28	LEU	-	expression tag	UNP P17065
M	29	GLY	-	expression tag	UNP P17065
M	30	SER	-	expression tag	UNP P17065
M	115	LEU	MET	engineered mutation	UNP P17065
N	26	GLY	-	expression tag	UNP P17065
N	27	PRO	-	expression tag	UNP P17065
N	28	LEU	-	expression tag	UNP P17065
N	29	GLY	-	expression tag	UNP P17065
N	30	SER	-	expression tag	UNP P17065
N	115	LEU	MET	engineered mutation	UNP P17065
O	26	GLY	-	expression tag	UNP P17065
O	27	PRO	-	expression tag	UNP P17065
O	28	LEU	-	expression tag	UNP P17065
O	29	GLY	-	expression tag	UNP P17065
O	30	SER	-	expression tag	UNP P17065
O	115	LEU	MET	engineered mutation	UNP P17065
P	26	GLY	-	expression tag	UNP P17065
P	27	PRO	-	expression tag	UNP P17065
P	28	LEU	-	expression tag	UNP P17065
P	29	GLY	-	expression tag	UNP P17065
P	30	SER	-	expression tag	UNP P17065
P	115	LEU	MET	engineered mutation	UNP P17065
Q	26	GLY	-	expression tag	UNP P17065
Q	27	PRO	-	expression tag	UNP P17065
Q	28	LEU	-	expression tag	UNP P17065
Q	29	GLY	-	expression tag	UNP P17065
Q	30	SER	-	expression tag	UNP P17065
Q	115	LEU	MET	engineered mutation	UNP P17065
R	26	GLY	-	expression tag	UNP P17065
R	27	PRO	-	expression tag	UNP P17065
R	28	LEU	-	expression tag	UNP P17065
R	29	GLY	-	expression tag	UNP P17065
R	30	SER	-	expression tag	UNP P17065
R	115	LEU	MET	engineered mutation	UNP P17065
S	26	GLY	-	expression tag	UNP P17065
S	27	PRO	-	expression tag	UNP P17065
S	28	LEU	-	expression tag	UNP P17065
S	29	GLY	-	expression tag	UNP P17065
S	30	SER	-	expression tag	UNP P17065
S	115	LEU	MET	engineered mutation	UNP P17065
T	26	GLY	-	expression tag	UNP P17065

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Chain	Residue	Modelled	Actual	Comment	Reference
T	27	PRO	-	expression tag	UNP P17065
T	28	LEU	-	expression tag	UNP P17065
T	29	GLY	-	expression tag	UNP P17065
T	30	SER	-	expression tag	UNP P17065
T	115	LEU	MET	engineered mutation	UNP P17065

- Molecule 2 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	17	Total O 17 17	0	0
2	B	14	Total O 14 14	0	0
2	C	12	Total O 12 12	0	0
2	D	11	Total O 11 11	0	0
2	E	17	Total O 17 17	0	0
2	F	9	Total O 9 9	0	0
2	G	12	Total O 12 12	0	0
2	H	10	Total O 10 10	0	0
2	I	6	Total O 6 6	0	0
2	J	11	Total O 11 11	0	0
2	K	20	Total O 20 20	0	0
2	L	17	Total O 17 17	0	0
2	M	14	Total O 14 14	0	0
2	N	16	Total O 16 16	0	0
2	O	11	Total O 11 11	0	0
2	P	16	Total O 16 16	0	0
2	Q	14	Total O 14 14	0	0

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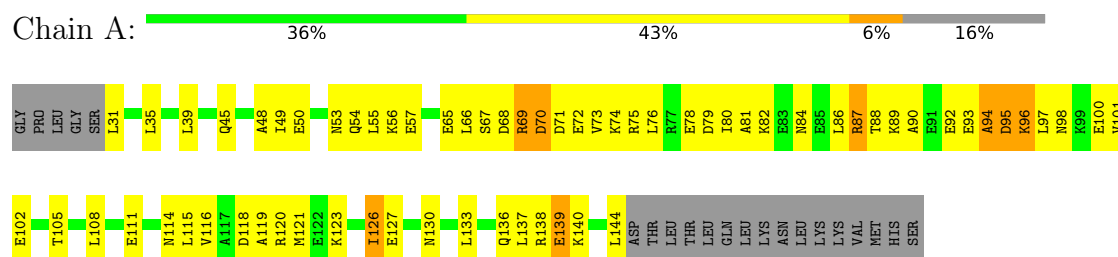
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	R	9	Total 9	O 9	0	0
2	S	14	Total 14	O 14	0	0
2	T	12	Total 12	O 12	0	0

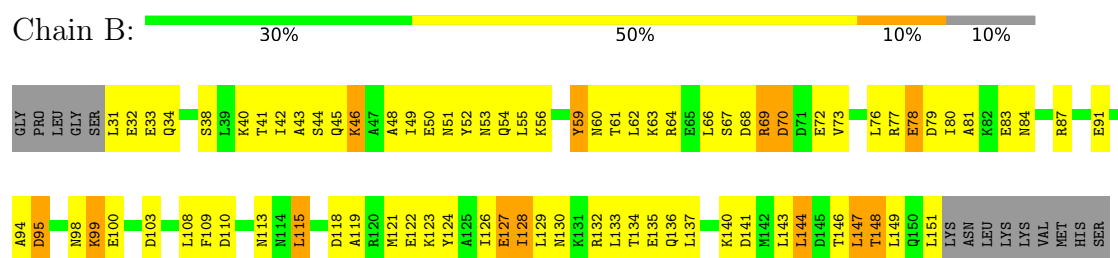
3 Residue-property plots [i](#)

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.

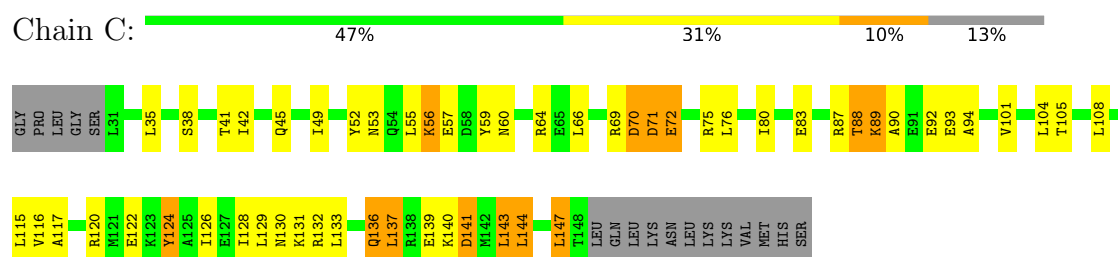
- Molecule 1: Rab guanine nucleotide exchange factor SEC2



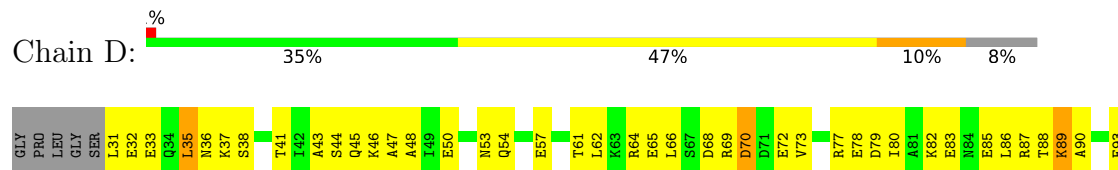
- Molecule 1: Rab guanine nucleotide exchange factor SEC2



- Molecule 1: Rab guanine nucleotide exchange factor SEC2



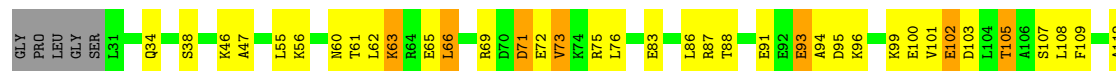
- Molecule 1: Rab guanine nucleotide exchange factor SEC2





- Molecule 1: Rab guanine nucleotide exchange factor SEC2

Chain E: 43% 36% 11% 8%



- Molecule 1: Rab guanine nucleotide exchange factor SEC2

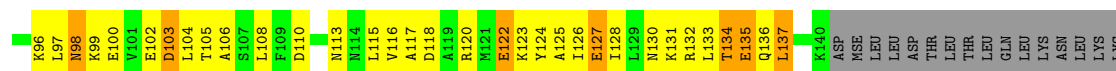
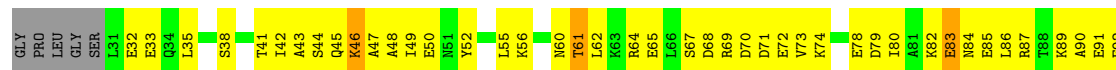
Chain F: 27% 56% 9% 8%



HIS
SER

- Molecule 1: Rab guanine nucleotide exchange factor SEC2

Chain G: 25% 49% 7% 19%

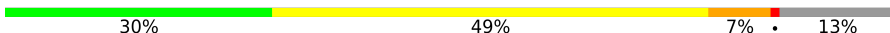


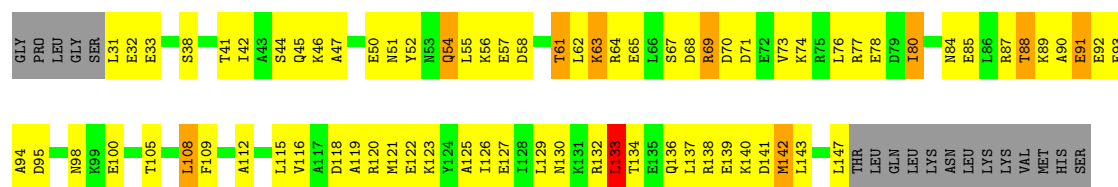
VAL
MET
HIS
SER

- Molecule 1: Rab guanine nucleotide exchange factor SEC2

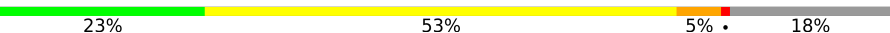
Chain H: 20% 51% 8% 21%

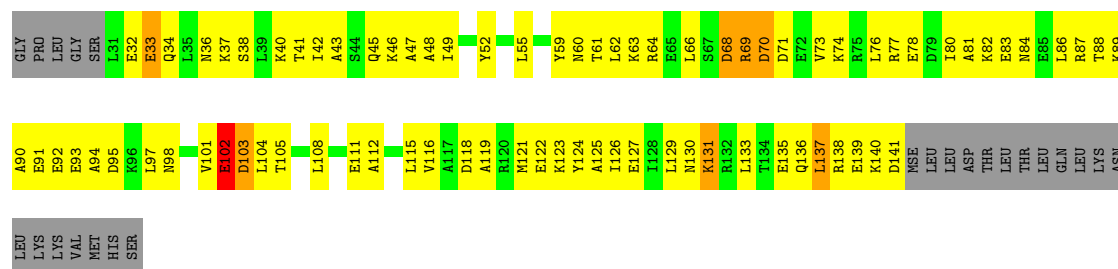


Chain M:  30% 49% 7% • 13%

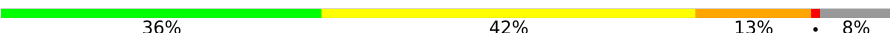


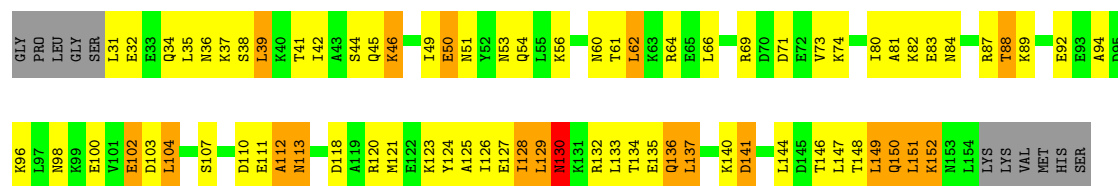
• Molecule 1: Rab guanine nucleotide exchange factor SEC2

Chain N:  23% 53% 5% • 18%

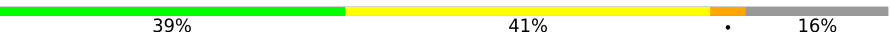


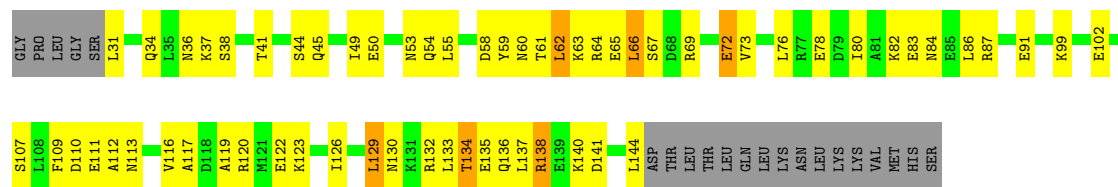
• Molecule 1: Rab guanine nucleotide exchange factor SEC2

Chain O:  36% 42% 13% • 8%

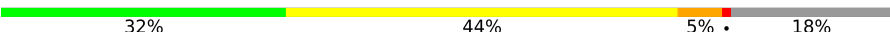


• Molecule 1: Rab guanine nucleotide exchange factor SEC2

Chain P:  39% 41% • 16%



• Molecule 1: Rab guanine nucleotide exchange factor SEC2

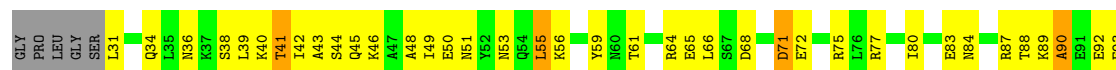
Chain Q:  32% 44% 5% • 18%





- Molecule 1: Rab guanine nucleotide exchange factor SEC2

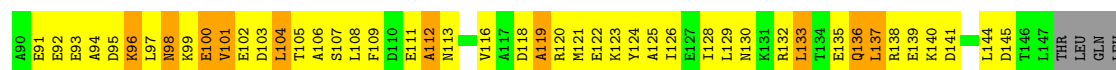
Chain R: 30% 44% 7% 18%



MET
HIS
SER

- Molecule 1: Rab guanine nucleotide exchange factor SEC2

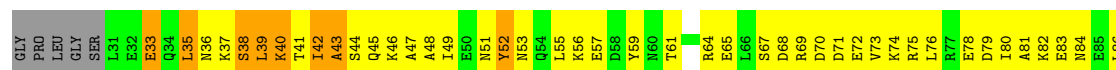
Chain S: 21% 54% 11% 13%



LYS
ASN
LEU
LYS
LYS
VAL
MET
HIS
SER

- Molecule 1: Rab guanine nucleotide exchange factor SEC2

Chain T: 25% 51% 8% 16%



LYS
VAL
MET
HIS
SER

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	101.94Å 176.57Å 181.45Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 50.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.00) 99.4 (50.00-3.00)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	0.08	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.33 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.229 , 0.285 0.234 , 0.282	Depositor DCC
R_{free} test set	6165 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	80.4	Xtriage
Anisotropy	0.332	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 134.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.034 for -h,l,k 0.034 for -h,-l,-k 0.499 for h,-k,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	19270	wwPDB-VP
Average B, all atoms (Å ²)	136.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 10.44% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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	0.66	0/939	1.15	16/1252 (1.3%)
1	B	0.66	0/994	1.16	14/1328 (1.1%)
1	C	0.55	0/969	1.11	14/1294 (1.1%)
1	D	0.57	0/1019	1.17	15/1361 (1.1%)
1	E	0.78	0/1019	1.20	15/1361 (1.1%)
1	F	0.84	0/1019	1.24	18/1361 (1.3%)
1	G	0.60	0/908	1.08	8/1212 (0.7%)
1	H	0.61	0/879	1.14	13/1175 (1.1%)
1	I	0.51	0/939	1.11	7/1252 (0.6%)
1	J	0.55	0/879	1.04	5/1175 (0.4%)
1	K	0.85	1/962 (0.1%)	1.21	13/1284 (1.0%)
1	L	0.75	0/939	1.08	5/1252 (0.4%)
1	M	0.60	0/962	1.18	14/1284 (1.1%)
1	N	0.60	0/916	1.09	7/1223 (0.6%)
1	O	0.67	0/1019	1.19	17/1361 (1.2%)
1	P	0.73	0/939	1.07	6/1252 (0.5%)
1	Q	0.61	0/916	1.12	10/1223 (0.8%)
1	R	0.57	0/916	1.05	10/1223 (0.8%)
1	S	0.49	0/962	1.11	12/1284 (0.9%)
1	T	0.48	0/939	1.09	10/1252 (0.8%)
All	All	0.65	1/19034 (0.0%)	1.13	229/25409 (0.9%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	48	ALA	CA-CB	-5.68	1.44	1.53

All (229) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	T	43	ALA	N-CA-C	-11.38	98.62	111.82
1	K	86	LEU	N-CA-C	-10.07	101.50	113.88
1	Q	108	LEU	N-CA-C	-9.50	100.61	110.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	56	LYS	N-CA-C	-9.41	101.05	112.54
1	P	138	ARG	N-CA-C	-9.41	101.93	113.41
1	T	38	SER	N-CA-C	-9.06	101.31	111.82
1	H	80	ILE	N-CA-C	-8.68	102.54	113.22
1	J	51	ASN	N-CA-C	-8.18	102.06	110.97
1	B	99	LYS	N-CA-C	-8.09	103.20	113.72
1	M	133	LEU	N-CA-C	-8.04	102.52	111.28
1	N	137	LEU	N-CA-C	-7.87	103.81	113.41
1	D	102	GLU	N-CA-C	-7.76	102.75	111.14
1	L	104	LEU	N-CA-C	-7.64	102.54	111.03
1	D	144	LEU	N-CA-C	-7.64	104.10	113.50
1	A	56	LYS	N-CA-C	-7.57	103.03	111.28
1	L	133	LEU	N-CA-C	-7.57	103.88	113.72
1	H	83	GLU	N-CA-C	-7.50	104.63	114.31
1	O	149	LEU	N-CA-C	-7.49	103.71	114.12
1	A	87	ARG	N-CA-C	-7.49	103.61	112.89
1	T	42	ILE	N-CA-C	-7.47	106.21	113.53
1	F	69	ARG	N-CA-C	-7.45	103.78	113.17
1	F	85	GLU	N-CA-C	-7.35	104.31	113.28
1	R	99	LYS	N-CA-C	-7.31	103.39	111.36
1	F	143	LEU	N-CA-C	-7.30	104.11	113.16
1	M	88	THR	N-CA-C	-7.19	103.53	111.36
1	I	33	GLU	N-CA-C	-7.16	104.42	113.01
1	F	141	ASP	N-CA-C	-7.14	104.17	113.17
1	B	81	ALA	N-CA-C	-7.12	104.59	113.28
1	C	88	THR	N-CA-C	-7.07	104.29	113.12
1	A	119	ALA	N-CA-C	-7.02	104.72	113.28
1	O	130	ASN	N-CA-C	-7.01	104.53	113.23
1	B	59	TYR	N-CA-C	-6.99	103.59	111.14
1	T	35	LEU	N-CA-C	-6.98	103.75	112.90
1	K	142	MSE	N-CA-C	-6.98	104.80	113.38
1	F	70	ASP	N-CA-C	-6.93	104.63	113.23
1	F	144	LEU	N-CA-C	-6.93	104.71	113.72
1	M	139	GLU	N-CA-C	-6.91	104.32	112.89
1	E	145	ASP	N-CA-C	-6.90	104.60	113.16
1	M	56	LYS	N-CA-C	-6.84	104.04	112.38
1	E	71	ASP	N-CA-C	-6.83	104.95	113.28
1	A	139	GLU	N-CA-C	-6.77	104.98	113.18
1	G	135	GLU	N-CA-C	-6.75	105.01	113.18
1	E	143	LEU	N-CA-C	-6.70	105.11	113.28
1	K	139	GLU	N-CA-C	-6.67	104.89	113.16
1	F	146	THR	N-CA-C	-6.65	104.64	112.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	147	LEU	N-CA-C	-6.65	105.28	113.19
1	F	147	LEU	N-CA-C	-6.63	104.94	113.16
1	M	100	GLU	N-CA-C	-6.63	105.73	113.88
1	K	138	ARG	N-CA-C	-6.62	105.82	114.04
1	D	132	ARG	N-CA-C	-6.62	104.14	111.82
1	C	70	ASP	N-CA-C	-6.61	105.04	113.23
1	C	143	LEU	N-CA-C	-6.61	104.45	113.30
1	O	151	LEU	N-CA-C	-6.59	105.27	113.38
1	A	70	ASP	N-CA-C	-6.56	104.22	111.82
1	G	134	THR	N-CA-C	-6.53	105.89	114.31
1	B	127	GLU	N-CA-C	-6.52	105.48	113.50
1	D	147	LEU	N-CA-C	-6.52	105.29	113.18
1	S	54	GLN	N-CA-C	-6.49	104.85	112.89
1	A	101	VAL	N-CA-C	-6.46	106.66	111.90
1	C	136	GLN	N-CA-C	-6.44	105.45	113.38
1	E	147	LEU	N-CA-C	-6.43	105.06	113.17
1	D	88	THR	N-CA-C	-6.43	105.07	114.39
1	E	130	ASN	N-CA-C	-6.40	105.22	113.16
1	S	104	LEU	N-CA-C	-6.39	104.58	112.38
1	K	143	LEU	N-CA-C	-6.39	105.06	112.92
1	H	107	SER	N-CA-C	-6.35	105.39	113.01
1	O	135	GLU	N-CA-C	-6.34	105.36	113.23
1	O	127	GLU	N-CA-C	-6.33	105.19	113.17
1	D	79	ASP	N-CA-C	-6.33	105.42	113.01
1	F	145	ASP	N-CA-C	-6.29	105.76	113.50
1	B	67	SER	N-CA-C	-6.29	105.67	113.15
1	O	96	LYS	N-CA-C	-6.27	103.76	111.40
1	E	129	LEU	N-CA-C	-6.26	105.64	113.28
1	E	72	GLU	N-CA-C	-6.26	105.80	113.50
1	S	70	ASP	N-CA-C	-6.25	104.52	111.71
1	N	68	ASP	N-CA-C	-6.21	104.77	112.72
1	R	55	LEU	N-CA-C	-6.20	104.42	112.23
1	B	115	LEU	N-CA-C	-6.20	104.63	111.82
1	Q	131	LYS	N-CA-C	-6.18	104.09	111.69
1	M	32	GLU	N-CA-C	-6.16	104.87	112.38
1	I	138	ARG	N-CA-C	-6.13	105.93	113.41
1	O	129	LEU	N-CA-C	-6.12	105.81	113.28
1	T	40	LYS	N-CA-C	-6.12	104.88	112.90
1	F	56	LYS	N-CA-C	-6.10	104.55	112.23
1	P	134	THR	N-CA-C	-6.09	104.64	111.28
1	O	120	ARG	N-CA-C	-6.08	105.84	113.20
1	E	73	VAL	N-CA-C	-6.07	104.82	113.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	145	ASP	N-CA-C	-6.07	105.84	113.18
1	A	138	ARG	N-CA-C	-6.04	104.99	112.90
1	T	41	THR	N-CA-C	-6.00	105.92	113.18
1	M	67	SER	N-CA-C	-5.99	105.82	113.01
1	R	123	LYS	N-CA-C	-5.99	105.62	113.17
1	H	70	ASP	N-CA-C	-5.99	106.11	113.41
1	O	152	LYS	N-CA-C	-5.96	105.19	112.88
1	R	90	ALA	N-CA-C	-5.96	105.97	113.18
1	T	44	SER	N-CA-C	-5.95	105.28	112.54
1	M	70	ASP	N-CA-C	-5.95	105.52	112.89
1	D	89	LYS	N-CA-C	-5.95	105.69	113.12
1	B	95	ASP	N-CA-C	-5.94	105.69	113.12
1	C	124	TYR	N-CA-C	-5.92	106.19	113.41
1	G	127	GLU	N-CA-C	-5.90	105.93	113.01
1	K	130	ASN	N-CA-C	-5.89	105.92	113.23
1	B	33	GLU	N-CA-C	-5.89	105.95	113.02
1	R	106	ALA	N-CA-C	-5.89	104.81	112.23
1	F	138	ARG	N-CA-C	-5.88	104.95	111.71
1	K	57	GLU	N-CA-C	-5.87	104.80	111.14
1	F	153	ASN	N-CA-C	-5.86	106.77	114.04
1	A	95	ASP	N-CA-C	-5.84	105.98	113.23
1	H	114	ASN	N-CA-C	-5.83	105.27	112.38
1	F	135	GLU	N-CA-C	-5.82	106.16	113.20
1	O	136	GLN	N-CA-C	-5.81	106.19	113.28
1	N	81	ALA	N-CA-C	-5.78	106.57	113.97
1	Q	66	LEU	N-CA-C	-5.78	105.06	111.36
1	N	69	ARG	N-CA-C	-5.78	106.39	113.50
1	D	85	GLU	N-CA-C	-5.77	106.86	114.31
1	J	117	ALA	N-CA-C	-5.77	104.60	111.69
1	H	67	SER	N-CA-C	-5.76	105.95	112.87
1	D	145	ASP	N-CA-C	-5.76	106.26	113.28
1	H	45	GLN	N-CA-C	-5.75	104.99	112.23
1	A	94	ALA	N-CA-C	-5.73	106.83	113.88
1	P	54	GLN	N-CA-C	-5.73	104.94	111.07
1	F	132	ARG	N-CA-C	-5.73	106.38	113.19
1	A	100	GLU	N-CA-C	-5.71	106.08	113.16
1	B	100	GLU	N-CA-C	-5.71	105.42	112.90
1	Q	133	LEU	N-CA-C	-5.68	105.01	111.14
1	H	106	ALA	N-CA-C	-5.64	106.07	113.12
1	Q	90	ALA	N-CA-C	-5.63	106.25	113.23
1	B	128	ILE	N-CA-C	-5.62	104.87	111.00
1	S	37	LYS	N-CA-C	-5.62	104.54	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	127	GLU	N-CA-C	-5.62	104.78	111.69
1	O	104	LEU	N-CA-C	-5.62	104.85	110.97
1	I	57	GLU	N-CA-C	-5.61	105.31	111.82
1	D	131	LYS	N-CA-C	-5.60	104.80	111.69
1	P	129	LEU	N-CA-C	-5.59	105.19	111.28
1	G	47	ALA	N-CA-C	-5.59	106.30	113.23
1	Q	80	ILE	N-CA-C	-5.58	106.26	111.45
1	F	100	GLU	N-CA-C	-5.58	105.74	112.54
1	Q	113	ASN	N-CA-C	-5.57	105.13	111.14
1	H	88	THR	N-CA-C	-5.55	106.00	112.89
1	S	136	GLN	N-CA-C	-5.55	106.01	112.89
1	C	137	LEU	N-CA-C	-5.55	106.87	113.97
1	D	148	THR	N-CA-C	-5.54	105.88	113.30
1	D	70	ASP	N-CA-C	-5.53	106.31	113.16
1	F	79	ASP	N-CA-C	-5.53	105.41	111.82
1	R	138	ARG	N-CA-C	-5.52	106.39	113.01
1	Q	137	LEU	N-CA-C	-5.50	106.52	113.18
1	A	114	ASN	N-CA-C	-5.50	105.39	111.71
1	G	84	ASN	N-CA-C	-5.50	106.55	113.20
1	M	91	GLU	N-CA-C	-5.50	107.22	114.31
1	S	137	LEU	N-CA-C	-5.49	106.74	113.50
1	T	39	LEU	N-CA-C	-5.49	106.53	113.18
1	C	35	LEU	N-CA-C	-5.47	106.19	112.92
1	M	69	ARG	N-CA-C	-5.47	106.74	113.41
1	B	148	THR	N-CA-C	-5.46	106.63	113.72
1	B	69	ARG	N-CA-C	-5.46	105.88	112.54
1	B	144	LEU	N-CA-C	-5.44	107.29	114.31
1	A	96	LYS	N-CA-C	-5.44	106.48	113.01
1	M	54	GLN	N-CA-C	-5.44	106.65	113.28
1	I	117	ALA	N-CA-C	-5.43	105.05	110.97
1	E	141	ASP	N-CA-C	-5.43	106.79	113.41
1	N	131	LYS	N-CA-C	-5.43	105.44	111.36
1	O	88	THR	N-CA-C	-5.43	105.46	112.68
1	M	71	ASP	N-CA-C	-5.39	105.05	111.69
1	M	125	ALA	N-CA-C	-5.39	105.84	112.90
1	G	137	LEU	N-CA-C	-5.38	105.94	112.88
1	K	127	GLU	N-CA-C	-5.38	105.45	112.23
1	E	93	GLU	N-CA-C	-5.38	106.56	113.01
1	K	122	GLU	N-CA-C	-5.37	105.59	111.82
1	L	71	ASP	N-CA-C	-5.36	105.52	111.36
1	A	68	ASP	N-CA-C	-5.35	106.80	113.38
1	L	65	GLU	N-CA-C	-5.34	107.31	113.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	46	LYS	CA-C-N	5.34	127.75	120.54
1	K	46	LYS	C-N-CA	5.34	127.75	120.54
1	L	42	ILE	N-CA-C	-5.33	106.07	113.00
1	E	146	THR	N-CA-C	-5.33	106.16	113.30
1	F	142	MSE	N-CA-C	-5.33	106.80	113.72
1	R	50	GLU	N-CA-C	-5.30	105.91	112.38
1	D	100	GLU	N-CA-C	-5.29	106.84	113.72
1	H	90	ALA	N-CA-C	-5.28	105.66	112.68
1	C	71	ASP	N-CA-C	-5.28	106.35	112.89
1	J	81	ALA	N-CA-C	-5.26	106.37	112.89
1	J	38	SER	N-CA-C	-5.25	106.90	113.15
1	N	70	ASP	N-CA-C	-5.25	106.57	112.87
1	C	141	ASP	N-CA-C	-5.25	105.15	112.45
1	S	58	ASP	N-CA-C	-5.25	107.01	113.41
1	Q	132	ARG	N-CA-C	-5.23	106.40	112.89
1	O	94	ALA	N-CA-C	-5.22	106.94	113.72
1	E	66	LEU	N-CA-C	-5.21	106.99	113.19
1	S	96	LYS	N-CA-C	-5.20	105.73	111.71
1	J	77	ARG	N-CA-C	-5.20	106.20	112.54
1	O	46	LYS	N-CA-C	-5.18	105.28	111.03
1	Q	117	ALA	N-CA-C	-5.18	106.47	112.89
1	E	144	LEU	N-CA-C	-5.18	106.20	112.88
1	O	37	LYS	N-CA-C	-5.17	105.72	111.36
1	C	89	LYS	N-CA-C	-5.17	106.23	112.54
1	I	137	LEU	N-CA-C	-5.17	107.00	113.72
1	H	71	ASP	N-CA-C	-5.16	107.01	113.15
1	O	150	GLN	N-CA-C	-5.16	106.95	114.12
1	I	54	GLN	N-CA-C	-5.15	105.09	111.33
1	O	69	ARG	N-CA-C	-5.15	105.79	111.71
1	G	90	ALA	N-CA-C	-5.14	105.13	111.40
1	D	72	GLU	N-CA-C	-5.14	106.85	113.01
1	D	35	LEU	N-CA-C	-5.12	106.71	113.17
1	T	112	ALA	N-CA-C	-5.12	107.09	113.19
1	A	126	ILE	N-CA-C	-5.12	106.58	112.98
1	I	140	LYS	N-CA-C	-5.11	106.82	113.16
1	S	100	GLU	N-CA-C	-5.11	106.20	112.90
1	E	148	THR	N-CA-C	-5.11	107.43	113.97
1	C	144	LEU	N-CA-C	-5.10	105.96	113.61
1	C	147	LEU	N-CA-C	-5.10	107.03	113.20
1	P	62	LEU	N-CA-C	-5.09	106.23	112.90
1	F	152	LYS	N-CA-C	-5.09	106.48	113.30
1	R	107	SER	N-CA-C	-5.08	105.65	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	131	LYS	N-CA-C	-5.08	106.67	112.92
1	K	94	ALA	N-CA-C	-5.07	105.40	112.45
1	M	108	LEU	N-CA-C	-5.07	104.74	112.04
1	K	42	ILE	N-CA-C	-5.06	104.95	112.04
1	A	137	LEU	N-CA-C	-5.06	106.95	113.23
1	S	101	VAL	N-CA-C	-5.06	106.13	110.74
1	N	136	GLN	N-CA-C	-5.05	107.08	113.18
1	R	41	THR	N-CA-C	-5.04	103.85	111.56
1	E	63	LYS	N-CA-C	-5.03	107.27	113.41
1	T	95	ASP	N-CA-C	-5.03	106.25	112.38
1	P	72	GLU	N-CA-C	-5.03	105.71	111.14
1	G	83	GLU	N-CA-C	-5.02	105.51	111.69
1	A	69	ARG	N-CA-C	-5.01	107.33	113.50
1	S	39	LEU	N-CA-C	-5.01	106.27	112.38
1	R	89	LYS	N-CA-C	-5.00	107.22	113.38
1	H	132	ARG	N-CA-C	-5.00	105.92	112.23

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	938	0	945	63	0
1	B	993	0	1004	81	0
1	C	968	0	974	73	0
1	D	1018	0	1034	97	0
1	E	1018	0	1034	87	0
1	F	1018	0	1034	98	0
1	G	906	0	910	113	0
1	H	877	0	878	123	0
1	I	938	0	945	141	0
1	J	877	0	878	131	0
1	K	961	0	967	85	0
1	L	938	0	945	94	0
1	M	961	0	967	84	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	N	914	0	914	92	0
1	O	1018	0	1034	86	0
1	P	938	0	945	97	0
1	Q	914	0	914	104	0
1	R	914	0	914	102	0
1	S	961	0	967	118	0
1	T	938	0	945	97	0
2	A	17	0	0	3	0
2	B	14	0	0	9	0
2	C	12	0	0	2	0
2	D	11	0	0	6	0
2	E	17	0	0	6	0
2	F	9	0	0	2	0
2	G	12	0	0	9	0
2	H	10	0	0	3	0
2	I	6	0	0	2	0
2	J	11	0	0	8	0
2	K	20	0	0	1	0
2	L	17	0	0	10	0
2	M	14	0	0	8	0
2	N	16	0	0	4	0
2	O	11	0	0	5	0
2	P	16	0	0	2	0
2	Q	14	0	0	3	0
2	R	9	0	0	4	0
2	S	14	0	0	6	0
2	T	12	0	0	3	0
All	All	19270	0	19148	1588	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 42.

All (1588) 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:73:VAL:HG21	1:J:69:ARG:HD2	1.31	1.13
1:Q:126:ILE:HD13	1:R:126:ILE:HG21	1.32	1.10
1:M:133:LEU:HD12	1:N:133:LEU:HD22	1.33	1.09
1:L:110:ASP:HA	1:L:113:ASN:HD22	1.14	1.08
1:Q:133:LEU:HD22	1:R:133:LEU:HB2	1.32	1.08
1:M:133:LEU:HG	1:N:133:LEU:HD13	1.28	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:80:ILE:HD11	1:P:80:ILE:HG12	1.35	1.07
1:E:144:LEU:HD22	1:F:143:LEU:HD13	1.36	1.05
1:S:56:LYS:HG3	1:T:55:LEU:HD21	1.38	1.04
1:A:118:ASP:HA	1:A:121:MSE:HG3	1.39	1.04
1:I:51:ASN:HA	1:I:54:GLN:HB3	1.40	1.04
1:E:144:LEU:HD13	1:F:143:LEU:HB3	1.36	1.03
1:O:147:LEU:HD23	1:P:144:LEU:HD11	1.41	1.02
1:S:137:LEU:HD13	1:T:137:LEU:HD22	1.44	1.00
1:E:133:LEU:HD13	1:F:133:LEU:HD11	1.43	0.97
1:C:126:ILE:HB	1:D:126:ILE:HG13	1.43	0.96
1:Q:133:LEU:HD13	1:R:133:LEU:HD13	1.44	0.96
1:G:105:THR:HG21	1:R:42:ILE:HG12	1.48	0.95
1:T:49:ILE:HD12	2:T:163:HOH:O	1.66	0.95
1:C:133:LEU:HD13	1:D:133:LEU:HD13	1.48	0.95
1:S:133:LEU:HD13	1:T:133:LEU:HB2	1.47	0.95
1:O:137:LEU:HD21	1:P:137:LEU:HD22	1.47	0.94
1:A:130:ASN:HD21	1:B:130:ASN:HB2	1.33	0.93
1:J:50:GLU:HA	1:J:53:ASN:HB2	1.51	0.92
1:G:98:ASN:HA	2:G:167:HOH:O	1.66	0.92
1:K:137:LEU:HD21	1:L:137:LEU:HG	1.49	0.92
1:N:135:GLU:HA	1:N:138:ARG:HG2	1.50	0.92
1:I:122:GLU:HG2	1:J:123:LYS:HE2	1.52	0.90
1:Q:87:ARG:HH21	1:R:87:ARG:HD2	1.36	0.90
1:K:80:ILE:HD11	1:L:80:ILE:HG12	1.53	0.89
1:I:58:ASP:HA	2:I:161:HOH:O	1.72	0.89
1:Q:130:ASN:HA	1:Q:133:LEU:HB3	1.53	0.89
2:O:164:HOH:O	1:P:133:LEU:HD21	1.74	0.88
1:T:139:GLU:O	1:T:143:LEU:HG	1.74	0.88
1:E:133:LEU:HB2	1:F:133:LEU:HD21	1.53	0.87
1:N:33:GLU:HB3	2:N:162:HOH:O	1.72	0.87
1:Q:51:ASN:HA	1:Q:54:GLN:HG2	1.56	0.87
1:G:131:LYS:O	1:G:135:GLU:HB2	1.72	0.87
1:C:141:ASP:N	1:D:140:LYS:HZ1	1.73	0.86
1:I:42:ILE:HA	1:I:45:GLN:HG2	1.57	0.86
1:A:130:ASN:HD21	1:B:130:ASN:CB	1.90	0.84
1:L:37:LYS:HE2	2:L:165:HOH:O	1.78	0.84
1:L:73:VAL:O	1:L:77:ARG:HB2	1.77	0.84
1:G:116:VAL:HG11	1:Q:51:ASN:HB3	1.60	0.84
1:I:86:LEU:O	1:I:89:LYS:HG2	1.79	0.83
1:C:133:LEU:HB2	1:D:133:LEU:HD22	1.61	0.83
1:M:140:LYS:HD3	1:N:140:LYS:HB3	1.61	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:137:LEU:CD2	1:P:137:LEU:HD22	2.09	0.83
1:C:108:LEU:HD13	1:Q:46:LYS:HA	1.61	0.82
1:D:50:GLU:HG2	1:D:54:GLN:HE21	1.44	0.82
1:G:130:ASN:HD21	1:H:130:ASN:ND2	1.77	0.82
1:J:129:LEU:HD11	1:J:133:LEU:HD22	1.60	0.82
1:O:130:ASN:CG	1:P:130:ASN:HD21	1.88	0.82
1:T:136:GLN:O	1:T:140:LYS:HB2	1.79	0.81
1:I:99:LYS:HA	1:I:102:GLU:HB2	1.61	0.81
1:K:126:ILE:HD13	1:K:129:LEU:HD12	1.62	0.81
1:I:132:ARG:HB3	1:I:136:GLN:NE2	1.95	0.81
1:N:64:ARG:O	1:N:68:ASP:HB2	1.81	0.81
1:T:133:LEU:HD12	1:T:137:LEU:HG	1.61	0.81
1:G:124:TYR:O	1:G:127:GLU:HG2	1.80	0.81
1:C:144:LEU:HD13	1:D:147:LEU:HD13	1.64	0.80
1:I:133:LEU:HB3	1:J:133:LEU:HD23	1.62	0.80
1:B:38:SER:O	1:B:42:ILE:HG12	1.82	0.80
1:H:128:ILE:HG23	1:H:132:ARG:HG3	1.64	0.80
2:O:170:HOH:O	1:P:137:LEU:HD13	1.80	0.80
1:M:133:LEU:CD1	1:N:133:LEU:HD22	2.11	0.80
1:I:133:LEU:HD13	1:J:129:LEU:HG	1.63	0.79
1:C:69:ARG:HB3	2:D:166:HOH:O	1.81	0.79
1:A:144:LEU:HD13	1:B:144:LEU:HD22	1.65	0.79
1:S:135:GLU:HA	1:S:138:ARG:HB2	1.64	0.79
1:L:110:ASP:HA	1:L:113:ASN:ND2	1.96	0.79
1:M:130:ASN:HA	1:M:133:LEU:HB2	1.65	0.79
1:E:93:GLU:HG2	1:E:96:LYS:HD2	1.63	0.78
1:E:83:GLU:O	1:E:87:ARG:HG2	1.83	0.78
1:O:61:THR:HA	1:O:64:ARG:HD2	1.66	0.78
1:O:130:ASN:ND2	1:P:130:ASN:HD21	1.82	0.78
1:S:83:GLU:O	1:S:87:ARG:HG2	1.82	0.78
1:I:79:ASP:O	1:I:83:GLU:HG2	1.84	0.78
1:K:87:ARG:HH21	1:L:87:ARG:HG2	1.50	0.77
1:C:133:LEU:CD1	1:D:133:LEU:HD13	2.15	0.77
1:E:147:LEU:HD23	1:F:147:LEU:HD23	1.66	0.77
1:C:143:LEU:HD23	1:D:144:LEU:HD21	1.67	0.77
1:N:124:TYR:HA	1:N:127:GLU:OE2	1.84	0.77
1:P:133:LEU:O	1:P:137:LEU:HG	1.85	0.77
1:T:140:LYS:O	1:T:144:LEU:HB2	1.85	0.77
1:T:43:ALA:HA	1:T:46:LYS:HE3	1.67	0.77
1:I:126:ILE:CG2	1:J:126:ILE:HG21	2.15	0.76
1:P:49:ILE:HG12	1:P:53:ASN:HD21	1.50	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:133:LEU:HD13	1:F:133:LEU:CD1	2.15	0.76
1:I:129:LEU:O	1:I:133:LEU:HG	1.85	0.76
2:M:174:HOH:O	1:N:76:LEU:HD13	1.84	0.76
1:A:87:ARG:HH21	1:B:87:ARG:HB3	1.50	0.76
1:G:132:ARG:O	1:G:136:GLN:HG3	1.86	0.76
1:C:129:LEU:HD23	1:D:130:ASN:OD1	1.85	0.76
1:S:97:LEU:O	1:S:101:VAL:HG23	1.86	0.76
1:A:144:LEU:HD11	1:B:147:LEU:HG	1.68	0.75
1:D:132:ARG:HG2	1:D:136:GLN:HE21	1.50	0.75
1:E:128:ILE:HD13	1:E:131:LYS:HD2	1.68	0.75
1:B:41:THR:O	1:B:45:GLN:HG3	1.86	0.75
1:Q:131:LYS:HD2	2:Q:171:HOH:O	1.84	0.75
1:B:73:VAL:O	1:B:77:ARG:HB2	1.87	0.75
1:C:136:GLN:HB3	1:D:137:LEU:HD21	1.69	0.75
1:J:108:LEU:HA	1:J:111:GLU:OE1	1.87	0.75
1:G:62:LEU:HB2	1:H:62:LEU:HD23	1.68	0.74
1:H:132:ARG:C	1:H:134:THR:H	1.94	0.74
1:O:126:ILE:HG22	1:P:126:ILE:HG22	1.69	0.74
1:I:116:VAL:O	1:I:119:ALA:HB3	1.87	0.74
1:J:47:ALA:O	1:J:51:ASN:HB2	1.86	0.74
1:S:125:ALA:O	1:S:129:LEU:HG	1.87	0.74
1:Q:133:LEU:HD13	1:R:133:LEU:CD1	2.16	0.74
1:S:137:LEU:HD13	1:T:137:LEU:CD2	2.17	0.74
1:M:133:LEU:HD23	2:M:168:HOH:O	1.88	0.74
1:H:99:LYS:CG	1:H:100:GLU:H	2.01	0.74
1:G:99:LYS:O	1:G:103:ASP:HB2	1.88	0.74
1:G:108:LEU:HD23	1:H:108:LEU:HG	1.70	0.74
1:L:50:GLU:O	1:L:54:GLN:HG3	1.87	0.73
1:H:44:SER:O	1:H:48:ALA:HB2	1.88	0.73
1:H:131:LYS:O	1:H:135:GLU:HG3	1.87	0.73
1:I:49:ILE:HA	1:I:52:TYR:HB3	1.68	0.73
1:Q:133:LEU:CD2	1:R:133:LEU:HB2	2.15	0.73
1:A:140:LYS:HZ1	1:B:140:LYS:C	1.95	0.73
1:Q:80:ILE:O	1:Q:84:ASN:HB2	1.88	0.73
1:G:41:THR:HG22	1:G:45:GLN:HE21	1.54	0.73
1:J:69:ARG:HD3	2:J:162:HOH:O	1.89	0.73
1:K:87:ARG:NH2	1:L:87:ARG:HG2	2.03	0.73
1:J:95:ASP:HA	1:J:98:ASN:HD22	1.53	0.73
1:S:126:ILE:CG2	1:T:126:ILE:HG21	2.19	0.73
1:Q:137:LEU:HD13	1:R:137:LEU:HD13	1.70	0.73
1:T:33:GLU:OE1	1:T:36:ASN:HB3	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:38:SER:O	1:F:42:ILE:HG12	1.89	0.73
1:I:45:GLN:HG3	1:I:46:LYS:N	2.04	0.73
1:I:132:ARG:HB3	1:I:136:GLN:HE21	1.53	0.72
1:O:98:ASN:O	1:O:102:GLU:HB3	1.90	0.72
1:I:56:LYS:HE3	1:J:55:LEU:HD11	1.72	0.72
1:A:88:THR:O	1:A:92:GLU:HG3	1.90	0.72
1:K:140:LYS:NZ	1:L:140:LYS:HB3	2.05	0.72
1:F:109:PHE:O	1:F:113:ASN:HB2	1.89	0.72
1:O:62:LEU:HD23	1:P:62:LEU:HD12	1.71	0.72
1:J:81:ALA:HA	1:J:84:ASN:HD22	1.53	0.72
1:D:146:THR:HA	1:D:149:LEU:HB3	1.72	0.71
1:R:111:GLU:HA	1:R:114:ASN:HB3	1.70	0.71
1:T:67:SER:HA	1:T:70:ASP:OD2	1.89	0.71
1:A:82:LYS:O	1:A:86:LEU:HG	1.90	0.71
1:G:137:LEU:HD21	1:H:137:LEU:HD22	1.71	0.71
1:F:88:THR:HG22	1:F:92:GLU:OE2	1.90	0.71
1:I:130:ASN:HD21	1:J:126:ILE:HD12	1.54	0.71
1:C:124:TYR:O	1:C:128:ILE:HG13	1.91	0.71
1:D:89:LYS:O	1:D:93:GLU:HG2	1.91	0.71
1:H:128:ILE:HA	1:H:131:LYS:HB2	1.72	0.71
1:O:147:LEU:CD2	1:P:144:LEU:HD11	2.19	0.71
1:M:134:THR:O	1:M:138:ARG:HB2	1.90	0.71
1:Q:126:ILE:HG21	1:R:126:ILE:HD12	1.73	0.71
1:G:98:ASN:CA	2:G:167:HOH:O	2.31	0.71
1:G:133:LEU:HG	1:H:133:LEU:HG	1.72	0.71
1:K:144:LEU:HD11	1:L:144:LEU:HG	1.73	0.71
1:O:80:ILE:CD1	1:P:80:ILE:HG12	2.17	0.71
1:Q:76:LEU:O	1:Q:80:ILE:HG13	1.91	0.71
2:A:176:HOH:O	1:B:144:LEU:HD22	1.90	0.71
1:B:44:SER:O	1:B:48:ALA:HB2	1.91	0.70
1:J:50:GLU:HB3	1:J:54:GLN:HG3	1.72	0.70
1:M:90:ALA:HA	1:M:93:GLU:CD	2.16	0.70
1:N:118:ASP:O	1:N:122:GLU:HG2	1.90	0.70
1:N:133:LEU:O	1:N:137:LEU:N	2.24	0.70
1:Q:133:LEU:HB2	1:R:133:LEU:HD22	1.71	0.70
1:E:147:LEU:HD13	1:E:147:LEU:O	1.90	0.70
1:G:137:LEU:HD21	1:H:137:LEU:CD2	2.21	0.70
1:R:61:THR:O	1:R:65:GLU:HG3	1.91	0.70
1:R:84:ASN:HA	1:R:87:ARG:HG2	1.74	0.70
1:Q:66:LEU:HG	1:Q:70:ASP:OD2	1.91	0.70
1:F:41:THR:HG22	1:F:45:GLN:HE21	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:93:GLU:O	1:D:96:LYS:HG2	1.92	0.70
1:D:33:GLU:OE2	1:D:37:LYS:HB2	1.92	0.70
1:I:59:TYR:CE2	1:I:63:LYS:HE3	2.27	0.70
1:T:81:ALA:HA	1:T:84:ASN:HD22	1.57	0.70
1:E:134:THR:HG22	1:E:138:ARG:HE	1.56	0.69
1:G:41:THR:HG22	1:G:45:GLN:NE2	2.07	0.69
1:S:126:ILE:HG21	1:T:126:ILE:HG21	1.72	0.69
1:H:92:GLU:HG3	1:H:93:GLU:H	1.57	0.69
1:S:137:LEU:HD22	1:T:137:LEU:HD21	1.73	0.69
1:D:130:ASN:HA	1:D:133:LEU:HB3	1.73	0.69
1:H:99:LYS:CG	1:H:100:GLU:N	2.55	0.69
1:R:31:LEU:N	2:R:166:HOH:O	2.24	0.69
1:G:62:LEU:CD1	1:H:63:LYS:HG3	2.23	0.69
1:C:126:ILE:HB	1:D:126:ILE:CG1	2.21	0.69
1:J:59:TYR:O	1:J:63:LYS:HB2	1.92	0.69
1:J:64:ARG:O	1:J:68:ASP:HB2	1.93	0.69
1:O:88:THR:O	1:O:92:GLU:HG3	1.91	0.69
1:Q:140:LYS:HB3	1:R:140:LYS:HE2	1.74	0.69
1:S:37:LYS:O	1:S:41:THR:HG23	1.92	0.69
1:D:50:GLU:HG2	1:D:54:GLN:NE2	2.08	0.69
1:H:80:ILE:O	1:H:84:ASN:HB2	1.93	0.69
1:O:137:LEU:HD13	1:O:141:ASP:OD1	1.93	0.69
1:I:109:PHE:O	1:I:112:ALA:HB3	1.93	0.68
1:C:87:ARG:HB2	1:D:87:ARG:NH1	2.08	0.68
2:C:169:HOH:O	1:D:133:LEU:HD21	1.93	0.68
1:S:104:LEU:O	1:S:108:LEU:HB2	1.93	0.68
1:J:115:LEU:HA	1:J:118:ASP:HB3	1.76	0.68
1:S:133:LEU:HD13	1:T:133:LEU:CB	2.24	0.68
1:I:42:ILE:HG12	1:I:45:GLN:HE21	1.58	0.68
1:M:73:VAL:HG12	2:M:162:HOH:O	1.92	0.68
1:C:41:THR:O	1:C:45:GLN:HG3	1.93	0.68
1:H:47:ALA:HA	1:H:50:GLU:HB3	1.76	0.68
1:H:100:GLU:HB2	1:R:39:LEU:HD21	1.75	0.68
1:L:38:SER:O	1:L:42:ILE:HG12	1.93	0.68
1:P:80:ILE:HG22	1:P:84:ASN:HD22	1.59	0.68
1:J:45:GLN:C	1:J:49:ILE:HG12	2.17	0.68
1:S:95:ASP:O	1:S:98:ASN:HB3	1.93	0.68
1:I:73:VAL:HG21	1:J:69:ARG:CD	2.19	0.68
1:J:56:LYS:HG3	1:J:60:ASN:HD21	1.58	0.68
1:M:63:LYS:HG3	1:N:62:LEU:HD11	1.76	0.68
1:J:60:ASN:HA	1:J:63:LYS:HB3	1.76	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:67:SER:HA	1:J:70:ASP:OD2	1.94	0.68
1:M:116:VAL:HG22	1:N:115:LEU:CD2	2.24	0.68
1:R:83:GLU:O	1:R:87:ARG:HB3	1.94	0.68
1:Q:124:TYR:O	1:Q:127:GLU:HG2	1.94	0.68
1:A:87:ARG:HH21	1:B:87:ARG:CB	2.07	0.67
1:N:32:GLU:C	1:N:34:GLN:H	2.02	0.67
1:I:73:VAL:CG2	1:J:69:ARG:HD2	2.17	0.67
1:I:140:LYS:HZ2	1:J:137:LEU:HD22	1.60	0.67
1:T:76:LEU:O	1:T:80:ILE:HG13	1.94	0.67
1:K:55:LEU:HD23	1:L:55:LEU:HD23	1.75	0.67
1:Q:126:ILE:HG21	1:R:126:ILE:CG2	2.25	0.67
1:Q:133:LEU:CD1	1:R:133:LEU:HD13	2.21	0.67
1:E:95:ASP:O	1:E:99:LYS:HB3	1.95	0.67
1:I:58:ASP:O	1:I:62:LEU:HG	1.94	0.67
1:L:83:GLU:O	1:L:87:ARG:HG3	1.95	0.67
1:Q:127:GLU:O	1:Q:131:LYS:HB2	1.94	0.67
1:G:128:ILE:HG22	1:G:132:ARG:HH21	1.59	0.67
1:D:131:LYS:O	1:D:135:GLU:HG3	1.95	0.67
1:E:131:LYS:C	1:E:133:LEU:H	2.02	0.67
1:I:113:ASN:N	1:I:113:ASN:HD22	1.92	0.67
1:O:50:GLU:O	1:O:54:GLN:HG2	1.95	0.67
1:C:132:ARG:O	1:C:136:GLN:HB2	1.95	0.66
1:I:132:ARG:O	1:I:136:GLN:HB2	1.95	0.66
1:K:144:LEU:HG	1:L:144:LEU:HD21	1.76	0.66
1:E:147:LEU:HD23	1:F:147:LEU:CD2	2.25	0.66
1:P:83:GLU:O	1:P:87:ARG:HG2	1.95	0.66
1:R:131:LYS:O	1:R:135:GLU:HG2	1.94	0.66
1:B:45:GLN:O	1:B:48:ALA:HB3	1.95	0.66
1:F:133:LEU:O	1:F:136:GLN:HB3	1.95	0.66
1:S:56:LYS:CG	1:T:55:LEU:HD21	2.22	0.66
1:S:93:GLU:O	1:S:97:LEU:HG	1.96	0.66
1:R:97:LEU:O	1:R:101:VAL:HG23	1.95	0.66
1:O:144:LEU:CD1	1:P:144:LEU:HD13	2.26	0.66
1:K:65:GLU:O	1:K:69:ARG:HG2	1.96	0.66
1:T:35:LEU:HD23	1:T:35:LEU:O	1.94	0.66
1:H:92:GLU:HG3	1:H:93:GLU:N	2.10	0.66
1:K:132:ARG:O	1:K:136:GLN:HG3	1.95	0.66
1:Q:54:GLN:HG3	1:Q:55:LEU:N	2.09	0.66
1:D:64:ARG:O	1:D:68:ASP:HB2	1.96	0.66
1:I:36:ASN:HD21	1:I:40:LYS:HE3	1.61	0.66
1:G:105:THR:HG23	1:H:108:LEU:CD2	2.26	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:123:LYS:O	1:I:127:GLU:HB2	1.96	0.65
1:J:111:GLU:HG2	1:J:112:ALA:N	2.10	0.65
1:R:41:THR:HG22	1:R:45:GLN:NE2	2.11	0.65
1:S:72:GLU:HA	1:S:75:ARG:HB2	1.76	0.65
1:K:147:LEU:HD22	1:L:144:LEU:HD11	1.77	0.65
1:S:100:GLU:O	1:S:104:LEU:HG	1.97	0.65
1:E:133:LEU:CD1	1:F:133:LEU:HD11	2.21	0.65
1:G:130:ASN:HD21	1:H:130:ASN:HD21	1.43	0.65
1:R:71:ASP:O	1:R:75:ARG:HG3	1.96	0.65
1:B:147:LEU:HD13	1:B:147:LEU:O	1.97	0.65
1:K:140:LYS:O	1:K:140:LYS:HG2	1.96	0.65
1:S:140:LYS:HD3	1:T:141:ASP:OD1	1.96	0.65
1:F:31:LEU:HD12	1:F:34:GLN:HE21	1.61	0.65
1:L:108:LEU:HD13	1:L:108:LEU:O	1.96	0.65
1:M:46:LYS:O	1:M:50:GLU:HB2	1.97	0.65
1:M:109:PHE:HA	1:N:108:LEU:HD21	1.79	0.65
1:P:119:ALA:HA	1:P:122:GLU:HG2	1.77	0.65
1:I:38:SER:O	1:I:42:ILE:HG13	1.95	0.65
1:G:126:ILE:HB	1:H:126:ILE:HD13	1.79	0.65
1:I:86:LEU:HD22	1:I:89:LYS:NZ	2.12	0.65
1:H:64:ARG:O	1:H:68:ASP:HB2	1.97	0.65
1:H:99:LYS:HG3	1:H:100:GLU:N	2.11	0.65
1:I:137:LEU:HD11	2:J:166:HOH:O	1.95	0.65
1:K:83:GLU:HG3	1:L:87:ARG:NH1	2.12	0.65
1:D:66:LEU:O	1:D:70:ASP:HB2	1.97	0.65
1:G:44:SER:O	1:G:48:ALA:HB2	1.97	0.65
1:O:62:LEU:HB3	1:P:62:LEU:HD12	1.79	0.65
1:J:35:LEU:HD23	1:J:35:LEU:O	1.95	0.65
1:R:87:ARG:HG3	1:R:88:THR:N	2.11	0.65
1:I:55:LEU:HD11	1:J:52:TYR:CZ	2.31	0.64
1:O:107:SER:O	1:O:111:GLU:HB2	1.96	0.64
1:J:126:ILE:HG23	1:J:130:ASN:OD1	1.97	0.64
1:S:69:ARG:O	1:S:73:VAL:HG23	1.97	0.64
1:C:116:VAL:HG13	1:D:115:LEU:HD21	1.77	0.64
1:G:116:VAL:HB	1:Q:51:ASN:ND2	2.13	0.64
1:J:61:THR:HA	1:J:64:ARG:HD2	1.78	0.64
1:K:74:LYS:O	1:K:78:GLU:HG3	1.97	0.64
1:E:94:ALA:HA	2:E:175:HOH:O	1.96	0.64
1:M:126:ILE:HG22	1:N:126:ILE:CG2	2.28	0.64
1:S:73:VAL:O	1:S:77:ARG:HG3	1.97	0.64
1:E:133:LEU:CB	1:F:133:LEU:HD21	2.26	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Q:72:GLU:O	1:Q:76:LEU:HG	1.97	0.64
1:I:134:THR:O	1:I:138:ARG:HG3	1.97	0.64
1:M:143:LEU:O	1:M:147:LEU:HG	1.97	0.64
1:Q:126:ILE:HG21	1:R:126:ILE:HG23	1.79	0.64
1:R:130:ASN:OD1	1:R:133:LEU:HD23	1.97	0.64
1:S:97:LEU:O	1:S:101:VAL:N	2.31	0.64
1:S:116:VAL:O	1:S:119:ALA:HB3	1.98	0.64
1:S:133:LEU:HD23	1:T:129:LEU:HD22	1.79	0.64
1:D:83:GLU:HG3	2:D:164:HOH:O	1.96	0.64
1:S:120:ARG:O	1:S:124:TYR:HB2	1.98	0.64
1:A:80:ILE:HD11	1:B:80:ILE:HD12	1.78	0.63
1:N:66:LEU:C	1:N:68:ASP:H	2.04	0.63
1:K:81:ALA:O	1:K:85:GLU:HB2	1.98	0.63
1:C:117:ALA:O	1:C:120:ARG:HG2	1.99	0.63
2:C:169:HOH:O	1:D:133:LEU:HD11	1.98	0.63
1:I:76:LEU:HD11	1:J:77:ARG:HE	1.63	0.63
1:L:140:LYS:O	1:L:140:LYS:HG2	1.98	0.63
1:O:60:ASN:HB3	1:O:64:ARG:NH2	2.13	0.63
1:P:49:ILE:HG23	1:P:50:GLU:N	2.13	0.63
1:F:40:LYS:O	1:F:44:SER:HB2	1.98	0.63
1:Q:87:ARG:NH2	1:R:87:ARG:HB2	2.13	0.63
1:R:64:ARG:HD3	2:R:163:HOH:O	1.97	0.63
1:H:87:ARG:O	1:H:91:GLU:HG3	1.99	0.63
1:N:97:LEU:O	1:N:101:VAL:HG23	1.97	0.63
1:Q:125:ALA:HA	1:Q:128:ILE:HD12	1.81	0.63
1:T:132:ARG:HB3	1:T:136:GLN:OE1	1.98	0.63
1:H:50:GLU:O	1:H:54:GLN:HG3	1.98	0.63
1:M:108:LEU:CD2	1:N:105:THR:HG23	2.29	0.63
1:R:127:GLU:O	1:R:131:LYS:HB2	1.99	0.63
1:Q:61:THR:HA	1:Q:64:ARG:NE	2.14	0.63
1:B:50:GLU:O	1:B:54:GLN:HG3	1.99	0.62
1:E:137:LEU:HD21	1:F:137:LEU:HD21	1.81	0.62
1:G:133:LEU:C	1:H:133:LEU:HD21	2.24	0.62
1:K:131:LYS:HG2	1:K:135:GLU:OE2	1.99	0.62
1:N:74:LYS:O	1:N:78:GLU:HG2	1.99	0.62
1:N:125:ALA:O	1:N:129:LEU:HG	1.99	0.62
1:P:133:LEU:HA	1:P:136:GLN:HB3	1.79	0.62
1:G:55:LEU:HD23	1:H:55:LEU:HD23	1.80	0.62
1:L:93:GLU:O	1:L:97:LEU:HG	1.99	0.62
1:M:88:THR:O	1:M:92:GLU:HG3	1.98	0.62
1:H:41:THR:O	1:H:45:GLN:HG3	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:97:LEU:HD13	1:R:36:ASN:OD1	1.99	0.62
1:K:83:GLU:HG3	1:L:87:ARG:HH12	1.65	0.62
1:O:35:LEU:HD12	1:O:38:SER:HB2	1.81	0.62
1:R:133:LEU:HD12	1:R:133:LEU:O	1.99	0.62
1:E:137:LEU:O	1:E:141:ASP:HB2	1.99	0.62
1:G:98:ASN:N	2:G:167:HOH:O	2.33	0.62
1:J:65:GLU:HA	1:J:68:ASP:HB3	1.80	0.62
1:S:133:LEU:HD11	2:T:168:HOH:O	1.98	0.62
1:A:144:LEU:HD22	1:B:144:LEU:HD21	1.80	0.62
1:A:72:GLU:O	1:A:76:LEU:HG	1.99	0.62
1:F:132:ARG:HD3	1:F:132:ARG:O	2.00	0.62
1:H:36:ASN:O	1:H:39:LEU:HB3	1.99	0.62
1:K:72:GLU:O	1:K:76:LEU:HG	2.00	0.62
1:K:144:LEU:HG	1:L:144:LEU:CD2	2.30	0.62
1:P:133:LEU:HD13	1:P:136:GLN:OE1	2.00	0.62
1:I:32:GLU:HG2	1:I:35:LEU:HD12	1.82	0.62
1:L:136:GLN:HG2	2:L:166:HOH:O	2.00	0.62
1:K:46:LYS:HE2	1:K:50:GLU:OE1	2.00	0.62
1:T:127:GLU:O	1:T:131:LYS:HG3	1.99	0.62
1:Q:105:THR:HG23	1:R:108:LEU:HD12	1.82	0.62
1:G:122:GLU:O	1:G:126:ILE:HG13	1.99	0.61
1:E:134:THR:HG21	1:E:138:ARG:HH21	1.63	0.61
1:L:88:THR:O	1:L:92:GLU:HG3	2.00	0.61
1:S:109:PHE:O	1:S:112:ALA:HB3	2.00	0.61
1:D:132:ARG:O	1:D:136:GLN:HG3	2.00	0.61
1:J:97:LEU:O	1:J:100:GLU:HB3	2.00	0.61
1:M:138:ARG:HG2	1:M:142:MSE:HG3	1.82	0.61
1:I:122:GLU:HG3	1:I:126:ILE:HD12	1.82	0.61
1:Q:108:LEU:HD23	1:Q:108:LEU:C	2.25	0.61
1:A:123:LYS:O	1:A:127:GLU:HB2	2.00	0.61
1:I:86:LEU:HD22	1:I:89:LYS:HZ2	1.64	0.61
1:J:72:GLU:O	1:J:76:LEU:HB2	2.01	0.61
1:Q:87:ARG:O	1:Q:91:GLU:HG3	2.01	0.61
1:R:41:THR:O	1:R:45:GLN:HG3	2.00	0.61
1:R:119:ALA:O	1:R:123:LYS:HG3	2.00	0.61
1:I:92:GLU:O	1:I:95:ASP:HB3	1.99	0.61
1:M:94:ALA:O	1:M:98:ASN:HB2	2.00	0.61
1:S:46:LYS:HE3	1:S:50:GLU:OE1	2.01	0.61
1:A:144:LEU:HD13	1:B:144:LEU:CD2	2.30	0.61
1:M:129:LEU:HG	1:N:130:ASN:HD22	1.65	0.61
1:N:66:LEU:O	1:N:70:ASP:HB2	2.00	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:44:SER:O	1:R:48:ALA:HB2	2.00	0.61
1:S:56:LYS:HG3	1:T:55:LEU:CD2	2.23	0.61
1:S:133:LEU:HB2	1:T:133:LEU:HD22	1.82	0.61
1:E:69:ARG:HD3	2:E:169:HOH:O	2.00	0.61
1:E:100:GLU:HA	1:E:103:ASP:OD2	2.01	0.61
1:L:108:LEU:HD13	1:L:108:LEU:C	2.26	0.61
1:K:137:LEU:HD21	1:L:137:LEU:CG	2.28	0.60
1:N:41:THR:O	1:N:45:GLN:HG3	2.01	0.60
1:D:112:ALA:O	1:D:116:VAL:HG23	2.00	0.60
1:J:45:GLN:O	1:J:49:ILE:HG12	2.01	0.60
1:Q:126:ILE:CG2	1:R:126:ILE:HD12	2.32	0.60
1:S:88:THR:HG22	1:S:92:GLU:OE2	2.01	0.60
1:T:89:LYS:O	1:T:93:GLU:HG3	2.02	0.60
1:P:65:GLU:O	1:P:69:ARG:HG2	2.01	0.60
1:P:120:ARG:NH2	1:P:123:LYS:HZ3	1.99	0.60
1:I:140:LYS:HD2	1:J:137:LEU:HD22	1.83	0.60
1:L:68:ASP:HA	1:L:71:ASP:HB3	1.84	0.60
1:Q:133:LEU:HD22	1:R:133:LEU:CB	2.21	0.60
1:T:42:ILE:O	1:T:45:GLN:HB3	2.00	0.60
1:T:97:LEU:O	1:T:101:VAL:HG23	2.01	0.60
1:I:55:LEU:O	1:I:59:TYR:N	2.26	0.60
1:I:74:LYS:O	1:I:78:GLU:HG2	2.01	0.60
1:I:130:ASN:ND2	1:I:133:LEU:HD12	2.17	0.60
1:T:42:ILE:HA	1:T:45:GLN:HB2	1.83	0.60
1:B:76:LEU:O	1:B:80:ILE:HG12	2.02	0.60
1:J:108:LEU:O	1:J:111:GLU:HG2	2.01	0.60
1:K:67:SER:O	1:K:70:ASP:HB2	2.01	0.60
1:R:102:GLU:O	1:R:106:ALA:N	2.34	0.60
1:S:36:ASN:HD21	1:S:40:LYS:HE3	1.66	0.60
1:N:38:SER:O	1:N:42:ILE:HG13	2.01	0.60
1:C:104:LEU:HD13	1:Q:43:ALA:HA	1.84	0.60
1:C:141:ASP:CG	1:D:140:LYS:HZ2	2.10	0.60
1:F:116:VAL:HG12	1:F:116:VAL:O	2.00	0.60
1:N:42:ILE:HA	1:N:45:GLN:HE21	1.66	0.60
1:T:36:ASN:HA	1:T:39:LEU:HB2	1.84	0.60
1:D:116:VAL:HG13	1:Q:52:TYR:OH	2.02	0.60
1:L:100:GLU:O	1:L:104:LEU:HG	2.01	0.60
1:M:120:ARG:HA	1:M:123:LYS:HD2	1.83	0.60
1:S:76:LEU:O	1:S:80:ILE:HG13	2.01	0.60
1:D:117:ALA:O	1:D:121:MSE:HG2	2.00	0.60
1:H:111:GLU:HB2	1:R:49:ILE:HD11	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:135:GLU:HG2	1:P:138:ARG:CZ	2.31	0.60
1:S:106:ALA:O	1:S:109:PHE:HB3	2.01	0.60
1:A:55:LEU:HD22	1:B:52:TYR:CE1	2.37	0.59
1:G:32:GLU:O	1:G:35:LEU:HB3	2.02	0.59
1:D:132:ARG:HG2	1:D:136:GLN:NE2	2.16	0.59
1:G:62:LEU:HD13	1:H:63:LYS:HG3	1.84	0.59
1:I:66:LEU:HD12	1:I:70:ASP:OD1	2.02	0.59
1:T:132:ARG:HB2	2:T:168:HOH:O	2.00	0.59
1:E:63:LYS:HA	1:F:62:LEU:HD21	1.84	0.59
1:E:137:LEU:HD22	1:F:140:LYS:HZ2	1.65	0.59
1:F:47:ALA:HA	1:F:50:GLU:HB2	1.83	0.59
1:F:76:LEU:O	1:F:80:ILE:HG12	2.02	0.59
1:K:141:ASP:OD1	1:L:140:LYS:HE2	2.03	0.59
1:P:59:TYR:CG	1:P:59:TYR:O	2.55	0.59
1:A:133:LEU:HD13	2:B:166:HOH:O	2.02	0.59
1:I:47:ALA:O	1:I:51:ASN:ND2	2.36	0.59
1:D:65:GLU:HA	1:D:68:ASP:HB3	1.84	0.59
1:K:86:LEU:O	1:K:89:LYS:HB3	2.02	0.59
1:A:71:ASP:O	1:A:75:ARG:HG3	2.03	0.59
1:N:130:ASN:O	1:N:133:LEU:HB3	2.03	0.59
1:O:41:THR:O	1:O:45:GLN:HG3	2.03	0.59
1:E:137:LEU:HD22	1:F:140:LYS:NZ	2.18	0.59
1:I:130:ASN:HA	1:I:133:LEU:HB2	1.83	0.59
1:J:56:LYS:HG3	1:J:60:ASN:ND2	2.18	0.59
1:S:137:LEU:HD11	1:T:140:LYS:NZ	2.18	0.59
1:C:38:SER:O	1:C:41:THR:HG22	2.02	0.59
1:C:116:VAL:HG22	1:D:115:LEU:HD23	1.85	0.59
1:G:60:ASN:O	1:G:64:ARG:HG3	2.02	0.59
1:G:137:LEU:HD11	1:H:133:LEU:CD1	2.33	0.59
1:K:144:LEU:CD1	1:L:144:LEU:HG	2.32	0.59
1:R:64:ARG:O	1:R:68:ASP:HB2	2.03	0.59
1:G:69:ARG:HD2	1:H:70:ASP:HA	1.85	0.59
1:I:36:ASN:ND2	1:I:40:LYS:HE3	2.18	0.59
1:J:115:LEU:O	1:J:118:ASP:HB3	2.03	0.59
1:N:89:LYS:O	1:N:93:GLU:HG2	2.03	0.59
1:S:79:ASP:O	1:S:83:GLU:HG2	2.01	0.59
1:H:132:ARG:HA	1:H:135:GLU:HB2	1.84	0.59
1:I:76:LEU:HA	1:I:79:ASP:OD2	2.03	0.59
1:K:140:LYS:HZ3	1:L:140:LYS:HB3	1.67	0.59
1:C:88:THR:O	1:C:92:GLU:HG3	2.03	0.58
1:I:59:TYR:CE1	1:J:62:LEU:HD22	2.37	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:126:ILE:HG22	1:O:126:ILE:O	2.03	0.58
1:R:108:LEU:O	1:R:112:ALA:HB2	2.03	0.58
1:F:80:ILE:O	1:F:84:ASN:HB2	2.03	0.58
1:G:69:ARG:O	1:G:73:VAL:HG23	2.03	0.58
1:I:49:ILE:HA	1:I:52:TYR:CB	2.33	0.58
1:I:58:ASP:O	1:I:61:THR:HB	2.03	0.58
1:I:87:ARG:HD3	1:J:87:ARG:NH2	2.18	0.58
1:M:137:LEU:HD11	1:N:140:LYS:HD2	1.85	0.58
1:P:120:ARG:NH2	1:P:123:LYS:NZ	2.50	0.58
1:Q:96:LYS:O	1:Q:100:GLU:HG3	2.04	0.58
1:K:97:LEU:O	1:K:100:GLU:HB3	2.04	0.58
1:L:110:ASP:O	1:L:113:ASN:HB2	2.04	0.58
1:P:80:ILE:HG22	1:P:84:ASN:ND2	2.18	0.58
1:Q:128:ILE:HG12	2:Q:171:HOH:O	2.03	0.58
1:S:123:LYS:NZ	2:S:170:HOH:O	2.34	0.58
1:B:79:ASP:O	1:B:83:GLU:HG3	2.04	0.58
1:D:82:LYS:O	1:D:86:LEU:HG	2.02	0.58
1:I:96:LYS:HG3	1:I:97:LEU:N	2.19	0.58
1:K:133:LEU:HD23	1:K:136:GLN:OE1	2.04	0.58
1:N:83:GLU:O	1:N:87:ARG:HG2	2.02	0.58
1:P:49:ILE:HG23	1:P:50:GLU:H	1.69	0.58
1:Q:61:THR:HA	1:Q:64:ARG:HE	1.68	0.58
1:S:33:GLU:O	1:S:37:LYS:N	2.34	0.58
1:E:144:LEU:CD1	1:F:143:LEU:HB3	2.24	0.58
1:I:51:ASN:CA	1:I:54:GLN:HB3	2.25	0.58
1:I:80:ILE:CD1	1:J:76:LEU:HD22	2.33	0.58
1:M:65:GLU:HA	1:M:68:ASP:OD2	2.04	0.58
1:D:126:ILE:HD13	1:D:126:ILE:O	2.03	0.58
1:C:136:GLN:O	1:D:137:LEU:HD11	2.04	0.58
1:F:41:THR:HG22	1:F:45:GLN:NE2	2.19	0.58
1:H:100:GLU:OE1	1:R:39:LEU:HD21	2.03	0.58
1:G:70:ASP:O	1:G:74:LYS:HG3	2.03	0.58
1:G:108:LEU:HD21	1:H:108:LEU:O	2.03	0.58
1:G:120:ARG:O	1:G:124:TYR:HB2	2.03	0.58
1:I:61:THR:HG22	1:I:65:GLU:OE2	2.03	0.58
1:G:62:LEU:HD11	1:H:63:LYS:HG3	1.85	0.58
1:H:123:LYS:O	1:H:127:GLU:HG2	2.03	0.58
1:P:36:ASN:C	1:P:38:SER:H	2.12	0.58
1:A:98:ASN:O	1:A:102:GLU:HB2	2.04	0.58
1:A:105:THR:HG23	1:B:108:LEU:HD23	1.84	0.58
1:P:113:ASN:HA	1:P:116:VAL:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:61:THR:HA	1:T:64:ARG:HE	1.69	0.58
1:J:42:ILE:O	1:J:45:GLN:HB2	2.03	0.57
1:D:44:SER:O	1:D:48:ALA:HB2	2.04	0.57
1:K:140:LYS:HE2	1:L:140:LYS:HG2	1.84	0.57
1:L:78:GLU:C	1:L:80:ILE:H	2.12	0.57
1:O:129:LEU:O	1:O:133:LEU:HB2	2.05	0.57
1:E:133:LEU:HB2	1:F:133:LEU:CD2	2.28	0.57
1:H:106:ALA:O	1:H:109:PHE:HB3	2.03	0.57
1:O:73:VAL:HG11	1:P:72:GLU:OE1	2.04	0.57
1:S:133:LEU:CD2	1:T:129:LEU:HD22	2.33	0.57
1:I:80:ILE:HG12	1:J:80:ILE:HG13	1.85	0.57
1:J:136:GLN:HB2	2:J:166:HOH:O	2.03	0.57
1:A:45:GLN:O	1:A:48:ALA:HB3	2.04	0.57
1:D:53:ASN:O	1:D:57:GLU:HG3	2.04	0.57
1:H:99:LYS:HG2	1:H:100:GLU:H	1.68	0.57
1:I:113:ASN:H	1:I:113:ASN:ND2	2.01	0.57
1:A:73:VAL:HG11	1:B:72:GLU:OE1	2.04	0.57
1:N:80:ILE:O	1:N:84:ASN:HB2	2.04	0.57
1:Q:36:ASN:O	1:Q:40:LYS:HG3	2.04	0.57
1:S:52:TYR:CE1	1:T:51:ASN:HB3	2.39	0.57
1:S:133:LEU:HD13	1:T:133:LEU:HD13	1.86	0.57
1:A:130:ASN:ND2	1:B:130:ASN:HD22	2.02	0.57
1:J:49:ILE:HG22	1:J:50:GLU:N	2.19	0.57
1:O:102:GLU:HG3	1:O:103:ASP:N	2.18	0.57
1:K:123:LYS:O	1:K:127:GLU:N	2.38	0.57
1:L:73:VAL:N	2:L:173:HOH:O	2.38	0.57
1:Q:129:LEU:HG	2:R:165:HOH:O	2.05	0.57
1:Q:132:ARG:O	1:Q:136:GLN:N	2.38	0.57
1:C:38:SER:HA	1:C:41:THR:HG22	1.85	0.57
1:I:113:ASN:N	1:I:113:ASN:ND2	2.52	0.57
1:O:38:SER:O	1:O:42:ILE:HG13	2.05	0.57
1:S:88:THR:O	1:S:92:GLU:HG2	2.05	0.57
1:A:144:LEU:HD11	1:B:147:LEU:CG	2.35	0.56
1:G:108:LEU:CD2	1:H:108:LEU:HG	2.35	0.56
1:K:103:ASP:O	1:K:104:LEU:C	2.48	0.56
1:M:112:ALA:CB	1:N:108:LEU:HD11	2.35	0.56
1:B:31:LEU:O	1:B:34:GLN:HB3	2.06	0.56
1:C:38:SER:O	1:C:42:ILE:HG13	2.05	0.56
1:E:86:LEU:C	1:E:88:THR:H	2.13	0.56
1:K:62:LEU:HD21	1:L:63:LYS:CA	2.35	0.56
1:M:61:THR:HG22	1:M:62:LEU:HD12	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:66:LEU:HA	1:P:66:LEU:HD23	1.87	0.56
1:O:110:ASP:HA	1:O:113:ASN:HD22	1.69	0.56
1:B:95:ASP:O	1:B:99:LYS:HG2	2.06	0.56
1:B:134:THR:N	2:B:166:HOH:O	2.37	0.56
1:C:139:GLU:O	1:C:143:LEU:HB2	2.05	0.56
1:G:82:LYS:HA	1:G:85:GLU:HB3	1.87	0.56
1:G:96:LYS:O	1:G:100:GLU:HG2	2.05	0.56
1:K:124:TYR:O	1:K:128:ILE:HG13	2.05	0.56
1:N:135:GLU:CA	1:N:138:ARG:HG2	2.32	0.56
1:S:36:ASN:O	1:S:40:LYS:HG3	2.05	0.56
1:F:31:LEU:CD1	1:F:34:GLN:HE21	2.18	0.56
1:I:137:LEU:HD21	1:J:136:GLN:OE1	2.05	0.56
1:J:111:GLU:CG	1:J:112:ALA:N	2.68	0.56
1:R:116:VAL:HG12	1:R:120:ARG:HG3	1.88	0.56
1:D:43:ALA:HA	1:D:46:LYS:HB3	1.87	0.56
1:F:132:ARG:O	1:F:136:GLN:HB2	2.06	0.56
1:O:46:LYS:NZ	2:O:163:HOH:O	2.39	0.56
1:D:113:ASN:HA	1:R:51:ASN:HD21	1.70	0.56
1:C:133:LEU:HB2	1:D:133:LEU:CD2	2.34	0.56
1:D:103:ASP:OD1	1:D:104:LEU:N	2.39	0.56
1:N:42:ILE:HA	1:N:45:GLN:NE2	2.20	0.56
1:O:35:LEU:HA	1:O:38:SER:HB2	1.88	0.56
1:O:140:LYS:O	1:P:140:LYS:HE2	2.06	0.56
1:O:140:LYS:HZ1	1:P:141:ASP:CG	2.14	0.56
1:P:120:ARG:HH22	1:P:123:LYS:HZ3	1.53	0.56
1:I:42:ILE:HG12	1:I:45:GLN:NE2	2.19	0.56
1:L:78:GLU:C	1:L:80:ILE:N	2.63	0.56
1:O:144:LEU:HD13	1:P:144:LEU:HD22	1.88	0.56
1:S:87:ARG:O	1:S:91:GLU:HG3	2.05	0.56
1:S:113:ASN:HA	1:S:116:VAL:CG2	2.36	0.56
1:B:123:LYS:O	1:B:123:LYS:HG2	2.06	0.56
1:D:98:ASN:HD21	1:Q:35:LEU:HD12	1.71	0.56
1:G:133:LEU:O	1:H:133:LEU:HD11	2.06	0.56
1:L:83:GLU:HB3	1:L:87:ARG:HE	1.71	0.56
1:P:126:ILE:HD13	1:P:129:LEU:HD12	1.88	0.56
1:S:133:LEU:HD12	1:S:133:LEU:O	2.05	0.56
1:T:53:ASN:O	1:T:57:GLU:N	2.38	0.56
1:Q:65:GLU:O	1:Q:69:ARG:HG2	2.06	0.55
1:G:64:ARG:O	1:G:67:SER:HB3	2.06	0.55
1:O:83:GLU:O	1:O:87:ARG:HG2	2.06	0.55
1:I:94:ALA:HA	1:I:97:LEU:HB2	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:61:THR:O	1:J:64:ARG:HB2	2.06	0.55
1:C:115:LEU:C	1:C:115:LEU:HD23	2.32	0.55
1:I:63:LYS:O	1:I:66:LEU:HB3	2.07	0.55
1:I:130:ASN:HD22	1:I:133:LEU:HD12	1.70	0.55
1:F:96:LYS:O	1:F:100:GLU:HG3	2.06	0.55
1:H:128:ILE:C	1:H:130:ASN:H	2.13	0.55
1:P:113:ASN:HB2	2:P:162:HOH:O	2.07	0.55
1:E:139:GLU:HG3	1:E:140:LYS:N	2.22	0.55
1:I:84:ASN:HA	1:I:87:ARG:HD2	1.89	0.55
1:H:88:THR:HA	1:H:91:GLU:OE1	2.07	0.55
1:I:91:GLU:O	1:I:95:ASP:HB2	2.06	0.55
1:P:82:LYS:O	1:P:86:LEU:HB2	2.07	0.55
1:J:56:LYS:HE2	2:J:164:HOH:O	2.07	0.55
1:S:99:LYS:O	1:S:103:ASP:HB2	2.07	0.55
1:F:105:THR:O	1:F:106:ALA:C	2.49	0.55
1:G:123:LYS:NZ	1:H:122:GLU:HB3	2.22	0.55
1:I:135:GLU:HG2	1:I:138:ARG:HD2	1.89	0.55
1:M:41:THR:O	1:M:45:GLN:HG3	2.07	0.55
1:Q:56:LYS:HD2	1:R:55:LEU:HD11	1.89	0.55
1:T:79:ASP:O	1:T:83:GLU:HG3	2.06	0.55
1:D:36:ASN:C	1:D:38:SER:N	2.63	0.55
1:J:134:THR:C	1:J:136:GLN:H	2.15	0.55
1:M:51:ASN:HA	1:M:54:GLN:HG2	1.89	0.55
1:O:140:LYS:NZ	1:P:141:ASP:CG	2.65	0.55
1:Q:118:ASP:C	1:Q:120:ARG:H	2.15	0.55
1:M:42:ILE:C	1:M:44:SER:H	2.14	0.54
1:T:71:ASP:O	1:T:75:ARG:HG2	2.07	0.54
1:C:89:LYS:HA	1:C:92:GLU:OE1	2.07	0.54
1:K:55:LEU:HD22	1:L:52:TYR:CE1	2.42	0.54
1:M:116:VAL:HA	1:N:115:LEU:HD21	1.89	0.54
1:N:43:ALA:C	1:N:45:GLN:H	2.14	0.54
1:O:148:THR:HG22	1:O:148:THR:O	2.07	0.54
1:H:66:LEU:C	1:H:68:ASP:H	2.13	0.54
1:K:134:THR:O	1:K:138:ARG:HG3	2.06	0.54
1:R:100:GLU:HB2	2:R:169:HOH:O	2.07	0.54
1:S:53:ASN:O	1:S:57:GLU:HB2	2.06	0.54
1:S:64:ARG:O	1:S:68:ASP:HB2	2.08	0.54
1:I:86:LEU:HB3	1:I:89:LYS:HE2	1.89	0.54
1:S:40:LYS:HA	2:S:167:HOH:O	2.06	0.54
1:S:132:ARG:O	1:S:136:GLN:N	2.35	0.54
1:S:36:ASN:ND2	1:S:40:LYS:HE3	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:88:THR:O	1:T:92:GLU:HG3	2.07	0.54
1:B:83:GLU:HB3	2:B:168:HOH:O	2.06	0.54
1:D:46:LYS:HG3	1:D:47:ALA:N	2.23	0.54
1:T:42:ILE:C	1:T:45:GLN:H	2.16	0.54
1:C:136:GLN:CB	1:D:137:LEU:HD21	2.38	0.54
1:H:64:ARG:HD3	2:H:165:HOH:O	2.07	0.54
1:I:80:ILE:HD13	1:J:76:LEU:HD22	1.89	0.54
1:S:133:LEU:CD1	1:T:133:LEU:HB2	2.31	0.54
1:A:55:LEU:HD23	1:B:55:LEU:HD23	1.90	0.54
1:B:46:LYS:C	1:B:48:ALA:H	2.16	0.54
1:M:55:LEU:C	1:M:57:GLU:H	2.15	0.54
1:G:52:TYR:CE2	1:G:56:LYS:HD2	2.43	0.54
1:H:99:LYS:HG3	1:H:100:GLU:H	1.72	0.54
1:L:73:VAL:O	1:L:77:ARG:CB	2.54	0.54
1:N:90:ALA:O	1:N:94:ALA:HB3	2.08	0.54
1:P:60:ASN:O	1:P:63:LYS:N	2.41	0.54
1:Q:46:LYS:HG3	1:Q:47:ALA:N	2.23	0.54
1:A:92:GLU:C	1:A:94:ALA:H	2.15	0.54
1:D:96:LYS:HG3	1:D:97:LEU:N	2.23	0.54
1:H:66:LEU:C	1:H:68:ASP:N	2.65	0.54
1:I:126:ILE:HG22	1:I:126:ILE:O	2.07	0.54
1:I:131:LYS:O	1:I:135:GLU:HB2	2.08	0.54
1:K:137:LEU:HD22	2:L:166:HOH:O	2.08	0.54
1:M:89:LYS:C	1:M:91:GLU:H	2.16	0.54
1:C:141:ASP:CG	1:D:140:LYS:NZ	2.66	0.53
1:I:42:ILE:C	1:I:44:SER:N	2.64	0.53
1:I:140:LYS:NZ	1:J:137:LEU:HD22	2.23	0.53
1:Q:136:GLN:O	1:Q:140:LYS:HG3	2.08	0.53
1:B:133:LEU:HB2	2:B:166:HOH:O	2.08	0.53
1:F:136:GLN:C	1:F:137:LEU:HD23	2.34	0.53
1:G:102:GLU:O	1:G:106:ALA:HB2	2.08	0.53
1:C:90:ALA:HA	1:C:93:GLU:HG2	1.90	0.53
1:C:137:LEU:O	1:D:140:LYS:NZ	2.41	0.53
1:E:131:LYS:C	1:E:133:LEU:N	2.65	0.53
1:J:81:ALA:HA	1:J:84:ASN:ND2	2.23	0.53
1:A:130:ASN:ND2	1:B:130:ASN:HB2	2.15	0.53
1:M:73:VAL:O	1:M:77:ARG:HB2	2.08	0.53
1:M:132:ARG:C	2:M:163:HOH:O	2.50	0.53
1:T:124:TYR:HA	1:T:127:GLU:CD	2.33	0.53
1:I:42:ILE:C	1:I:44:SER:H	2.16	0.53
1:J:45:GLN:O	1:J:46:LYS:C	2.51	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:98:ASN:C	1:S:98:ASN:ND2	2.65	0.53
1:C:105:THR:HG23	1:D:105:THR:CG2	2.39	0.53
1:E:56:LYS:O	1:E:60:ASN:ND2	2.41	0.53
1:L:61:THR:O	1:L:65:GLU:HB2	2.08	0.53
1:A:140:LYS:HE2	1:B:140:LYS:O	2.08	0.53
1:E:69:ARG:HD2	1:F:70:ASP:OD1	2.09	0.53
1:F:111:GLU:O	1:F:114:ASN:HB3	2.09	0.53
1:F:116:VAL:O	1:F:116:VAL:CG1	2.57	0.53
1:I:45:GLN:HG3	1:I:46:LYS:H	1.73	0.53
1:J:49:ILE:C	1:J:51:ASN:N	2.63	0.53
1:Q:135:GLU:O	1:Q:139:GLU:HG3	2.09	0.53
1:S:126:ILE:HA	1:S:129:LEU:CG	2.38	0.53
1:G:83:GLU:O	1:G:87:ARG:HG2	2.07	0.53
1:I:120:ARG:NH1	2:I:162:HOH:O	2.41	0.53
1:K:62:LEU:HD21	1:L:63:LYS:N	2.24	0.53
1:N:112:ALA:O	1:N:116:VAL:HG23	2.09	0.53
1:O:147:LEU:HD23	1:P:144:LEU:CD1	2.28	0.53
1:J:92:GLU:O	1:J:96:LYS:HG3	2.07	0.53
1:T:89:LYS:HA	1:T:92:GLU:OE1	2.09	0.53
1:I:71:ASP:O	1:I:75:ARG:N	2.41	0.53
1:J:56:LYS:NZ	1:J:59:TYR:HE2	2.07	0.53
1:O:49:ILE:HG22	1:O:53:ASN:ND2	2.24	0.53
1:R:90:ALA:O	1:R:94:ALA:HB2	2.08	0.53
1:B:49:ILE:O	1:B:50:GLU:C	2.52	0.52
1:C:66:LEU:HD11	1:D:69:ARG:HD2	1.89	0.52
1:D:45:GLN:O	1:D:48:ALA:HB3	2.10	0.52
1:E:137:LEU:CD2	1:F:140:LYS:HZ2	2.23	0.52
1:E:144:LEU:HD21	1:F:143:LEU:HD22	1.91	0.52
1:M:122:GLU:HG2	1:N:123:LYS:NZ	2.24	0.52
1:N:69:ARG:O	1:N:73:VAL:HG23	2.09	0.52
1:Q:41:THR:O	1:Q:44:SER:HB2	2.09	0.52
1:S:36:ASN:HA	1:S:39:LEU:HB3	1.90	0.52
1:S:71:ASP:O	1:S:75:ARG:N	2.41	0.52
1:T:80:ILE:O	1:T:83:GLU:HB2	2.08	0.52
1:A:79:ASP:C	1:A:81:ALA:H	2.17	0.52
1:G:127:GLU:O	1:G:131:LYS:HG3	2.10	0.52
1:L:69:ARG:N	2:L:161:HOH:O	2.42	0.52
1:S:126:ILE:HG23	1:S:129:LEU:HD12	1.91	0.52
1:B:46:LYS:HE3	1:B:50:GLU:OE1	2.09	0.52
1:F:57:GLU:O	1:F:60:ASN:HB2	2.09	0.52
1:P:135:GLU:HA	1:P:138:ARG:HG3	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:107:SER:O	1:S:111:GLU:HG2	2.09	0.52
1:T:113:ASN:CG	1:T:114:ASN:N	2.68	0.52
1:A:70:ASP:OD1	1:B:69:ARG:CZ	2.57	0.52
1:F:148:THR:HG22	1:F:152:LYS:HE3	1.90	0.52
1:J:38:SER:O	1:J:42:ILE:HG12	2.10	0.52
1:K:133:LEU:O	1:K:137:LEU:HG	2.09	0.52
1:Q:38:SER:O	1:Q:42:ILE:HG12	2.09	0.52
1:S:71:ASP:CG	1:S:72:GLU:N	2.67	0.52
1:M:126:ILE:HG22	1:N:126:ILE:HG22	1.91	0.52
1:N:59:TYR:CZ	1:N:63:LYS:HE3	2.45	0.52
1:S:62:LEU:HD11	1:T:59:TYR:CE1	2.45	0.52
1:T:39:LEU:O	1:T:43:ALA:HB2	2.09	0.52
1:T:56:LYS:O	1:T:59:TYR:HB3	2.10	0.52
1:C:144:LEU:CD1	1:D:147:LEU:HD13	2.39	0.52
1:E:137:LEU:HD21	1:F:137:LEU:CD2	2.39	0.52
1:F:46:LYS:HG2	1:F:50:GLU:OE2	2.10	0.52
1:H:38:SER:O	1:H:42:ILE:HG13	2.10	0.52
1:M:46:LYS:HB2	2:M:173:HOH:O	2.10	0.52
1:Q:134:THR:O	1:Q:138:ARG:HG3	2.10	0.52
1:C:76:LEU:O	1:C:80:ILE:HG12	2.09	0.52
1:H:122:GLU:OE2	1:R:59:TYR:HE2	1.91	0.52
1:J:50:GLU:O	1:J:54:GLN:N	2.42	0.52
1:K:138:ARG:O	1:K:142:MSE:HG3	2.10	0.52
1:L:56:LYS:HE3	1:L:59:TYR:CD2	2.45	0.52
1:Q:115:LEU:O	1:Q:118:ASP:HB3	2.09	0.52
1:R:48:ALA:O	1:R:51:ASN:HB2	2.10	0.52
1:D:90:ALA:HB1	2:D:169:HOH:O	2.10	0.52
1:L:68:ASP:C	2:L:161:HOH:O	2.52	0.52
1:M:55:LEU:C	1:M:57:GLU:N	2.60	0.52
1:M:116:VAL:HG22	1:N:115:LEU:HD22	1.91	0.52
1:A:39:LEU:O	1:A:39:LEU:HD23	2.10	0.52
1:G:125:ALA:O	1:G:128:ILE:HB	2.10	0.52
1:K:115:LEU:CD2	1:L:116:VAL:HG22	2.40	0.52
1:H:85:GLU:O	1:H:89:LYS:HG3	2.10	0.52
1:J:69:ARG:O	1:J:73:VAL:HG23	2.10	0.52
1:K:49:ILE:HG22	1:K:53:ASN:OD1	2.10	0.52
1:K:131:LYS:O	1:K:135:GLU:HG3	2.11	0.52
1:M:69:ARG:O	1:M:73:VAL:HG23	2.10	0.52
1:M:118:ASP:O	1:M:121:MSE:HB2	2.10	0.52
1:N:32:GLU:C	1:N:34:GLN:N	2.68	0.52
1:O:35:LEU:HD12	1:O:38:SER:CB	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:130:ASN:HD22	1:P:126:ILE:HG23	1.75	0.52
1:I:126:ILE:HG22	1:J:126:ILE:HG13	1.92	0.51
1:K:115:LEU:HD21	1:L:116:VAL:HG22	1.93	0.51
1:K:140:LYS:HE3	1:L:141:ASP:CG	2.36	0.51
1:M:133:LEU:HD21	2:N:172:HOH:O	2.09	0.51
1:O:81:ALA:C	1:O:83:GLU:H	2.17	0.51
1:S:137:LEU:HG	1:S:141:ASP:OD2	2.10	0.51
1:A:140:LYS:HZ1	1:B:141:ASP:N	2.08	0.51
1:E:65:GLU:O	1:E:69:ARG:HG2	2.10	0.51
1:I:130:ASN:C	1:I:132:ARG:N	2.67	0.51
1:N:32:GLU:HG3	1:N:33:GLU:H	1.74	0.51
1:P:87:ARG:O	1:P:91:GLU:HG3	2.10	0.51
1:T:92:GLU:O	1:T:96:LYS:HG3	2.10	0.51
1:T:135:GLU:O	1:T:139:GLU:HB2	2.10	0.51
1:C:80:ILE:HD11	1:D:80:ILE:HG12	1.92	0.51
1:D:133:LEU:HD12	1:D:133:LEU:O	2.11	0.51
1:I:120:ARG:O	1:I:124:TYR:HB2	2.10	0.51
1:O:100:GLU:O	1:O:104:LEU:HG	2.11	0.51
1:Q:132:ARG:HA	1:Q:135:GLU:HB2	1.92	0.51
1:R:123:LYS:O	1:R:127:GLU:OE1	2.29	0.51
1:A:120:ARG:HH11	1:A:123:LYS:HD3	1.75	0.51
1:G:80:ILE:HD11	1:H:80:ILE:CD1	2.40	0.51
1:G:115:LEU:HD11	1:H:116:VAL:HG22	1.92	0.51
1:N:32:GLU:HG3	1:N:33:GLU:N	2.26	0.51
1:N:59:TYR:CE2	1:N:63:LYS:HE3	2.45	0.51
1:P:134:THR:O	1:P:138:ARG:HG3	2.10	0.51
1:I:49:ILE:O	1:I:52:TYR:HB3	2.10	0.51
1:J:120:ARG:NH1	1:J:123:LYS:HZ2	2.07	0.51
1:J:137:LEU:N	2:J:165:HOH:O	2.42	0.51
1:O:34:GLN:HG3	1:O:35:LEU:N	2.26	0.51
1:T:52:TYR:O	1:T:56:LYS:N	2.41	0.51
1:I:130:ASN:C	1:I:132:ARG:H	2.17	0.51
1:P:136:GLN:O	1:P:137:LEU:HD23	2.11	0.51
1:H:108:LEU:O	1:H:112:ALA:HB2	2.10	0.51
1:I:53:ASN:HA	1:I:56:LYS:HB2	1.93	0.51
1:J:111:GLU:O	1:J:114:ASN:HB3	2.10	0.51
1:M:109:PHE:CA	1:N:108:LEU:HD21	2.40	0.51
1:Q:140:LYS:HZ2	1:R:137:LEU:CG	2.24	0.51
1:A:49:ILE:O	1:A:50:GLU:C	2.54	0.51
1:A:80:ILE:HD11	1:B:80:ILE:CD1	2.40	0.51
1:I:76:LEU:CD1	1:J:77:ARG:HE	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:111:GLU:HA	1:J:114:ASN:HB3	1.92	0.51
1:O:31:LEU:O	1:O:34:GLN:HG2	2.11	0.51
1:P:45:GLN:O	1:P:49:ILE:HG22	2.10	0.51
1:F:82:LYS:C	1:F:84:ASN:H	2.19	0.51
1:I:82:LYS:O	1:I:85:GLU:HB3	2.11	0.51
1:J:119:ALA:C	1:J:121:MSE:N	2.69	0.51
1:P:136:GLN:C	1:P:137:LEU:HD23	2.35	0.51
1:M:63:LYS:HG3	1:N:62:LEU:CD1	2.40	0.51
1:M:118:ASP:C	1:M:121:MSE:HB2	2.36	0.51
1:N:94:ALA:O	1:N:98:ASN:ND2	2.44	0.51
1:E:147:LEU:HG	1:F:146:THR:CG2	2.42	0.50
1:H:111:GLU:CB	1:R:49:ILE:HD11	2.40	0.50
1:E:128:ILE:O	1:E:131:LYS:HB2	2.11	0.50
1:G:56:LYS:HG2	2:G:171:HOH:O	2.10	0.50
1:G:91:GLU:CG	1:H:87:ARG:HH22	2.24	0.50
1:M:108:LEU:HD22	1:N:105:THR:HG23	1.93	0.50
1:Q:61:THR:O	1:Q:65:GLU:HG3	2.12	0.50
1:Q:140:LYS:HB3	1:R:140:LYS:CE	2.41	0.50
1:E:61:THR:O	1:E:65:GLU:HG3	2.11	0.50
1:G:123:LYS:HG3	2:G:172:HOH:O	2.12	0.50
1:H:95:ASP:HA	1:H:98:ASN:HB3	1.93	0.50
1:L:56:LYS:O	1:L:56:LYS:HG3	2.11	0.50
1:O:56:LYS:HA	1:P:55:LEU:HD21	1.91	0.50
1:P:50:GLU:HA	1:P:53:ASN:HD22	1.76	0.50
1:P:116:VAL:HG23	1:P:117:ALA:N	2.26	0.50
1:S:50:GLU:O	1:S:50:GLU:HG2	2.11	0.50
1:T:37:LYS:O	1:T:40:LYS:HB3	2.11	0.50
1:B:69:ARG:NE	2:B:161:HOH:O	2.44	0.50
1:G:100:GLU:O	1:G:104:LEU:HB2	2.11	0.50
1:I:47:ALA:O	1:I:50:GLU:HG2	2.12	0.50
1:J:56:LYS:HZ2	1:J:59:TYR:HE2	1.56	0.50
1:S:126:ILE:HG22	1:T:126:ILE:HG21	1.91	0.50
1:B:132:ARG:HA	1:B:135:GLU:HG2	1.94	0.50
1:M:138:ARG:O	1:M:142:MSE:HB2	2.11	0.50
1:R:124:TYR:O	1:R:127:GLU:HB2	2.11	0.50
1:C:116:VAL:HG22	1:D:115:LEU:CD2	2.41	0.50
1:C:141:ASP:CA	1:D:140:LYS:HZ1	2.25	0.50
1:G:79:ASP:O	1:G:83:GLU:N	2.45	0.50
1:I:69:ARG:HA	1:I:72:GLU:HG2	1.94	0.50
1:K:120:ARG:HH11	1:K:123:LYS:HD2	1.77	0.50
1:O:130:ASN:ND2	1:P:130:ASN:ND2	2.56	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:45:GLN:HA	1:G:48:ALA:HB3	1.94	0.50
1:G:87:ARG:HD2	1:H:87:ARG:NE	2.26	0.50
1:G:123:LYS:HE2	1:H:123:LYS:HA	1.93	0.50
1:J:65:GLU:O	1:J:69:ARG:HB2	2.12	0.50
1:L:87:ARG:O	1:L:91:GLU:HG3	2.11	0.50
1:M:123:LYS:O	1:M:127:GLU:HG3	2.12	0.50
1:Q:105:THR:HG23	1:R:108:LEU:CD1	2.42	0.50
1:Q:116:VAL:HG12	1:Q:116:VAL:O	2.10	0.50
1:S:52:TYR:CE1	1:T:55:LEU:HD22	2.47	0.50
1:F:83:GLU:O	1:F:87:ARG:HG2	2.12	0.50
1:I:113:ASN:HD22	1:I:113:ASN:H	1.59	0.50
1:A:89:LYS:HG3	1:A:90:ALA:N	2.27	0.50
1:H:61:THR:HG22	1:H:61:THR:O	2.12	0.50
1:H:108:LEU:HD13	1:R:46:LYS:HA	1.93	0.50
1:H:132:ARG:C	1:H:134:THR:N	2.66	0.50
1:I:73:VAL:O	1:I:77:ARG:HD2	2.12	0.50
1:M:116:VAL:O	1:M:119:ALA:HB3	2.12	0.50
1:N:119:ALA:O	1:N:123:LYS:HG2	2.11	0.50
1:O:110:ASP:HA	1:O:113:ASN:ND2	2.26	0.50
1:F:140:LYS:CG	1:F:143:LEU:HD12	2.42	0.49
1:G:91:GLU:HG3	1:H:87:ARG:HH22	1.76	0.49
1:G:98:ASN:O	1:G:102:GLU:HB3	2.12	0.49
1:G:110:ASP:O	1:G:113:ASN:HB2	2.12	0.49
1:I:130:ASN:HD22	1:I:130:ASN:N	2.08	0.49
1:I:140:LYS:HD2	1:J:137:LEU:CD2	2.42	0.49
1:J:56:LYS:O	1:J:60:ASN:ND2	2.45	0.49
1:P:34:GLN:NE2	2:P:165:HOH:O	2.44	0.49
1:A:80:ILE:N	1:A:80:ILE:HD12	2.26	0.49
1:E:147:LEU:HB2	1:F:147:LEU:HD21	1.94	0.49
1:I:130:ASN:OD1	1:J:126:ILE:HD11	2.11	0.49
1:M:115:LEU:CD2	1:N:112:ALA:HB1	2.42	0.49
1:N:47:ALA:O	1:N:48:ALA:C	2.54	0.49
1:D:109:PHE:C	1:D:111:GLU:H	2.18	0.49
1:J:34:GLN:O	1:J:34:GLN:HG3	2.13	0.49
1:K:140:LYS:HE2	1:L:140:LYS:CG	2.42	0.49
1:L:83:GLU:C	1:L:85:GLU:H	2.21	0.49
1:A:69:ARG:NH1	1:B:70:ASP:OD1	2.45	0.49
1:B:78:GLU:HG2	1:B:79:ASP:N	2.26	0.49
1:C:72:GLU:HB3	1:D:73:VAL:HG22	1.93	0.49
1:E:91:GLU:HA	1:E:94:ALA:HB2	1.93	0.49
1:E:112:ALA:O	1:E:116:VAL:HG23	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:118:ASP:O	1:E:120:ARG:N	2.46	0.49
1:G:38:SER:O	1:G:42:ILE:HG13	2.12	0.49
1:J:73:VAL:O	1:J:77:ARG:HG3	2.12	0.49
1:O:129:LEU:HA	1:O:132:ARG:HG2	1.94	0.49
1:Q:99:LYS:HA	1:Q:102:GLU:HB3	1.94	0.49
1:Q:133:LEU:HB2	1:R:133:LEU:HD13	1.93	0.49
1:T:45:GLN:O	1:T:49:ILE:HG13	2.13	0.49
1:A:108:LEU:HD21	1:B:109:PHE:HA	1.95	0.49
1:E:63:LYS:CA	1:F:62:LEU:HD21	2.42	0.49
1:G:134:THR:HA	1:G:137:LEU:HG	1.95	0.49
1:N:66:LEU:C	1:N:68:ASP:N	2.71	0.49
1:R:92:GLU:O	1:R:96:LYS:HG3	2.12	0.49
1:S:144:LEU:HD11	1:T:144:LEU:CD1	2.41	0.49
1:B:146:THR:C	1:B:148:THR:H	2.20	0.49
1:E:134:THR:CG2	1:E:138:ARG:HE	2.24	0.49
1:F:41:THR:O	1:F:45:GLN:HG3	2.13	0.49
1:J:56:LYS:NZ	1:J:59:TYR:CE2	2.81	0.49
1:N:88:THR:O	1:N:92:GLU:HG3	2.12	0.49
1:S:98:ASN:C	1:S:98:ASN:HD22	2.17	0.49
1:B:128:ILE:CG2	1:B:129:LEU:N	2.75	0.49
1:K:144:LEU:CG	1:L:144:LEU:HG	2.43	0.49
1:L:42:ILE:HG22	1:L:42:ILE:O	2.13	0.49
1:P:36:ASN:C	1:P:38:SER:N	2.71	0.49
1:Q:118:ASP:C	1:Q:120:ARG:N	2.70	0.49
1:S:126:ILE:HA	1:S:129:LEU:HD12	1.94	0.49
1:I:87:ARG:O	1:I:91:GLU:HG3	2.13	0.49
1:B:143:LEU:O	1:B:144:LEU:HD23	2.13	0.49
1:D:36:ASN:C	1:D:38:SER:H	2.21	0.49
1:F:55:LEU:O	1:F:55:LEU:HG	2.12	0.49
1:G:61:THR:HG22	1:G:62:LEU:N	2.28	0.49
1:G:133:LEU:HB3	1:H:133:LEU:CD2	2.43	0.49
1:S:99:LYS:HA	1:S:102:GLU:HG2	1.95	0.49
1:I:52:TYR:CE1	1:J:55:LEU:HD12	2.47	0.49
1:M:80:ILE:O	1:M:84:ASN:HB2	2.13	0.49
1:N:101:VAL:HG12	1:N:101:VAL:O	2.13	0.49
1:T:82:LYS:O	1:T:86:LEU:HG	2.13	0.49
1:T:93:GLU:HA	1:T:96:LYS:HD2	1.95	0.49
1:T:117:ALA:O	1:T:121:MSE:HG3	2.12	0.49
1:D:41:THR:O	1:D:45:GLN:HG3	2.12	0.48
1:F:123:LYS:O	1:F:127:GLU:HG2	2.13	0.48
1:N:33:GLU:O	1:N:33:GLU:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:134:THR:HG23	2:O:164:HOH:O	2.12	0.48
1:O:148:THR:O	1:O:152:LYS:HE3	2.12	0.48
1:H:35:LEU:HG	2:H:164:HOH:O	2.12	0.48
1:H:89:LYS:HA	1:H:92:GLU:OE2	2.13	0.48
1:M:118:ASP:HA	1:M:121:MSE:HB2	1.95	0.48
1:D:45:GLN:HA	1:D:48:ALA:HB3	1.94	0.48
1:K:92:GLU:C	1:K:94:ALA:H	2.20	0.48
1:L:80:ILE:HG22	1:L:84:ASN:ND2	2.28	0.48
1:N:82:LYS:O	1:N:86:LEU:HG	2.13	0.48
1:S:103:ASP:C	1:S:105:THR:N	2.65	0.48
1:S:135:GLU:O	1:S:139:GLU:HG3	2.13	0.48
1:T:111:GLU:C	1:T:113:ASN:H	2.20	0.48
1:B:46:LYS:C	1:B:48:ALA:N	2.70	0.48
1:C:71:ASP:O	1:C:75:ARG:HG3	2.13	0.48
1:G:133:LEU:O	1:H:133:LEU:HD21	2.13	0.48
2:K:177:HOH:O	1:L:73:VAL:HG11	2.13	0.48
1:O:132:ARG:O	1:O:136:GLN:HG2	2.13	0.48
1:Q:140:LYS:HZ2	1:R:137:LEU:HD21	1.78	0.48
1:S:126:ILE:HG12	1:S:129:LEU:HD12	1.95	0.48
1:D:126:ILE:O	1:D:130:ASN:HB2	2.13	0.48
1:J:56:LYS:HD2	1:J:59:TYR:CD2	2.48	0.48
1:O:81:ALA:C	1:O:83:GLU:N	2.69	0.48
1:Q:44:SER:C	1:Q:46:LYS:N	2.70	0.48
1:F:143:LEU:C	1:F:146:THR:HG22	2.39	0.48
1:G:137:LEU:HD22	1:H:137:LEU:HD13	1.96	0.48
1:H:83:GLU:O	1:H:87:ARG:HB2	2.14	0.48
1:E:109:PHE:O	1:E:113:ASN:HB2	2.13	0.48
1:H:73:VAL:O	1:H:77:ARG:HB2	2.14	0.48
1:I:133:LEU:HD11	1:J:130:ASN:OD1	2.13	0.48
1:J:41:THR:O	1:J:44:SER:HB3	2.13	0.48
1:N:91:GLU:O	1:N:95:ASP:HB2	2.14	0.48
1:R:41:THR:HG22	1:R:45:GLN:HE21	1.77	0.48
1:S:94:ALA:O	1:S:97:LEU:HB2	2.13	0.48
1:H:109:PHE:C	1:H:109:PHE:CD2	2.91	0.48
1:M:140:LYS:HD3	1:N:140:LYS:CB	2.38	0.48
1:T:40:LYS:HA	1:T:43:ALA:HB3	1.95	0.48
1:T:92:GLU:O	1:T:96:LYS:HE3	2.13	0.48
1:G:46:LYS:HD2	1:G:46:LYS:O	2.14	0.48
1:G:49:ILE:O	1:G:50:GLU:C	2.57	0.48
1:H:99:LYS:C	1:H:101:VAL:N	2.69	0.48
1:I:124:TYR:O	1:I:128:ILE:HG12	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:37:LYS:C	1:J:39:LEU:H	2.21	0.48
1:L:67:SER:O	1:L:71:ASP:HB2	2.14	0.48
2:O:164:HOH:O	1:P:133:LEU:CD2	2.47	0.48
1:S:52:TYR:OH	1:S:56:LYS:HE3	2.14	0.48
1:S:105:THR:O	1:S:109:PHE:N	2.33	0.48
1:G:72:GLU:OE2	1:H:73:VAL:HG13	2.13	0.48
1:J:45:GLN:HA	1:J:45:GLN:OE1	2.14	0.48
1:K:140:LYS:O	1:K:144:LEU:HD13	2.14	0.48
1:N:43:ALA:C	1:N:45:GLN:N	2.72	0.48
1:T:40:LYS:HA	1:T:43:ALA:CB	2.44	0.48
1:C:80:ILE:HD11	1:D:80:ILE:HD11	1.96	0.47
1:D:98:ASN:C	1:D:100:GLU:H	2.20	0.47
1:E:46:LYS:HD3	1:E:47:ALA:N	2.29	0.47
1:M:42:ILE:C	1:M:44:SER:N	2.70	0.47
1:N:69:ARG:C	1:N:71:ASP:N	2.71	0.47
1:R:68:ASP:O	1:R:71:ASP:HB2	2.14	0.47
1:A:76:LEU:HD21	1:B:77:ARG:HH11	1.77	0.47
1:B:126:ILE:O	1:B:126:ILE:HG22	2.13	0.47
1:B:136:GLN:O	1:B:136:GLN:HG2	2.12	0.47
1:J:119:ALA:O	1:J:121:MSE:N	2.47	0.47
1:L:32:GLU:O	1:L:36:ASN:HB2	2.14	0.47
1:A:79:ASP:C	1:A:81:ALA:N	2.70	0.47
1:D:125:ALA:O	1:D:129:LEU:HB2	2.14	0.47
1:E:141:ASP:CG	1:F:140:LYS:NZ	2.73	0.47
1:F:132:ARG:HD3	1:F:132:ARG:C	2.39	0.47
1:I:76:LEU:HD23	1:I:79:ASP:OD2	2.15	0.47
1:J:60:ASN:O	1:J:64:ARG:HG3	2.14	0.47
1:L:41:THR:O	1:L:45:GLN:HG3	2.13	0.47
1:S:82:LYS:NZ	2:S:166:HOH:O	2.43	0.47
1:A:126:ILE:HG22	1:A:126:ILE:O	2.13	0.47
1:C:80:ILE:HD11	1:D:80:ILE:CD1	2.43	0.47
1:G:115:LEU:CD1	1:H:116:VAL:HG22	2.44	0.47
1:Q:140:LYS:NZ	1:R:137:LEU:HG	2.30	0.47
1:B:72:GLU:O	1:B:76:LEU:HG	2.14	0.47
1:C:147:LEU:HD23	2:D:168:HOH:O	2.14	0.47
1:H:100:GLU:HB2	1:R:39:LEU:HD11	1.96	0.47
1:I:130:ASN:ND2	1:I:130:ASN:N	2.60	0.47
1:J:49:ILE:O	1:J:52:TYR:N	2.48	0.47
1:J:60:ASN:O	1:J:64:ARG:N	2.48	0.47
1:P:41:THR:O	1:P:44:SER:HB3	2.14	0.47
1:S:98:ASN:O	1:S:102:GLU:HG2	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:S:113:ASN:HA	1:S:116:VAL:HG23	1.95	0.47
1:S:130:ASN:OD1	1:T:129:LEU:HD13	2.15	0.47
1:T:46:LYS:C	1:T:48:ALA:H	2.23	0.47
1:A:80:ILE:HG22	1:A:80:ILE:O	2.15	0.47
1:F:88:THR:O	1:F:92:GLU:HG3	2.14	0.47
1:K:80:ILE:HG23	1:K:84:ASN:ND2	2.29	0.47
1:N:87:ARG:NE	2:N:168:HOH:O	2.48	0.47
1:O:39:LEU:HD12	1:O:42:ILE:HD12	1.95	0.47
1:O:41:THR:O	1:O:44:SER:HB3	2.14	0.47
1:Q:81:ALA:HA	1:Q:84:ASN:HB3	1.96	0.47
1:T:37:LYS:C	1:T:40:LYS:H	2.23	0.47
1:B:87:ARG:O	1:B:91:GLU:HG3	2.15	0.47
1:B:124:TYR:O	1:B:127:GLU:N	2.44	0.47
1:C:104:LEU:HD13	1:Q:43:ALA:CA	2.44	0.47
1:D:73:VAL:O	1:D:77:ARG:HG3	2.15	0.47
1:E:55:LEU:HD22	1:F:52:TYR:CZ	2.50	0.47
1:H:66:LEU:O	1:H:70:ASP:N	2.47	0.47
1:I:89:LYS:CG	1:I:90:ALA:N	2.77	0.47
1:K:137:LEU:HD13	2:L:166:HOH:O	2.13	0.47
1:N:104:LEU:HD12	1:N:104:LEU:O	2.15	0.47
1:O:49:ILE:C	1:O:51:ASN:H	2.23	0.47
1:Q:65:GLU:HA	1:Q:68:ASP:OD2	2.14	0.47
1:Q:124:TYR:O	1:Q:128:ILE:HG13	2.15	0.47
1:D:113:ASN:HA	1:R:51:ASN:ND2	2.30	0.47
1:G:43:ALA:C	1:G:45:GLN:H	2.21	0.47
1:H:113:ASN:C	1:H:115:LEU:N	2.72	0.47
1:I:109:PHE:O	1:I:113:ASN:ND2	2.47	0.47
1:O:130:ASN:CG	1:P:130:ASN:ND2	2.66	0.47
1:P:37:LYS:O	1:P:37:LYS:HG2	2.15	0.47
1:S:133:LEU:HD12	1:S:133:LEU:C	2.39	0.47
1:C:101:VAL:HG22	1:Q:39:LEU:HD13	1.97	0.47
1:K:111:GLU:O	1:K:115:LEU:HB2	2.15	0.47
1:L:72:GLU:C	2:L:173:HOH:O	2.57	0.47
1:M:54:GLN:O	1:M:57:GLU:HB3	2.14	0.47
1:P:60:ASN:C	1:P:62:LEU:N	2.71	0.47
1:B:84:ASN:ND2	2:B:168:HOH:O	2.47	0.47
1:C:136:GLN:C	1:D:137:LEU:HD11	2.40	0.47
1:G:126:ILE:HG21	1:H:126:ILE:HG23	1.96	0.47
1:M:52:TYR:CE1	1:N:55:LEU:HD22	2.50	0.47
1:Q:115:LEU:O	1:Q:115:LEU:HD13	2.15	0.47
1:R:40:LYS:HA	1:R:40:LYS:HD2	1.70	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:93:GLU:HG2	1:E:96:LYS:CD	2.39	0.46
1:E:137:LEU:CD2	1:F:137:LEU:HD21	2.45	0.46
1:G:123:LYS:HZ1	1:H:122:GLU:HB3	1.80	0.46
1:I:49:ILE:CA	1:I:52:TYR:HB3	2.41	0.46
1:I:108:LEU:HD21	1:J:105:THR:HG23	1.98	0.46
1:J:86:LEU:O	1:J:90:ALA:HB2	2.15	0.46
1:J:117:ALA:O	1:J:121:MSE:HG2	2.14	0.46
1:K:120:ARG:NH1	1:K:123:LYS:NZ	2.63	0.46
1:N:43:ALA:HA	1:N:46:LYS:HB3	1.98	0.46
1:O:89:LYS:HA	1:O:92:GLU:OE1	2.15	0.46
1:O:144:LEU:HD11	1:P:144:LEU:HD13	1.96	0.46
1:S:140:LYS:O	1:S:140:LYS:HG2	2.16	0.46
1:G:97:LEU:C	2:G:167:HOH:O	2.58	0.46
1:I:51:ASN:O	1:I:55:LEU:HG	2.16	0.46
1:J:97:LEU:O	1:J:101:VAL:N	2.41	0.46
1:M:87:ARG:O	1:M:91:GLU:HB2	2.16	0.46
1:S:46:LYS:HE3	1:S:50:GLU:HB2	1.97	0.46
1:T:74:LYS:O	1:T:78:GLU:N	2.43	0.46
1:E:133:LEU:HD12	1:E:133:LEU:O	2.15	0.46
1:F:65:GLU:O	1:F:69:ARG:HG2	2.15	0.46
1:G:98:ASN:ND2	1:R:34:GLN:HB3	2.30	0.46
1:H:65:GLU:C	1:H:68:ASP:HB3	2.40	0.46
1:K:126:ILE:CD1	1:K:129:LEU:HD12	2.38	0.46
1:M:55:LEU:HD22	1:N:52:TYR:CE1	2.51	0.46
1:P:64:ARG:O	1:P:67:SER:N	2.43	0.46
1:H:111:GLU:O	1:R:49:ILE:HD12	2.16	0.46
1:I:137:LEU:HD13	2:J:165:HOH:O	2.14	0.46
1:L:96:LYS:O	1:L:97:LEU:HD23	2.16	0.46
1:M:89:LYS:O	1:M:93:GLU:HG2	2.16	0.46
1:O:49:ILE:C	1:O:51:ASN:N	2.73	0.46
1:T:118:ASP:O	1:T:121:MSE:HB2	2.15	0.46
1:E:69:ARG:CD	2:E:169:HOH:O	2.60	0.46
1:G:105:THR:OG1	1:H:105:THR:HG23	2.15	0.46
1:I:61:THR:O	1:I:65:GLU:HG3	2.15	0.46
1:S:52:TYR:CD1	1:T:51:ASN:HB3	2.50	0.46
1:T:120:ARG:O	1:T:124:TYR:HD1	1.98	0.46
1:E:95:ASP:O	1:E:99:LYS:CB	2.61	0.46
1:G:80:ILE:HD11	1:H:80:ILE:HD13	1.97	0.46
1:J:56:LYS:O	1:J:59:TYR:HB3	2.16	0.46
1:J:56:LYS:HD2	1:J:59:TYR:HD2	1.80	0.46
1:L:56:LYS:HA	1:L:56:LYS:HD2	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:126:ILE:HG22	1:M:126:ILE:O	2.14	0.46
1:E:146:THR:HG22	1:E:146:THR:O	2.15	0.46
1:R:45:GLN:O	1:R:48:ALA:HB3	2.16	0.46
1:S:47:ALA:HB2	2:S:164:HOH:O	2.15	0.46
1:B:83:GLU:CB	2:B:168:HOH:O	2.64	0.46
1:K:80:ILE:HD11	1:L:80:ILE:CG1	2.36	0.46
1:K:113:ASN:O	1:K:117:ALA:HB2	2.15	0.46
1:S:102:GLU:O	1:S:106:ALA:N	2.46	0.46
1:S:137:LEU:HD11	1:T:140:LYS:HZ2	1.79	0.46
1:T:83:GLU:O	1:T:87:ARG:HG2	2.16	0.46
1:C:115:LEU:C	1:C:117:ALA:H	2.24	0.46
1:E:118:ASP:O	1:E:119:ALA:C	2.59	0.46
1:G:82:LYS:O	1:G:86:LEU:HG	2.16	0.46
1:I:96:LYS:O	1:I:100:GLU:HG2	2.15	0.46
1:Q:108:LEU:C	1:Q:108:LEU:CD2	2.89	0.46
1:S:61:THR:HG22	1:S:65:GLU:OE2	2.16	0.46
1:A:136:GLN:HA	1:A:139:GLU:HB3	1.96	0.46
1:C:140:LYS:C	1:D:140:LYS:HZ1	2.24	0.46
1:E:62:LEU:HD21	1:F:63:LYS:CA	2.46	0.46
1:E:76:LEU:HD11	1:F:77:ARG:HG2	1.97	0.46
1:E:101:VAL:HG23	1:E:102:GLU:N	2.31	0.46
1:G:74:LYS:O	1:G:78:GLU:HG3	2.16	0.46
1:G:118:ASP:O	1:G:122:GLU:HB2	2.17	0.46
1:I:130:ASN:HD21	1:J:126:ILE:CD1	2.24	0.46
1:L:96:LYS:C	1:L:97:LEU:HD23	2.41	0.46
1:N:121:MSE:C	1:N:123:LYS:H	2.23	0.46
1:R:134:THR:O	1:R:138:ARG:HG3	2.14	0.46
1:S:126:ILE:HA	1:S:129:LEU:HB2	1.98	0.46
1:A:39:LEU:HD23	1:A:39:LEU:C	2.41	0.45
1:A:93:GLU:HA	1:A:96:LYS:HB3	1.98	0.45
1:C:49:ILE:HG22	1:C:53:ASN:ND2	2.32	0.45
1:D:132:ARG:HA	1:D:135:GLU:OE1	2.15	0.45
1:G:68:ASP:HA	1:G:71:ASP:HB2	1.97	0.45
1:G:69:ARG:HG3	1:H:69:ARG:O	2.16	0.45
1:G:87:ARG:O	1:G:91:GLU:HG3	2.16	0.45
1:I:140:LYS:CD	1:J:137:LEU:HD22	2.45	0.45
1:K:62:LEU:HD23	1:L:62:LEU:HB2	1.97	0.45
1:K:143:LEU:C	1:K:144:LEU:HD12	2.41	0.45
1:N:60:ASN:O	1:N:64:ARG:HG2	2.16	0.45
1:P:64:ARG:O	1:P:65:GLU:C	2.59	0.45
1:S:96:LYS:O	1:S:100:GLU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:132:ARG:HB3	1:T:136:GLN:CD	2.40	0.45
1:B:151:LEU:HD12	2:B:169:HOH:O	2.17	0.45
1:H:60:ASN:C	1:H:62:LEU:N	2.73	0.45
1:L:124:TYR:HA	1:L:127:GLU:HB3	1.98	0.45
1:M:76:LEU:C	1:M:78:GLU:H	2.24	0.45
1:O:147:LEU:HG	1:O:151:LEU:HD12	1.98	0.45
1:A:80:ILE:O	1:A:84:ASN:HB2	2.16	0.45
1:B:137:LEU:HB3	1:B:141:ASP:OD2	2.17	0.45
1:C:80:ILE:CD1	1:D:80:ILE:HG12	2.47	0.45
1:I:65:GLU:O	1:I:69:ARG:HG3	2.15	0.45
1:O:133:LEU:HD23	1:P:133:LEU:HB3	1.98	0.45
1:Q:87:ARG:HA	1:Q:90:ALA:HB3	1.98	0.45
1:T:111:GLU:C	1:T:113:ASN:N	2.74	0.45
1:C:60:ASN:O	1:C:64:ARG:HG3	2.16	0.45
1:C:122:GLU:HG3	1:Q:63:LYS:NZ	2.31	0.45
1:I:133:LEU:HD22	1:J:130:ASN:HA	1.97	0.45
1:J:124:TYR:HA	1:J:127:GLU:HG2	1.98	0.45
1:J:135:GLU:HG3	1:J:135:GLU:O	2.16	0.45
1:M:58:ASP:O	1:M:62:LEU:HD13	2.16	0.45
1:O:49:ILE:O	1:O:51:ASN:N	2.50	0.45
1:A:80:ILE:N	1:A:80:ILE:CD1	2.79	0.45
1:D:145:ASP:HA	1:D:148:THR:HG22	1.99	0.45
1:E:61:THR:O	1:E:61:THR:HG22	2.17	0.45
1:H:60:ASN:C	1:H:62:LEU:H	2.25	0.45
1:J:112:ALA:O	1:J:116:VAL:HG23	2.16	0.45
1:O:146:THR:HA	1:O:149:LEU:HB3	1.99	0.45
1:P:99:LYS:HA	1:P:102:GLU:HG2	1.97	0.45
1:F:73:VAL:O	1:F:77:ARG:HB2	2.17	0.45
1:H:46:LYS:HG2	1:H:47:ALA:N	2.30	0.45
1:L:95:ASP:C	1:L:97:LEU:H	2.24	0.45
1:A:53:ASN:O	1:A:57:GLU:HB2	2.16	0.45
1:E:144:LEU:CD2	1:F:143:LEU:HD13	2.25	0.45
1:G:69:ARG:N	2:G:162:HOH:O	2.49	0.45
1:G:82:LYS:O	1:G:85:GLU:HB3	2.17	0.45
1:K:120:ARG:NH1	1:K:123:LYS:HZ3	2.15	0.45
1:M:31:LEU:C	1:M:33:GLU:N	2.74	0.45
1:N:121:MSE:C	1:N:123:LYS:N	2.72	0.45
1:S:41:THR:O	1:S:44:SER:HB2	2.17	0.45
1:C:101:VAL:CG2	1:Q:39:LEU:HD13	2.45	0.45
1:E:142:MSE:HA	1:E:145:ASP:HB2	1.98	0.45
1:G:41:THR:O	1:G:45:GLN:HG3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:71:ASP:C	1:N:73:VAL:N	2.74	0.45
1:O:133:LEU:CD2	1:P:133:LEU:HB3	2.47	0.45
1:D:96:LYS:CG	1:D:97:LEU:N	2.80	0.45
1:E:69:ARG:O	1:E:73:VAL:HG23	2.17	0.45
1:G:56:LYS:CG	2:G:171:HOH:O	2.63	0.45
1:H:70:ASP:C	1:H:72:GLU:H	2.23	0.45
1:H:96:LYS:O	1:H:99:LYS:HG2	2.17	0.45
1:I:104:LEU:O	1:I:108:LEU:HB2	2.16	0.45
1:J:45:GLN:O	1:J:49:ILE:N	2.33	0.45
1:J:118:ASP:O	1:J:121:MSE:HB2	2.16	0.45
1:O:32:GLU:HA	1:O:32:GLU:OE1	2.17	0.45
1:S:99:LYS:HA	1:S:102:GLU:CG	2.47	0.45
1:B:146:THR:C	1:B:148:THR:N	2.75	0.45
1:F:101:VAL:O	1:F:102:GLU:C	2.60	0.45
1:G:126:ILE:HG22	1:H:126:ILE:HG12	1.98	0.45
1:G:133:LEU:HG	1:H:133:LEU:CG	2.45	0.45
1:I:44:SER:O	1:I:45:GLN:C	2.60	0.45
1:J:49:ILE:C	1:J:51:ASN:H	2.23	0.45
1:C:90:ALA:O	1:C:94:ALA:HB2	2.17	0.44
1:D:98:ASN:C	1:D:100:GLU:N	2.73	0.44
1:E:151:LEU:HG	1:F:150:GLN:HE22	1.83	0.44
1:F:140:LYS:HG2	1:F:143:LEU:HD12	1.99	0.44
1:G:130:ASN:ND2	1:H:130:ASN:HD21	2.12	0.44
1:G:137:LEU:HD11	1:H:133:LEU:HD11	1.99	0.44
1:I:102:GLU:O	1:I:106:ALA:HB2	2.16	0.44
1:K:92:GLU:C	1:K:94:ALA:N	2.75	0.44
1:N:77:ARG:O	1:N:80:ILE:HB	2.18	0.44
1:O:148:THR:O	1:O:152:LYS:HB2	2.17	0.44
1:S:133:LEU:CD1	1:T:133:LEU:HD13	2.45	0.44
1:T:93:GLU:HA	1:T:96:LYS:CD	2.46	0.44
1:C:55:LEU:C	1:C:57:GLU:N	2.74	0.44
1:C:136:GLN:O	1:C:140:LYS:HD2	2.17	0.44
1:D:117:ALA:O	1:D:121:MSE:CG	2.63	0.44
1:E:115:LEU:HD21	1:F:116:VAL:HG23	2.00	0.44
1:G:42:ILE:O	1:G:45:GLN:HB2	2.17	0.44
1:H:45:GLN:O	1:H:48:ALA:HB3	2.18	0.44
1:H:92:GLU:CG	1:H:93:GLU:N	2.80	0.44
1:H:93:GLU:OE1	1:H:96:LYS:HD3	2.18	0.44
1:I:44:SER:O	1:I:48:ALA:N	2.42	0.44
1:M:54:GLN:C	1:M:57:GLU:HB3	2.42	0.44
1:O:123:LYS:O	1:O:124:TYR:C	2.61	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:ASN:ND2	1:B:130:ASN:ND2	2.64	0.44
1:H:108:LEU:HD13	1:R:46:LYS:CA	2.47	0.44
1:H:122:GLU:CD	1:R:56:LYS:HZ1	2.23	0.44
1:K:52:TYR:CE2	1:K:56:LYS:HE3	2.53	0.44
1:M:74:LYS:HA	2:M:162:HOH:O	2.17	0.44
1:N:137:LEU:O	1:N:141:ASP:OD2	2.34	0.44
1:O:126:ILE:HG22	1:P:126:ILE:CG2	2.44	0.44
1:P:109:PHE:O	1:P:110:ASP:C	2.61	0.44
1:N:62:LEU:O	1:N:63:LYS:C	2.60	0.44
1:N:80:ILE:O	1:N:80:ILE:HG22	2.18	0.44
1:N:135:GLU:O	1:N:139:GLU:N	2.51	0.44
1:B:134:THR:C	1:B:136:GLN:H	2.24	0.44
1:B:146:THR:O	1:B:149:LEU:HB3	2.18	0.44
1:E:147:LEU:HG	1:F:146:THR:HG23	1.99	0.44
1:F:66:LEU:HG	1:F:66:LEU:O	2.18	0.44
1:P:130:ASN:N	1:P:130:ASN:HD22	2.16	0.44
1:Q:134:THR:O	1:Q:138:ARG:CG	2.66	0.44
1:S:42:ILE:C	1:S:44:SER:N	2.75	0.44
1:S:43:ALA:HB1	2:S:165:HOH:O	2.16	0.44
1:A:116:VAL:O	1:A:120:ARG:HG2	2.17	0.44
1:G:133:LEU:HB3	1:H:133:LEU:HD21	2.00	0.44
1:P:31:LEU:HD23	1:P:34:GLN:NE2	2.32	0.44
1:R:120:ARG:C	1:R:122:GLU:H	2.26	0.44
1:I:73:VAL:O	1:I:73:VAL:HG12	2.17	0.44
1:I:123:LYS:O	1:I:127:GLU:CB	2.64	0.44
1:K:87:ARG:C	1:K:89:LYS:H	2.26	0.44
1:L:124:TYR:O	1:L:128:ILE:HG22	2.17	0.44
1:P:112:ALA:O	1:P:116:VAL:HG13	2.18	0.44
1:Q:132:ARG:O	1:Q:136:GLN:HG3	2.18	0.44
1:R:108:LEU:O	1:R:112:ALA:CB	2.65	0.44
1:C:116:VAL:HG12	1:C:116:VAL:O	2.17	0.44
1:D:53:ASN:N	1:D:53:ASN:HD22	2.15	0.44
1:F:47:ALA:O	1:F:48:ALA:C	2.61	0.44
1:I:43:ALA:O	1:I:47:ALA:HB2	2.18	0.44
1:I:62:LEU:HD11	1:J:59:TYR:CE1	2.53	0.44
1:J:56:LYS:CE	2:J:164:HOH:O	2.65	0.44
1:K:99:LYS:HD3	1:K:102:GLU:OE2	2.17	0.44
1:L:83:GLU:C	1:L:85:GLU:N	2.74	0.44
1:M:38:SER:O	1:M:42:ILE:HG13	2.17	0.44
1:N:71:ASP:C	1:N:73:VAL:H	2.25	0.44
1:N:87:ARG:CZ	2:N:168:HOH:O	2.66	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:135:GLU:HA	1:P:138:ARG:CG	2.48	0.44
1:S:92:GLU:HG3	1:S:93:GLU:N	2.33	0.44
1:F:49:ILE:O	1:F:50:GLU:C	2.61	0.44
1:I:97:LEU:HA	1:I:100:GLU:CG	2.48	0.44
1:L:50:GLU:HG2	1:L:54:GLN:NE2	2.32	0.44
1:M:108:LEU:HD23	1:N:108:LEU:HD23	1.99	0.44
1:Q:54:GLN:HG3	1:Q:55:LEU:H	1.79	0.44
1:Q:66:LEU:HD12	1:R:66:LEU:HD23	1.98	0.44
1:Q:140:LYS:HD2	1:R:137:LEU:HD11	2.00	0.44
1:S:42:ILE:C	1:S:44:SER:H	2.25	0.44
1:B:69:ARG:CD	2:B:161:HOH:O	2.66	0.43
1:D:130:ASN:ND2	2:D:162:HOH:O	2.50	0.43
1:E:120:ARG:NH1	1:E:123:LYS:HD2	2.33	0.43
1:I:126:ILE:HG21	1:J:126:ILE:HG21	1.95	0.43
1:J:120:ARG:HH12	1:J:123:LYS:HZ2	1.66	0.43
1:M:85:GLU:HA	1:M:88:THR:OG1	2.18	0.43
1:O:148:THR:HA	1:O:151:LEU:HB2	2.00	0.43
1:T:52:TYR:O	1:T:53:ASN:C	2.60	0.43
1:A:31:LEU:O	1:A:35:LEU:HB2	2.18	0.43
1:B:56:LYS:HA	1:B:59:TYR:HB3	2.00	0.43
1:C:52:TYR:O	1:C:56:LYS:HB2	2.18	0.43
1:I:53:ASN:O	1:I:57:GLU:N	2.46	0.43
1:I:88:THR:HG22	1:I:92:GLU:OE1	2.18	0.43
1:M:140:LYS:HE3	1:M:140:LYS:HB2	1.85	0.43
1:O:128:ILE:O	1:O:128:ILE:CG2	2.64	0.43
1:P:76:LEU:C	1:P:78:GLU:H	2.26	0.43
1:P:132:ARG:O	1:P:132:ARG:HG2	2.18	0.43
1:S:38:SER:HA	1:S:41:THR:HG23	1.99	0.43
1:G:98:ASN:HD21	1:R:34:GLN:HB3	1.84	0.43
1:H:46:LYS:C	1:H:48:ALA:N	2.73	0.43
1:I:48:ALA:O	1:I:52:TYR:N	2.49	0.43
1:K:71:ASP:O	1:K:72:GLU:C	2.61	0.43
1:L:66:LEU:C	1:L:68:ASP:N	2.76	0.43
1:Q:51:ASN:O	1:Q:54:GLN:HG3	2.18	0.43
1:S:72:GLU:HB3	2:S:169:HOH:O	2.18	0.43
1:T:65:GLU:O	1:T:69:ARG:HG2	2.17	0.43
1:G:33:GLU:HG3	2:G:168:HOH:O	2.17	0.43
1:I:47:ALA:C	1:I:50:GLU:HG2	2.43	0.43
1:J:50:GLU:CA	1:J:53:ASN:HB2	2.36	0.43
1:T:137:LEU:N	1:T:137:LEU:HD23	2.34	0.43
1:B:134:THR:C	1:B:136:GLN:N	2.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:130:ASN:HD22	1:E:130:ASN:HA	1.59	0.43
1:F:136:GLN:O	1:F:136:GLN:HG3	2.18	0.43
1:J:122:GLU:O	1:J:125:ALA:HB3	2.17	0.43
1:K:111:GLU:C	1:K:113:ASN:H	2.24	0.43
1:K:120:ARG:HD3	1:K:120:ARG:HA	1.81	0.43
1:L:78:GLU:O	1:L:80:ILE:N	2.51	0.43
1:N:69:ARG:C	1:N:71:ASP:H	2.25	0.43
1:P:107:SER:O	1:P:111:GLU:HG2	2.19	0.43
1:P:113:ASN:HA	1:P:116:VAL:CG2	2.48	0.43
1:T:72:GLU:O	1:T:73:VAL:C	2.60	0.43
1:E:62:LEU:HD21	1:F:63:LYS:HB2	1.99	0.43
1:F:130:ASN:N	1:F:130:ASN:HD22	2.16	0.43
1:J:127:GLU:O	1:J:131:LYS:HG3	2.18	0.43
1:J:130:ASN:O	1:J:134:THR:HG23	2.18	0.43
1:K:55:LEU:CD2	1:L:55:LEU:HD23	2.44	0.43
1:M:76:LEU:C	1:M:78:GLU:N	2.76	0.43
1:S:72:GLU:CA	1:S:75:ARG:HB2	2.45	0.43
1:S:137:LEU:HD22	1:T:137:LEU:CD2	2.46	0.43
1:B:115:LEU:O	1:B:119:ALA:HB2	2.19	0.43
1:F:129:LEU:O	1:F:133:LEU:HB2	2.19	0.43
1:G:99:LYS:O	1:G:100:GLU:C	2.62	0.43
1:O:81:ALA:O	1:O:83:GLU:N	2.52	0.43
1:O:112:ALA:O	1:O:113:ASN:C	2.61	0.43
1:O:130:ASN:ND2	1:P:126:ILE:HG23	2.32	0.43
1:Q:130:ASN:OD1	1:Q:133:LEU:HD23	2.19	0.43
1:R:127:GLU:OE1	1:R:127:GLU:N	2.49	0.43
1:G:82:LYS:C	1:G:85:GLU:HB3	2.44	0.43
1:H:74:LYS:O	1:H:78:GLU:HG3	2.18	0.43
1:J:45:GLN:C	1:J:47:ALA:N	2.73	0.43
1:J:129:LEU:CD1	1:J:133:LEU:HD22	2.42	0.43
1:K:144:LEU:HG	1:L:144:LEU:CG	2.48	0.43
1:K:144:LEU:HG	1:L:144:LEU:HG	2.01	0.43
1:M:126:ILE:HG22	1:N:126:ILE:HG21	2.01	0.43
2:M:174:HOH:O	1:N:76:LEU:CD1	2.57	0.43
1:N:135:GLU:O	1:N:139:GLU:HG3	2.18	0.43
1:Q:66:LEU:HA	1:R:66:LEU:CD2	2.49	0.43
1:Q:76:LEU:HD11	1:R:77:ARG:CZ	2.49	0.43
1:R:56:LYS:HG3	1:R:56:LYS:O	2.19	0.43
1:B:53:ASN:C	1:B:55:LEU:H	2.27	0.43
1:B:62:LEU:O	1:B:64:ARG:N	2.52	0.43
1:C:45:GLN:O	1:C:49:ILE:HG13	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:66:LEU:O	1:I:70:ASP:N	2.47	0.43
1:I:106:ALA:O	1:I:109:PHE:HB3	2.19	0.43
1:J:53:ASN:O	1:J:54:GLN:C	2.62	0.43
1:L:118:ASP:OD1	1:L:118:ASP:C	2.62	0.43
1:M:55:LEU:HD23	1:N:55:LEU:HD23	2.00	0.43
1:M:80:ILE:HD11	1:N:80:ILE:CG1	2.49	0.43
1:R:46:LYS:HD3	1:R:46:LYS:C	2.44	0.43
1:C:115:LEU:HD23	1:C:116:VAL:N	2.33	0.43
1:E:93:GLU:HA	1:E:96:LYS:HG3	2.00	0.43
1:H:36:ASN:HB3	2:H:164:HOH:O	2.18	0.43
1:P:60:ASN:O	1:P:64:ARG:HG3	2.18	0.43
1:S:118:ASP:O	1:S:121:MSE:HB2	2.18	0.43
1:T:132:ARG:O	1:T:136:GLN:HG3	2.19	0.43
1:A:74:LYS:O	1:A:78:GLU:HG3	2.19	0.42
1:F:39:LEU:O	1:F:42:ILE:N	2.52	0.42
1:F:115:LEU:C	1:F:117:ALA:N	2.76	0.42
1:G:133:LEU:CG	1:H:133:LEU:HG	2.44	0.42
1:H:104:LEU:CD1	1:R:43:ALA:HB2	2.49	0.42
1:I:32:GLU:C	1:I:34:GLN:N	2.76	0.42
1:S:38:SER:HA	1:S:41:THR:CG2	2.49	0.42
1:A:66:LEU:HD12	1:B:69:ARG:HG3	2.00	0.42
1:E:102:GLU:HA	1:E:105:THR:OG1	2.20	0.42
1:E:108:LEU:CD2	1:F:108:LEU:HD23	2.49	0.42
1:E:141:ASP:CG	1:F:140:LYS:HZ3	2.27	0.42
1:F:69:ARG:HA	1:F:69:ARG:HD3	1.82	0.42
1:G:102:GLU:HB2	1:R:38:SER:OG	2.18	0.42
1:H:65:GLU:HA	1:H:68:ASP:CB	2.49	0.42
1:J:65:GLU:HA	1:J:68:ASP:CB	2.47	0.42
1:B:53:ASN:C	1:B:55:LEU:N	2.76	0.42
1:C:80:ILE:HD11	1:D:80:ILE:CG1	2.49	0.42
1:C:83:GLU:O	1:C:83:GLU:HG2	2.19	0.42
1:D:31:LEU:O	1:D:35:LEU:HG	2.20	0.42
1:E:133:LEU:HD12	1:E:137:LEU:HD12	1.99	0.42
1:I:122:GLU:CG	1:J:123:LYS:HE2	2.37	0.42
1:J:126:ILE:O	1:J:129:LEU:N	2.52	0.42
1:P:135:GLU:HA	1:P:138:ARG:CD	2.49	0.42
1:Q:81:ALA:O	1:Q:85:GLU:N	2.53	0.42
1:R:93:GLU:O	1:R:93:GLU:HG2	2.19	0.42
1:S:97:LEU:HA	1:S:100:GLU:HB3	2.00	0.42
1:S:126:ILE:CG2	1:T:126:ILE:HD13	2.50	0.42
1:B:59:TYR:HD2	1:B:60:ASN:ND2	2.16	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:122:GLU:HG3	1:Q:63:LYS:HZ1	1.84	0.42
1:D:109:PHE:C	1:D:111:GLU:N	2.78	0.42
1:F:61:THR:O	1:F:65:GLU:HG3	2.19	0.42
1:G:72:GLU:OE2	1:H:73:VAL:HG22	2.19	0.42
1:L:46:LYS:O	1:L:46:LYS:HG2	2.20	0.42
1:C:72:GLU:HG2	1:D:73:VAL:CG1	2.49	0.42
1:F:46:LYS:O	1:F:50:GLU:HG3	2.20	0.42
1:F:134:THR:C	1:F:136:GLN:H	2.26	0.42
1:J:111:GLU:HG2	1:J:112:ALA:H	1.79	0.42
1:K:133:LEU:HD22	1:L:137:LEU:HD12	2.00	0.42
1:S:122:GLU:O	1:S:126:ILE:HG13	2.20	0.42
1:G:120:ARG:HH12	1:Q:58:ASP:CG	2.28	0.42
1:L:62:LEU:O	1:L:66:LEU:N	2.49	0.42
1:M:134:THR:O	1:M:138:ARG:N	2.52	0.42
1:O:147:LEU:HG	1:O:151:LEU:CD1	2.49	0.42
1:T:38:SER:O	1:T:42:ILE:HD12	2.20	0.42
1:F:118:ASP:O	1:F:119:ALA:C	2.61	0.42
1:H:49:ILE:C	1:H:51:ASN:N	2.74	0.42
1:H:89:LYS:C	1:H:92:GLU:HG2	2.45	0.42
1:H:99:LYS:C	1:H:101:VAL:H	2.28	0.42
1:I:55:LEU:HD11	1:J:52:TYR:CE1	2.55	0.42
1:J:87:ARG:O	1:J:91:GLU:HG3	2.20	0.42
1:K:123:LYS:O	1:K:127:GLU:HB2	2.19	0.42
1:N:131:LYS:O	1:N:135:GLU:HG3	2.20	0.42
1:S:54:GLN:O	1:S:58:ASP:OD2	2.38	0.42
1:T:33:GLU:O	1:T:37:LYS:N	2.50	0.42
1:E:126:ILE:HG22	1:F:126:ILE:CG2	2.49	0.42
1:E:128:ILE:CD1	1:E:131:LYS:HD2	2.41	0.42
1:F:72:GLU:O	1:F:76:LEU:HG	2.20	0.42
1:F:150:GLN:O	1:F:151:LEU:HD23	2.20	0.42
1:K:141:ASP:OD1	1:L:140:LYS:CE	2.66	0.42
1:O:73:VAL:HG23	1:P:73:VAL:HG23	2.02	0.42
1:E:62:LEU:HD21	1:F:63:LYS:CB	2.50	0.42
1:E:93:GLU:CG	1:E:96:LYS:HD2	2.42	0.42
1:G:56:LYS:HA	1:H:55:LEU:HD21	2.02	0.42
1:G:130:ASN:HB3	1:H:129:LEU:CD2	2.50	0.42
1:I:66:LEU:O	1:I:70:ASP:HB2	2.20	0.42
1:J:108:LEU:O	1:J:109:PHE:C	2.62	0.42
1:K:66:LEU:HA	1:L:66:LEU:CD1	2.49	0.42
1:L:97:LEU:O	1:L:101:VAL:HG23	2.19	0.42
1:M:132:ARG:HB2	2:M:163:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:138:ARG:O	1:M:142:MSE:N	2.48	0.42
1:Q:76:LEU:HD11	1:R:77:ARG:NE	2.34	0.42
1:A:144:LEU:HD13	2:A:176:HOH:O	2.19	0.42
1:A:144:LEU:HB2	2:A:176:HOH:O	2.20	0.42
1:G:87:ARG:HD2	1:H:87:ARG:HE	1.85	0.42
1:I:103:ASP:O	1:I:104:LEU:C	2.62	0.42
1:K:125:ALA:O	1:K:129:LEU:HG	2.20	0.42
1:O:56:LYS:O	1:O:56:LYS:HG3	2.19	0.42
1:O:84:ASN:O	1:O:88:THR:N	2.53	0.42
1:R:120:ARG:C	1:R:122:GLU:N	2.77	0.42
1:S:103:ASP:O	1:S:107:SER:N	2.46	0.42
1:I:93:GLU:C	1:I:95:ASP:N	2.75	0.41
1:K:137:LEU:CD2	2:L:166:HOH:O	2.66	0.41
1:L:96:LYS:O	1:L:96:LYS:HG2	2.20	0.41
1:M:87:ARG:HA	1:M:90:ALA:HB3	2.01	0.41
1:P:31:LEU:CD2	1:P:34:GLN:NE2	2.82	0.41
1:P:73:VAL:O	1:P:73:VAL:HG12	2.19	0.41
1:Q:77:ARG:HH21	1:R:72:GLU:CD	2.28	0.41
1:R:92:GLU:HG3	1:R:93:GLU:N	2.35	0.41
1:T:61:THR:HA	1:T:64:ARG:NE	2.34	0.41
1:T:74:LYS:O	1:T:78:GLU:HG3	2.20	0.41
1:T:75:ARG:O	1:T:78:GLU:HB2	2.20	0.41
1:T:110:ASP:O	1:T:113:ASN:HB3	2.20	0.41
1:A:65:GLU:C	1:A:67:SER:N	2.77	0.41
1:B:61:THR:O	1:B:61:THR:HG22	2.20	0.41
1:C:126:ILE:HG23	2:Q:162:HOH:O	2.20	0.41
1:D:78:GLU:C	1:D:80:ILE:N	2.77	0.41
1:D:98:ASN:ND2	1:Q:35:LEU:HD12	2.33	0.41
1:F:31:LEU:N	2:F:169:HOH:O	2.52	0.41
1:L:83:GLU:O	1:L:87:ARG:N	2.52	0.41
1:O:62:LEU:HB3	1:P:62:LEU:CD1	2.49	0.41
1:O:133:LEU:HD23	1:P:133:LEU:HD23	2.01	0.41
1:O:147:LEU:O	1:O:151:LEU:HG	2.19	0.41
1:P:58:ASP:C	1:P:60:ASN:N	2.77	0.41
1:S:126:ILE:HA	1:S:129:LEU:HG	2.02	0.41
1:A:111:GLU:O	1:A:115:LEU:HB2	2.21	0.41
1:D:103:ASP:CG	1:D:104:LEU:N	2.78	0.41
1:D:145:ASP:O	1:D:149:LEU:HB2	2.20	0.41
1:E:46:LYS:NZ	2:E:170:HOH:O	2.51	0.41
1:H:113:ASN:O	1:H:116:VAL:N	2.53	0.41
1:I:99:LYS:HA	1:I:102:GLU:CB	2.42	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:66:LEU:HD13	1:L:66:LEU:HA	2.01	0.41
1:L:56:LYS:HE3	1:L:59:TYR:CE2	2.56	0.41
1:P:120:ARG:HH21	1:P:123:LYS:NZ	2.17	0.41
1:Q:80:ILE:HG12	1:R:80:ILE:HG12	2.02	0.41
1:R:99:LYS:HG3	1:R:100:GLU:N	2.34	0.41
1:R:99:LYS:O	1:R:102:GLU:HB3	2.21	0.41
1:S:38:SER:O	1:S:42:ILE:HG13	2.21	0.41
1:S:137:LEU:HB2	1:T:137:LEU:HD21	2.02	0.41
1:D:98:ASN:O	1:D:101:VAL:N	2.44	0.41
1:I:100:GLU:O	1:I:103:ASP:HB3	2.21	0.41
1:O:60:ASN:HB3	1:O:64:ARG:CZ	2.50	0.41
1:P:62:LEU:HD13	1:P:62:LEU:O	2.20	0.41
1:R:66:LEU:HD23	1:R:66:LEU:HA	1.92	0.41
1:C:66:LEU:O	1:C:70:ASP:CG	2.63	0.41
1:E:128:ILE:HD13	1:E:128:ILE:HA	1.91	0.41
1:F:101:VAL:C	1:F:103:ASP:N	2.76	0.41
1:F:131:LYS:C	1:F:133:LEU:H	2.27	0.41
1:F:136:GLN:O	1:F:137:LEU:HD23	2.20	0.41
1:G:115:LEU:C	1:G:117:ALA:N	2.77	0.41
1:H:90:ALA:C	1:H:92:GLU:N	2.76	0.41
1:H:108:LEU:CD1	1:R:46:LYS:HA	2.50	0.41
1:I:50:GLU:O	1:I:54:GLN:N	2.53	0.41
1:I:140:LYS:HZ1	1:J:137:LEU:HD13	1.85	0.41
1:L:73:VAL:CA	2:L:173:HOH:O	2.69	0.41
1:M:47:ALA:O	1:M:50:GLU:N	2.54	0.41
1:P:49:ILE:CG2	1:P:50:GLU:N	2.83	0.41
1:R:88:THR:O	1:R:88:THR:HG22	2.19	0.41
1:S:103:ASP:C	1:S:105:THR:H	2.27	0.41
1:C:89:LYS:O	1:C:93:GLU:HG2	2.20	0.41
1:E:136:GLN:NE2	2:E:171:HOH:O	2.52	0.41
1:E:137:LEU:C	1:E:139:GLU:H	2.27	0.41
1:J:56:LYS:HA	1:J:59:TYR:HB3	2.02	0.41
1:J:129:LEU:O	1:J:130:ASN:C	2.63	0.41
1:K:90:ALA:C	1:K:92:GLU:N	2.77	0.41
1:L:111:GLU:HA	1:L:114:ASN:HD22	1.86	0.41
1:P:49:ILE:HG12	1:P:53:ASN:ND2	2.28	0.41
1:Q:41:THR:O	1:Q:45:GLN:HG3	2.20	0.41
1:Q:46:LYS:HD2	1:Q:46:LYS:C	2.46	0.41
1:Q:56:LYS:O	1:Q:56:LYS:HG3	2.21	0.41
1:Q:133:LEU:HG	1:Q:134:THR:N	2.34	0.41
1:S:86:LEU:O	1:S:89:LYS:HE2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:LEU:HD22	1:B:144:LEU:CD2	2.48	0.41
1:E:87:ARG:NE	1:F:87:ARG:HG3	2.36	0.41
1:G:45:GLN:O	1:G:48:ALA:HB3	2.21	0.41
1:G:82:LYS:CA	1:G:85:GLU:HB3	2.51	0.41
1:G:89:LYS:O	1:G:92:GLU:HB3	2.21	0.41
1:H:90:ALA:O	1:H:94:ALA:CB	2.68	0.41
1:H:106:ALA:C	1:H:108:LEU:N	2.77	0.41
1:J:100:GLU:O	1:J:104:LEU:HG	2.21	0.41
1:O:146:THR:O	1:O:150:GLN:HG3	2.20	0.41
1:T:115:LEU:HD23	1:T:115:LEU:HA	1.90	0.41
1:F:133:LEU:HD12	1:F:133:LEU:HA	1.91	0.41
1:F:148:THR:O	1:F:152:LYS:HB2	2.19	0.41
1:G:69:ARG:HH11	1:H:73:VAL:HG21	1.85	0.41
1:J:71:ASP:O	1:J:75:ARG:N	2.54	0.41
1:J:119:ALA:O	1:J:120:ARG:C	2.62	0.41
1:J:126:ILE:C	1:J:128:ILE:N	2.79	0.41
1:K:140:LYS:O	1:K:140:LYS:CG	2.67	0.41
1:L:68:ASP:HA	1:L:71:ASP:CB	2.50	0.41
1:N:32:GLU:O	1:N:34:GLN:N	2.54	0.41
1:O:140:LYS:NZ	1:P:141:ASP:OD2	2.54	0.41
1:P:58:ASP:C	1:P:60:ASN:H	2.28	0.41
1:Q:44:SER:O	1:Q:45:GLN:C	2.62	0.41
1:Q:120:ARG:HA	1:Q:120:ARG:HD2	1.78	0.41
1:Q:140:LYS:HZ2	1:R:137:LEU:CD2	2.32	0.41
1:R:132:ARG:HA	1:R:135:GLU:HG2	2.03	0.41
1:S:55:LEU:O	1:S:59:TYR:N	2.50	0.41
1:T:70:ASP:O	1:T:71:ASP:C	2.63	0.41
1:A:80:ILE:O	1:A:80:ILE:CG2	2.69	0.41
1:A:95:ASP:C	1:A:97:LEU:H	2.28	0.41
1:B:94:ALA:O	1:B:98:ASN:HB2	2.21	0.41
1:B:118:ASP:OD1	1:B:118:ASP:C	2.64	0.41
1:D:45:GLN:HA	1:D:48:ALA:CB	2.51	0.41
1:E:86:LEU:C	1:E:88:THR:N	2.76	0.41
1:F:51:ASN:ND2	2:F:161:HOH:O	2.54	0.41
1:I:103:ASP:O	1:I:106:ALA:N	2.54	0.41
1:I:123:LYS:O	1:I:127:GLU:N	2.54	0.41
1:J:115:LEU:CA	1:J:118:ASP:HB3	2.50	0.41
1:K:68:ASP:C	1:K:70:ASP:H	2.28	0.41
1:K:118:ASP:HA	1:K:121:MSE:HB2	2.02	0.41
1:K:120:ARG:NH1	1:K:123:LYS:HD2	2.35	0.41
1:L:31:LEU:C	1:L:33:GLU:N	2.78	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:31:LEU:C	1:L:33:GLU:H	2.28	0.41
1:L:60:ASN:O	1:L:64:ARG:HG2	2.21	0.41
1:M:119:ALA:C	1:M:121:MSE:N	2.77	0.41
1:O:125:ALA:O	1:O:129:LEU:HG	2.21	0.41
1:P:113:ASN:CA	1:P:116:VAL:HG22	2.49	0.41
1:Q:101:VAL:O	1:Q:105:THR:CB	2.68	0.41
1:R:128:ILE:O	1:R:128:ILE:HG22	2.21	0.41
1:T:43:ALA:O	1:T:46:LYS:HG3	2.20	0.41
1:F:53:ASN:O	1:F:54:GLN:C	2.62	0.41
1:M:47:ALA:HA	1:M:50:GLU:CB	2.51	0.41
1:M:62:LEU:O	1:M:64:ARG:N	2.54	0.41
1:M:65:GLU:O	1:M:68:ASP:HB2	2.21	0.41
1:N:36:ASN:O	1:N:37:LYS:C	2.64	0.41
1:P:60:ASN:O	1:P:61:THR:C	2.63	0.41
1:S:33:GLU:OE2	1:S:37:LYS:HB2	2.21	0.41
1:S:64:ARG:O	1:S:68:ASP:N	2.54	0.41
1:S:137:LEU:HD11	1:T:140:LYS:HZ3	1.87	0.41
1:A:49:ILE:HG22	1:A:53:ASN:HD22	1.86	0.40
1:E:94:ALA:CA	2:E:175:HOH:O	2.64	0.40
1:F:105:THR:OG1	1:F:106:ALA:N	2.54	0.40
1:I:137:LEU:HD22	1:J:133:LEU:O	2.21	0.40
1:J:47:ALA:HB1	2:J:161:HOH:O	2.21	0.40
1:K:83:GLU:CG	1:L:87:ARG:NH1	2.82	0.40
1:M:73:VAL:O	1:M:77:ARG:CB	2.69	0.40
1:N:92:GLU:O	1:N:95:ASP:HB3	2.22	0.40
1:Q:56:LYS:HB2	1:R:55:LEU:HD21	2.03	0.40
1:Q:101:VAL:O	1:Q:105:THR:HB	2.20	0.40
1:R:116:VAL:O	1:R:120:ARG:HG3	2.21	0.40
1:A:72:GLU:OE1	1:B:73:VAL:HG11	2.22	0.40
1:B:51:ASN:HA	1:B:54:GLN:HB2	2.03	0.40
1:C:140:LYS:C	1:D:140:LYS:HE2	2.46	0.40
1:M:89:LYS:C	1:M:91:GLU:N	2.79	0.40
1:O:126:ILE:O	1:O:126:ILE:CG2	2.68	0.40
1:P:41:THR:O	1:P:45:GLN:HG3	2.21	0.40
1:P:64:ARG:C	1:P:66:LEU:N	2.79	0.40
1:P:76:LEU:C	1:P:78:GLU:N	2.78	0.40
1:B:32:GLU:OE1	1:B:32:GLU:HA	2.22	0.40
1:C:59:TYR:CE1	1:D:62:LEU:HD12	2.56	0.40
1:C:129:LEU:C	2:D:162:HOH:O	2.65	0.40
1:D:142:MSE:O	1:D:146:THR:N	2.55	0.40
1:E:66:LEU:HA	1:F:66:LEU:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:80:ILE:O	1:K:84:ASN:HB2	2.21	0.40
1:L:125:ALA:C	1:L:126:ILE:HD12	2.47	0.40
1:R:102:GLU:O	1:R:106:ALA:CB	2.70	0.40
1:T:128:ILE:HA	1:T:131:LYS:HD2	2.02	0.40
1:B:43:ALA:O	1:B:46:LYS:N	2.54	0.40
1:B:66:LEU:C	1:B:68:ASP:H	2.29	0.40
1:D:61:THR:O	1:D:64:ARG:HB2	2.22	0.40
1:D:83:GLU:O	1:D:87:ARG:HB2	2.21	0.40
1:E:34:GLN:O	1:E:38:SER:HB2	2.21	0.40
1:G:116:VAL:CG1	1:Q:51:ASN:HB3	2.43	0.40
1:H:85:GLU:C	1:H:87:ARG:H	2.28	0.40
1:N:49:ILE:H	1:N:49:ILE:HG13	1.75	0.40
1:N:102:GLU:O	1:N:103:ASP:C	2.63	0.40
1:O:71:ASP:O	1:O:74:LYS:HB3	2.21	0.40
1:Q:126:ILE:CG2	1:R:126:ILE:HG23	2.50	0.40
1:Q:133:LEU:HB2	1:R:133:LEU:CD2	2.47	0.40
1:S:124:TYR:O	1:S:128:ILE:HG13	2.21	0.40
1:D:53:ASN:N	1:D:53:ASN:ND2	2.70	0.40
1:G:65:GLU:O	1:G:69:ARG:HB2	2.22	0.40
1:G:130:ASN:HD21	1:H:130:ASN:CG	2.26	0.40
1:I:140:LYS:NZ	1:J:137:LEU:HD13	2.36	0.40
1:J:134:THR:C	1:J:136:GLN:N	2.79	0.40
1:K:120:ARG:HH11	1:K:123:LYS:CD	2.34	0.40
1:M:132:ARG:O	1:M:136:GLN:HG2	2.21	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	112/135 (83%)	102 (91%)	10 (9%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	119/135 (88%)	105 (88%)	11 (9%)	3 (2%)	4	23
1	C	116/135 (86%)	105 (90%)	11 (10%)	0	100	100
1	D	122/135 (90%)	108 (88%)	12 (10%)	2 (2%)	7	34
1	E	122/135 (90%)	112 (92%)	7 (6%)	3 (2%)	4	23
1	F	122/135 (90%)	107 (88%)	12 (10%)	3 (2%)	4	23
1	G	108/135 (80%)	89 (82%)	18 (17%)	1 (1%)	14	48
1	H	105/135 (78%)	80 (76%)	23 (22%)	2 (2%)	6	30
1	I	112/135 (83%)	96 (86%)	16 (14%)	0	100	100
1	J	105/135 (78%)	86 (82%)	14 (13%)	5 (5%)	2	11
1	K	115/135 (85%)	97 (84%)	17 (15%)	1 (1%)	14	48
1	L	112/135 (83%)	102 (91%)	10 (9%)	0	100	100
1	M	115/135 (85%)	105 (91%)	8 (7%)	2 (2%)	7	32
1	N	109/135 (81%)	88 (81%)	18 (16%)	3 (3%)	4	21
1	O	122/135 (90%)	106 (87%)	12 (10%)	4 (3%)	3	17
1	P	112/135 (83%)	104 (93%)	8 (7%)	0	100	100
1	Q	109/135 (81%)	96 (88%)	12 (11%)	1 (1%)	14	48
1	R	109/135 (81%)	97 (89%)	11 (10%)	1 (1%)	14	48
1	S	115/135 (85%)	102 (89%)	11 (10%)	2 (2%)	7	32
1	T	112/135 (83%)	94 (84%)	16 (14%)	2 (2%)	6	31
All	All	2273/2700 (84%)	1981 (87%)	257 (11%)	35 (2%)	8	35

All (35) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	32	GLU
1	O	113	ASN
1	T	52	TYR
1	D	104	LEU
1	E	119	ALA
1	H	33	GLU
1	S	112	ALA
1	S	119	ALA
1	B	46	LYS
1	B	63	LYS
1	F	50	GLU

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Mol	Chain	Res	Type
1	F	53	ASN
1	F	121	MSE
1	J	48	ALA
1	J	49	ILE
1	N	33	GLU
1	O	50	GLU
1	O	112	ALA
1	T	47	ALA
1	E	118	ASP
1	G	122	GLU
1	Q	122	GLU
1	E	75	ARG
1	J	47	ALA
1	J	120	ARG
1	M	63	LYS
1	N	40	LYS
1	N	102	GLU
1	R	53	ASN
1	B	110	ASP
1	H	101	VAL
1	J	53	ASN
1	K	104	LEU
1	O	82	LYS
1	M	80	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	103/120 (86%)	102 (99%)	1 (1%)	68	84
1	B	110/120 (92%)	103 (94%)	7 (6%)	16	48
1	C	107/120 (89%)	105 (98%)	2 (2%)	50	76
1	D	113/120 (94%)	110 (97%)	3 (3%)	39	71
1	E	113/120 (94%)	104 (92%)	9 (8%)	11	38

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	113/120 (94%)	110 (97%)	3 (3%)	39	71
1	G	99/120 (82%)	95 (96%)	4 (4%)	28	62
1	H	96/120 (80%)	93 (97%)	3 (3%)	35	68
1	I	103/120 (86%)	97 (94%)	6 (6%)	18	51
1	J	96/120 (80%)	93 (97%)	3 (3%)	35	68
1	K	106/120 (88%)	104 (98%)	2 (2%)	50	76
1	L	103/120 (86%)	98 (95%)	5 (5%)	22	56
1	M	106/120 (88%)	100 (94%)	6 (6%)	18	52
1	N	100/120 (83%)	96 (96%)	4 (4%)	28	62
1	O	113/120 (94%)	103 (91%)	10 (9%)	9	35
1	P	103/120 (86%)	102 (99%)	1 (1%)	68	84
1	Q	100/120 (83%)	96 (96%)	4 (4%)	28	62
1	R	100/120 (83%)	96 (96%)	4 (4%)	28	62
1	S	106/120 (88%)	103 (97%)	3 (3%)	38	70
1	T	103/120 (86%)	97 (94%)	6 (6%)	18	51
All	All	2093/2400 (87%)	2007 (96%)	86 (4%)	27	61

All (86) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	54	GLN
1	B	40	LYS
1	B	70	ASP
1	B	78	GLU
1	B	103	ASP
1	B	113	ASN
1	B	121	MSE
1	B	122	GLU
1	C	72	GLU
1	C	130	ASN
1	D	103	ASP
1	D	118	ASP
1	D	126	ILE
1	E	71	ASP
1	E	102	GLU
1	E	105	THR
1	E	107	SER

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Mol	Chain	Res	Type
1	E	122	GLU
1	E	128	ILE
1	E	130	ASN
1	E	133	LEU
1	E	141	ASP
1	F	34	GLN
1	F	71	ASP
1	F	79	ASP
1	G	46	LYS
1	G	61	THR
1	G	98	ASN
1	G	103	ASP
1	H	76	LEU
1	H	102	GLU
1	H	109	PHE
1	I	54	GLN
1	I	68	ASP
1	I	70	ASP
1	I	113	ASN
1	I	114	ASN
1	I	141	ASP
1	J	49	ILE
1	J	76	LEU
1	J	118	ASP
1	K	54	GLN
1	K	100	GLU
1	L	46	LYS
1	L	121	MSE
1	L	137	LEU
1	L	142	MSE
1	L	144	LEU
1	M	61	THR
1	M	95	ASP
1	M	105	THR
1	M	133	LEU
1	M	141	ASP
1	M	142	MSE
1	N	61	THR
1	N	102	GLU
1	N	103	ASP
1	N	111	GLU
1	O	36	ASN

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Mol	Chain	Res	Type
1	O	39	LEU
1	O	62	LEU
1	O	102	GLU
1	O	118	ASP
1	O	121	MSE
1	O	128	ILE
1	O	130	ASN
1	O	137	LEU
1	O	141	ASP
1	P	66	LEU
1	Q	54	GLN
1	Q	71	ASP
1	Q	108	LEU
1	Q	133	LEU
1	R	71	ASP
1	R	98	ASN
1	R	127	GLU
1	R	133	LEU
1	S	68	ASP
1	S	98	ASN
1	S	133	LEU
1	T	33	GLU
1	T	68	ASP
1	T	103	ASP
1	T	129	LEU
1	T	137	LEU
1	T	144	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (97) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN
1	A	53	ASN
1	A	54	GLN
1	A	60	ASN
1	A	113	ASN
1	A	130	ASN
1	A	136	GLN
1	B	36	ASN
1	B	45	GLN
1	B	51	ASN
1	B	54	GLN

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Mol	Chain	Res	Type
1	B	60	ASN
1	B	84	ASN
1	B	113	ASN
1	B	114	ASN
1	C	45	GLN
1	C	53	ASN
1	C	84	ASN
1	D	51	ASN
1	D	53	ASN
1	D	54	GLN
1	D	60	ASN
1	D	84	ASN
1	D	98	ASN
1	D	114	ASN
1	D	136	GLN
1	E	60	ASN
1	E	84	ASN
1	E	114	ASN
1	E	130	ASN
1	E	150	GLN
1	F	34	GLN
1	F	36	ASN
1	F	45	GLN
1	F	51	ASN
1	F	53	ASN
1	F	60	ASN
1	F	84	ASN
1	F	130	ASN
1	F	150	GLN
1	G	45	GLN
1	G	53	ASN
1	G	60	ASN
1	G	98	ASN
1	G	113	ASN
1	H	51	ASN
1	H	53	ASN
1	H	54	GLN
1	H	98	ASN
1	H	113	ASN
1	H	130	ASN
1	I	36	ASN
1	I	45	GLN

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Mol	Chain	Res	Type
1	I	54	GLN
1	I	60	ASN
1	I	113	ASN
1	I	114	ASN
1	I	130	ASN
1	I	136	GLN
1	J	36	ASN
1	J	60	ASN
1	J	84	ASN
1	J	98	ASN
1	J	114	ASN
1	K	60	ASN
1	K	84	ASN
1	L	54	GLN
1	L	84	ASN
1	L	98	ASN
1	L	113	ASN
1	L	114	ASN
1	M	54	GLN
1	M	84	ASN
1	M	98	ASN
1	M	114	ASN
1	N	45	GLN
1	N	98	ASN
1	N	130	ASN
1	O	45	GLN
1	O	53	ASN
1	O	54	GLN
1	O	113	ASN
1	O	130	ASN
1	O	150	GLN
1	P	34	GLN
1	P	53	ASN
1	P	84	ASN
1	P	130	ASN
1	Q	51	ASN
1	R	34	GLN
1	R	45	GLN
1	S	53	ASN
1	S	84	ASN
1	S	98	ASN
1	T	51	ASN

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Mol	Chain	Res	Type
1	T	60	ASN
1	T	84	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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	112/135 (82%)	-1.19	0 100 100	44, 113, 189, 200	0
1	B	119/135 (88%)	-1.20	0 100 100	46, 110, 198, 200	0
1	C	116/135 (85%)	-1.02	0 100 100	77, 151, 200, 200	0
1	D	122/135 (90%)	-0.97	1 (0%) 82 64	61, 152, 199, 200	0
1	E	122/135 (90%)	-1.25	0 100 100	32, 104, 198, 200	0
1	F	122/135 (90%)	-1.31	0 100 100	20, 108, 193, 200	0
1	G	109/135 (80%)	-1.20	0 100 100	69, 128, 187, 200	0
1	H	106/135 (78%)	-1.17	0 100 100	70, 128, 192, 200	0
1	I	112/135 (82%)	-1.02	0 100 100	96, 178, 200, 200	0
1	J	106/135 (78%)	-1.12	0 100 100	65, 168, 199, 200	0
1	K	115/135 (85%)	-1.26	0 100 100	15, 115, 193, 200	0
1	L	112/135 (82%)	-1.14	0 100 100	32, 115, 185, 200	0
1	M	115/135 (85%)	-1.10	0 100 100	52, 136, 196, 200	0
1	N	110/135 (81%)	-1.07	0 100 100	38, 142, 192, 200	0
1	O	122/135 (90%)	-1.15	0 100 100	50, 126, 197, 200	0
1	P	112/135 (82%)	-1.22	0 100 100	50, 111, 184, 198	0
1	Q	110/135 (81%)	-1.22	0 100 100	59, 133, 198, 200	0
1	R	110/135 (81%)	-1.05	0 100 100	48, 147, 198, 200	0
1	S	115/135 (85%)	-0.81	0 100 100	108, 177, 200, 200	0
1	T	112/135 (82%)	-0.98	0 100 100	109, 169, 200, 200	0
All	All	2279/2700 (84%)	-1.12	1 (0%) 100 100	15, 138, 199, 200	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	149	LEU	2.9

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.