



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 10:43 PM UTC

PDB ID : 1GYT / pdb_00001gyt
Title : E. coli Aminopeptidase A (PepA)
Authors : Straeter, N.
Deposited on : 2002-04-29
Resolution : 2.50 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

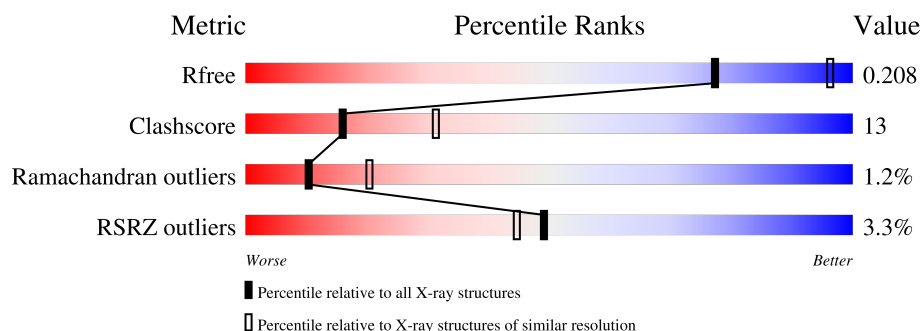
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	503	3% 71% 26% .
1	B	503	3% 76% 22% .
1	C	503	3% 74% 24% .
1	D	503	3% 71% 26% .
1	E	503	3% 77% 21% .
1	F	503	3% 78% 20% .

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Mol	Chain	Length	Quality of chain
1	G	503	2% 79% 19%
1	H	503	6% 70% 26%
1	I	503	2% 82% 16%
1	J	503	2% 75% 22%
1	K	503	3% 73% 25%
1	L	503	8% 69% 27%

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 49952 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 CYTOSOL AMINOPEPTIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	503	Total	C	N	O	S	0	0	0
			3846	2401	691	729	25			
1	B	503	Total	C	N	O	S	0	0	0
			3846	2401	691	729	25			
1	C	503	Total	C	N	O	S	0	0	0
			3846	2401	691	729	25			
1	D	503	Total	C	N	O	S	0	0	0
			3846	2401	691	729	25			
1	E	503	Total	C	N	O	S	0	0	0
			3846	2401	691	729	25			
1	F	503	Total	C	N	O	S	0	0	0
			3846	2401	691	729	25			
1	G	503	Total	C	N	O	S	0	0	0
			3846	2401	691	729	25			
1	H	503	Total	C	N	O	S	0	0	0
			3846	2401	691	729	25			
1	I	503	Total	C	N	O	S	0	0	0
			3846	2401	691	729	25			
1	J	503	Total	C	N	O	S	0	0	0
			3846	2401	691	729	25			
1	K	503	Total	C	N	O	S	0	0	0
			3846	2401	691	729	25			
1	L	503	Total	C	N	O	S	0	0	0
			3846	2401	691	729	25			

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

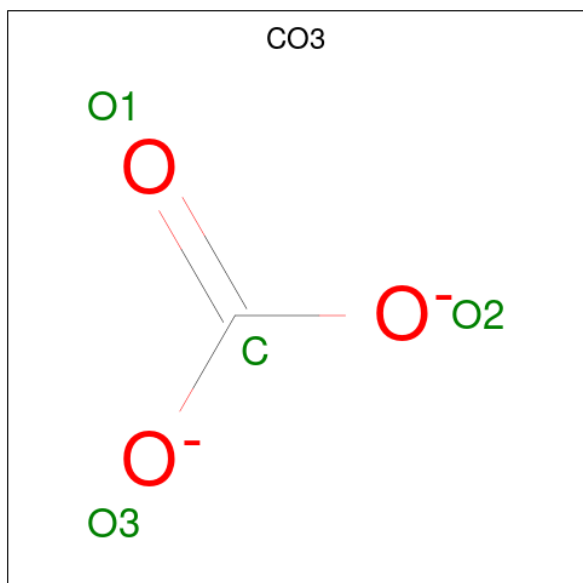
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	C	2	Total 2	Zn 2	0	0
2	D	2	Total 2	Zn 2	0	0
2	E	2	Total 2	Zn 2	0	0
2	F	2	Total 2	Zn 2	0	0
2	G	2	Total 2	Zn 2	0	0
2	H	2	Total 2	Zn 2	0	0
2	I	2	Total 2	Zn 2	0	0
2	J	2	Total 2	Zn 2	0	0
2	K	2	Total 2	Zn 2	0	0
2	L	2	Total 2	Zn 2	0	0

- Molecule 3 is CARBONATE ION (CCD ID: CO3) (formula: CO₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 4	C 1	O 3	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 4 1 3	0	0
3	C	1	Total C O 4 1 3	0	0
3	D	1	Total C O 4 1 3	0	0
3	E	1	Total C O 4 1 3	0	0
3	F	1	Total C O 4 1 3	0	0
3	G	1	Total C O 4 1 3	0	0
3	H	1	Total C O 4 1 3	0	0
3	I	1	Total C O 4 1 3	0	0
3	J	1	Total C O 4 1 3	0	0
3	K	1	Total C O 4 1 3	0	0
3	L	1	Total C O 4 1 3	0	0

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Cl 1 1	0	0
4	F	1	Total Cl 1 1	0	0
4	G	1	Total Cl 1 1	0	0
4	K	1	Total Cl 1 1	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	256	Total O 256 256	0	0
5	B	341	Total O 341 341	0	0

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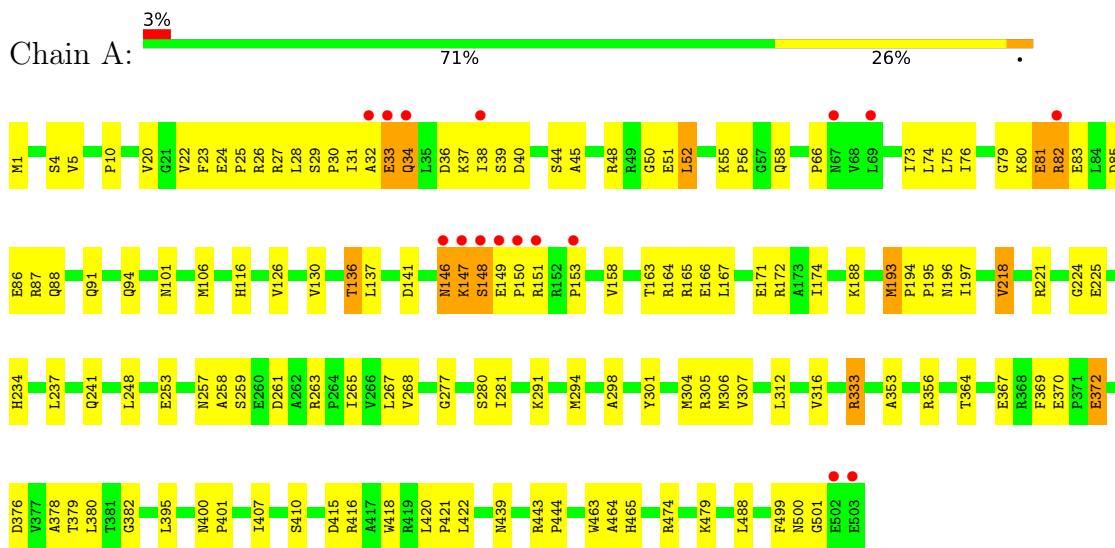
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	318	Total 318	O 318	0	0
5	D	310	Total 310	O 310	0	0
5	E	345	Total 345	O 345	0	0
5	F	304	Total 304	O 304	0	0
5	G	374	Total 374	O 374	0	0
5	H	203	Total 203	O 203	0	0
5	I	398	Total 398	O 398	0	0
5	J	313	Total 313	O 313	0	0
5	K	273	Total 273	O 273	0	0
5	L	289	Total 289	O 289	0	0

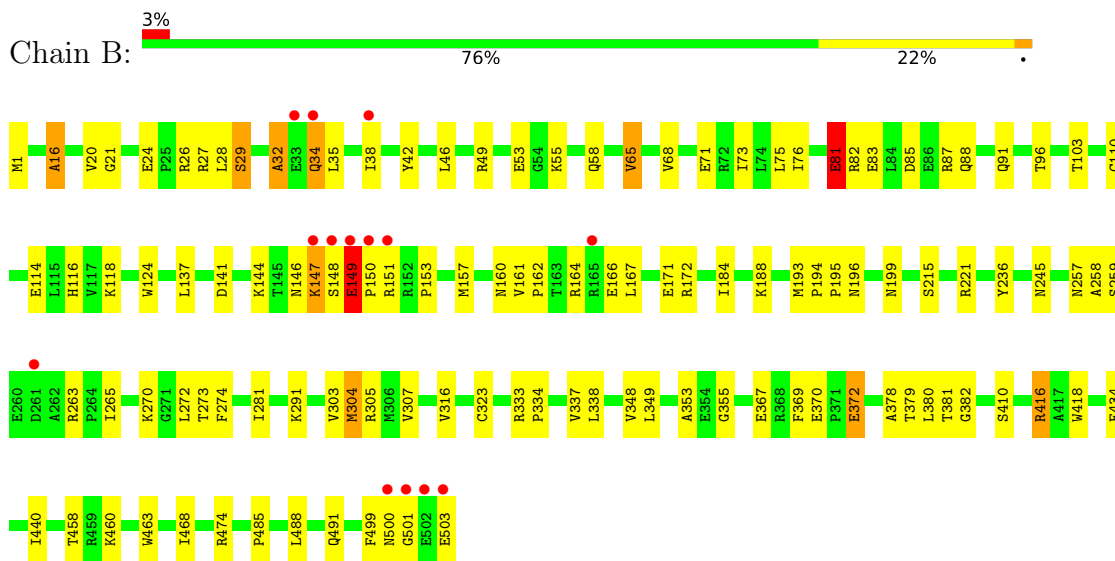
3 Residue-property plots [i](#)

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: CYTOSOL AMINOPEPTIDASE

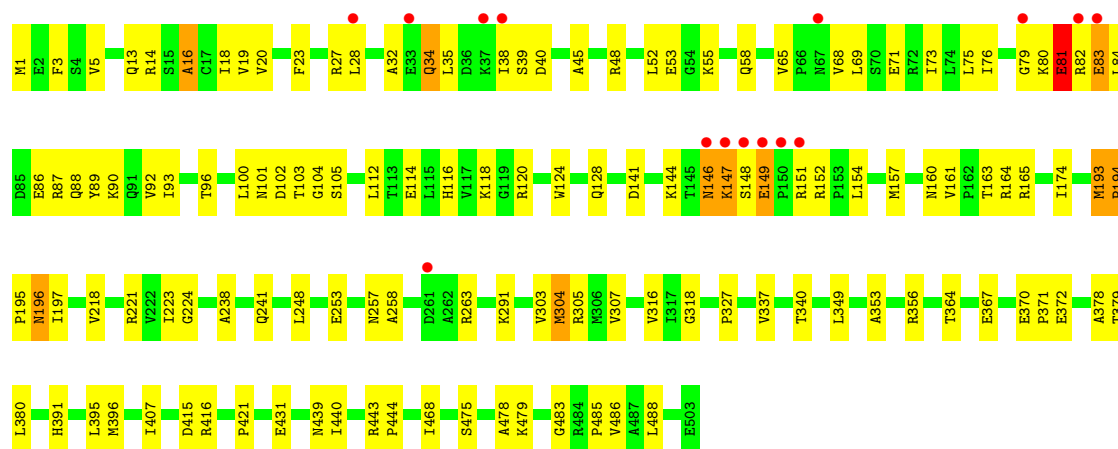


• Molecule 1: CYTOSOL AMINOPEPTIDASE

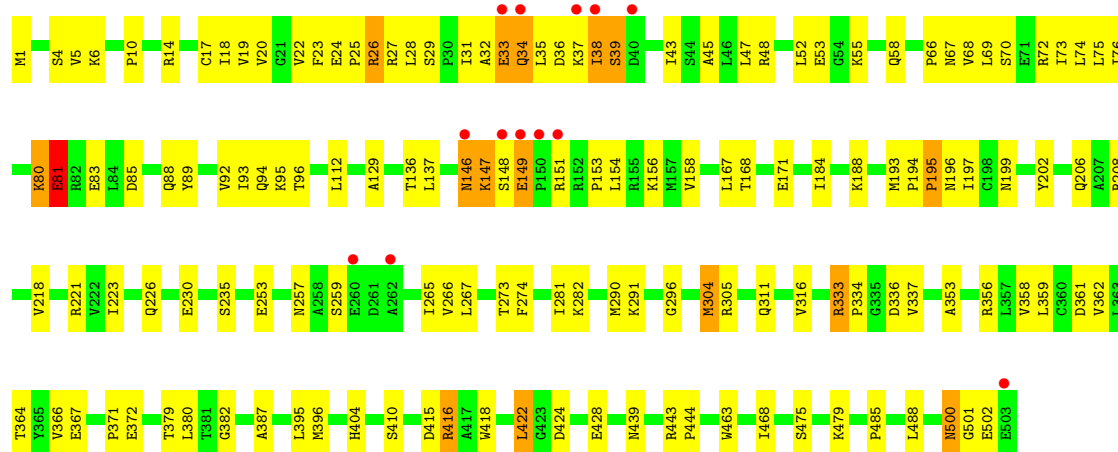


• Molecule 1: CYTOSOL AMINOPEPTIDASE

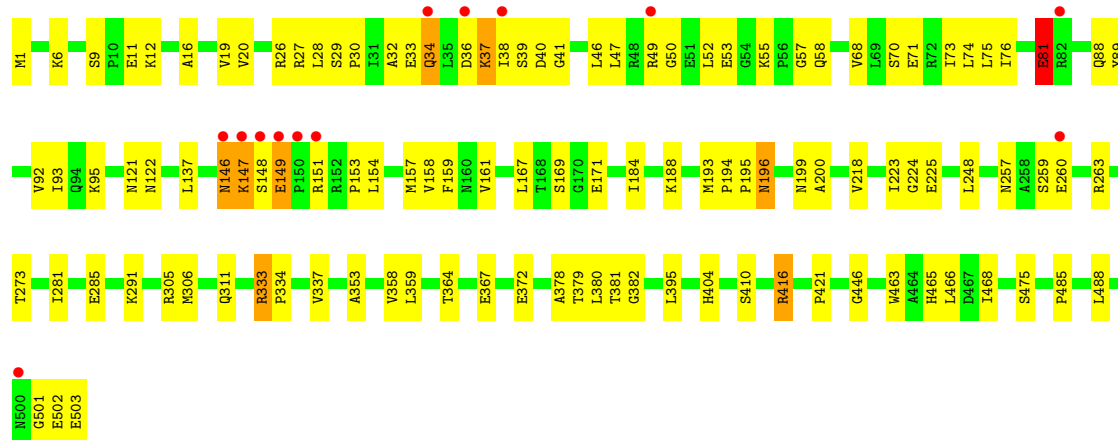
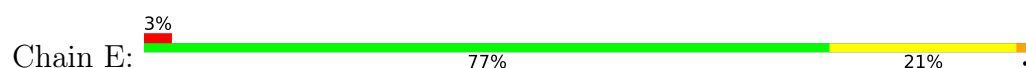




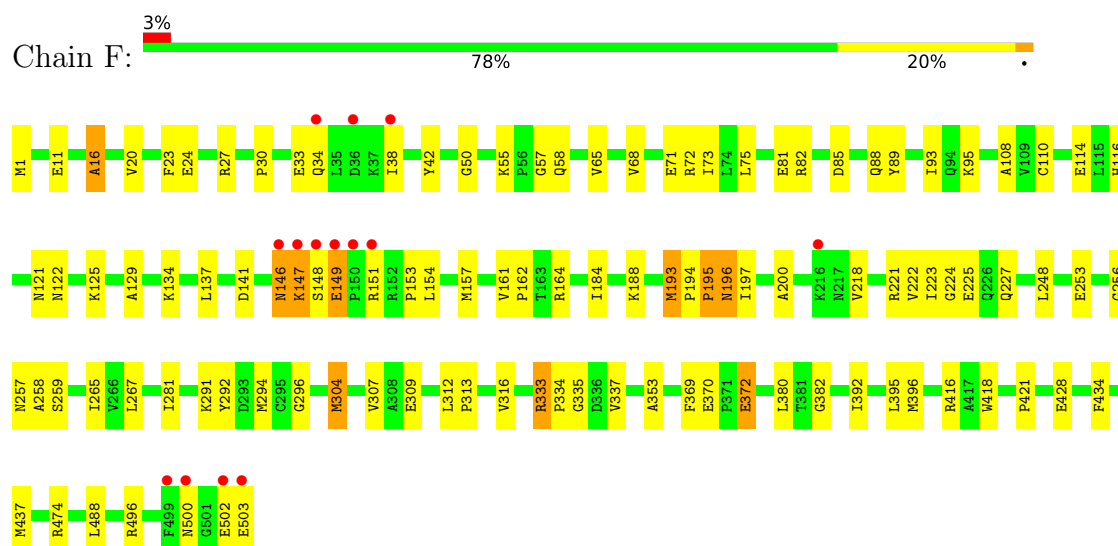
• Molecule 1: CYTOSOL AMINOPEPTIDASE



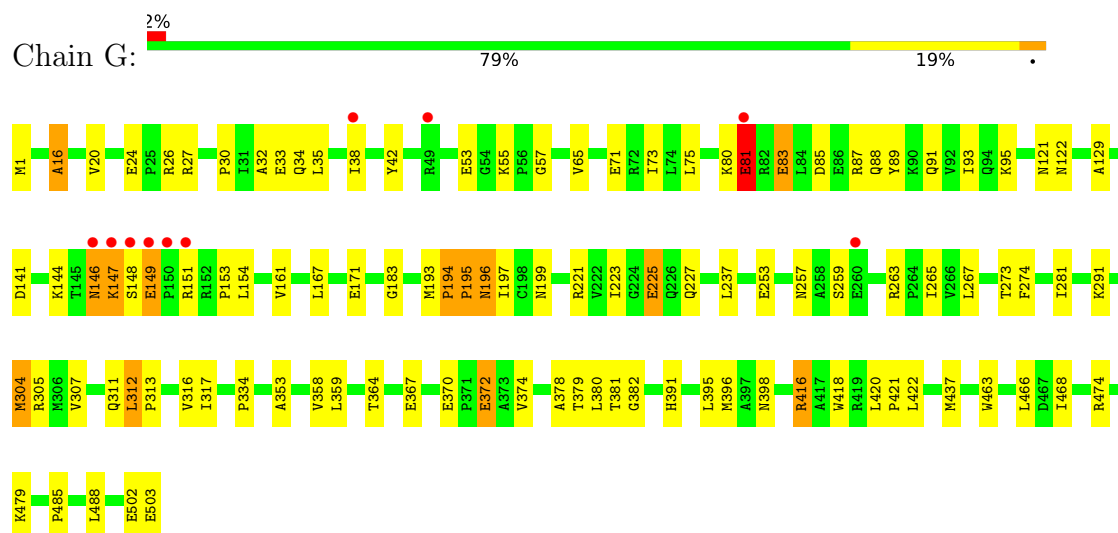
• Molecule 1: CYTOSOL AMINOPEPTIDASE



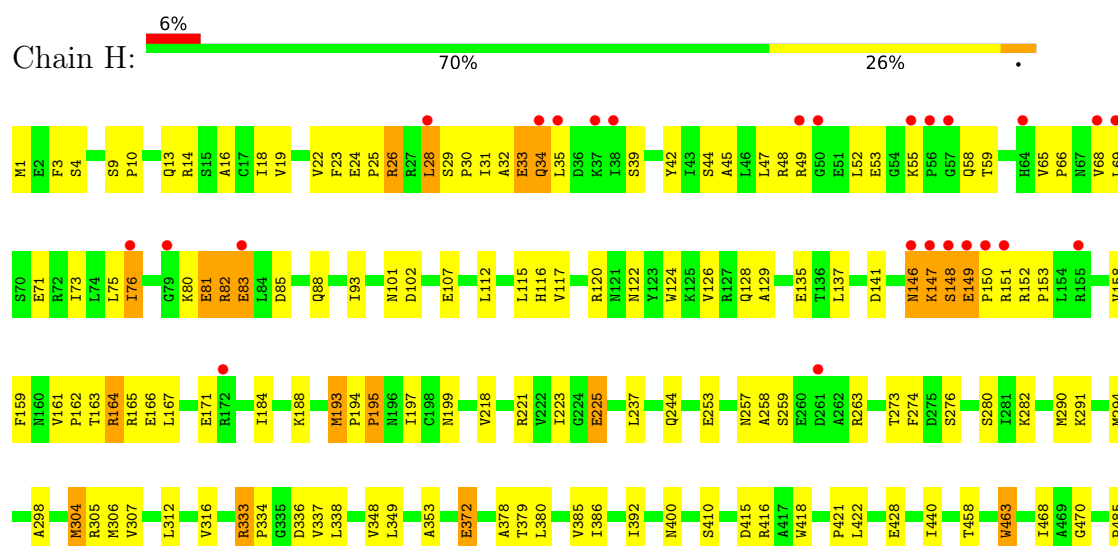
• Molecule 1: CYTOSOL AMINOPEPTIDASE



• Molecule 1: CYTOSOL AMINOPEPTIDASE

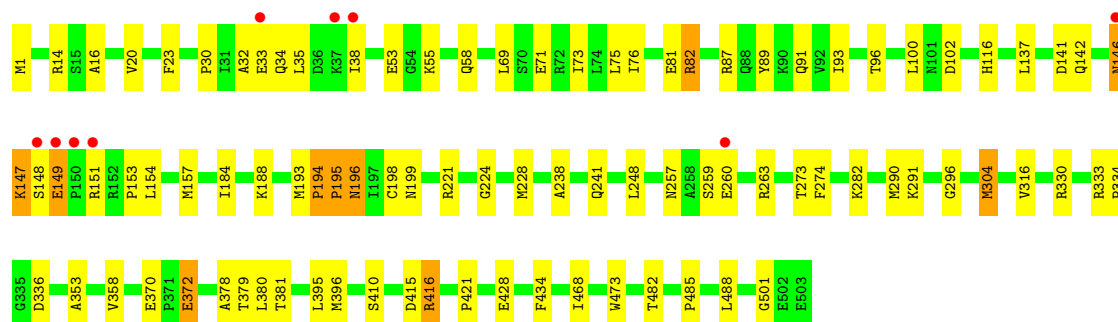
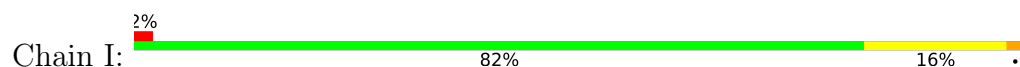


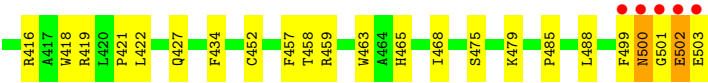
• Molecule 1: CYTOSOL AMINOPEPTIDASE



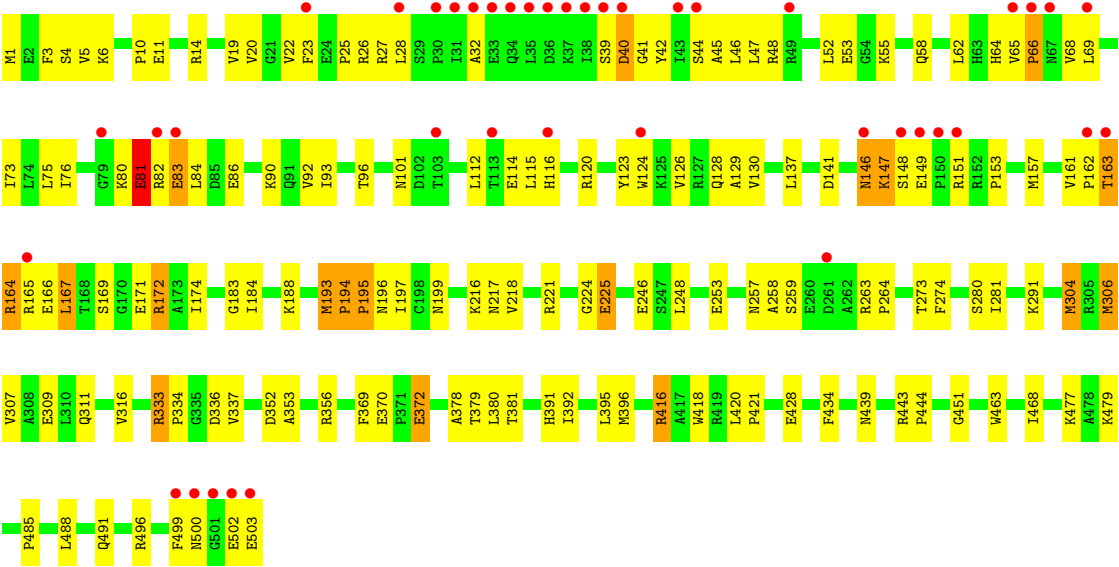


• Molecule 1: CYTOSOL AMINOPEPTIDASE





● Molecule 1: CYTOSOL AMINOPEPTIDASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	178.00Å 178.00Å 244.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	30.00 – 2.50 30.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.9 (30.00-2.50) 99.8 (30.00-2.50)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.63 (at 2.51Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.165 , 0.209 0.165 , 0.208	Depositor DCC
R_{free} test set	14839 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	18.7	Xtriage
Anisotropy	0.335	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 55.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.002 for -h,-k,l 0.016 for h,-h-k,-l 0.007 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	49952	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.69% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, CO3, CL

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	0.73	0/3909	1.13	31/5277 (0.6%)
1	B	0.83	1/3909 (0.0%)	1.14	29/5277 (0.5%)
1	C	0.81	2/3909 (0.1%)	1.13	22/5277 (0.4%)
1	D	0.78	1/3909 (0.0%)	1.14	29/5277 (0.5%)
1	E	0.80	0/3909	1.13	28/5277 (0.5%)
1	F	0.77	2/3909 (0.1%)	1.12	20/5277 (0.4%)
1	G	0.81	2/3909 (0.1%)	1.12	29/5277 (0.5%)
1	H	0.71	1/3909 (0.0%)	1.13	31/5277 (0.6%)
1	I	0.87	1/3909 (0.0%)	1.14	21/5277 (0.4%)
1	J	0.80	2/3909 (0.1%)	1.13	25/5277 (0.5%)
1	K	0.76	2/3909 (0.1%)	1.13	28/5277 (0.5%)
1	L	0.82	2/3909 (0.1%)	1.14	33/5277 (0.6%)
All	All	0.79	16/46908 (0.0%)	1.13	326/63324 (0.5%)

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	304	MET	SD-CE	-9.67	1.55	1.79
1	I	304	MET	SD-CE	-9.55	1.55	1.79
1	C	304	MET	SD-CE	-8.93	1.57	1.79
1	F	304	MET	SD-CE	-8.71	1.57	1.79
1	B	304	MET	SD-CE	-8.47	1.58	1.79
1	D	304	MET	SD-CE	-7.61	1.60	1.79
1	K	1	MET	SD-CE	7.50	1.98	1.79
1	L	304	MET	SD-CE	-6.46	1.63	1.79
1	J	304	MET	SD-CE	-6.18	1.64	1.79
1	H	304	MET	SD-CE	-5.98	1.64	1.79
1	C	193	MET	SD-CE	-5.79	1.65	1.79
1	L	306	MET	SD-CE	-5.73	1.65	1.79
1	K	106	MET	SD-CE	5.69	1.93	1.79
1	J	193	MET	SD-CE	-5.57	1.65	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	437	MET	SD-CE	5.32	1.92	1.79
1	G	437	MET	SD-CE	5.16	1.92	1.79

All (326) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	193	MET	CA-C-N	12.97	129.00	119.66
1	F	193	MET	C-N-CA	12.97	129.00	119.66
1	H	501	GLY	N-CA-C	-10.11	99.33	114.90
1	K	416	ARG	N-CA-C	9.91	123.83	110.35
1	C	34	GLN	N-CA-C	-9.68	101.61	113.41
1	D	501	GLY	N-CA-C	-9.63	103.23	114.69
1	H	416	ARG	N-CA-C	9.08	122.70	110.35
1	J	193	MET	CA-C-N	9.01	126.14	119.66
1	J	193	MET	C-N-CA	9.01	126.14	119.66
1	D	416	ARG	N-CA-C	9.00	123.18	110.50
1	A	193	MET	CA-C-N	8.96	126.11	119.66
1	A	193	MET	C-N-CA	8.96	126.11	119.66
1	E	358	VAL	N-CA-C	-8.90	102.19	110.82
1	G	416	ARG	N-CA-C	8.89	122.43	110.35
1	L	416	ARG	N-CA-C	8.84	123.05	110.23
1	F	416	ARG	N-CA-C	8.79	122.30	110.35
1	E	416	ARG	N-CA-C	8.71	122.20	110.35
1	B	34	GLN	N-CA-C	-8.65	101.76	111.71
1	J	353	ALA	N-CA-C	-8.36	100.12	110.65
1	J	416	ARG	N-CA-C	8.18	121.47	110.35
1	J	195	PRO	CA-C-N	8.07	131.09	120.28
1	J	195	PRO	C-N-CA	8.07	131.09	120.28
1	C	416	ARG	N-CA-C	7.97	121.18	110.35
1	I	194	PRO	CA-C-N	7.96	127.62	119.82
1	I	194	PRO	C-N-CA	7.96	127.62	119.82
1	A	380	LEU	N-CA-C	7.93	123.04	113.12
1	H	34	GLN	N-CA-C	-7.89	102.37	110.97
1	C	372	GLU	N-CA-C	-7.89	102.76	111.36
1	I	501	GLY	N-CA-C	-7.85	105.34	114.69
1	B	193	MET	CA-C-N	7.84	125.31	119.66
1	B	193	MET	C-N-CA	7.84	125.31	119.66
1	B	291	LYS	N-CA-C	-7.84	102.97	112.54
1	K	265	ILE	N-CA-C	-7.76	97.26	108.36
1	C	353	ALA	N-CA-C	-7.74	100.90	110.65
1	A	416	ARG	N-CA-C	7.72	120.84	110.35
1	B	416	ARG	N-CA-C	7.69	121.34	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	196	ASN	N-CA-CB	-7.64	98.43	110.28
1	G	195	PRO	CA-C-N	7.52	131.74	120.31
1	G	195	PRO	C-N-CA	7.52	131.74	120.31
1	I	291	LYS	N-CA-C	-7.50	104.00	113.01
1	E	193	MET	CA-C-N	7.50	125.06	119.66
1	E	193	MET	C-N-CA	7.50	125.06	119.66
1	A	382	GLY	N-CA-C	-7.48	103.35	113.37
1	I	353	ALA	N-CA-C	-7.47	101.23	110.65
1	G	83	GLU	N-CA-C	-7.46	104.14	112.57
1	D	380	LEU	N-CA-C	7.42	122.72	112.04
1	H	372	GLU	N-CA-C	-7.35	102.23	112.45
1	L	164	ARG	N-CA-C	-7.30	103.97	114.12
1	I	416	ARG	N-CA-C	7.27	120.23	110.35
1	B	32	ALA	N-CA-C	7.26	119.28	111.36
1	L	291	LYS	N-CA-C	-7.24	103.71	112.54
1	D	422	LEU	N-CA-C	-7.23	99.10	109.29
1	E	380	LEU	N-CA-C	7.21	122.43	112.04
1	K	353	ALA	N-CA-C	-7.20	101.69	111.55
1	E	334	PRO	N-CA-C	-7.19	99.95	111.03
1	B	333	ARG	N-CA-C	7.17	121.86	109.82
1	H	333	ARG	N-CA-C	7.17	121.56	109.09
1	D	195	PRO	CA-C-N	7.14	130.42	120.29
1	D	195	PRO	C-N-CA	7.14	130.42	120.29
1	D	353	ALA	N-CA-C	-7.13	101.78	111.55
1	H	193	MET	CA-C-N	7.10	124.77	119.66
1	H	193	MET	C-N-CA	7.10	124.77	119.66
1	B	281	ILE	N-CA-C	7.09	119.85	109.63
1	A	34	GLN	N-CA-C	-7.09	103.24	110.97
1	B	334	PRO	N-CA-C	-7.09	100.12	111.03
1	H	164	ARG	N-CA-C	-7.05	104.55	113.01
1	L	195	PRO	CA-C-N	7.04	129.60	120.44
1	L	195	PRO	C-N-CA	7.04	129.60	120.44
1	F	380	LEU	N-CA-C	7.03	122.03	112.68
1	F	353	ALA	N-CA-C	-7.03	101.79	110.65
1	I	381	THR	N-CA-C	7.00	120.08	109.23
1	H	353	ALA	N-CA-C	-6.99	101.85	110.65
1	E	501	GLY	N-CA-C	-6.98	105.84	114.92
1	J	378	ALA	N-CA-C	6.97	120.67	108.75
1	F	291	LYS	N-CA-C	-6.96	104.75	113.18
1	G	81	GLU	N-CA-C	6.96	125.63	110.80
1	K	194	PRO	CA-C-N	6.96	126.66	119.56
1	K	194	PRO	C-N-CA	6.96	126.66	119.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	225	GLU	N-CA-C	6.94	118.85	111.28
1	G	265	ILE	N-CA-C	-6.94	97.86	107.99
1	E	291	LYS	N-CA-C	-6.92	104.71	113.01
1	E	195	PRO	CA-C-N	6.90	130.08	120.29
1	E	195	PRO	C-N-CA	6.90	130.08	120.29
1	D	81	GLU	N-CA-C	6.89	125.48	110.80
1	I	378	ALA	N-CA-C	6.88	120.52	108.75
1	C	380	LEU	N-CA-C	6.85	121.90	112.04
1	F	372	GLU	N-CA-C	-6.84	103.93	112.90
1	D	38	ILE	N-CA-C	-6.81	105.95	111.81
1	I	333	ARG	N-CA-C	6.80	120.92	109.09
1	K	501	GLY	N-CA-C	-6.79	97.10	113.18
1	J	379	THR	N-CA-C	-6.77	96.78	108.56
1	L	334	PRO	N-CA-C	-6.77	100.60	111.03
1	B	161	VAL	CA-C-N	6.76	128.29	119.84
1	B	161	VAL	C-N-CA	6.76	128.29	119.84
1	D	358	VAL	N-CA-C	-6.76	104.26	110.82
1	F	333	ARG	N-CA-C	6.75	120.84	109.09
1	I	358	VAL	N-CA-C	-6.75	104.28	110.82
1	B	265	ILE	N-CA-C	-6.70	98.78	108.36
1	J	380	LEU	N-CA-C	6.70	121.68	112.04
1	D	80	LYS	N-CA-C	6.67	119.40	108.52
1	D	281	ILE	N-CA-C	6.67	119.05	109.51
1	F	382	GLY	N-CA-C	-6.66	104.45	113.37
1	L	183	GLY	N-CA-C	-6.64	104.80	112.50
1	G	353	ALA	N-CA-C	-6.61	102.32	110.65
1	E	359	LEU	N-CA-C	6.59	118.47	111.28
1	B	380	LEU	N-CA-C	6.58	121.51	112.04
1	G	291	LYS	N-CA-C	-6.57	104.52	112.54
1	F	296	GLY	N-CA-C	-6.57	104.55	112.49
1	I	193	MET	CA-C-N	6.55	124.37	119.66
1	I	193	MET	C-N-CA	6.55	124.37	119.66
1	J	327	PRO	N-CA-C	-6.54	101.63	111.57
1	E	379	THR	N-CA-C	-6.53	97.15	108.52
1	L	281	ILE	N-CA-C	6.53	119.03	109.63
1	I	334	PRO	N-CA-C	-6.51	101.00	111.03
1	L	353	ALA	N-CA-C	-6.50	102.46	110.65
1	E	382	GLY	N-CA-C	-6.49	104.68	113.37
1	J	281	ILE	N-CA-C	6.48	118.96	109.63
1	D	334	PRO	N-CA-C	-6.46	101.06	111.14
1	I	379	THR	N-CA-C	-6.46	97.28	108.52
1	L	372	GLU	N-CA-C	-6.46	103.52	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	500	ASN	N-CA-C	6.45	119.62	111.69
1	K	291	LYS	N-CA-C	-6.44	104.68	112.54
1	H	244	GLN	N-CA-C	-6.42	105.41	113.18
1	K	334	PRO	N-CA-C	-6.39	101.17	111.14
1	C	81	GLU	N-CA-C	6.38	124.38	110.80
1	H	195	PRO	CA-C-N	6.36	129.97	120.31
1	H	195	PRO	C-N-CA	6.36	129.97	120.31
1	A	265	ILE	N-CA-C	-6.34	99.29	108.36
1	A	195	PRO	CA-C-N	6.33	128.76	120.28
1	A	195	PRO	C-N-CA	6.33	128.76	120.28
1	B	353	ALA	N-CA-C	-6.32	102.69	110.65
1	C	194	PRO	CA-C-N	6.31	126.00	119.82
1	C	194	PRO	C-N-CA	6.31	126.00	119.82
1	L	333	ARG	N-CA-C	6.31	120.41	109.82
1	J	372	GLU	N-CA-C	-6.30	104.49	111.36
1	I	380	LEU	N-CA-C	6.30	121.11	112.04
1	L	194	PRO	CA-C-N	6.29	125.98	119.82
1	L	194	PRO	C-N-CA	6.29	125.98	119.82
1	H	194	PRO	CA-C-N	6.27	125.95	119.56
1	H	194	PRO	C-N-CA	6.27	125.95	119.56
1	B	16	ALA	N-CA-C	-6.24	104.77	112.38
1	K	218	VAL	N-CA-C	6.21	116.81	107.75
1	L	193	MET	CA-C-N	6.19	124.12	119.66
1	L	193	MET	C-N-CA	6.19	124.12	119.66
1	I	372	GLU	N-CA-C	-6.19	104.08	111.69
1	L	163	THR	CB-CA-C	-6.18	106.67	114.40
1	K	152	ARG	CA-C-N	-6.18	113.32	119.56
1	K	152	ARG	C-N-CA	-6.18	113.32	119.56
1	D	379	THR	N-CA-C	-6.16	97.80	108.52
1	E	333	ARG	N-CA-C	6.16	120.17	109.82
1	F	161	VAL	CA-C-N	6.16	127.53	119.84
1	F	161	VAL	C-N-CA	6.16	127.53	119.84
1	I	296	GLY	N-CA-C	-6.14	105.06	112.49
1	K	281	ILE	N-CA-C	6.14	118.47	109.63
1	A	51	GLU	N-CA-C	6.13	120.49	113.19
1	D	359	LEU	N-CA-C	6.13	118.76	111.71
1	K	380	LEU	N-CA-C	6.13	120.86	112.04
1	H	380	LEU	N-CA-C	6.12	120.77	113.12
1	G	422	LEU	N-CA-C	-6.10	99.43	109.80
1	J	424	ASP	N-CA-C	6.10	118.71	111.33
1	H	83	GLU	N-CA-C	-6.08	103.36	112.54
1	A	291	LYS	N-CA-C	-6.07	105.14	112.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	16	ALA	N-CA-C	-6.06	104.98	112.38
1	J	196	ASN	N-CA-CB	-6.06	101.21	110.12
1	H	291	LYS	N-CA-C	-6.05	105.16	112.54
1	B	379	THR	N-CA-C	-6.05	98.00	108.52
1	F	281	ILE	N-CA-C	6.05	118.16	109.51
1	F	195	PRO	CA-C-N	6.04	129.49	120.31
1	F	195	PRO	C-N-CA	6.04	129.49	120.31
1	H	400	ASN	CA-C-N	-6.04	112.35	119.05
1	H	400	ASN	C-N-CA	-6.04	112.35	119.05
1	C	196	ASN	N-CA-CB	-6.04	101.22	110.16
1	L	381	THR	N-CA-C	6.03	119.32	109.06
1	C	161	VAL	CA-C-N	6.01	126.18	119.32
1	C	161	VAL	C-N-CA	6.01	126.18	119.32
1	H	379	THR	N-CA-C	-6.01	98.07	108.52
1	E	281	ILE	N-CA-C	6.00	118.27	109.63
1	H	218	VAL	N-CA-C	6.00	116.50	108.11
1	G	312	LEU	CA-C-N	5.99	127.33	119.84
1	G	312	LEU	C-N-CA	5.99	127.33	119.84
1	J	291	LYS	N-CA-C	-5.98	105.83	113.01
1	D	265	ILE	N-CA-C	-5.98	99.81	108.36
1	A	39	SER	N-CA-C	-5.97	105.18	112.88
1	H	378	ALA	N-CA-C	5.97	118.95	108.75
1	G	281	ILE	N-CA-C	5.96	118.22	109.63
1	I	195	PRO	CA-C-N	5.96	128.75	120.29
1	I	195	PRO	C-N-CA	5.96	128.75	120.29
1	A	379	THR	N-CA-C	-5.96	98.16	108.52
1	L	380	LEU	N-CA-C	5.95	120.60	112.04
1	G	380	LEU	N-CA-C	5.93	120.57	112.68
1	K	379	THR	N-CA-C	-5.92	98.21	108.52
1	G	334	PRO	N-CA-C	-5.90	101.94	111.03
1	G	194	PRO	CA-C-N	5.87	127.18	119.84
1	G	194	PRO	C-N-CA	5.87	127.18	119.84
1	D	218	VAL	N-CA-C	5.87	116.32	108.11
1	B	215	SER	N-CA-C	5.85	119.52	112.38
1	D	333	ARG	N-CA-C	5.85	119.27	109.09
1	D	463	TRP	N-CA-C	5.84	118.28	109.23
1	B	149	GLU	CA-C-N	5.84	127.14	119.84
1	B	149	GLU	C-N-CA	5.84	127.14	119.84
1	F	16	ALA	N-CA-C	-5.80	105.47	112.54
1	C	102	ASP	N-CA-C	-5.79	105.88	113.17
1	J	391	HIS	N-CA-C	5.78	120.47	113.41
1	G	225	GLU	N-CA-C	5.78	117.58	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	195	PRO	CA-C-N	5.77	128.48	120.29
1	C	195	PRO	C-N-CA	5.77	128.48	120.29
1	A	33	GLU	N-CA-C	-5.76	105.52	112.54
1	L	167	LEU	N-CA-C	-5.76	104.97	112.23
1	L	378	ALA	N-CA-C	5.75	117.87	108.55
1	A	234	HIS	N-CA-C	5.74	118.48	111.82
1	A	333	ARG	N-CA-C	5.71	119.21	109.06
1	A	280	SER	N-CA-C	-5.70	101.86	110.70
1	F	225	GLU	N-CA-C	5.70	117.49	111.28
1	G	183	GLY	N-CA-C	-5.70	105.48	112.77
1	A	29	SER	CA-C-N	5.68	125.80	119.32
1	A	29	SER	C-N-CA	5.68	125.80	119.32
1	J	333	ARG	N-CA-C	5.68	118.97	109.09
1	H	276	SER	N-CA-C	-5.67	106.32	113.18
1	D	291	LYS	N-CA-C	-5.65	105.64	112.54
1	J	417	ALA	N-CA-C	-5.65	100.70	109.24
1	A	353	ALA	N-CA-C	-5.64	102.84	110.68
1	B	81	GLU	N-CA-C	5.64	122.81	110.80
1	L	379	THR	N-CA-C	-5.64	97.38	107.98
1	A	136	THR	N-CA-C	5.63	117.42	111.28
1	D	424	ASP	N-CA-C	5.62	117.40	111.28
1	E	225	GLU	N-CA-C	5.61	117.40	111.28
1	K	280	SER	N-CA-C	-5.61	102.01	110.70
1	B	236	TYR	N-CA-C	-5.58	105.19	111.28
1	E	71	GLU	N-CA-C	5.57	118.28	111.82
1	A	277	GLY	N-CA-C	-5.57	108.06	114.69
1	F	334	PRO	N-CA-C	-5.56	102.47	111.14
1	A	372	GLU	N-CA-C	-5.55	105.24	112.23
1	E	378	ALA	N-CA-C	5.55	118.24	108.75
1	B	382	GLY	N-CA-C	-5.54	107.46	114.16
1	G	378	ALA	N-CA-C	5.52	118.19	108.75
1	K	382	GLY	N-CA-C	-5.51	105.98	113.37
1	B	434	PHE	N-CA-C	5.50	121.77	114.12
1	L	352	ASP	N-CA-C	-5.48	106.60	113.28
1	E	463	TRP	N-CA-C	5.47	117.71	109.23
1	G	420	LEU	N-CA-C	-5.47	102.58	110.40
1	E	218	VAL	N-CA-C	5.46	115.75	108.11
1	L	420	LEU	N-CA-C	-5.46	102.59	110.40
1	D	296	GLY	N-CA-C	-5.46	105.89	112.49
1	G	379	THR	N-CA-C	-5.45	97.74	107.98
1	C	327	PRO	N-CA-C	-5.44	103.02	111.13
1	E	446	GLY	N-CA-C	5.42	120.48	113.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	263	ARG	CA-C-N	-5.42	115.00	120.31
1	K	263	ARG	C-N-CA	-5.42	115.00	120.31
1	D	382	GLY	N-CA-C	-5.42	106.11	113.37
1	D	39	SER	N-CA-C	-5.41	106.45	113.16
1	A	24	GLU	N-CA-C	-5.41	103.22	109.93
1	H	76	ILE	N-CA-C	5.41	115.91	108.12
1	K	378	ALA	N-CA-C	5.41	117.31	108.55
1	C	38	ILE	N-CA-C	-5.41	107.16	111.81
1	K	197	ILE	N-CA-C	-5.41	107.35	111.62
1	C	415	ASP	N-CA-C	-5.40	100.92	108.54
1	J	277	GLY	N-CA-C	-5.37	108.30	114.69
1	J	420	LEU	N-CA-C	-5.35	101.92	110.10
1	B	65	VAL	N-CA-C	-5.35	104.05	109.02
1	A	378	ALA	N-CA-C	5.34	117.89	108.75
1	K	14	ARG	N-CA-C	-5.32	101.04	108.54
1	L	225	GLU	N-CA-C	5.30	117.75	111.33
1	C	291	LYS	N-CA-C	-5.30	106.07	112.54
1	C	379	THR	N-CA-C	-5.30	99.30	108.52
1	E	196	ASN	N-CA-CB	-5.29	102.33	110.16
1	E	381	THR	N-CA-C	5.29	118.07	109.24
1	G	359	LEU	N-CA-C	5.29	117.12	111.36
1	A	261	ASP	N-CA-C	-5.28	106.15	112.59
1	H	463	TRP	N-CA-C	5.28	117.28	108.99
1	D	387	ALA	N-CA-C	5.28	116.84	111.14
1	E	81	GLU	N-CA-C	5.26	122.00	110.80
1	C	391	HIS	N-CA-C	5.26	119.79	112.90
1	E	50	GLY	N-CA-C	5.24	123.08	115.32
1	K	276	SER	N-CA-C	-5.24	106.66	113.16
1	F	196	ASN	N-CA-CB	-5.24	102.16	110.28
1	L	169	SER	N-CA-C	-5.22	105.67	111.36
1	A	218	VAL	N-CA-C	5.22	115.48	108.17
1	E	353	ALA	N-CA-C	-5.22	104.39	111.55
1	L	81	GLU	N-CA-C	5.22	121.93	110.80
1	B	372	GLU	N-CA-C	-5.22	105.27	111.69
1	J	34	GLN	N-CA-C	-5.22	105.59	111.28
1	L	451	GLY	N-CA-C	-5.22	106.45	112.50
1	B	378	ALA	N-CA-C	5.20	117.64	108.75
1	C	16	ALA	N-CA-C	-5.20	106.19	112.54
1	D	372	GLU	N-CA-C	-5.20	105.69	111.36
1	K	172	ARG	N-CA-C	-5.20	105.69	111.36
1	D	34	GLN	CA-C-N	5.19	128.20	120.31
1	D	34	GLN	C-N-CA	5.19	128.20	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	264	PRO	N-CA-C	5.19	121.56	112.01
1	L	391	HIS	N-CA-C	5.18	119.69	112.90
1	G	381	THR	N-CA-C	5.17	117.88	109.24
1	K	76	ILE	N-CA-C	5.17	115.57	108.12
1	H	280	SER	N-CA-C	-5.15	102.72	110.70
1	G	382	GLY	N-CA-C	-5.14	106.51	113.24
1	I	102	ASP	N-CA-C	-5.14	106.79	113.16
1	C	378	ALA	N-CA-C	5.13	117.53	108.75
1	G	358	VAL	N-CA-C	-5.13	105.41	111.00
1	E	34	GLN	N-CA-C	-5.12	105.78	111.36
1	H	102	ASP	N-CA-C	-5.12	107.08	113.38
1	B	381	THR	N-CA-C	5.12	117.75	109.06
1	G	372	GLU	N-CA-C	-5.12	105.40	111.69
1	K	422	LEU	N-CA-C	-5.11	101.12	109.80
1	L	172	ARG	N-CA-C	-5.11	105.72	111.28
1	A	281	ILE	N-CA-C	5.10	116.97	109.63
1	H	71	GLU	N-CA-C	5.09	118.75	112.54
1	B	29	SER	CA-C-N	5.08	125.11	119.32
1	B	29	SER	C-N-CA	5.08	125.11	119.32
1	L	218	VAL	N-CA-C	5.08	115.22	108.11
1	K	81	GLU	N-CA-C	5.07	121.61	110.80
1	E	16	ALA	N-CA-C	-5.06	106.20	112.38
1	L	280	SER	N-CA-C	-5.06	102.03	109.62
1	I	196	ASN	N-CA-CB	-5.06	102.67	110.16
1	K	120	ARG	N-CA-C	5.05	116.65	108.41
1	K	296	GLY	N-CA-C	-5.05	106.67	112.73
1	G	391	HIS	N-CA-C	5.05	119.51	112.90
1	J	194	PRO	CA-C-N	5.04	124.71	119.56
1	J	194	PRO	C-N-CA	5.04	124.71	119.56
1	J	43	ILE	N-CA-C	5.04	115.27	110.53
1	A	420	LEU	N-CA-C	-5.04	102.39	110.10
1	H	334	PRO	N-CA-C	-5.04	103.28	111.03
1	A	422	LEU	N-CA-C	-5.03	102.13	109.63
1	L	463	TRP	N-CA-C	5.03	117.02	109.23
1	A	148	SER	N-CA-C	-5.01	105.27	113.19
1	F	265	ILE	N-CA-C	-5.01	100.68	107.99
1	H	422	LEU	N-CA-C	-5.00	102.23	109.29
1	J	426	TYR	N-CA-C	-5.00	105.54	111.69

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	3846	0	3866	115	0
1	B	3846	0	3866	100	1
1	C	3846	0	3866	114	0
1	D	3846	0	3866	113	1
1	E	3846	0	3866	83	0
1	F	3846	0	3866	102	0
1	G	3846	0	3866	93	0
1	H	3846	0	3866	124	0
1	I	3846	0	3866	72	0
1	J	3846	0	3866	118	0
1	K	3846	0	3866	105	0
1	L	3846	0	3866	133	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
2	D	2	0	0	0	0
2	E	2	0	0	0	0
2	F	2	0	0	0	0
2	G	2	0	0	0	0
2	H	2	0	0	0	0
2	I	2	0	0	0	0
2	J	2	0	0	0	0
2	K	2	0	0	0	0
2	L	2	0	0	0	0
3	A	4	0	0	0	0
3	B	4	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
3	E	4	0	0	0	0
3	F	4	0	0	0	0
3	G	4	0	0	0	0
3	H	4	0	0	0	0
3	I	4	0	0	0	0
3	J	4	0	0	0	0
3	K	4	0	0	0	0
3	L	4	0	0	0	0
4	B	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	F	1	0	0	0	0
4	G	1	0	0	0	0
4	K	1	0	0	0	0
5	A	256	0	0	6	0
5	B	341	0	0	10	0
5	C	318	0	0	9	0
5	D	310	0	0	6	0
5	E	345	0	0	7	0
5	F	304	0	0	7	0
5	G	374	0	0	3	0
5	H	203	0	0	3	0
5	I	398	0	0	4	0
5	J	313	0	0	6	0
5	K	273	0	0	8	0
5	L	289	0	0	6	0
All	All	49952	0	46392	1220	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 13.

All (1220) 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:B:27:ARG:HH22	1:B:81:GLU:HG3	1.10	1.16
1:E:27:ARG:HH22	1:E:81:GLU:HG3	1.12	1.12
1:D:27:ARG:HH22	1:D:81:GLU:HG3	1.03	1.09
1:C:103:THR:HG22	1:C:105:SER:H	1.18	1.07
1:L:163:THR:HG22	1:L:164:ARG:H	1.14	1.07
1:L:26:ARG:HH21	1:L:53:GLU:HG2	1.21	1.03
1:D:27:ARG:NH2	1:D:81:GLU:HG3	1.75	1.02
1:F:30:PRO:HA	1:F:33:GLU:HG3	1.42	0.99
1:F:55:LYS:H	1:F:58:GLN:NE2	1.62	0.98
1:F:55:LYS:H	1:F:58:GLN:HE21	1.10	0.98
1:I:55:LYS:H	1:I:58:GLN:NE2	1.60	0.98
1:K:55:LYS:H	1:K:58:GLN:HE21	1.04	0.95
1:H:163:THR:HG22	1:H:165:ARG:H	1.31	0.95
1:L:499:PHE:HZ	1:L:502:GLU:HG2	1.28	0.95
1:B:1:MET:HE3	1:B:137:LEU:HD11	1.49	0.94
1:A:55:LYS:HB2	1:A:58:GLN:HE21	1.33	0.94
1:G:27:ARG:NH2	1:G:81:GLU:HG3	1.82	0.93
1:G:85:ASP:H	1:G:88:GLN:HE21	1.04	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:27:ARG:NH2	1:C:81:GLU:HG3	1.82	0.93
1:H:82:ARG:HA	1:H:116:HIS:HD2	1.34	0.93
1:C:82:ARG:CZ	1:C:116:HIS:CE1	2.54	0.91
1:I:55:LYS:H	1:I:58:GLN:HE21	1.04	0.91
1:F:55:LYS:N	1:F:58:GLN:HE21	1.70	0.90
1:J:304:MET:HE2	1:J:304:MET:HA	1.54	0.90
1:K:305:ARG:HG2	1:K:305:ARG:HH11	1.35	0.90
1:H:257:ASN:C	1:H:257:ASN:HD22	1.79	0.89
1:L:172:ARG:HD3	1:L:502:GLU:OE2	1.72	0.89
1:A:333:ARG:HG2	1:A:333:ARG:HH11	1.37	0.88
1:F:110:CYS:HB2	1:F:157:MET:HE2	1.56	0.88
1:L:263:ARG:NH1	1:L:372:GLU:HG2	1.89	0.88
1:A:500:ASN:HD22	1:A:501:GLY:N	1.71	0.88
1:C:86:GLU:OE2	1:C:120:ARG:HD2	1.72	0.88
1:E:27:ARG:NH2	1:E:81:GLU:HG3	1.88	0.88
1:B:49:ARG:HH22	1:F:71:GLU:HB2	1.40	0.86
1:I:53:GLU:HG2	1:K:151:ARG:HH12	1.40	0.85
1:I:55:LYS:N	1:I:58:GLN:HE21	1.73	0.85
1:B:55:LYS:HB2	1:B:58:GLN:HE21	1.40	0.85
1:B:110:CYS:HB2	1:B:157:MET:HE2	1.57	0.85
1:J:27:ARG:HH12	1:J:81:GLU:HG3	1.42	0.85
1:J:257:ASN:C	1:J:257:ASN:HD22	1.82	0.85
1:H:148:SER:O	1:H:149:GLU:HG2	1.78	0.84
1:F:33:GLU:HB3	5:F:938:HOH:O	1.76	0.84
1:J:146:ASN:HB2	5:L:798:HOH:O	1.77	0.84
1:B:82:ARG:HH21	1:B:116:HIS:CE1	1.94	0.83
1:H:161:VAL:HB	1:H:166:GLU:HB2	1.60	0.83
1:L:163:THR:HG22	1:L:164:ARG:N	1.94	0.83
1:D:221:ARG:HH21	1:D:253:GLU:CD	1.86	0.83
1:J:257:ASN:ND2	1:J:259:SER:H	1.76	0.83
1:D:304:MET:HE1	1:D:316:VAL:CG1	2.08	0.82
1:K:55:LYS:H	1:K:58:GLN:NE2	1.77	0.82
1:G:85:ASP:H	1:G:88:GLN:NE2	1.76	0.82
1:G:148:SER:O	1:G:149:GLU:HG2	1.79	0.82
1:B:167:LEU:O	1:B:171:GLU:HG3	1.80	0.82
1:I:76:ILE:HD13	1:I:96:THR:OG1	1.80	0.82
1:J:146:ASN:O	1:J:147:LYS:O	1.97	0.82
1:G:151:ARG:HD3	1:G:153:PRO:HD3	1.60	0.81
1:D:304:MET:HE1	1:D:316:VAL:HG11	1.62	0.81
1:A:304:MET:HE1	1:A:316:VAL:HG11	1.62	0.81
1:B:27:ARG:HH22	1:B:81:GLU:CG	1.93	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:257:ASN:ND2	1:I:259:SER:H	1.77	0.81
1:I:1:MET:HE3	1:I:137:LEU:HD11	1.61	0.81
1:J:53:GLU:HB3	1:J:58:GLN:HE22	1.45	0.80
1:K:55:LYS:N	1:K:58:GLN:HE21	1.79	0.80
1:K:27:ARG:HH22	1:K:81:GLU:HG3	1.46	0.80
1:K:1:MET:HE3	1:K:137:LEU:HD11	1.64	0.80
1:B:53:GLU:HG2	1:F:151:ARG:HH12	1.46	0.80
1:H:82:ARG:HA	1:H:116:HIS:CD2	2.16	0.80
1:B:257:ASN:C	1:B:257:ASN:HD22	1.89	0.80
1:B:257:ASN:HD22	1:B:258:ALA:N	1.80	0.79
1:B:27:ARG:NH2	1:B:81:GLU:HG3	1.95	0.79
1:G:27:ARG:HH22	1:G:81:GLU:HG3	1.48	0.79
1:A:148:SER:O	1:A:149:GLU:HG2	1.84	0.78
1:J:114:GLU:HG3	5:J:751:HOH:O	1.82	0.78
1:B:141:ASP:HB3	1:B:147:LYS:HD3	1.65	0.78
1:H:1:MET:HE3	1:H:137:LEU:HD11	1.64	0.78
1:I:395:LEU:HD12	1:I:396:MET:N	1.97	0.78
1:C:305:ARG:HD2	5:C:811:HOH:O	1.83	0.77
1:K:193:MET:CE	1:K:197:ILE:HG21	2.13	0.77
1:G:364:THR:O	1:G:367:GLU:HG2	1.84	0.77
1:L:148:SER:O	1:L:149:GLU:HG2	1.85	0.77
1:C:27:ARG:HH22	1:C:81:GLU:HG3	1.49	0.77
1:H:162:PRO:HD2	1:H:166:GLU:HG3	1.67	0.76
1:L:499:PHE:CZ	1:L:502:GLU:HG2	2.17	0.76
1:L:5:VAL:O	1:L:6:LYS:HG3	1.85	0.76
1:L:304:MET:HE1	1:L:316:VAL:HG11	1.68	0.76
1:D:148:SER:O	1:D:149:GLU:HG2	1.85	0.75
1:K:27:ARG:NH2	1:K:81:GLU:HG3	2.01	0.75
1:G:141:ASP:O	1:G:147:LYS:HE2	1.85	0.75
1:I:53:GLU:CG	1:K:151:ARG:HH12	1.98	0.75
1:E:55:LYS:H	1:E:58:GLN:NE2	1.84	0.75
1:B:85:ASP:H	1:B:88:GLN:HE21	1.35	0.75
1:H:257:ASN:HD22	1:H:258:ALA:N	1.85	0.75
1:F:257:ASN:HD22	1:F:258:ALA:N	1.85	0.75
1:E:55:LYS:N	1:E:58:GLN:HE21	1.85	0.74
1:G:93:ILE:HD13	1:G:129:ALA:CB	2.17	0.74
1:L:20:VAL:HG23	1:L:75:LEU:HD13	1.70	0.74
1:G:53:GLU:HG2	1:J:151:ARG:HH12	1.52	0.74
1:I:257:ASN:HD21	1:I:259:SER:HB3	1.50	0.74
1:A:241:GLN:HG3	5:A:880:HOH:O	1.88	0.74
1:F:304:MET:HE1	1:F:316:VAL:CG1	2.18	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:304:MET:HE1	1:L:316:VAL:CG1	2.18	0.73
1:G:221:ARG:HH21	1:G:253:GLU:CD	1.97	0.73
1:K:89:TYR:CZ	1:K:93:ILE:HD11	2.24	0.73
1:L:47:LEU:HD22	1:L:52:LEU:HB3	1.69	0.73
1:D:257:ASN:ND2	1:D:259:SER:H	1.87	0.73
1:A:55:LYS:HB2	1:A:58:GLN:NE2	2.02	0.72
1:B:110:CYS:HB2	1:B:157:MET:CE	2.18	0.72
1:K:305:ARG:HG2	1:K:305:ARG:NH1	2.02	0.72
1:J:27:ARG:NH1	1:J:81:GLU:HG3	2.04	0.72
1:J:304:MET:HE2	1:J:304:MET:CA	2.19	0.72
1:C:76:ILE:HD13	1:C:96:THR:OG1	1.90	0.72
1:B:82:ARG:NH2	1:B:116:HIS:CE1	2.57	0.72
1:F:148:SER:O	1:F:149:GLU:HG2	1.89	0.72
1:F:30:PRO:HA	1:F:33:GLU:CG	2.18	0.72
1:F:257:ASN:HD22	1:F:257:ASN:C	1.96	0.72
1:J:82:ARG:C	1:J:84:LEU:H	1.97	0.72
1:I:330:ARG:NH1	5:I:701:HOH:O	2.21	0.72
1:E:475:SER:HB2	5:E:731:HOH:O	1.90	0.72
1:L:55:LYS:H	1:L:58:GLN:NE2	1.87	0.72
1:C:304:MET:HE1	1:C:316:VAL:HG12	1.71	0.71
1:C:164:ARG:NH1	1:C:164:ARG:HB3	2.06	0.71
1:K:85:ASP:H	1:K:88:GLN:HE21	1.36	0.71
1:A:474:ARG:HH11	1:A:474:ARG:HG2	1.54	0.71
1:E:404:HIS:HB3	5:E:990:HOH:O	1.90	0.71
1:B:49:ARG:NH2	1:F:71:GLU:HB2	2.05	0.71
1:H:304:MET:HE1	1:H:316:VAL:HG11	1.73	0.71
1:A:257:ASN:HD22	1:A:258:ALA:N	1.88	0.71
1:J:148:SER:O	1:J:149:GLU:HG2	1.90	0.71
1:A:257:ASN:HD22	1:A:257:ASN:C	1.99	0.70
1:B:257:ASN:ND2	1:B:259:SER:H	1.89	0.70
1:C:263:ARG:HG3	1:C:263:ARG:HH11	1.54	0.70
1:H:304:MET:HE1	1:H:316:VAL:CG1	2.21	0.70
1:I:148:SER:O	1:I:149:GLU:HG2	1.90	0.70
1:L:1:MET:HE3	1:L:137:LEU:HD11	1.72	0.70
1:A:172:ARG:HD3	1:A:499:PHE:HE1	1.54	0.70
1:E:39:SER:O	1:E:40:ASP:HB2	1.92	0.70
1:E:55:LYS:H	1:E:58:GLN:HE21	1.40	0.70
1:F:221:ARG:HG2	1:F:221:ARG:HH11	1.57	0.70
1:C:304:MET:HE3	1:C:318:GLY:HA3	1.72	0.70
1:L:82:ARG:NH1	1:L:116:HIS:NE2	2.39	0.70
1:L:309:GLU:HG2	5:L:934:HOH:O	1.90	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:307:VAL:HG23	1:A:312:LEU:HD12	1.73	0.69
1:C:395:LEU:HD12	1:C:396:MET:N	2.07	0.69
1:G:1:MET:HE1	1:G:154:LEU:HD23	1.73	0.69
1:G:85:ASP:OD1	1:G:88:GLN:HG3	1.91	0.69
1:B:162:PRO:HD2	1:B:166:GLU:HG3	1.74	0.69
1:H:257:ASN:ND2	1:H:259:SER:H	1.90	0.69
1:L:44:SER:O	1:L:48:ARG:HG3	1.92	0.69
1:G:146:ASN:O	1:G:147:LYS:HG2	1.92	0.69
1:I:194:PRO:HD3	5:I:811:HOH:O	1.91	0.69
1:K:33:GLU:OE2	1:K:37:LYS:HE3	1.93	0.69
1:J:89:TYR:CZ	1:J:93:ILE:HD11	2.28	0.69
1:K:172:ARG:HD2	1:K:502:GLU:OE2	1.93	0.69
1:D:311:GLN:HG2	5:D:894:HOH:O	1.93	0.68
1:D:364:THR:O	1:D:367:GLU:HG2	1.93	0.68
1:L:257:ASN:C	1:L:257:ASN:HD22	1.98	0.68
1:K:364:THR:O	1:K:367:GLU:HG2	1.93	0.68
1:E:20:VAL:HG23	1:E:75:LEU:HD13	1.76	0.68
1:H:85:ASP:OD1	1:H:88:GLN:HG3	1.94	0.68
1:L:66:PRO:O	1:L:68:VAL:HG23	1.92	0.68
1:A:305:ARG:HG2	1:A:305:ARG:HH11	1.58	0.68
1:L:163:THR:HB	1:L:166:GLU:OE2	1.94	0.68
1:J:193:MET:HE3	1:J:194:PRO:HD2	1.74	0.67
1:F:333:ARG:HG2	1:F:333:ARG:HH11	1.60	0.67
1:G:257:ASN:HD22	1:G:259:SER:H	1.40	0.67
1:B:148:SER:O	1:B:149:GLU:HG2	1.94	0.67
1:A:364:THR:O	1:A:367:GLU:HG2	1.94	0.67
1:D:1:MET:HE3	1:D:137:LEU:HD11	1.75	0.67
1:E:148:SER:O	1:E:149:GLU:HG2	1.94	0.67
1:H:164:ARG:HB3	1:H:164:ARG:NH1	2.09	0.67
1:B:55:LYS:CB	1:B:58:GLN:HE21	2.08	0.67
1:B:55:LYS:H	1:B:58:GLN:NE2	1.92	0.67
1:C:141:ASP:O	1:C:147:LYS:HE2	1.94	0.67
1:C:194:PRO:HD3	5:C:737:HOH:O	1.94	0.67
1:C:364:THR:O	1:C:367:GLU:HG2	1.95	0.67
1:D:76:ILE:HD13	1:D:96:THR:OG1	1.94	0.67
1:L:26:ARG:HH21	1:L:53:GLU:CG	2.02	0.67
1:A:20:VAL:HG23	1:A:75:LEU:HD13	1.77	0.66
1:L:184:ILE:O	1:L:188:LYS:HG3	1.95	0.66
1:D:267:LEU:HD12	1:D:304:MET:HE3	1.77	0.66
1:B:304:MET:HE1	1:B:316:VAL:HG12	1.76	0.66
1:D:55:LYS:H	1:D:58:GLN:HE21	1.42	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:135:GLU:OE2	1:H:188:LYS:NZ	2.29	0.66
1:H:307:VAL:HG23	1:H:312:LEU:HD12	1.77	0.66
1:J:144:LYS:O	1:J:147:LYS:HE3	1.96	0.66
1:J:333:ARG:HD2	1:J:333:ARG:N	2.11	0.66
1:E:364:THR:O	1:E:367:GLU:HG2	1.96	0.66
1:H:257:ASN:C	1:H:257:ASN:ND2	2.52	0.66
1:D:23:PHE:CE1	1:D:81:GLU:HA	2.31	0.66
1:D:53:GLU:HB2	1:D:58:GLN:HE22	1.60	0.66
1:I:488:LEU:C	1:I:488:LEU:HD23	2.21	0.66
1:G:122:ASN:HD21	1:G:161:VAL:HG12	1.62	0.65
1:K:53:GLU:HB2	1:K:58:GLN:HE22	1.60	0.65
1:C:1:MET:HE1	1:C:154:LEU:HD23	1.78	0.65
1:G:257:ASN:ND2	1:G:259:SER:H	1.92	0.65
1:K:120:ARG:HD3	1:K:128:GLN:HE22	1.61	0.65
1:K:34:GLN:O	1:K:38:ILE:HG12	1.96	0.65
1:L:82:ARG:HD2	1:L:116:HIS:CD2	2.32	0.65
1:L:141:ASP:HB3	1:L:147:LYS:HD3	1.77	0.65
1:C:124:TRP:CH2	1:C:128:GLN:HG2	2.32	0.65
1:E:146:ASN:O	1:E:147:LYS:O	2.14	0.65
1:I:34:GLN:O	1:I:38:ILE:HG12	1.96	0.65
1:C:103:THR:CG2	1:C:105:SER:H	2.04	0.65
1:A:82:ARG:HA	1:A:116:HIS:HD2	1.62	0.65
1:J:68:VAL:HG12	1:J:70:SER:H	1.61	0.65
1:C:257:ASN:HD22	1:C:258:ALA:N	1.95	0.64
1:E:305:ARG:HH11	1:E:305:ARG:HG2	1.63	0.64
1:H:120:ARG:HD3	1:H:128:GLN:HE22	1.61	0.64
1:J:257:ASN:HD22	1:J:258:ALA:N	1.95	0.64
1:K:164:ARG:HG3	1:K:167:LEU:HD12	1.80	0.64
1:H:221:ARG:NH2	1:H:253:GLU:OE2	2.25	0.64
1:K:73:ILE:HG22	1:K:75:LEU:HD22	1.78	0.64
1:K:172:ARG:HD3	1:K:499:PHE:HE1	1.63	0.64
1:I:263:ARG:CB	1:I:372:GLU:HB2	2.28	0.64
1:K:475:SER:HB3	5:K:796:HOH:O	1.98	0.64
1:B:304:MET:HE1	1:B:316:VAL:CG1	2.27	0.64
1:E:68:VAL:HG12	1:E:70:SER:H	1.62	0.64
1:F:304:MET:HE1	1:F:316:VAL:HG11	1.79	0.64
1:C:90:LYS:HE2	1:C:128:GLN:CD	2.23	0.64
1:D:488:LEU:C	1:D:488:LEU:HD23	2.22	0.64
1:A:23:PHE:CE2	1:A:81:GLU:HG2	2.32	0.64
1:E:184:ILE:O	1:E:188:LYS:HG3	1.97	0.64
1:F:82:ARG:HA	1:F:116:HIS:CD2	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:73:ILE:HG22	1:L:75:LEU:HD22	1.80	0.64
1:L:42:TYR:CD2	1:L:65:VAL:HG13	2.32	0.63
1:I:421:PRO:HD3	1:J:418:TRP:CE2	2.33	0.63
1:B:32:ALA:O	1:B:35:LEU:HB3	1.99	0.63
1:D:28:LEU:HG	1:D:32:ALA:HB3	1.80	0.63
1:K:27:ARG:HH22	1:K:81:GLU:CG	2.12	0.63
1:F:1:MET:HE3	1:F:137:LEU:HD11	1.81	0.63
1:H:81:GLU:O	1:H:83:GLU:HG3	1.98	0.63
1:E:305:ARG:NH2	5:E:701:HOH:O	2.32	0.63
1:B:468:ILE:HG21	1:B:485:PRO:HD3	1.80	0.63
1:J:82:ARG:NH1	1:J:116:HIS:CE1	2.66	0.63
1:K:395:LEU:HD12	1:K:396:MET:N	2.13	0.63
1:L:90:LYS:NZ	5:L:702:HOH:O	2.31	0.63
1:A:27:ARG:HH22	1:A:81:GLU:HG3	1.63	0.63
1:G:305:ARG:HG2	1:G:305:ARG:HH11	1.62	0.63
1:L:172:ARG:HD3	1:L:502:GLU:CD	2.24	0.63
1:D:193:MET:HE3	1:D:194:PRO:HD2	1.80	0.63
1:H:9:SER:O	1:H:13:GLN:HG2	1.99	0.62
1:H:23:PHE:CZ	1:H:81:GLU:HG2	2.34	0.62
1:A:500:ASN:HD22	1:A:501:GLY:H	1.45	0.62
1:E:121:ASN:HD22	1:E:503:GLU:HG2	1.64	0.62
1:E:257:ASN:HD22	1:E:259:SER:H	1.47	0.62
1:I:76:ILE:CD1	1:I:96:THR:OG1	2.47	0.62
1:B:55:LYS:HB2	1:B:58:GLN:NE2	2.14	0.62
1:H:32:ALA:O	1:H:35:LEU:N	2.32	0.62
1:H:468:ILE:HG21	1:H:485:PRO:HD3	1.82	0.62
1:I:55:LYS:HB2	1:I:58:GLN:HE21	1.64	0.62
1:B:55:LYS:H	1:B:58:GLN:HE21	1.47	0.62
1:I:151:ARG:HD3	1:I:153:PRO:HD3	1.82	0.62
1:J:221:ARG:NH2	1:J:253:GLU:OE2	2.33	0.62
1:K:194:PRO:HD3	5:K:769:HOH:O	1.98	0.62
1:A:23:PHE:CZ	1:A:81:GLU:HG2	2.34	0.62
1:A:305:ARG:HG2	1:A:305:ARG:NH1	2.15	0.62
1:A:305:ARG:HD2	5:A:852:HOH:O	2.00	0.62
1:A:474:ARG:HG2	1:A:474:ARG:NH1	2.15	0.62
1:A:27:ARG:NH2	1:A:81:GLU:HG3	2.15	0.62
1:A:221:ARG:HH21	1:A:253:GLU:CD	2.07	0.62
1:C:82:ARG:C	1:C:84:LEU:H	2.07	0.62
1:J:257:ASN:HD21	1:J:259:SER:HB3	1.63	0.62
1:A:94:GLN:HG3	1:A:136:THR:OG1	1.99	0.62
1:D:32:ALA:O	1:D:35:LEU:N	2.33	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:73:ILE:HG22	1:B:75:LEU:HD22	1.80	0.61
1:F:50:GLY:HA2	5:F:795:HOH:O	1.99	0.61
1:E:20:VAL:CG2	1:E:75:LEU:HD13	2.30	0.61
1:F:30:PRO:CA	1:F:33:GLU:HG3	2.26	0.61
1:F:304:MET:HE1	1:F:316:VAL:HG12	1.81	0.61
1:J:10:PRO:HG2	1:J:31:ILE:CG2	2.30	0.61
1:F:82:ARG:HA	1:F:116:HIS:HD2	1.64	0.61
1:L:372:GLU:CD	1:L:496:ARG:HH12	2.08	0.61
1:D:257:ASN:C	1:D:257:ASN:HD22	2.08	0.61
1:K:55:LYS:O	1:K:58:GLN:HG3	2.00	0.61
1:A:166:GLU:H	1:A:166:GLU:CD	2.09	0.61
1:B:34:GLN:O	1:B:38:ILE:HG12	2.00	0.61
1:C:475:SER:HB3	5:C:791:HOH:O	2.00	0.61
1:D:221:ARG:NH2	1:D:253:GLU:OE2	2.27	0.61
1:B:501:GLY:C	1:B:503:GLU:H	2.07	0.61
1:B:303:VAL:O	1:B:307:VAL:HG12	1.99	0.61
1:C:92:VAL:CG1	1:C:112:LEU:HD13	2.31	0.61
1:G:151:ARG:HE	1:G:153:PRO:CG	2.14	0.61
1:J:304:MET:HE1	1:J:316:VAL:HG11	1.83	0.61
1:I:1:MET:HE1	1:I:154:LEU:HD23	1.83	0.60
1:F:194:PRO:HB2	1:F:196:ASN:HB3	1.82	0.60
1:G:27:ARG:HH22	1:G:81:GLU:CG	2.14	0.60
1:J:257:ASN:HD22	1:J:259:SER:H	1.49	0.60
1:C:82:ARG:NE	1:C:116:HIS:CE1	2.69	0.60
1:C:103:THR:HG22	1:C:105:SER:N	2.03	0.60
1:I:55:LYS:HB2	1:I:58:GLN:NE2	2.16	0.60
1:F:110:CYS:HB2	1:F:157:MET:CE	2.30	0.60
1:J:21:GLY:O	1:J:29:SER:HB2	2.02	0.60
1:E:6:LYS:HD2	1:E:158:VAL:HG11	1.82	0.60
1:H:59:THR:HG22	1:H:76:ILE:HG12	1.83	0.60
1:L:146:ASN:O	1:L:147:LYS:O	2.17	0.60
1:C:45:ALA:HA	1:C:48:ARG:NH1	2.17	0.60
1:F:395:LEU:HD12	1:F:396:MET:N	2.16	0.60
1:G:53:GLU:HG2	1:J:151:ARG:NH1	2.16	0.60
1:G:221:ARG:NH2	1:G:253:GLU:OE2	2.30	0.60
1:L:224:GLY:HA2	1:L:248:LEU:HD23	1.84	0.60
1:L:395:LEU:HD12	1:L:396:MET:N	2.17	0.60
1:A:73:ILE:HG22	1:A:75:LEU:HD22	1.82	0.60
1:B:410:SER:HB2	1:B:416:ARG:HA	1.84	0.60
1:C:14:ARG:HE	1:C:69:LEU:HD13	1.67	0.60
1:D:184:ILE:O	1:D:188:LYS:HG3	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:263:ARG:HB3	1:I:372:GLU:HB2	1.84	0.60
1:L:82:ARG:C	1:L:84:LEU:H	2.10	0.60
1:F:184:ILE:O	1:F:188:LYS:HG3	2.00	0.60
1:D:304:MET:HE1	1:D:316:VAL:HG12	1.83	0.60
1:E:30:PRO:HA	1:E:33:GLU:HG3	1.83	0.60
1:D:24:GLU:OE2	1:D:55:LYS:HG2	2.02	0.59
1:F:193:MET:HE1	1:F:197:ILE:HG21	1.83	0.59
1:F:372:GLU:OE1	1:F:496:ARG:NH1	2.32	0.59
1:I:55:LYS:CB	1:I:58:GLN:HE21	2.15	0.59
1:D:146:ASN:O	1:D:147:LYS:HG3	2.01	0.59
1:E:311:GLN:HG2	5:E:919:HOH:O	2.02	0.59
1:F:221:ARG:HG2	1:F:221:ARG:NH1	2.16	0.59
1:G:93:ILE:HD13	1:G:129:ALA:HB2	1.83	0.59
1:H:49:ARG:NH2	1:L:64:HIS:NE2	2.50	0.59
1:J:333:ARG:HD3	1:J:336:ASP:OD1	2.01	0.59
1:K:84:LEU:HD12	1:K:88:GLN:HB2	1.84	0.59
1:L:257:ASN:HD22	1:L:258:ALA:N	2.00	0.59
1:F:34:GLN:O	1:F:38:ILE:HG12	2.03	0.59
1:D:55:LYS:HB2	1:D:58:GLN:HE21	1.68	0.59
1:K:263:ARG:HB2	1:K:372:GLU:HB2	1.84	0.59
1:E:263:ARG:HB2	1:E:372:GLU:HB2	1.84	0.59
1:J:20:VAL:HG23	1:J:75:LEU:HD13	1.84	0.59
1:L:216:LYS:NZ	1:L:311:GLN:NE2	2.50	0.59
1:L:333:ARG:HD2	1:L:336:ASP:OD1	2.02	0.59
1:A:304:MET:HE1	1:A:316:VAL:CG1	2.32	0.59
1:C:101:ASN:O	1:C:151:ARG:HD3	2.03	0.59
1:K:257:ASN:C	1:K:257:ASN:HD22	2.09	0.59
1:C:146:ASN:O	1:C:147:LYS:O	2.21	0.59
1:F:55:LYS:HB2	1:F:58:GLN:NE2	2.18	0.59
1:J:474:ARG:HG2	1:J:474:ARG:HH11	1.67	0.59
1:K:479:LYS:HE3	5:K:905:HOH:O	2.02	0.59
1:A:167:LEU:O	1:A:171:GLU:HG3	2.03	0.58
1:B:85:ASP:H	1:B:88:GLN:NE2	1.99	0.58
1:D:151:ARG:HD3	1:D:153:PRO:HD3	1.85	0.58
1:I:224:GLY:HA2	1:I:248:LEU:HD23	1.84	0.58
1:B:116:HIS:HB2	5:B:837:HOH:O	2.02	0.58
1:K:84:LEU:CD1	1:K:88:GLN:HB2	2.33	0.58
1:F:11:GLU:OE2	1:F:34:GLN:NE2	2.37	0.58
1:H:14:ARG:HG2	1:H:69:LEU:HB3	1.85	0.58
1:L:45:ALA:HA	1:L:48:ARG:NH1	2.19	0.58
1:L:163:THR:CG2	1:L:164:ARG:H	1.91	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:141:ASP:HB3	1:F:147:LYS:HD3	1.84	0.58
1:J:488:LEU:C	1:J:488:LEU:HD23	2.27	0.58
1:A:500:ASN:ND2	1:A:501:GLY:N	2.49	0.58
1:E:53:GLU:HB3	1:E:58:GLN:HE22	1.67	0.58
1:K:488:LEU:HD23	1:K:488:LEU:C	2.28	0.58
1:L:257:ASN:ND2	1:L:259:SER:H	2.02	0.58
1:B:20:VAL:HG23	1:B:75:LEU:HD13	1.86	0.58
1:C:488:LEU:C	1:C:488:LEU:HD23	2.27	0.58
1:E:1:MET:HE1	1:E:154:LEU:HD23	1.85	0.58
1:F:93:ILE:HD13	1:F:129:ALA:CB	2.33	0.58
1:K:172:ARG:HD3	1:K:499:PHE:CE1	2.38	0.58
1:E:74:LEU:HG	1:E:76:ILE:CD1	2.34	0.57
1:E:337:VAL:O	1:F:196:ASN:ND2	2.37	0.57
1:G:263:ARG:HB2	1:G:372:GLU:HB2	1.86	0.57
1:B:184:ILE:O	1:B:188:LYS:HG3	2.04	0.57
1:J:90:LYS:HE2	1:J:128:GLN:CD	2.28	0.57
1:G:167:LEU:O	1:G:171:GLU:HG3	2.04	0.57
1:G:305:ARG:HG2	1:G:305:ARG:NH1	2.20	0.57
1:J:166:GLU:N	1:J:166:GLU:OE1	2.37	0.57
1:J:263:ARG:NH1	1:J:372:GLU:HG2	2.19	0.57
1:K:114:GLU:OE2	1:K:160:ASN:ND2	2.31	0.57
1:E:121:ASN:ND2	1:E:503:GLU:HG2	2.19	0.57
1:G:27:ARG:HH21	1:G:81:GLU:HG3	1.68	0.57
1:A:81:GLU:O	1:A:83:GLU:HG3	2.04	0.57
1:B:20:VAL:CG2	1:B:75:LEU:HD13	2.35	0.57
1:B:87:ARG:O	1:B:91:GLN:HG3	2.05	0.57
1:D:10:PRO:HG2	1:D:31:ILE:HG22	1.87	0.57
1:J:122:ASN:HD21	1:J:161:VAL:HG12	1.68	0.57
1:D:5:VAL:O	1:D:6:LYS:HG3	2.04	0.57
1:F:193:MET:CE	1:F:197:ILE:HG21	2.35	0.57
1:A:4:SER:OG	1:A:158:VAL:HG22	2.04	0.57
1:H:306:MET:HE3	1:H:307:VAL:N	2.20	0.57
1:D:257:ASN:HD22	1:D:259:SER:H	1.51	0.57
1:F:27:ARG:HH22	1:F:81:GLU:HG3	1.69	0.57
1:A:164:ARG:HH11	1:A:164:ARG:HB3	1.70	0.56
1:A:188:LYS:HE2	5:A:713:HOH:O	2.04	0.56
1:C:55:LYS:HD2	1:C:58:GLN:NE2	2.20	0.56
1:I:416:ARG:HD2	5:I:734:HOH:O	2.04	0.56
1:A:1:MET:HE3	1:A:137:LEU:HD11	1.86	0.56
1:C:82:ARG:O	1:C:84:LEU:N	2.33	0.56
1:C:193:MET:CE	1:C:197:ILE:HG21	2.34	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:4:SER:OG	1:D:158:VAL:HG22	2.04	0.56
1:H:163:THR:HG22	1:H:164:ARG:N	2.20	0.56
1:I:141:ASP:HB3	1:I:147:LYS:HD3	1.86	0.56
1:J:55:LYS:H	1:J:58:GLN:HE21	1.52	0.56
1:A:25:PRO:O	1:A:27:ARG:N	2.39	0.56
1:C:304:MET:HE3	1:C:318:GLY:CA	2.36	0.56
1:D:14:ARG:NE	1:D:69:LEU:HD13	2.20	0.56
1:D:89:TYR:CZ	1:D:93:ILE:HD11	2.41	0.56
1:E:224:GLY:HA2	1:E:248:LEU:HD23	1.88	0.56
1:F:121:ASN:O	1:F:125:LYS:HG3	2.04	0.56
1:H:502:GLU:HG2	1:H:502:GLU:O	2.05	0.56
1:A:163:THR:HG23	1:A:166:GLU:OE2	2.06	0.56
1:I:195:PRO:HB3	1:I:274:PHE:HB2	1.87	0.56
1:D:93:ILE:HD13	1:D:129:ALA:CB	2.35	0.56
1:J:141:ASP:HB3	1:J:147:LYS:HD3	1.88	0.56
1:C:305:ARG:NH1	1:C:305:ARG:HG2	2.19	0.56
1:D:24:GLU:OE1	1:D:80:LYS:HE2	2.06	0.56
1:H:161:VAL:HB	1:H:166:GLU:CB	2.33	0.56
1:J:221:ARG:HH21	1:J:253:GLU:CD	2.13	0.56
1:K:86:GLU:OE2	1:K:120:ARG:HD2	2.06	0.56
1:E:1:MET:HE3	1:E:137:LEU:HD11	1.87	0.56
1:H:53:GLU:HG3	1:L:151:ARG:NH2	2.20	0.56
1:I:257:ASN:HD22	1:I:259:SER:H	1.50	0.56
1:K:167:LEU:O	1:K:171:GLU:HG3	2.06	0.56
1:E:30:PRO:HA	1:E:33:GLU:CG	2.36	0.56
1:G:311:GLN:HG2	5:G:818:HOH:O	2.06	0.56
1:G:488:LEU:C	1:G:488:LEU:HD23	2.31	0.56
1:J:241:GLN:HG2	1:J:330:ARG:O	2.06	0.56
1:A:421:PRO:HD3	1:F:418:TRP:CE2	2.41	0.55
1:L:65:VAL:HG21	1:L:73:ILE:HD12	1.88	0.55
1:G:87:ARG:O	1:G:91:GLN:HG3	2.06	0.55
1:L:263:ARG:HH12	1:L:372:GLU:HG2	1.71	0.55
1:D:333:ARG:HD2	1:D:336:ASP:OD1	2.06	0.55
1:H:146:ASN:ND2	5:H:703:HOH:O	2.40	0.55
1:J:195:PRO:HB2	1:L:333:ARG:HD3	1.87	0.55
1:L:76:ILE:HD12	1:L:96:THR:OG1	2.07	0.55
1:A:45:ALA:HA	1:A:48:ARG:NH1	2.22	0.55
1:E:74:LEU:HG	1:E:76:ILE:HD12	1.89	0.55
1:H:163:THR:HG22	1:H:165:ARG:N	2.13	0.55
1:C:305:ARG:HG2	1:C:305:ARG:HH11	1.71	0.55
1:G:16:ALA:HA	1:G:71:GLU:CG	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:184:ILE:O	1:K:188:LYS:HG3	2.06	0.55
1:L:416:ARG:NH1	5:L:705:HOH:O	2.40	0.55
1:A:443:ARG:N	1:A:444:PRO:CD	2.70	0.55
1:C:79:GLY:C	1:C:80:LYS:HG3	2.30	0.55
1:F:108:ALA:HB3	1:F:157:MET:HE3	1.88	0.55
1:J:81:GLU:C	1:J:83:GLU:H	2.14	0.55
1:L:47:LEU:CD2	1:L:52:LEU:HB3	2.34	0.55
1:C:103:THR:CG2	1:C:104:GLY:N	2.70	0.55
1:E:257:ASN:ND2	1:E:259:SER:H	2.05	0.55
1:F:57:GLY:O	1:F:95:LYS:HE2	2.07	0.55
1:F:218:VAL:HA	1:F:253:GLU:O	2.07	0.55
1:L:500:ASN:O	1:L:503:GLU:HG2	2.07	0.55
1:G:141:ASP:HB3	1:G:147:LYS:HD3	1.89	0.55
1:K:502:GLU:C	1:K:503:GLU:HG2	2.32	0.55
1:E:11:GLU:HG2	1:E:12:LYS:HG3	1.88	0.54
1:D:395:LEU:HD12	1:D:396:MET:N	2.22	0.54
1:E:34:GLN:O	1:E:38:ILE:HG12	2.08	0.54
1:H:337:VAL:O	1:I:196:ASN:ND2	2.40	0.54
1:K:502:GLU:O	1:K:503:GLU:HG2	2.08	0.54
1:A:146:ASN:O	1:A:147:LYS:O	2.26	0.54
1:C:86:GLU:HG2	5:C:937:HOH:O	2.06	0.54
1:A:80:LYS:O	1:A:83:GLU:HB2	2.07	0.54
1:J:85:ASP:OD1	1:J:88:GLN:HG3	2.06	0.54
1:A:126:VAL:O	1:A:130:VAL:HG23	2.07	0.54
1:G:34:GLN:O	1:G:38:ILE:HG12	2.06	0.54
1:K:53:GLU:CB	1:K:58:GLN:HE22	2.20	0.54
1:L:503:GLU:OE1	1:L:503:GLU:HA	2.06	0.54
1:D:68:VAL:HG12	1:D:70:SER:H	1.72	0.54
1:G:304:MET:HE1	1:G:316:VAL:CG1	2.38	0.54
1:J:73:ILE:HG22	1:J:75:LEU:HD22	1.90	0.54
1:A:10:PRO:HG2	1:A:31:ILE:HG22	1.89	0.54
1:I:16:ALA:HA	1:I:71:GLU:HG3	1.89	0.54
1:J:88:GLN:HA	1:J:91:GLN:OE1	2.08	0.54
1:F:16:ALA:HA	1:F:71:GLU:HG2	1.90	0.54
1:J:22:VAL:HG22	1:J:28:LEU:HD12	1.89	0.54
1:J:124:TRP:CH2	1:J:128:GLN:HG2	2.43	0.54
1:K:119:GLY:C	1:K:120:ARG:HG2	2.32	0.54
1:A:81:GLU:O	1:A:83:GLU:N	2.40	0.54
1:C:151:ARG:O	1:C:152:ARG:HD3	2.08	0.54
1:J:196:ASN:ND2	1:L:337:VAL:O	2.41	0.54
1:K:257:ASN:HD22	1:K:258:ALA:N	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:434:PHE:HE2	1:L:479:LYS:HD2	1.72	0.54
1:C:364:THR:O	1:C:367:GLU:CG	2.56	0.53
1:K:76:ILE:CD1	1:K:96:THR:OG1	2.57	0.53
1:F:151:ARG:HE	1:F:153:PRO:HG2	1.73	0.53
1:F:500:ASN:HB2	1:F:503:GLU:O	2.07	0.53
1:L:123:TYR:CG	1:L:502:GLU:HB2	2.43	0.53
1:A:488:LEU:HD23	1:A:488:LEU:C	2.34	0.53
1:E:488:LEU:C	1:E:488:LEU:HD23	2.32	0.53
1:H:167:LEU:O	1:H:171:GLU:HG3	2.09	0.53
1:E:305:ARG:HG2	1:E:305:ARG:NH1	2.22	0.53
1:D:85:ASP:OD1	1:D:88:GLN:HG3	2.08	0.53
1:H:53:GLU:OE2	1:L:151:ARG:HG3	2.08	0.53
1:H:500:ASN:C	1:H:502:GLU:N	2.64	0.53
1:A:164:ARG:HB3	1:A:164:ARG:NH1	2.22	0.53
1:G:141:ASP:HB3	1:G:147:LYS:CD	2.39	0.53
1:I:87:ARG:O	1:I:91:GLN:HG3	2.09	0.53
1:K:93:ILE:HD13	1:K:129:ALA:CB	2.38	0.53
1:L:151:ARG:HD3	1:L:153:PRO:HD3	1.91	0.53
1:L:193:MET:CE	1:L:197:ILE:HG21	2.38	0.53
1:A:20:VAL:CG2	1:A:75:LEU:HD13	2.39	0.53
1:D:19:VAL:CG1	1:D:76:ILE:HD12	2.39	0.53
1:D:235:SER:HB3	1:D:361:ASP:OD2	2.09	0.53
1:J:257:ASN:C	1:J:257:ASN:ND2	2.56	0.53
1:L:73:ILE:HG22	1:L:75:LEU:CD2	2.39	0.53
1:L:80:LYS:O	1:L:83:GLU:HB2	2.08	0.53
1:C:82:ARG:CZ	1:C:116:HIS:HE1	2.17	0.53
1:D:38:ILE:HG22	1:D:67:ASN:HB2	1.91	0.53
1:H:23:PHE:CE2	1:H:81:GLU:HG2	2.44	0.53
1:L:216:LYS:NZ	1:L:311:GLN:HE22	2.07	0.53
1:A:74:LEU:HG	1:A:76:ILE:CD1	2.39	0.53
1:A:224:GLY:HA2	1:A:248:LEU:HD23	1.90	0.53
1:B:68:VAL:HA	5:B:709:HOH:O	2.07	0.53
1:B:503:GLU:HA	5:B:734:HOH:O	2.09	0.53
1:C:13:GLN:O	1:C:69:LEU:HB2	2.09	0.53
1:E:169:SER:HB2	1:E:502:GLU:CG	2.39	0.52
1:F:20:VAL:HG23	1:F:75:LEU:HD13	1.91	0.52
1:I:263:ARG:HB2	1:I:372:GLU:HB2	1.90	0.52
1:A:82:ARG:HA	1:A:116:HIS:CD2	2.44	0.52
1:B:65:VAL:HG21	1:B:73:ILE:HD12	1.92	0.52
1:C:27:ARG:HH22	1:C:81:GLU:CG	2.22	0.52
1:D:55:LYS:HB2	1:D:58:GLN:NE2	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:156:LYS:HD3	5:D:960:HOH:O	2.08	0.52
1:F:23:PHE:CZ	1:F:81:GLU:HG2	2.44	0.52
1:H:22:VAL:CG2	1:H:75:LEU:HD12	2.39	0.52
1:H:28:LEU:HG	1:H:29:SER:N	2.24	0.52
1:H:257:ASN:HD21	1:H:259:SER:H	1.57	0.52
1:H:305:ARG:HH11	1:H:305:ARG:HG2	1.74	0.52
1:J:10:PRO:HG2	1:J:31:ILE:HG22	1.91	0.52
1:C:100:LEU:O	1:C:103:THR:HB	2.09	0.52
1:G:146:ASN:O	1:G:147:LYS:O	2.27	0.52
1:G:395:LEU:HD12	1:G:466:LEU:HD23	1.92	0.52
1:L:19:VAL:HG11	1:L:96:THR:HG23	1.91	0.52
1:C:88:GLN:HB3	5:C:957:HOH:O	2.08	0.52
1:C:193:MET:CE	1:C:197:ILE:CG2	2.88	0.52
1:D:32:ALA:O	1:D:34:GLN:N	2.42	0.52
1:L:10:PRO:HD2	1:L:11:GLU:OE1	2.10	0.52
1:D:196:ASN:ND2	1:F:337:VAL:O	2.42	0.52
1:E:29:SER:O	1:E:32:ALA:HB3	2.10	0.52
1:E:157:MET:HE3	1:E:159:PHE:CE1	2.44	0.52
1:H:421:PRO:HD3	1:K:418:TRP:CE2	2.45	0.52
1:A:193:MET:HE1	1:A:197:ILE:HG21	1.92	0.52
1:J:257:ASN:HD21	1:J:259:SER:CB	2.23	0.52
1:C:19:VAL:CG1	1:C:76:ILE:HD12	2.40	0.52
1:C:193:MET:HE1	1:C:197:ILE:HG21	1.91	0.52
1:F:307:VAL:HG23	1:F:312:LEU:HD12	1.91	0.52
1:K:468:ILE:HG21	1:K:485:PRO:HD3	1.91	0.52
1:B:53:GLU:HB2	1:B:58:GLN:HE22	1.75	0.52
1:B:146:ASN:O	1:B:147:LYS:O	2.28	0.52
1:F:224:GLY:HA2	1:F:248:LEU:HD23	1.92	0.52
1:J:28:LEU:HG	1:J:32:ALA:CB	2.40	0.52
1:A:221:ARG:NH2	1:A:253:GLU:OE2	2.41	0.51
1:B:305:ARG:HD2	5:B:747:HOH:O	2.09	0.51
1:F:146:ASN:O	1:F:147:LYS:O	2.27	0.51
1:H:161:VAL:CB	1:H:166:GLU:HB2	2.36	0.51
1:L:65:VAL:HG13	1:L:66:PRO:HD2	1.93	0.51
1:G:73:ILE:HG22	1:G:75:LEU:HD22	1.91	0.51
1:H:18:ILE:HD11	1:H:35:LEU:HD21	1.91	0.51
1:A:38:ILE:HG22	1:A:38:ILE:O	2.10	0.51
1:B:85:ASP:CG	1:B:88:GLN:HG3	2.36	0.51
1:I:184:ILE:O	1:I:188:LYS:HG3	2.10	0.51
1:L:124:TRP:HH2	1:L:491:GLN:OE1	1.94	0.51
1:G:121:ASN:HD22	1:G:503:GLU:HG2	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:225:GLU:HG2	1:K:237:LEU:CD2	2.41	0.51
1:L:193:MET:HE3	1:L:197:ILE:CG2	2.41	0.51
1:B:144:LYS:NZ	5:B:708:HOH:O	2.44	0.51
1:E:33:GLU:O	1:E:37:LYS:HG3	2.11	0.51
1:F:392:ILE:HG21	1:F:418:TRP:HB2	1.93	0.51
1:J:257:ASN:ND2	1:J:259:SER:N	2.53	0.51
1:C:257:ASN:HD22	1:C:257:ASN:C	2.19	0.51
1:L:23:PHE:CE1	1:L:81:GLU:HA	2.46	0.51
1:A:87:ARG:HH22	1:F:428:GLU:CD	2.18	0.51
1:J:55:LYS:H	1:J:58:GLN:NE2	2.08	0.51
1:A:28:LEU:HD11	1:A:32:ALA:HB1	1.92	0.51
1:B:85:ASP:OD1	1:B:88:GLN:HG3	2.11	0.51
1:E:200:ALA:HB3	5:E:810:HOH:O	2.11	0.51
1:F:223:ILE:HD12	1:F:223:ILE:N	2.25	0.51
1:E:76:ILE:HG21	1:E:92:VAL:HG13	1.94	0.50
1:K:282:LYS:HE3	1:K:290:MET:SD	2.51	0.50
1:F:1:MET:HE1	1:F:154:LEU:HD23	1.93	0.50
1:J:305:ARG:NH1	1:J:309:GLU:OE1	2.35	0.50
1:C:304:MET:HE1	1:C:316:VAL:CG1	2.39	0.50
1:J:84:LEU:HD12	1:J:88:GLN:HB2	1.91	0.50
1:D:20:VAL:HG23	1:D:75:LEU:HD13	1.94	0.50
1:G:193:MET:CE	1:G:197:ILE:HG21	2.41	0.50
1:I:142:GLN:H	1:I:142:GLN:CD	2.17	0.50
1:C:148:SER:O	1:C:149:GLU:HG2	2.12	0.50
1:G:374:VAL:O	1:G:463:TRP:HA	2.11	0.50
1:J:85:ASP:H	1:J:88:GLN:HE21	1.59	0.50
1:L:84:LEU:CD2	1:L:115:LEU:HD13	2.41	0.50
1:E:30:PRO:O	1:E:33:GLU:HG3	2.11	0.50
1:K:85:ASP:H	1:K:88:GLN:NE2	2.05	0.50
1:K:193:MET:CE	1:K:197:ILE:CG2	2.87	0.50
1:L:199:ASN:C	1:L:273:THR:HG21	2.37	0.50
1:C:16:ALA:HA	1:C:71:GLU:HG3	1.93	0.50
1:C:28:LEU:HD11	1:C:32:ALA:HB1	1.94	0.50
1:D:193:MET:HE2	1:D:197:ILE:HG21	1.94	0.50
1:I:146:ASN:O	1:I:147:LYS:O	2.30	0.50
1:J:92:VAL:CG1	1:J:112:LEU:HD13	2.42	0.50
1:L:257:ASN:C	1:L:257:ASN:ND2	2.68	0.50
1:C:263:ARG:HG3	1:C:263:ARG:NH1	2.25	0.50
1:E:89:TYR:CE1	1:E:93:ILE:HD11	2.47	0.50
1:G:304:MET:HE1	1:G:316:VAL:HG12	1.94	0.50
1:H:93:ILE:HD12	1:H:129:ALA:CB	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:4:SER:HA	1:L:174:ILE:HD13	1.94	0.50
1:L:488:LEU:C	1:L:488:LEU:HD23	2.37	0.50
1:C:223:ILE:N	1:C:223:ILE:HD12	2.27	0.49
1:G:151:ARG:HE	1:G:153:PRO:HG3	1.77	0.49
1:H:141:ASP:O	1:H:147:LYS:HE3	2.11	0.49
1:K:259:SER:C	1:K:261:ASP:H	2.20	0.49
1:K:305:ARG:HH11	1:K:305:ARG:CG	2.15	0.49
1:H:53:GLU:HB2	1:H:58:GLN:HE22	1.76	0.49
1:L:41:GLY:O	1:L:45:ALA:HB2	2.12	0.49
1:L:304:MET:HE1	1:L:316:VAL:HG12	1.94	0.49
1:A:263:ARG:HB3	1:A:372:GLU:HB2	1.93	0.49
1:B:338:LEU:HD22	1:B:348:VAL:CG2	2.42	0.49
1:D:36:ASP:OD1	1:D:43:ILE:HB	2.12	0.49
1:D:193:MET:HE1	1:D:197:ILE:CD1	2.42	0.49
1:D:410:SER:HB2	1:D:415:ASP:O	2.13	0.49
1:G:193:MET:HE1	1:G:197:ILE:HG21	1.94	0.49
1:G:257:ASN:HD22	1:G:257:ASN:C	2.20	0.49
1:H:24:GLU:OE2	1:H:55:LYS:HA	2.13	0.49
1:K:221:ARG:HD2	5:K:845:HOH:O	2.11	0.49
1:K:330:ARG:NH1	5:K:706:HOH:O	2.44	0.49
1:B:195:PRO:HB3	1:B:274:PHE:HB2	1.94	0.49
1:B:474:ARG:HG2	1:B:474:ARG:HH11	1.77	0.49
1:D:468:ILE:HG21	1:D:485:PRO:HD3	1.94	0.49
1:F:488:LEU:HD23	1:F:488:LEU:C	2.38	0.49
1:H:52:LEU:CD2	1:H:75:LEU:HB3	2.42	0.49
1:H:164:ARG:HB3	1:H:164:ARG:CZ	2.42	0.49
1:H:294:MET:O	1:H:294:MET:HE2	2.13	0.49
1:J:47:LEU:HD22	1:J:52:LEU:HB3	1.94	0.49
1:A:356:ARG:HD2	1:A:439:ASN:O	2.12	0.49
1:D:226:GLN:O	1:D:230:GLU:HG3	2.11	0.49
1:F:85:ASP:OD1	1:F:88:GLN:HG3	2.12	0.49
1:H:23:PHE:CE1	1:H:81:GLU:HG2	2.48	0.49
1:L:28:LEU:HD11	1:L:32:ALA:HB1	1.94	0.49
1:L:82:ARG:CG	1:L:116:HIS:HD2	2.24	0.49
1:B:16:ALA:HA	1:B:71:GLU:CG	2.42	0.49
1:F:502:GLU:O	1:F:502:GLU:HG3	2.13	0.49
1:G:479:LYS:HD2	1:I:434:PHE:HE2	1.77	0.49
1:L:39:SER:O	1:L:40:ASP:HB2	2.11	0.49
1:L:101:ASN:HA	1:L:153:PRO:HD2	1.95	0.49
1:B:28:LEU:HG	1:B:32:ALA:HB3	1.94	0.49
1:C:23:PHE:CE1	1:C:81:GLU:HA	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:223:ILE:N	1:E:223:ILE:HD12	2.27	0.49
1:G:53:GLU:CG	1:J:151:ARG:HH12	2.21	0.49
1:H:45:ALA:O	1:H:48:ARG:HB2	2.13	0.49
1:I:304:MET:HE1	1:I:316:VAL:CG1	2.43	0.49
1:K:337:VAL:O	1:L:196:ASN:ND2	2.46	0.49
1:L:167:LEU:O	1:L:171:GLU:HG3	2.13	0.49
1:L:416:ARG:HG3	5:L:854:HOH:O	2.12	0.49
1:A:257:ASN:C	1:A:257:ASN:ND2	2.66	0.49
1:C:84:LEU:O	1:C:118:LYS:HG3	2.13	0.49
1:G:196:ASN:HB2	1:I:336:ASP:OD1	2.12	0.49
1:G:225:GLU:HG2	1:G:237:LEU:CD2	2.42	0.49
1:H:418:TRP:CE2	1:K:421:PRO:HD3	2.47	0.49
1:D:479:LYS:HE3	5:D:928:HOH:O	2.13	0.49
1:G:16:ALA:HA	1:G:71:GLU:HG3	1.95	0.49
1:A:418:TRP:CE2	1:F:421:PRO:HD3	2.48	0.49
1:D:29:SER:O	1:D:32:ALA:HB3	2.13	0.49
1:I:30:PRO:O	1:I:33:GLU:HG2	2.12	0.49
1:B:21:GLY:O	1:B:29:SER:HB2	2.13	0.48
1:B:103:THR:O	1:B:153:PRO:HG2	2.13	0.48
1:D:18:ILE:HD11	1:D:35:LEU:HD21	1.95	0.48
1:E:49:ARG:O	1:E:49:ARG:HG3	2.12	0.48
1:A:85:ASP:OD1	1:A:88:GLN:HG3	2.13	0.48
1:D:80:LYS:HB2	1:D:83:GLU:CD	2.38	0.48
1:E:57:GLY:O	1:E:95:LYS:HE2	2.13	0.48
1:I:410:SER:HB2	1:I:415:ASP:O	2.13	0.48
1:J:333:ARG:N	1:J:333:ARG:CD	2.77	0.48
1:B:172:ARG:HD2	1:B:499:PHE:CE1	2.48	0.48
1:C:53:GLU:HG2	1:E:151:ARG:HH12	1.77	0.48
1:C:349:LEU:HB2	1:C:440:ILE:HG12	1.95	0.48
1:G:395:LEU:HG	1:G:396:MET:N	2.28	0.48
1:A:268:VAL:O	1:A:376:ASP:HA	2.13	0.48
1:B:257:ASN:C	1:B:257:ASN:ND2	2.60	0.48
1:C:18:ILE:HD11	1:C:35:LEU:HD21	1.95	0.48
1:C:218:VAL:HA	1:C:253:GLU:O	2.13	0.48
1:D:55:LYS:H	1:D:58:GLN:NE2	2.10	0.48
1:I:55:LYS:CA	1:I:58:GLN:HE21	2.25	0.48
1:I:395:LEU:HD12	1:I:395:LEU:C	2.38	0.48
1:K:502:GLU:HA	1:K:502:GLU:OE1	2.12	0.48
1:L:194:PRO:HB2	1:L:196:ASN:HB3	1.95	0.48
1:A:81:GLU:C	1:A:83:GLU:H	2.21	0.48
1:A:410:SER:HB2	1:A:415:ASP:O	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:488:LEU:HD23	1:E:488:LEU:O	2.14	0.48
1:G:121:ASN:ND2	1:G:503:GLU:HG2	2.28	0.48
1:H:338:LEU:HD22	1:H:348:VAL:CG2	2.44	0.48
1:J:333:ARG:HB2	1:J:334:PRO:HD2	1.94	0.48
1:J:474:ARG:HD2	5:J:795:HOH:O	2.13	0.48
1:B:110:CYS:CB	1:B:157:MET:HE2	2.36	0.48
1:G:146:ASN:C	1:G:147:LYS:HG2	2.38	0.48
1:H:10:PRO:HG2	1:H:31:ILE:O	2.14	0.48
1:I:263:ARG:NH1	1:I:370:GLU:HB2	2.28	0.48
1:L:55:LYS:H	1:L:58:GLN:HE21	1.61	0.48
1:C:164:ARG:HB3	1:C:164:ARG:HH11	1.74	0.48
1:H:68:VAL:HG11	1:H:73:ILE:HD11	1.95	0.48
1:J:304:MET:HA	1:J:307:VAL:HG12	1.95	0.48
1:K:277:GLY:HA2	1:K:352:ASP:OD1	2.14	0.48
1:L:3:PHE:HA	1:L:157:MET:O	2.14	0.48
1:A:87:ARG:O	1:A:91:GLN:HG3	2.13	0.48
1:A:163:THR:CG2	1:A:166:GLU:OE2	2.62	0.48
1:B:257:ASN:HD21	1:B:259:SER:H	1.60	0.48
1:E:73:ILE:HG22	1:E:75:LEU:HD22	1.96	0.48
1:F:200:ALA:HB1	1:F:248:LEU:HB2	1.96	0.48
1:F:474:ARG:HB3	1:F:474:ARG:NH1	2.29	0.48
1:H:4:SER:OG	1:H:158:VAL:HG22	2.13	0.48
1:H:14:ARG:HE	1:H:69:LEU:HD13	1.78	0.48
1:H:124:TRP:HE1	1:H:503:GLU:CD	2.22	0.48
1:J:27:ARG:HH22	1:J:81:GLU:HB2	1.78	0.48
1:A:81:GLU:C	1:A:83:GLU:N	2.72	0.48
1:B:141:ASP:CB	1:B:147:LYS:HD3	2.37	0.48
1:B:199:ASN:C	1:B:273:THR:HG21	2.38	0.48
1:B:418:TRP:CE2	1:E:421:PRO:HD3	2.49	0.48
1:C:87:ARG:HH22	1:D:428:GLU:CD	2.21	0.48
1:D:410:SER:HB2	1:D:416:ARG:HA	1.96	0.48
1:E:167:LEU:O	1:E:171:GLU:HG3	2.14	0.48
1:E:263:ARG:CB	1:E:372:GLU:HB2	2.44	0.48
1:G:30:PRO:HA	1:G:33:GLU:HG3	1.96	0.48
1:H:117:VAL:HG12	1:H:120:ARG:HG3	1.96	0.48
1:H:257:ASN:ND2	1:H:259:SER:N	2.58	0.48
1:K:259:SER:O	1:K:261:ASP:N	2.47	0.48
1:L:82:ARG:CD	1:L:116:HIS:CD2	2.96	0.48
1:B:151:ARG:HE	1:B:153:PRO:HG3	1.79	0.48
1:B:474:ARG:HD2	5:B:788:HOH:O	2.13	0.48
1:C:73:ILE:HG22	1:C:75:LEU:HD22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:163:THR:OG1	1:C:165:ARG:HB2	2.14	0.48
1:D:76:ILE:CD1	1:D:96:THR:OG1	2.61	0.48
1:D:475:SER:HB2	5:D:791:HOH:O	2.14	0.48
1:I:221:ARG:HD2	5:I:1006:HOH:O	2.13	0.48
1:J:47:LEU:CD2	1:J:52:LEU:HB3	2.44	0.48
1:J:84:LEU:CD2	1:J:115:LEU:HD13	2.44	0.48
1:K:304:MET:HA	1:K:307:VAL:HG12	1.95	0.48
1:E:28:LEU:HG	1:E:32:ALA:HB3	1.95	0.47
1:F:193:MET:CE	1:F:197:ILE:CG2	2.92	0.47
1:D:199:ASN:C	1:D:273:THR:HG21	2.38	0.47
1:D:282:LYS:HE3	1:D:290:MET:SD	2.54	0.47
1:E:468:ILE:HG21	1:E:485:PRO:HD3	1.96	0.47
1:G:93:ILE:CD1	1:G:129:ALA:HB2	2.44	0.47
1:H:392:ILE:HG21	1:H:418:TRP:HB2	1.96	0.47
1:J:18:ILE:CD1	1:J:35:LEU:HD21	2.44	0.47
1:J:257:ASN:HD21	1:J:259:SER:H	1.55	0.47
1:K:165:ARG:HB2	1:K:165:ARG:CZ	2.44	0.47
1:D:33:GLU:O	1:D:37:LYS:HG3	2.15	0.47
1:D:68:VAL:HG11	1:D:73:ILE:HD11	1.95	0.47
1:K:221:ARG:HH21	1:K:253:GLU:CD	2.21	0.47
1:K:502:GLU:O	1:K:503:GLU:CB	2.61	0.47
1:C:483:GLY:O	1:C:486:VAL:HG23	2.14	0.47
1:D:47:LEU:CD2	1:D:52:LEU:HB3	2.45	0.47
1:I:263:ARG:HH11	1:I:370:GLU:HB2	1.78	0.47
1:I:468:ILE:HG21	1:I:485:PRO:HD3	1.96	0.47
1:B:32:ALA:O	1:B:35:LEU:CB	2.63	0.47
1:D:202:TYR:O	1:D:206:GLN:HG2	2.14	0.47
1:D:500:ASN:HB3	1:D:502:GLU:H	1.79	0.47
1:H:122:ASN:O	1:H:126:VAL:HG23	2.14	0.47
1:H:385:VAL:HG22	1:H:470:GLY:CA	2.44	0.47
1:L:126:VAL:O	1:L:130:VAL:HG23	2.14	0.47
1:L:225:GLU:HG3	1:L:246:GLU:HG3	1.96	0.47
1:A:474:ARG:NH1	1:A:474:ARG:CG	2.78	0.47
1:C:27:ARG:HH21	1:C:81:GLU:HG3	1.70	0.47
1:H:410:SER:HB2	1:H:415:ASP:O	2.14	0.47
1:A:196:ASN:ND2	1:C:337:VAL:O	2.47	0.47
1:B:305:ARG:HG2	1:B:305:ARG:HH11	1.79	0.47
1:B:474:ARG:HG2	1:B:474:ARG:NH1	2.29	0.47
1:C:82:ARG:C	1:C:84:LEU:N	2.73	0.47
1:E:306:MET:HE3	1:E:306:MET:HB3	1.83	0.47
1:G:195:PRO:HB3	1:G:274:PHE:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:19:VAL:CG1	1:H:76:ILE:HD12	2.45	0.47
1:H:24:GLU:OE1	1:H:80:LYS:HE3	2.15	0.47
1:H:184:ILE:O	1:H:188:LYS:HG3	2.15	0.47
1:H:223:ILE:N	1:H:223:ILE:HD12	2.30	0.47
1:L:221:ARG:HH21	1:L:253:GLU:CD	2.23	0.47
1:A:44:SER:O	1:A:48:ARG:HG3	2.15	0.47
1:B:164:ARG:HB3	1:B:164:ARG:NH1	2.30	0.47
1:D:208:ARG:HD2	5:D:715:HOH:O	2.13	0.47
1:D:479:LYS:HD2	1:F:434:PHE:HE2	1.80	0.47
1:J:108:ALA:HB3	1:J:157:MET:HE3	1.96	0.47
1:D:38:ILE:HG22	1:D:67:ASN:CB	2.44	0.47
1:D:80:LYS:O	1:D:83:GLU:HG2	2.15	0.47
1:D:337:VAL:O	1:E:196:ASN:ND2	2.47	0.47
1:F:114:GLU:HG2	1:F:162:PRO:HG3	1.96	0.47
1:A:500:ASN:ND2	1:A:500:ASN:C	2.73	0.47
1:B:55:LYS:N	1:B:58:GLN:HE21	2.12	0.47
1:B:305:ARG:HG2	1:B:305:ARG:NH1	2.30	0.47
1:D:193:MET:HE2	1:D:197:ILE:CG2	2.44	0.47
1:G:20:VAL:HG23	1:G:75:LEU:HD13	1.97	0.47
1:H:82:ARG:HG2	1:H:116:HIS:CD2	2.49	0.47
1:I:199:ASN:C	1:I:273:THR:HG21	2.40	0.47
1:A:369:PHE:O	1:A:370:GLU:C	2.57	0.46
1:G:144:LYS:O	1:G:147:LYS:HE3	2.15	0.46
1:G:196:ASN:HB2	1:I:336:ASP:CG	2.41	0.46
1:H:47:LEU:CD2	1:H:52:LEU:HB3	2.45	0.46
1:H:80:LYS:HB3	1:H:83:GLU:OE2	2.15	0.46
1:H:82:ARG:HG2	1:H:116:HIS:CG	2.50	0.46
1:L:19:VAL:HG11	1:L:96:THR:CG2	2.44	0.46
1:L:42:TYR:CD2	1:L:66:PRO:HD2	2.51	0.46
1:L:120:ARG:HD3	1:L:128:GLN:HE22	1.79	0.46
1:A:101:ASN:O	1:A:151:ARG:HD3	2.16	0.46
1:C:65:VAL:HG21	1:C:73:ILE:HD12	1.98	0.46
1:E:395:LEU:HD13	1:E:466:LEU:CD2	2.45	0.46
1:F:257:ASN:ND2	1:F:259:SER:H	2.13	0.46
1:G:257:ASN:HD21	1:G:259:SER:HB2	1.79	0.46
1:G:418:TRP:CE2	1:L:421:PRO:HD3	2.50	0.46
1:H:44:SER:O	1:H:48:ARG:HG3	2.15	0.46
1:L:86:GLU:CD	1:L:120:ARG:HH11	2.23	0.46
1:L:216:LYS:HZ3	1:L:311:GLN:NE2	2.13	0.46
1:A:163:THR:OG1	1:A:164:ARG:N	2.48	0.46
1:E:169:SER:HB2	1:E:502:GLU:HG2	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:87:ARG:HH22	1:L:428:GLU:CD	2.22	0.46
1:H:3:PHE:HD2	1:H:159:PHE:CE2	2.33	0.46
1:H:80:LYS:O	1:H:83:GLU:HB2	2.15	0.46
1:A:267:LEU:HD12	1:A:304:MET:HE3	1.97	0.46
1:J:81:GLU:O	1:J:83:GLU:N	2.39	0.46
1:L:479:LYS:CE	5:L:908:HOH:O	2.63	0.46
1:A:500:ASN:HD22	1:A:500:ASN:C	2.15	0.46
1:D:73:ILE:HG22	1:D:75:LEU:HD22	1.97	0.46
1:D:305:ARG:HG2	1:D:305:ARG:HH11	1.81	0.46
1:G:89:TYR:CZ	1:G:93:ILE:HD11	2.51	0.46
1:K:148:SER:O	1:K:149:GLU:HG2	2.16	0.46
1:F:85:ASP:H	1:F:88:GLN:HE21	1.61	0.46
1:H:428:GLU:CD	1:K:87:ARG:HH22	2.24	0.46
1:B:29:SER:O	1:B:32:ALA:HB3	2.16	0.46
1:C:103:THR:HG22	1:C:104:GLY:N	2.31	0.46
1:D:362:VAL:O	1:D:366:VAL:HG13	2.16	0.46
1:A:74:LEU:HG	1:A:76:ILE:HD12	1.97	0.46
1:I:488:LEU:C	1:I:488:LEU:CD2	2.89	0.46
1:B:149:GLU:HA	1:B:150:PRO:HD3	1.86	0.46
1:C:141:ASP:HB3	1:C:147:LYS:CD	2.45	0.46
1:C:144:LYS:O	1:C:147:LYS:HE3	2.16	0.46
1:D:22:VAL:HG21	1:D:52:LEU:HD23	1.97	0.46
1:G:146:ASN:O	1:G:147:LYS:CG	2.61	0.46
1:H:32:ALA:O	1:H:34:GLN:N	2.49	0.46
1:L:27:ARG:NH2	1:L:81:GLU:OE2	2.48	0.46
1:C:356:ARG:HD2	1:C:439:ASN:O	2.16	0.45
1:F:55:LYS:CA	1:F:58:GLN:HE21	2.28	0.45
1:F:141:ASP:O	1:F:147:LYS:HE3	2.16	0.45
1:F:309:GLU:HG3	5:F:837:HOH:O	2.15	0.45
1:H:304:MET:HE1	1:H:316:VAL:HG12	1.95	0.45
1:J:25:PRO:C	1:J:26:ARG:HG2	2.41	0.45
1:K:369:PHE:O	1:K:370:GLU:C	2.57	0.45
1:B:76:ILE:HD13	1:B:96:THR:OG1	2.16	0.45
1:B:221:ARG:NH2	5:B:716:HOH:O	2.49	0.45
1:H:488:LEU:HD23	1:H:488:LEU:C	2.41	0.45
1:J:80:LYS:O	1:J:83:GLU:HB2	2.17	0.45
1:K:146:ASN:ND2	5:K:709:HOH:O	2.49	0.45
1:B:114:GLU:OE2	1:B:160:ASN:ND2	2.43	0.45
1:C:82:ARG:NH2	1:C:116:HIS:CE1	2.83	0.45
1:H:16:ALA:HB3	1:H:107:GLU:O	2.16	0.45
1:H:22:VAL:HG21	1:H:75:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:503:GLU:HG2	5:H:785:HOH:O	2.16	0.45
1:J:245:ASN:ND2	5:J:712:HOH:O	2.50	0.45
1:J:479:LYS:HD2	1:L:434:PHE:HE2	1.81	0.45
1:B:73:ILE:HG22	1:B:75:LEU:CD2	2.46	0.45
1:C:68:VAL:HG11	1:C:73:ILE:HD11	1.99	0.45
1:C:76:ILE:CD1	1:C:96:THR:OG1	2.62	0.45
1:F:20:VAL:HG23	1:F:75:LEU:CD1	2.47	0.45
1:H:30:PRO:HA	1:H:33:GLU:OE2	2.16	0.45
1:I:282:LYS:HE3	1:I:290:MET:SD	2.57	0.45
1:K:202:TYR:O	1:K:206:GLN:HG2	2.16	0.45
1:K:259:SER:C	1:K:261:ASP:N	2.73	0.45
1:L:163:THR:HG21	1:L:165:ARG:HG3	1.98	0.45
1:C:443:ARG:N	1:C:444:PRO:CD	2.80	0.45
1:D:195:PRO:HB3	1:D:274:PHE:HB2	1.98	0.45
1:H:26:ARG:HD3	1:H:47:LEU:O	2.15	0.45
1:K:221:ARG:NE	1:K:253:GLU:OE2	2.47	0.45
1:K:396:MET:HE3	1:K:465:HIS:CD2	2.51	0.45
1:L:55:LYS:HB2	1:L:58:GLN:NE2	2.32	0.45
1:A:56:PRO:HD3	1:A:79:GLY:HA2	1.99	0.45
1:H:195:PRO:HB3	1:H:274:PHE:HB2	1.97	0.45
1:L:46:LEU:HD13	1:L:62:LEU:HD21	1.97	0.45
1:L:55:LYS:N	1:L:58:GLN:HE21	2.15	0.45
1:F:55:LYS:O	1:F:58:GLN:HG3	2.17	0.45
1:H:199:ASN:C	1:H:273:THR:HG21	2.42	0.45
1:J:468:ILE:HG21	1:J:485:PRO:HD3	1.98	0.45
1:A:306:MET:HE3	1:A:307:VAL:N	2.32	0.45
1:B:488:LEU:C	1:B:488:LEU:HD23	2.42	0.45
1:C:154:LEU:HD21	1:C:157:MET:HE3	1.99	0.45
1:E:305:ARG:HD2	5:E:915:HOH:O	2.16	0.45
1:G:257:ASN:HD21	1:G:259:SER:CB	2.29	0.45
1:G:421:PRO:HD3	1:L:418:TRP:CE2	2.52	0.45
1:K:256:GLY:O	1:K:313:PRO:HA	2.17	0.45
1:A:395:LEU:HD23	1:A:407:ILE:HD11	1.99	0.45
1:B:42:TYR:CD2	1:B:65:VAL:HG13	2.52	0.45
1:D:194:PRO:HB3	1:F:335:GLY:O	2.17	0.45
1:E:89:TYR:CZ	1:E:93:ILE:HD11	2.52	0.45
1:E:257:ASN:HD22	1:E:257:ASN:C	2.25	0.45
1:G:30:PRO:O	1:G:33:GLU:HG3	2.16	0.45
1:J:117:VAL:O	1:J:118:LYS:C	2.59	0.45
1:A:294:MET:HE1	1:A:298:ALA:HB2	1.99	0.45
1:C:395:LEU:HD12	1:C:395:LEU:C	2.41	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:312:LEU:HA	1:G:313:PRO:HD3	1.68	0.45
1:I:198:CYS:O	1:I:273:THR:HB	2.17	0.45
1:L:124:TRP:HB3	1:L:128:GLN:NE2	2.32	0.45
1:C:16:ALA:HA	1:C:71:GLU:CG	2.47	0.44
1:C:52:LEU:CD1	1:C:58:GLN:HB3	2.47	0.44
1:D:92:VAL:HG12	1:D:112:LEU:HD13	1.99	0.44
1:E:199:ASN:C	1:E:273:THR:HG21	2.41	0.44
1:F:34:GLN:H	1:F:34:GLN:HG3	1.34	0.44
1:J:474:ARG:HH11	1:J:474:ARG:CG	2.30	0.44
1:B:501:GLY:C	1:B:503:GLU:N	2.75	0.44
1:D:404:HIS:HB3	5:D:974:HOH:O	2.17	0.44
1:E:333:ARG:CD	1:F:195:PRO:HB2	2.47	0.44
1:G:65:VAL:HG21	1:G:73:ILE:HD12	1.98	0.44
1:H:1:MET:HG3	1:H:3:PHE:CZ	2.53	0.44
1:H:163:THR:CG2	1:H:165:ARG:H	2.17	0.44
1:K:398:ASN:C	1:K:398:ASN:OD1	2.60	0.44
1:B:458:THR:HG21	1:B:463:TRP:CD1	2.52	0.44
1:H:386:ILE:HD13	1:K:386:ILE:HD13	1.98	0.44
1:J:167:LEU:O	1:J:171:GLU:HG3	2.17	0.44
1:J:195:PRO:HB3	1:J:274:PHE:HB2	1.98	0.44
1:J:304:MET:HE1	1:J:316:VAL:CG1	2.48	0.44
1:K:24:GLU:HA	1:K:25:PRO:HA	1.72	0.44
1:H:193:MET:HE3	1:H:197:ILE:CG2	2.48	0.44
1:H:305:ARG:HG2	1:H:305:ARG:NH1	2.32	0.44
1:J:271:GLY:O	1:J:322:GLY:HA2	2.17	0.44
1:A:301:TYR:CD1	1:A:301:TYR:C	2.95	0.44
1:C:20:VAL:HG23	1:C:75:LEU:HD13	1.98	0.44
1:D:45:ALA:HA	1:D:48:ARG:NH1	2.33	0.44
1:E:9:SER:HB2	1:E:11:GLU:OE1	2.18	0.44
1:E:55:LYS:HB2	1:E:58:GLN:NE2	2.31	0.44
1:H:112:LEU:HD22	1:H:115:LEU:HD11	1.98	0.44
1:H:294:MET:HE1	1:H:298:ALA:HB2	1.99	0.44
1:K:22:VAL:HG21	1:K:52:LEU:HD23	2.00	0.44
1:K:257:ASN:C	1:K:257:ASN:ND2	2.74	0.44
1:K:403:ALA:O	1:K:407:ILE:HG12	2.17	0.44
1:L:22:VAL:HG21	1:L:52:LEU:HD23	2.00	0.44
1:L:93:ILE:HD13	1:L:129:ALA:CB	2.47	0.44
1:A:28:LEU:HD11	1:A:32:ALA:CB	2.47	0.44
1:B:144:LYS:HD3	5:B:708:HOH:O	2.17	0.44
1:B:369:PHE:O	1:B:370:GLU:C	2.61	0.44
1:C:55:LYS:HB2	1:C:58:GLN:NE2	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:141:ASP:HB3	1:C:147:LYS:HD3	1.99	0.44
1:K:26:ARG:NE	1:K:53:GLU:OE2	2.49	0.44
1:A:30:PRO:HA	1:A:33:GLU:HG2	2.00	0.44
1:C:92:VAL:HG12	1:C:112:LEU:HD13	2.00	0.44
1:H:39:SER:O	1:H:42:TYR:HB2	2.18	0.44
1:J:474:ARG:CG	1:J:474:ARG:NH1	2.79	0.44
1:A:5:VAL:HG13	1:A:174:ILE:HD11	2.00	0.44
1:A:194:PRO:HB2	1:A:196:ASN:HB3	2.00	0.44
1:B:71:GLU:H	1:B:71:GLU:HG2	1.54	0.44
1:C:5:VAL:HG13	1:C:174:ILE:HD11	1.99	0.44
1:D:305:ARG:HG2	1:D:305:ARG:NH1	2.32	0.44
1:H:148:SER:O	1:H:149:GLU:CG	2.59	0.44
1:I:32:ALA:O	1:I:35:LEU:HB3	2.18	0.44
1:J:225:GLU:HG3	1:J:246:GLU:HG3	1.99	0.44
1:L:304:MET:HA	1:L:307:VAL:HG12	2.00	0.44
1:B:24:GLU:CD	1:B:55:LYS:HG2	2.42	0.44
1:D:356:ARG:HD2	1:D:439:ASN:O	2.18	0.44
1:G:193:MET:CE	1:G:197:ILE:CG2	2.96	0.44
1:K:395:LEU:HD12	1:K:395:LEU:C	2.43	0.44
1:K:400:ASN:HB2	1:K:401:PRO:HD3	2.00	0.44
1:L:193:MET:HE1	1:L:197:ILE:HG21	1.98	0.44
1:D:29:SER:O	1:D:32:ALA:N	2.48	0.43
1:D:85:ASP:H	1:D:88:GLN:HE21	1.66	0.43
1:H:151:ARG:HE	1:H:153:PRO:CG	2.31	0.43
1:I:71:GLU:H	1:I:71:GLU:HG2	1.60	0.43
1:I:73:ILE:HG22	1:I:75:LEU:HD22	2.00	0.43
1:K:221:ARG:NH2	1:K:253:GLU:OE2	2.50	0.43
1:K:459:ARG:HB2	5:K:749:HOH:O	2.18	0.43
1:A:172:ARG:HD3	1:A:499:PHE:CE1	2.43	0.43
1:C:114:GLU:OE2	1:C:160:ASN:ND2	2.40	0.43
1:F:71:GLU:HG3	1:F:72:ARG:NH1	2.32	0.43
1:I:257:ASN:ND2	1:I:259:SER:N	2.57	0.43
1:A:150:PRO:HG3	5:A:820:HOH:O	2.17	0.43
1:G:307:VAL:HG23	1:G:312:LEU:HD12	2.00	0.43
1:H:149:GLU:O	1:H:149:GLU:HG3	2.19	0.43
1:J:151:ARG:HD3	1:J:153:PRO:HD3	2.00	0.43
1:J:152:ARG:HB3	5:J:846:HOH:O	2.17	0.43
1:L:306:MET:HE3	1:L:307:VAL:N	2.33	0.43
1:F:85:ASP:H	1:F:88:GLN:NE2	2.16	0.43
1:B:500:ASN:ND2	5:B:710:HOH:O	2.46	0.43
1:C:421:PRO:HD3	1:D:418:TRP:CE2	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:55:LYS:N	1:E:58:GLN:NE2	2.51	0.43
1:F:1:MET:N	1:F:134:LYS:NZ	2.67	0.43
1:F:369:PHE:O	1:F:370:GLU:C	2.61	0.43
1:I:257:ASN:HD22	1:I:259:SER:N	2.16	0.43
1:J:21:GLY:O	1:J:29:SER:CB	2.66	0.43
1:J:223:ILE:N	1:J:223:ILE:HD12	2.33	0.43
1:L:193:MET:HE3	1:L:197:ILE:HG21	2.00	0.43
1:L:372:GLU:OE1	1:L:496:ARG:NH1	2.51	0.43
1:A:263:ARG:HD2	1:A:370:GLU:O	2.19	0.43
1:C:86:GLU:HB3	1:C:124:TRP:CH2	2.54	0.43
1:I:141:ASP:O	1:I:147:LYS:HE2	2.18	0.43
1:K:172:ARG:NH1	1:K:500:ASN:ND2	2.66	0.43
1:K:272:LEU:HA	1:K:323:CYS:O	2.18	0.43
1:L:25:PRO:O	1:L:26:ARG:HG2	2.19	0.43
1:L:114:GLU:HG2	1:L:162:PRO:HD3	2.00	0.43
1:L:369:PHE:O	1:L:370:GLU:C	2.62	0.43
1:A:151:ARG:HH12	1:D:53:GLU:HG2	1.82	0.43
1:B:26:ARG:NH2	1:B:53:GLU:OE2	2.44	0.43
1:B:81:GLU:C	1:B:83:GLU:H	2.26	0.43
1:G:263:ARG:NH1	1:G:370:GLU:HB2	2.34	0.43
1:H:1:MET:HG3	1:H:3:PHE:CE1	2.54	0.43
1:H:163:THR:CG2	1:H:164:ARG:N	2.82	0.43
1:L:14:ARG:CG	1:L:69:LEU:HD13	2.49	0.43
1:L:82:ARG:CD	1:L:116:HIS:HD2	2.31	0.43
1:A:86:GLU:H	1:A:86:GLU:HG2	1.65	0.43
1:A:141:ASP:HB3	1:A:147:LYS:HD3	2.00	0.43
1:B:337:VAL:O	1:C:196:ASN:ND2	2.51	0.43
1:E:121:ASN:HD22	1:E:503:GLU:CG	2.31	0.43
1:F:221:ARG:NH1	5:F:721:HOH:O	2.51	0.43
1:I:87:ARG:HH22	1:J:428:GLU:CD	2.25	0.43
1:J:10:PRO:HB2	1:J:35:LEU:HD13	2.01	0.43
1:B:272:LEU:HA	1:B:323:CYS:O	2.19	0.43
1:G:193:MET:HE3	1:G:197:ILE:HB	2.01	0.43
1:G:223:ILE:HG23	1:G:227:GLN:HB2	2.00	0.43
1:D:443:ARG:N	1:D:444:PRO:CD	2.81	0.43
1:G:32:ALA:O	1:G:35:LEU:HB3	2.19	0.43
1:J:20:VAL:CG2	1:J:75:LEU:HD13	2.48	0.43
1:J:28:LEU:HG	1:J:32:ALA:HB1	2.00	0.43
1:J:475:SER:HB2	5:J:735:HOH:O	2.18	0.43
1:C:116:HIS:HB2	5:C:717:HOH:O	2.18	0.42
1:C:468:ILE:HG21	1:C:485:PRO:HD3	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:410:SER:HB2	1:E:416:ARG:HA	2.01	0.42
1:G:30:PRO:HA	1:G:33:GLU:CG	2.48	0.42
1:H:282:LYS:NZ	5:H:707:HOH:O	2.46	0.42
1:I:16:ALA:HA	1:I:71:GLU:CG	2.48	0.42
1:E:68:VAL:HG21	1:E:73:ILE:HD11	2.02	0.42
1:G:151:ARG:HE	1:G:153:PRO:HG2	1.81	0.42
1:G:194:PRO:HA	1:G:195:PRO:HD3	1.87	0.42
1:H:30:PRO:O	1:H:33:GLU:HG2	2.19	0.42
1:H:349:LEU:HB2	1:H:440:ILE:HG12	2.02	0.42
1:D:85:ASP:H	1:D:88:GLN:NE2	2.16	0.42
1:D:488:LEU:C	1:D:488:LEU:CD2	2.92	0.42
1:E:36:ASP:C	1:E:38:ILE:H	2.27	0.42
1:F:267:LEU:HD12	1:F:304:MET:HE3	2.02	0.42
1:G:267:LEU:HD12	1:G:304:MET:HE3	2.01	0.42
1:H:282:LYS:HE3	1:H:290:MET:SD	2.60	0.42
1:H:333:ARG:HD2	1:H:336:ASP:OD1	2.20	0.42
1:K:26:ARG:NH2	1:K:53:GLU:OE2	2.49	0.42
1:C:478:ALA:O	1:C:479:LYS:C	2.61	0.42
1:D:39:SER:HA	1:D:66:PRO:O	2.19	0.42
1:E:36:ASP:OD1	1:E:41:GLY:HA2	2.19	0.42
1:F:267:LEU:HD12	1:F:304:MET:CE	2.50	0.42
1:I:238:ALA:O	1:I:241:GLN:HB2	2.19	0.42
1:L:164:ARG:NH1	1:L:164:ARG:HB3	2.34	0.42
1:A:50:GLY:O	1:D:151:ARG:NH2	2.52	0.42
1:B:46:LEU:HD23	1:B:49:ARG:HH11	1.84	0.42
1:B:257:ASN:ND2	1:B:259:SER:N	2.64	0.42
1:F:223:ILE:N	1:F:223:ILE:CD1	2.82	0.42
1:F:256:GLY:O	1:F:313:PRO:HA	2.20	0.42
1:G:24:GLU:OE2	1:G:55:LYS:HA	2.20	0.42
1:J:18:ILE:HD11	1:J:35:LEU:HD21	2.02	0.42
1:L:92:VAL:HG12	1:L:112:LEU:HD13	2.00	0.42
1:A:166:GLU:CD	1:A:166:GLU:N	2.77	0.42
1:C:305:ARG:HH11	1:C:305:ARG:CG	2.33	0.42
1:D:24:GLU:OE1	1:D:80:LYS:CE	2.68	0.42
1:F:55:LYS:HB2	1:F:58:GLN:HE21	1.84	0.42
1:G:57:GLY:O	1:G:95:LYS:HE2	2.20	0.42
1:J:10:PRO:HG2	1:J:31:ILE:HG23	2.01	0.42
1:J:28:LEU:HG	1:J:32:ALA:HB3	2.01	0.42
1:J:68:VAL:HG21	1:J:73:ILE:HD11	2.02	0.42
1:J:333:ARG:HD2	1:J:333:ARG:H	1.85	0.42
1:J:333:ARG:HB2	1:J:334:PRO:CD	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:474:ARG:HG2	1:J:474:ARG:NH1	2.33	0.42
1:L:55:LYS:H	1:L:58:GLN:HE22	1.64	0.42
1:C:238:ALA:O	1:C:241:GLN:HB2	2.20	0.42
1:C:395:LEU:HD23	1:C:407:ILE:CD1	2.50	0.42
1:D:80:LYS:O	1:D:83:GLU:CG	2.68	0.42
1:E:194:PRO:HB2	1:E:196:ASN:HB3	2.01	0.42
1:G:42:TYR:CE1	1:J:64:HIS:HD2	2.37	0.42
1:G:468:ILE:HG21	1:G:485:PRO:HD3	2.02	0.42
1:H:151:ARG:O	1:H:152:ARG:HD3	2.20	0.42
1:C:32:ALA:C	1:C:34:GLN:H	2.28	0.42
1:D:55:LYS:N	1:D:58:GLN:HE21	2.14	0.42
1:F:24:GLU:CD	1:F:55:LYS:HG2	2.45	0.42
1:F:55:LYS:CB	1:F:58:GLN:NE2	2.82	0.42
1:G:253:GLU:HG2	1:G:317:ILE:HG12	2.01	0.42
1:I:14:ARG:CZ	1:I:69:LEU:HD13	2.50	0.42
1:J:89:TYR:CZ	1:J:93:ILE:CD1	3.01	0.42
1:A:163:THR:HG23	1:A:165:ARG:HB2	2.01	0.42
1:A:395:LEU:HD11	1:A:464:ALA:HB1	2.02	0.42
1:C:257:ASN:C	1:C:257:ASN:ND2	2.78	0.42
1:G:27:ARG:HH22	1:G:81:GLU:CD	2.28	0.42
1:I:82:ARG:HG3	1:I:116:HIS:CG	2.55	0.42
1:A:31:ILE:O	1:A:34:GLN:HB2	2.20	0.41
1:A:263:ARG:CB	1:A:372:GLU:HB2	2.50	0.41
1:A:400:ASN:HB2	1:A:401:PRO:HD3	2.02	0.41
1:C:89:TYR:CZ	1:C:93:ILE:HD11	2.55	0.41
1:F:33:GLU:CB	5:F:938:HOH:O	2.49	0.41
1:F:68:VAL:HG11	1:F:73:ILE:HD11	2.02	0.41
1:F:395:LEU:HD12	1:F:396:MET:H	1.85	0.41
1:L:392:ILE:HG21	1:L:418:TRP:HB2	2.02	0.41
1:B:194:PRO:C	1:B:196:ASN:H	2.27	0.41
1:D:257:ASN:ND2	1:D:257:ASN:C	2.72	0.41
1:D:266:VAL:HG23	1:D:371:PRO:HB3	2.02	0.41
1:G:416:ARG:HD2	5:G:774:HOH:O	2.19	0.41
1:H:53:GLU:HG3	1:L:151:ARG:HH22	1.84	0.41
1:H:55:LYS:HB2	1:H:58:GLN:HE21	1.84	0.41
1:I:224:GLY:O	1:I:228:MET:HG3	2.20	0.41
1:J:39:SER:HA	1:J:66:PRO:O	2.20	0.41
1:L:443:ARG:N	1:L:444:PRO:CD	2.83	0.41
1:L:468:ILE:HG21	1:L:485:PRO:HD3	2.02	0.41
1:D:415:ASP:OD2	1:D:485:PRO:HA	2.20	0.41
1:F:223:ILE:HG23	1:F:227:GLN:HB3	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:42:TYR:CE1	1:J:64:HIS:CD2	3.09	0.41
1:H:146:ASN:O	1:H:147:LYS:O	2.38	0.41
1:H:304:MET:HA	1:H:304:MET:HE2	2.01	0.41
1:J:82:ARG:C	1:J:84:LEU:N	2.68	0.41
1:L:14:ARG:HG2	1:L:69:LEU:HD13	2.01	0.41
1:C:80:LYS:O	1:C:83:GLU:HB2	2.19	0.41
1:D:19:VAL:HG22	1:D:74:LEU:HB3	2.01	0.41
1:F:55:LYS:CB	1:F:58:GLN:HE21	2.33	0.41
1:F:222:VAL:C	1:F:223:ILE:HD12	2.46	0.41
1:F:304:MET:O	1:F:307:VAL:HG12	2.21	0.41
1:G:474:ARG:O	1:G:479:LYS:HA	2.20	0.41
1:G:502:GLU:HG3	5:G:781:HOH:O	2.19	0.41
1:L:195:PRO:HB3	1:L:274:PHE:HB2	2.03	0.41
1:C:221:ARG:NE	1:C:253:GLU:OE2	2.47	0.41
1:C:370:GLU:N	1:C:371:PRO:CD	2.84	0.41
1:F:110:CYS:CB	1:F:157:MET:HE2	2.37	0.41
1:G:199:ASN:C	1:G:273:THR:HG21	2.45	0.41
1:J:82:ARG:HD3	1:J:116:HIS:CD2	2.55	0.41
1:L:221:ARG:NH2	1:L:253:GLU:OE2	2.48	0.41
1:L:257:ASN:HD22	1:L:259:SER:H	1.68	0.41
1:B:258:ALA:O	1:B:259:SER:C	2.63	0.41
1:C:340:THR:HB	5:C:730:HOH:O	2.21	0.41
1:C:431:GLU:HG2	5:C:982:HOH:O	2.20	0.41
1:D:32:ALA:C	1:D:34:GLN:N	2.77	0.41
1:D:94:GLN:HG3	1:D:136:THR:OG1	2.21	0.41
1:D:95:LYS:HA	1:D:95:LYS:HD2	1.84	0.41
1:F:292:TYR:C	1:F:294:MET:H	2.27	0.41
1:H:101:ASN:OD1	1:H:153:PRO:HD2	2.21	0.41
1:J:55:LYS:N	1:J:58:GLN:HE21	2.16	0.41
1:J:311:GLN:NE2	5:J:719:HOH:O	2.54	0.41
1:K:16:ALA:HA	1:K:71:GLU:HG2	2.02	0.41
1:A:218:VAL:HA	1:A:253:GLU:O	2.21	0.41
1:A:463:TRP:CZ2	1:A:465:HIS:HB2	2.56	0.41
1:D:17:CYS:HA	1:D:72:ARG:O	2.21	0.41
1:E:151:ARG:HD3	1:E:153:PRO:HD3	2.02	0.41
1:H:53:GLU:HG3	1:L:151:ARG:CZ	2.50	0.41
1:K:458:THR:HG21	1:K:463:TRP:CD1	2.56	0.41
1:B:263:ARG:NH1	1:B:263:ARG:HG3	2.36	0.41
1:C:3:PHE:HA	1:C:157:MET:O	2.20	0.41
1:C:224:GLY:HA2	1:C:248:LEU:HD23	2.02	0.41
1:D:167:LEU:O	1:D:171:GLU:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:422:LEU:HD23	1:D:422:LEU:HA	1.92	0.41
1:F:27:ARG:NH2	1:F:81:GLU:HG3	2.35	0.41
1:G:80:LYS:HD2	1:G:83:GLU:OE1	2.20	0.41
1:H:65:VAL:HG13	1:H:66:PRO:HD2	2.02	0.41
1:H:85:ASP:H	1:H:88:GLN:HE21	1.69	0.41
1:H:263:ARG:HB2	1:H:372:GLU:HB2	2.02	0.41
1:H:458:THR:HG21	1:H:463:TRP:CD1	2.56	0.41
1:I:23:PHE:CZ	1:I:81:GLU:HG2	2.56	0.41
1:K:193:MET:HE2	1:K:197:ILE:HG21	2.00	0.41
1:L:45:ALA:HA	1:L:48:ARG:HH11	1.83	0.41
1:L:216:LYS:HE2	1:L:217:ASN:ND2	2.36	0.41
1:A:22:VAL:HG21	1:A:52:LEU:HD13	2.02	0.41
1:A:25:PRO:C	1:A:27:ARG:N	2.79	0.41
1:A:36:ASP:OD2	1:A:44:SER:N	2.51	0.41
1:A:106:MET:HA	1:A:153:PRO:O	2.21	0.41
1:A:258:ALA:O	1:A:259:SER:C	2.63	0.41
1:B:124:TRP:HH2	1:B:491:GLN:OE1	2.03	0.41
1:B:245:ASN:ND2	5:B:729:HOH:O	2.54	0.41
1:B:349:LEU:HB2	1:B:440:ILE:HG12	2.02	0.41
1:C:18:ILE:CD1	1:C:35:LEU:HD21	2.51	0.41
1:C:194:PRO:C	1:C:196:ASN:H	2.27	0.41
1:D:25:PRO:O	1:D:26:ARG:C	2.63	0.41
1:E:30:PRO:C	1:E:32:ALA:N	2.78	0.41
1:E:47:LEU:HD21	1:E:52:LEU:HB3	2.02	0.41
1:I:304:MET:HE1	1:I:316:VAL:HG11	2.02	0.41
1:J:100:LEU:HD11	1:J:157:MET:HE1	2.02	0.41
1:J:374:VAL:O	1:J:463:TRP:HA	2.21	0.41
1:K:55:LYS:O	1:K:56:PRO:C	2.64	0.41
1:K:165:ARG:HB2	1:K:165:ARG:NH1	2.36	0.41
1:L:5:VAL:C	1:L:6:LYS:HG3	2.45	0.41
1:L:6:LYS:O	1:L:161:VAL:HG22	2.20	0.41
1:A:74:LEU:HG	1:A:76:ILE:HD11	2.03	0.41
1:B:367:GLU:CD	1:B:460:LYS:HD2	2.46	0.41
1:D:443:ARG:NH2	1:E:285:GLU:OE1	2.54	0.41
1:E:19:VAL:CG1	1:E:76:ILE:HD13	2.51	0.41
1:H:193:MET:HE3	1:H:197:ILE:HG21	2.03	0.41
1:I:20:VAL:CG2	1:I:75:LEU:HD13	2.51	0.41
1:I:89:TYR:CZ	1:I:93:ILE:CD1	3.04	0.41
1:J:205:SER:O	1:J:209:GLN:HG3	2.21	0.41
1:K:193:MET:HE3	1:K:197:ILE:CG2	2.51	0.41
1:K:376:ASP:OD2	1:K:465:HIS:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:PRO:HG3	5:A:813:HOH:O	2.21	0.40
1:C:39:SER:O	1:C:40:ASP:HB2	2.21	0.40
1:F:42:TYR:CD2	1:F:65:VAL:HG13	2.55	0.40
1:F:89:TYR:CZ	1:F:93:ILE:HD11	2.56	0.40
1:G:398:ASN:OD1	1:G:398:ASN:C	2.63	0.40
1:H:25:PRO:O	1:H:26:ARG:C	2.63	0.40
1:I:473:TRP:HA	1:I:482:THR:HG23	2.03	0.40
1:J:218:VAL:HA	1:J:253:GLU:O	2.21	0.40
1:K:427:GLN:CD	1:K:452:CYS:HB3	2.46	0.40
1:L:82:ARG:C	1:L:84:LEU:N	2.74	0.40
1:A:193:MET:HE3	1:A:197:ILE:HB	2.04	0.40
1:A:479:LYS:CE	5:A:888:HOH:O	2.69	0.40
1:B:263:ARG:HG3	1:B:263:ARG:HH11	1.86	0.40
1:D:223:ILE:HD12	1:D:223:ILE:N	2.35	0.40
1:F:164:ARG:HG3	5:F:799:HOH:O	2.20	0.40
1:J:146:ASN:O	1:J:147:LYS:C	2.64	0.40
1:K:117:VAL:O	1:K:118:LYS:C	2.65	0.40
1:K:151:ARG:HD3	1:K:153:PRO:HD3	2.02	0.40
1:L:477:LYS:HA	1:L:477:LYS:HD2	1.86	0.40
1:A:38:ILE:O	1:A:38:ILE:CG2	2.69	0.40
1:A:193:MET:CE	1:A:197:ILE:HG21	2.50	0.40
1:B:270:LYS:HE3	1:B:355:GLY:CA	2.51	0.40
1:C:147:LYS:O	1:C:147:LYS:HG3	2.21	0.40
1:C:303:VAL:O	1:C:307:VAL:HG23	2.21	0.40
1:D:28:LEU:HD11	1:D:32:ALA:HB1	2.04	0.40
1:E:122:ASN:HD21	1:E:161:VAL:HG12	1.86	0.40
1:E:395:LEU:HD12	1:E:465:HIS:O	2.21	0.40
1:F:122:ASN:ND2	5:F:713:HOH:O	2.46	0.40
1:F:258:ALA:O	1:F:259:SER:C	2.62	0.40
1:G:148:SER:O	1:G:149:GLU:CG	2.60	0.40
1:H:163:THR:C	1:H:165:ARG:N	2.76	0.40
1:I:100:LEU:CD1	1:I:157:MET:HE1	2.52	0.40
1:I:428:GLU:CD	1:J:87:ARG:HH22	2.29	0.40
1:K:149:GLU:HA	1:K:150:PRO:HD3	1.84	0.40
1:K:360:CYS:HB2	1:K:457:PHE:CD2	2.56	0.40
1:K:395:LEU:O	1:K:419:ARG:HA	2.21	0.40
1:K:502:GLU:O	1:K:503:GLU:HB2	2.20	0.40
1:L:356:ARG:HD2	1:L:439:ASN:O	2.21	0.40
1:C:14:ARG:HG2	1:C:69:LEU:HB3	2.03	0.40
5:C:823:HOH:O	1:E:46:LEU:HG	2.21	0.40
1:H:225:GLU:HG2	1:H:237:LEU:CD2	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:82:ARG:O	1:J:84:LEU:N	2.53	0.40
1:J:392:ILE:HG21	1:J:418:TRP:HB2	2.03	0.40
1:K:85:ASP:OD1	1:K:88:GLN:HG3	2.22	0.40
1:K:121:ASN:OD1	1:K:121:ASN:C	2.65	0.40
1:K:263:ARG:HG3	5:K:949:HOH:O	2.21	0.40
1:A:193:MET:HA	1:A:194:PRO:HD3	1.84	0.40
1:A:225:GLU:HG2	1:A:237:LEU:CD2	2.51	0.40
1:D:194:PRO:HA	1:D:195:PRO:HD3	1.92	0.40
1:E:88:GLN:HG3	5:E:789:HOH:O	2.21	0.40
1:H:73:ILE:HG22	1:H:75:LEU:HD22	2.03	0.40
1:I:55:LYS:CB	1:I:58:GLN:NE2	2.80	0.40
1:J:5:VAL:HA	1:J:159:PHE:O	2.21	0.40
1:J:27:ARG:HH12	1:J:81:GLU:CG	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:372:GLU:OE2	1:D:168:THR:OG1[3_565]	2.18	0.02

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	501/503 (100%)	474 (95%)	18 (4%)	9 (2%)	6	12
1	B	501/503 (100%)	475 (95%)	22 (4%)	4 (1%)	16	31
1	C	501/503 (100%)	473 (94%)	23 (5%)	5 (1%)	12	24
1	D	501/503 (100%)	471 (94%)	23 (5%)	7 (1%)	9	17
1	E	501/503 (100%)	478 (95%)	16 (3%)	7 (1%)	9	17
1	F	501/503 (100%)	478 (95%)	20 (4%)	3 (1%)	21	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	G	501/503 (100%)	475 (95%)	21 (4%)	5 (1%)	12	24
1	H	501/503 (100%)	464 (93%)	26 (5%)	11 (2%)	5	9
1	I	501/503 (100%)	475 (95%)	21 (4%)	5 (1%)	12	24
1	J	501/503 (100%)	477 (95%)	18 (4%)	6 (1%)	10	20
1	K	501/503 (100%)	474 (95%)	21 (4%)	6 (1%)	10	20
1	L	501/503 (100%)	467 (93%)	28 (6%)	6 (1%)	10	20
All	All	6012/6036 (100%)	5681 (94%)	257 (4%)	74 (1%)	10	20

All (74) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	ARG
1	A	81	GLU
1	A	82	ARG
1	A	146	ASN
1	A	147	LYS
1	B	81	GLU
1	B	147	LYS
1	C	81	GLU
1	C	83	GLU
1	C	147	LYS
1	D	26	ARG
1	D	81	GLU
1	D	147	LYS
1	E	81	GLU
1	E	146	ASN
1	E	147	LYS
1	F	146	ASN
1	F	147	LYS
1	G	81	GLU
1	G	147	LYS
1	H	28	LEU
1	H	147	LYS
1	H	148	SER
1	I	147	LYS
1	J	146	ASN
1	J	147	LYS
1	K	81	GLU
1	K	147	LYS
1	K	500	ASN

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Mol	Chain	Res	Type
1	L	81	GLU
1	L	147	LYS
1	B	149	GLU
1	D	33	GLU
1	D	146	ASN
1	E	260	GLU
1	H	33	GLU
1	H	82	ARG
1	H	502	GLU
1	I	146	ASN
1	J	83	GLU
1	K	149	GLU
1	K	260	GLU
1	L	83	GLU
1	A	40	ASP
1	D	154	LEU
1	G	26	ARG
1	G	146	ASN
1	H	81	GLU
1	H	146	ASN
1	H	150	PRO
1	I	260	GLU
1	J	118	LYS
1	D	149	GLU
1	E	37	LYS
1	E	149	GLU
1	H	26	ARG
1	H	149	GLU
1	K	502	GLU
1	L	40	ASP
1	L	146	ASN
1	A	37	LYS
1	A	52	LEU
1	A	66	PRO
1	B	118	LYS
1	C	146	ASN
1	E	26	ARG
1	I	82	ARG
1	J	81	GLU
1	J	149	GLU
1	G	149	GLU
1	I	149	GLU

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Mol	Chain	Res	Type
1	F	149	GLU
1	L	66	PRO
1	C	149	GLU

5.3.2 Protein sidechains [i](#)

There are no protein residues with a non-rotameric sidechain to report in this entry.

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](#)

Of 40 ligands modelled in this entry, 28 are monoatomic - leaving 12 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	CO3	H	603	-	3,3,3	0.71	0	2,3,3	0.43	0
3	CO3	A	603	-	3,3,3	0.86	0	2,3,3	0.58	0
3	CO3	F	603	-	3,3,3	0.82	0	2,3,3	0.51	0
3	CO3	K	603	-	3,3,3	0.66	0	2,3,3	0.58	0
3	CO3	J	603	-	3,3,3	1.10	0	2,3,3	1.72	1 (50%)
3	CO3	B	603	-	3,3,3	0.81	0	2,3,3	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	CO3	D	603	-	3,3,3	0.58	0	2,3,3	2.07	1 (50%)
3	CO3	G	603	-	3,3,3	0.67	0	2,3,3	0.81	0
3	CO3	I	603	-	3,3,3	1.19	0	2,3,3	1.82	1 (50%)
3	CO3	E	603	-	3,3,3	0.51	0	2,3,3	0.53	0
3	CO3	C	603	-	3,3,3	1.17	0	2,3,3	2.10	1 (50%)
3	CO3	L	603	-	3,3,3	0.60	0	2,3,3	0.70	0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	603	CO3	O2-C-O1	2.45	125.94	119.68
3	D	603	CO3	O2-C-O1	2.41	125.83	119.68
3	J	603	CO3	O2-C-O1	2.15	125.19	119.68
3	I	603	CO3	O2-C-O1	2.11	125.06	119.68

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

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	503/503 (100%)	-0.21	16 (3%)	50	46	9, 25, 61, 73	0
1	B	503/503 (100%)	-0.52	14 (2%)	55	50	6, 17, 51, 72	0
1	C	503/503 (100%)	-0.42	15 (2%)	52	48	6, 18, 57, 74	0
1	D	503/503 (100%)	-0.42	13 (2%)	57	52	8, 19, 57, 71	0
1	E	503/503 (100%)	-0.51	13 (2%)	57	52	7, 18, 53, 71	0
1	F	503/503 (100%)	-0.41	14 (2%)	55	50	12, 24, 53, 72	0
1	G	503/503 (100%)	-0.60	10 (1%)	65	61	7, 18, 49, 69	0
1	H	503/503 (100%)	-0.02	30 (5%)	27	24	10, 28, 66, 74	0
1	I	503/503 (100%)	-0.69	9 (1%)	67	64	5, 15, 45, 69	0
1	J	503/503 (100%)	-0.50	8 (1%)	70	67	8, 18, 53, 73	0
1	K	503/503 (100%)	-0.40	14 (2%)	55	50	10, 24, 54, 69	0
1	L	503/503 (100%)	-0.14	41 (8%)	17	15	7, 19, 69, 77	0
All	All	6036/6036 (100%)	-0.40	197 (3%)	49	45	5, 21, 61, 77	0

All (197) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	150	PRO	4.9
1	L	500	ASN	4.9
1	H	150	PRO	4.7
1	L	502	GLU	4.6
1	F	150	PRO	4.5
1	B	150	PRO	4.4
1	B	149	GLU	4.3
1	E	150	PRO	4.1
1	C	149	GLU	4.1
1	L	150	PRO	4.0
1	L	66	PRO	4.0

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Mol	Chain	Res	Type	RSRZ
1	B	503	GLU	3.9
1	L	163	THR	3.9
1	A	150	PRO	3.9
1	C	148	SER	3.9
1	H	151	ARG	3.8
1	C	151	ARG	3.8
1	E	151	ARG	3.8
1	D	150	PRO	3.8
1	H	148	SER	3.7
1	F	151	ARG	3.7
1	G	150	PRO	3.7
1	J	148	SER	3.7
1	J	150	PRO	3.7
1	K	150	PRO	3.7
1	L	148	SER	3.6
1	H	146	ASN	3.6
1	F	149	GLU	3.6
1	A	146	ASN	3.6
1	B	148	SER	3.5
1	E	149	GLU	3.5
1	K	502	GLU	3.5
1	F	34	GLN	3.5
1	K	38	ILE	3.5
1	I	146	ASN	3.5
1	F	503	GLU	3.5
1	J	151	ARG	3.5
1	D	148	SER	3.5
1	D	149	GLU	3.4
1	L	30	PRO	3.4
1	K	503	GLU	3.3
1	F	148	SER	3.3
1	A	151	ARG	3.2
1	F	500	ASN	3.2
1	D	503	GLU	3.1
1	B	502	GLU	3.1
1	L	149	GLU	3.1
1	F	38	ILE	3.1
1	C	146	ASN	3.0
1	H	503	GLU	3.0
1	B	151	ARG	3.0
1	K	500	ASN	3.0
1	G	151	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	G	146	ASN	3.0
1	D	151	ARG	3.0
1	A	147	LYS	3.0
1	H	500	ASN	3.0
1	A	34	GLN	3.0
1	G	149	GLU	2.9
1	I	148	SER	2.9
1	H	34	GLN	2.9
1	C	82	ARG	2.9
1	I	150	PRO	2.9
1	L	162	PRO	2.8
1	K	151	ARG	2.8
1	A	38	ILE	2.8
1	A	149	GLU	2.8
1	L	165	ARG	2.8
1	L	37	LYS	2.7
1	A	33	GLU	2.7
1	B	33	GLU	2.7
1	B	500	ASN	2.7
1	D	260	GLU	2.7
1	J	149	GLU	2.7
1	C	79	GLY	2.7
1	I	151	ARG	2.7
1	I	149	GLU	2.7
1	L	33	GLU	2.7
1	C	38	ILE	2.7
1	F	146	ASN	2.7
1	H	69	LEU	2.7
1	J	82	ARG	2.7
1	L	261	ASP	2.6
1	H	499	PHE	2.6
1	L	67	ASN	2.6
1	I	260	GLU	2.6
1	K	501	GLY	2.6
1	L	79	GLY	2.6
1	L	501	GLY	2.6
1	E	82	ARG	2.6
1	H	49	ARG	2.6
1	E	146	ASN	2.6
1	L	43	ILE	2.6
1	C	33	GLU	2.6
1	H	149	GLU	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	501	GLY	2.6
1	A	503	GLU	2.6
1	L	83	GLU	2.6
1	K	146	ASN	2.6
1	B	34	GLN	2.6
1	E	34	GLN	2.6
1	G	148	SER	2.6
1	B	147	LYS	2.6
1	H	57	GLY	2.5
1	L	32	ALA	2.5
1	L	39	SER	2.5
1	C	83	GLU	2.5
1	K	36	ASP	2.5
1	E	500	ASN	2.5
1	B	38	ILE	2.5
1	L	124	TRP	2.5
1	D	38	ILE	2.4
1	A	82	ARG	2.4
1	L	113	THR	2.4
1	G	147	LYS	2.4
1	H	50	GLY	2.4
1	H	55	LYS	2.4
1	L	36	ASP	2.4
1	L	151	ARG	2.4
1	E	148	SER	2.4
1	K	57	GLY	2.4
1	E	38	ILE	2.4
1	L	38	ILE	2.4
1	D	262	ALA	2.4
1	A	502	GLU	2.4
1	L	503	GLU	2.4
1	L	28	LEU	2.4
1	L	40	ASP	2.4
1	L	65	VAL	2.4
1	L	82	ARG	2.3
1	L	499	PHE	2.3
1	D	146	ASN	2.3
1	I	33	GLU	2.3
1	A	148	SER	2.3
1	H	76	ILE	2.3
1	A	69	LEU	2.3
1	H	38	ILE	2.3

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Mol	Chain	Res	Type	RSRZ
1	F	147	LYS	2.3
1	D	34	GLN	2.3
1	I	38	ILE	2.3
1	L	35	LEU	2.3
1	H	502	GLU	2.3
1	H	155	ARG	2.3
1	G	38	ILE	2.2
1	H	37	LYS	2.2
1	H	147	LYS	2.2
1	C	261	ASP	2.2
1	F	36	ASP	2.2
1	E	260	GLU	2.2
1	G	81	GLU	2.2
1	A	32	ALA	2.2
1	L	34	GLN	2.2
1	K	148	SER	2.2
1	F	502	GLU	2.2
1	J	84	LEU	2.2
1	G	260	GLU	2.2
1	H	35	LEU	2.2
1	L	31	ILE	2.2
1	H	83	GLU	2.2
1	B	165	ARG	2.2
1	C	37	LYS	2.2
1	E	147	LYS	2.2
1	L	23	PHE	2.2
1	H	68	VAL	2.1
1	L	116	HIS	2.1
1	H	79	GLY	2.1
1	E	49	ARG	2.1
1	H	261	ASP	2.1
1	L	49	ARG	2.1
1	K	37	LYS	2.1
1	L	69	LEU	2.1
1	D	33	GLU	2.1
1	K	149	GLU	2.1
1	B	261	ASP	2.1
1	D	40	ASP	2.1
1	J	147	LYS	2.1
1	L	44	SER	2.1
1	A	153	PRO	2.1
1	A	67	ASN	2.1

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Mol	Chain	Res	Type	RSRZ
1	H	172	ARG	2.1
1	H	501	GLY	2.1
1	F	216	LYS	2.1
1	I	37	LYS	2.1
1	H	56	PRO	2.1
1	F	499	PHE	2.0
1	G	49	ARG	2.0
1	C	28	LEU	2.0
1	C	67	ASN	2.0
1	L	146	ASN	2.0
1	C	147	LYS	2.0
1	D	37	LYS	2.0
1	J	80	LYS	2.0
1	K	499	PHE	2.0
1	H	28	LEU	2.0
1	L	103	THR	2.0
1	E	36	ASP	2.0
1	H	64	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CO3	E	603	4/4	0.96	0.07	13,14,14,16	0
3	CO3	D	603	4/4	0.98	0.04	13,15,15,17	0
3	CO3	F	603	4/4	0.98	0.05	17,18,19,19	0
3	CO3	H	603	4/4	0.98	0.06	13,15,15,16	0
3	CO3	I	603	4/4	0.98	0.04	12,12,13,14	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	CO3	K	603	4/4	0.98	0.05	17,17,19,21	0
3	CO3	B	603	4/4	0.99	0.04	9,11,12,12	0
3	CO3	C	603	4/4	0.99	0.04	10,10,11,12	0
2	ZN	A	601	1/1	0.99	0.04	18,18,18,18	0
2	ZN	B	602	1/1	0.99	0.10	19,19,19,19	0
2	ZN	E	601	1/1	0.99	0.03	16,16,16,16	0
3	CO3	G	603	4/4	0.99	0.05	14,16,16,17	0
2	ZN	I	602	1/1	0.99	0.04	13,13,13,13	0
2	ZN	K	602	1/1	0.99	0.06	19,19,19,19	0
3	CO3	J	603	4/4	0.99	0.04	11,11,12,13	0
3	CO3	A	603	4/4	0.99	0.03	16,16,17,17	0
3	CO3	L	603	4/4	0.99	0.05	8,10,10,11	0
4	CL	B	604	1/1	0.99	0.14	9,9,9,9	0
4	CL	F	604	1/1	0.99	0.15	14,14,14,14	0
4	CL	G	604	1/1	0.99	0.15	9,9,9,9	0
4	CL	K	604	1/1	0.99	0.14	13,13,13,13	0
2	ZN	C	601	1/1	1.00	0.04	15,15,15,15	0
2	ZN	L	601	1/1	1.00	0.05	16,16,16,16	0
2	ZN	L	602	1/1	1.00	0.04	15,15,15,15	0
2	ZN	C	602	1/1	1.00	0.02	11,11,11,11	0
2	ZN	D	601	1/1	1.00	0.04	13,13,13,13	0
2	ZN	D	602	1/1	1.00	0.04	15,15,15,15	0
2	ZN	B	601	1/1	1.00	0.04	14,14,14,14	0
2	ZN	E	602	1/1	1.00	0.03	16,16,16,16	0
2	ZN	F	601	1/1	1.00	0.03	19,19,19,19	0
2	ZN	F	602	1/1	1.00	0.02	16,16,16,16	0
2	ZN	G	601	1/1	1.00	0.05	16,16,16,16	0
2	ZN	G	602	1/1	1.00	0.04	15,15,15,15	0
2	ZN	H	601	1/1	1.00	0.03	17,17,17,17	0
2	ZN	H	602	1/1	1.00	0.03	16,16,16,16	0
2	ZN	I	601	1/1	1.00	0.04	13,13,13,13	0
2	ZN	A	602	1/1	1.00	0.03	15,15,15,15	0
2	ZN	J	601	1/1	1.00	0.04	15,15,15,15	0
2	ZN	J	602	1/1	1.00	0.02	12,12,12,12	0
2	ZN	K	601	1/1	1.00	0.05	16,16,16,16	0

6.5 Other polymers

There are no such residues in this entry.