



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 01:11 PM UTC

PDB ID : 1IWA / pdb_00001iwa
Title : RUBISCO FROM GALDIERIA PARTITA
Authors : Okano, Y.; Mizohata, E.; Xie, Y.; Matsumura, H.; Sugawara, H.; Inoue, T.;
Yokota, A.; Kai, Y.
Deposited on : 2002-04-30
Resolution : 2.60 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:

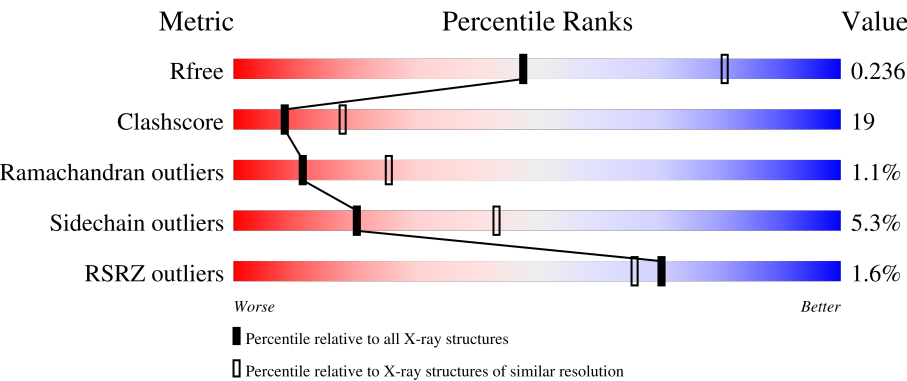
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	493	% 56%35% . .
1	C	493	% 65%26%5% .
1	E	493	% 60%31% . . .
1	G	493	5% 55%36%5% .
1	I	493	% 58%34% . .

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Mol	Chain	Length	Quality of chain
1	K	493	4% 54% 39% • • •
1	M	493	2% 61% 30% • •
1	O	493	% 57% 35% • •
2	B	138	67% 30% •
2	D	138	63% 33% •
2	F	138	65% 33% •
2	H	138	65% 33% •
2	J	138	71% 28% •
2	L	138	69% 28% •
2	N	138	63% 35% • •
2	P	138	% 62% 33% • •

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 42000 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 ribulose-1,5-bisphosphate carboxylase/oxygenase large subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	473	Total	C	N	O	S	0	0	0
			3712	2367	642	684	19			
1	C	473	Total	C	N	O	S	0	0	0
			3712	2367	642	684	19			
1	E	473	Total	C	N	O	S	0	0	0
			3712	2367	642	684	19			
1	G	473	Total	C	N	O	S	0	0	0
			3712	2367	642	684	19			
1	I	473	Total	C	N	O	S	0	0	0
			3712	2367	642	684	19			
1	K	473	Total	C	N	O	S	0	0	0
			3712	2367	642	684	19			
1	M	473	Total	C	N	O	S	0	0	0
			3712	2367	642	684	19			
1	O	473	Total	C	N	O	S	0	0	0
			3712	2367	642	684	19			

- Molecule 2 is a protein called ribulose-1,5-bisphosphate carboxylase/oxygenase small subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	138	Total	C	N	O	S	0	0	0
			1144	736	193	211	4			
2	D	138	Total	C	N	O	S	0	0	0
			1144	736	193	211	4			
2	F	138	Total	C	N	O	S	0	0	0
			1144	736	193	211	4			
2	H	138	Total	C	N	O	S	0	0	0
			1144	736	193	211	4			
2	J	138	Total	C	N	O	S	0	0	0
			1144	736	193	211	4			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	138	Total	C	N	O	S	0	0	0
			1144	736	193	211	4			
2	N	138	Total	C	N	O	S	0	0	0
			1144	736	193	211	4			
2	P	138	Total	C	N	O	S	0	0	0
			1144	736	193	211	4			

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		
3	E	1	Total	O	S	0	0
			5	4	1		
3	G	1	Total	O	S	0	0
			5	4	1		
3	I	1	Total	O	S	0	0
			5	4	1		
3	K	1	Total	O	S	0	0
			5	4	1		
3	M	1	Total	O	S	0	0
			5	4	1		
3	O	1	Total	O	S	0	0
			5	4	1		

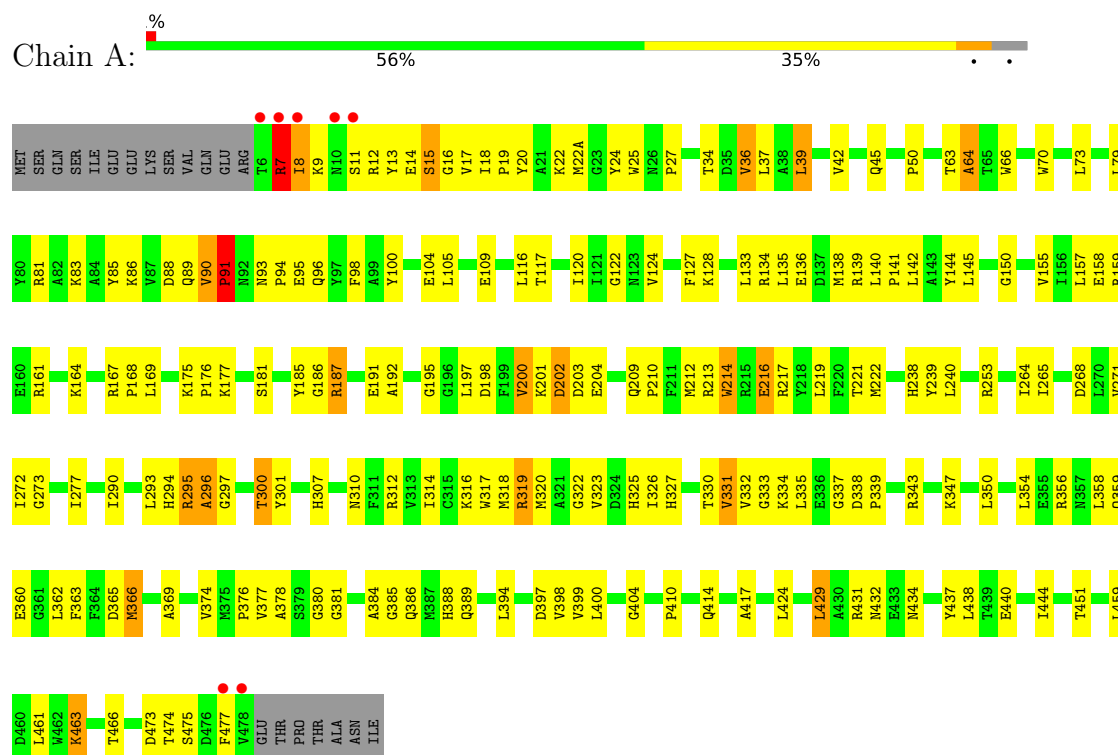
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	282	Total 282	O 282	0	0
4	B	102	Total 102	O 102	0	0
4	C	313	Total 313	O 313	0	0
4	D	117	Total 117	O 117	0	0
4	E	281	Total 281	O 281	0	0
4	F	113	Total 113	O 113	0	0
4	G	191	Total 191	O 191	0	0
4	H	120	Total 120	O 120	0	0
4	I	275	Total 275	O 275	0	0
4	J	145	Total 145	O 145	0	0
4	K	196	Total 196	O 196	0	0
4	L	143	Total 143	O 143	0	0
4	M	284	Total 284	O 284	0	0
4	N	134	Total 134	O 134	0	0
4	O	283	Total 283	O 283	0	0
4	P	133	Total 133	O 133	0	0

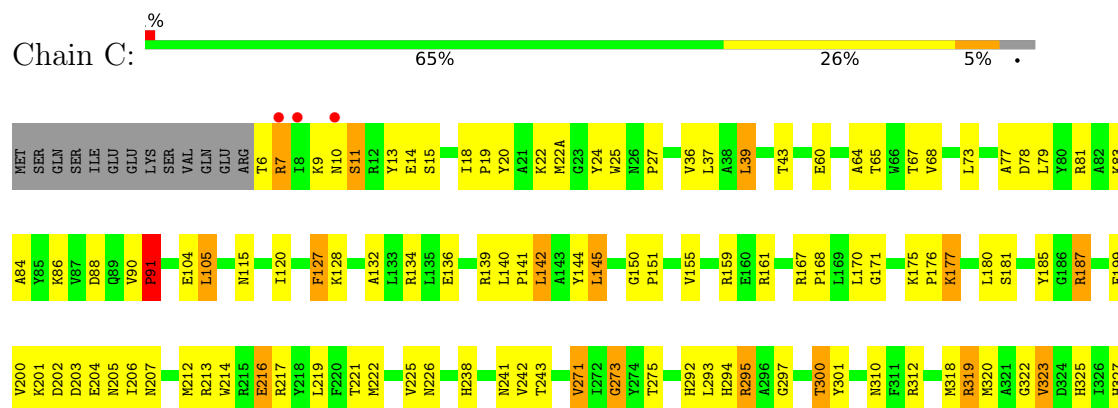
3 Residue-property plots

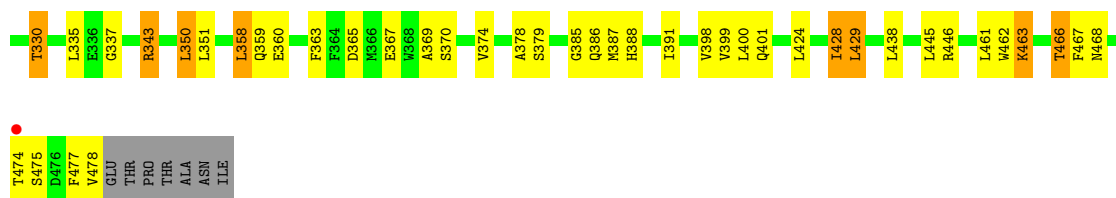
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: ribulose-1,5-bisphosphate carboxylase/oxygenase large subunit

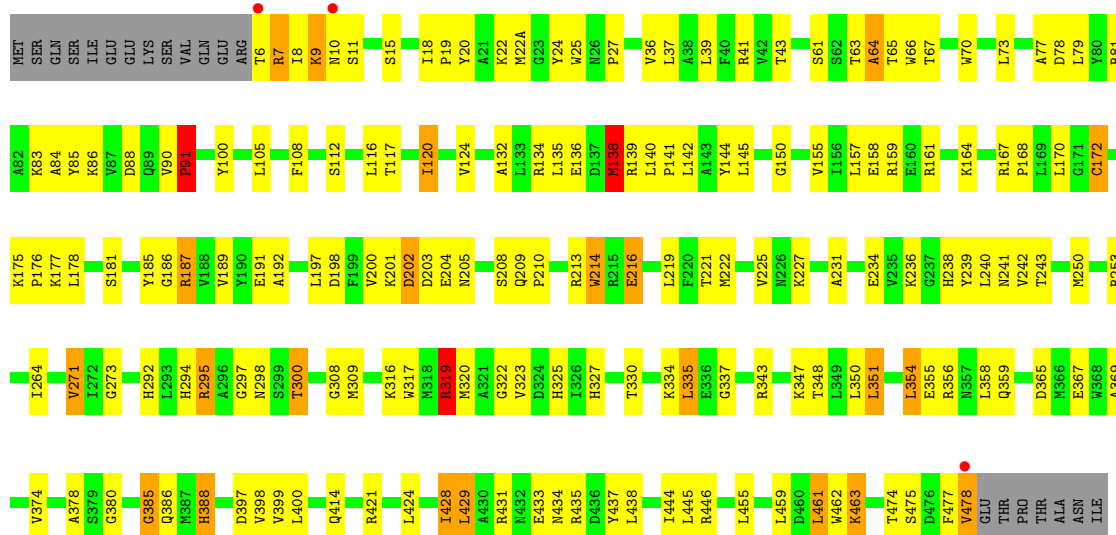


- Molecule 1: ribulose-1,5-bisphosphate carboxylase/oxygenase large subunit

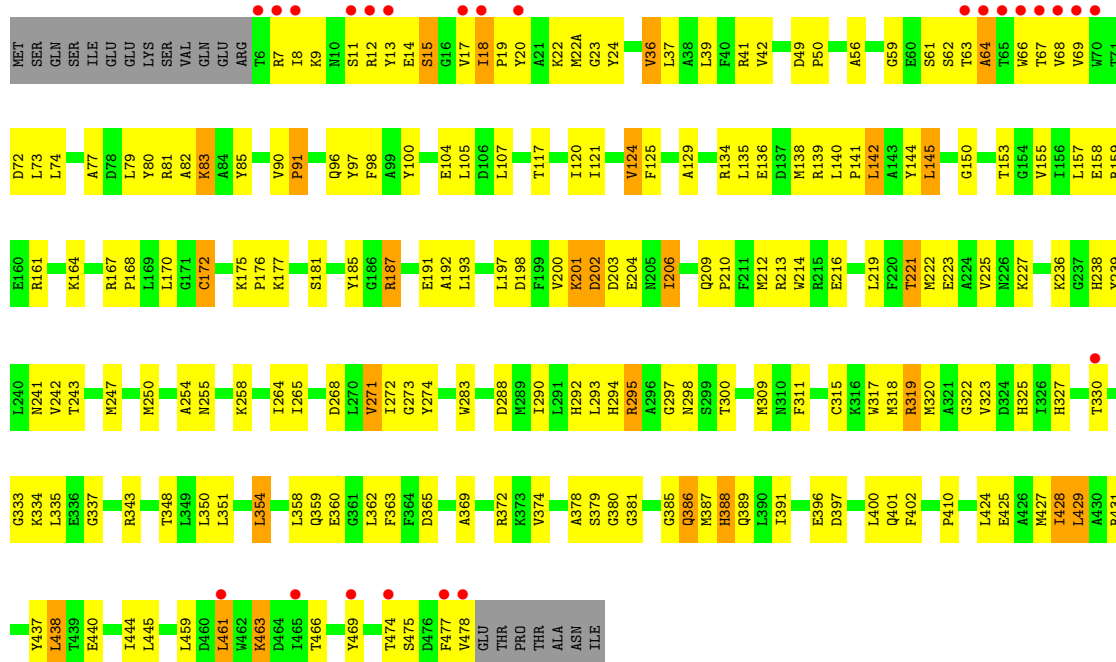




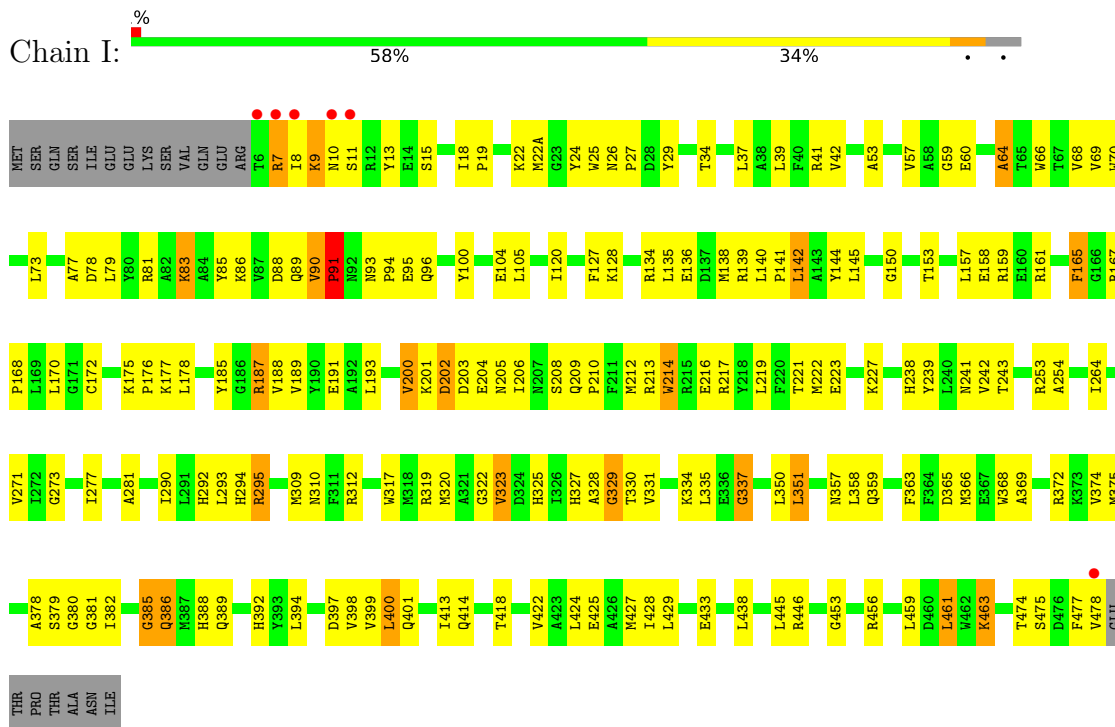
- Molecule 1: ribulose-1,5-bisphosphate carboxylase/oxygenase large subunit



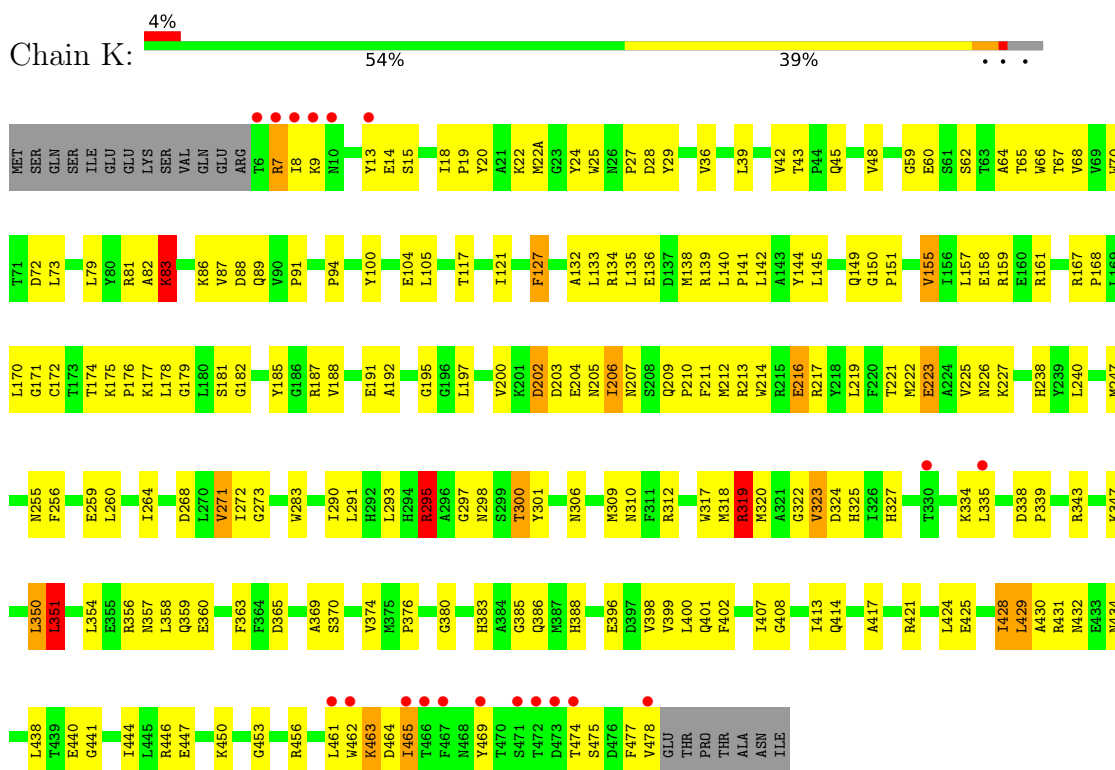
- Molecule 1: ribulose-1,5-bisphosphate carboxylase/oxygenase large subunit



- Molecule 1: ribulose-1,5-bisphosphate carboxylase/oxygenase large subunit

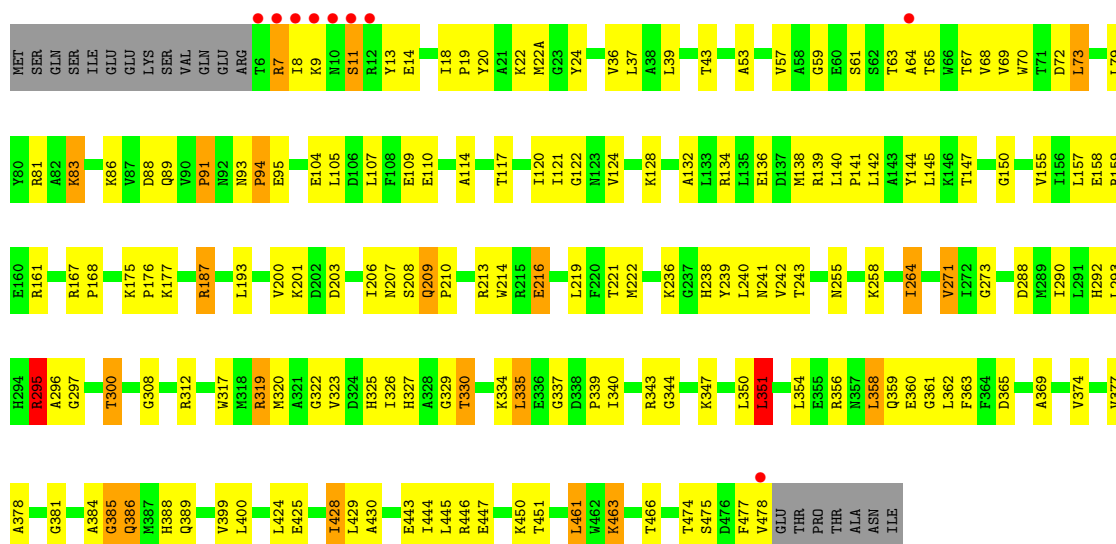


- Molecule 1: ribulose-1,5-bisphosphate carboxylase/oxygenase large subunit

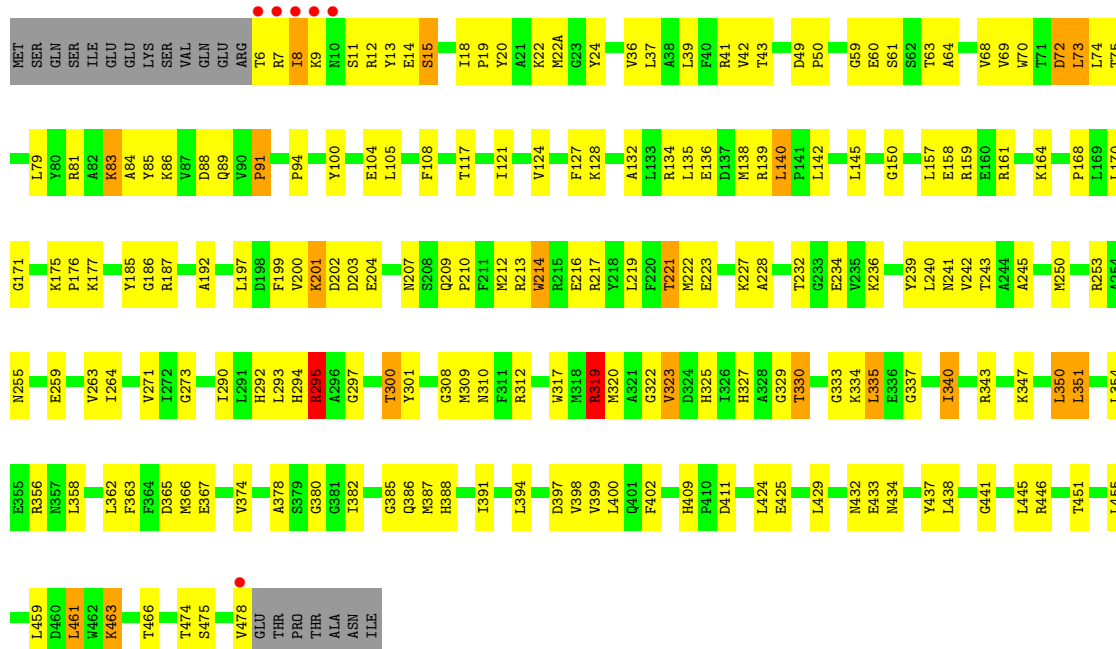


- Molecule 1: ribulose-1,5-bisphosphate carboxylase/oxygenase large subunit

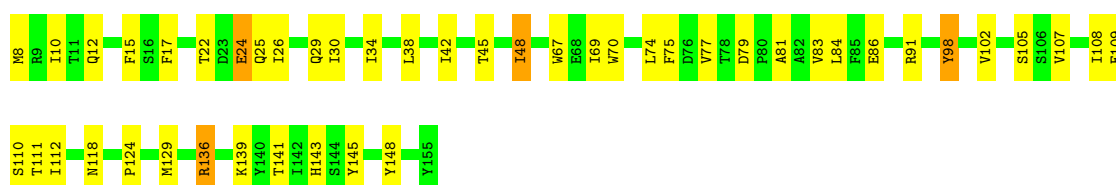




• Molecule 1: ribulose-1,5-bisphosphate carboxylase/oxygenase large subunit

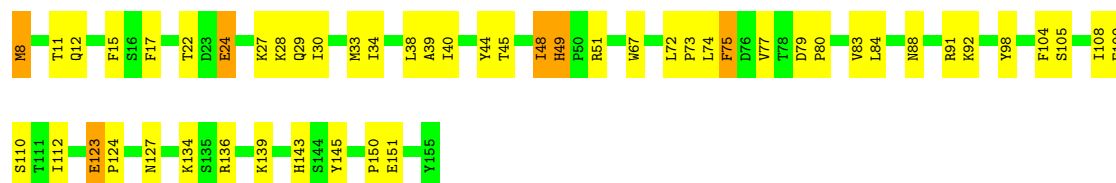


• Molecule 2: ribulose-1,5-bisphosphate carboxylase/oxygenase small subunit



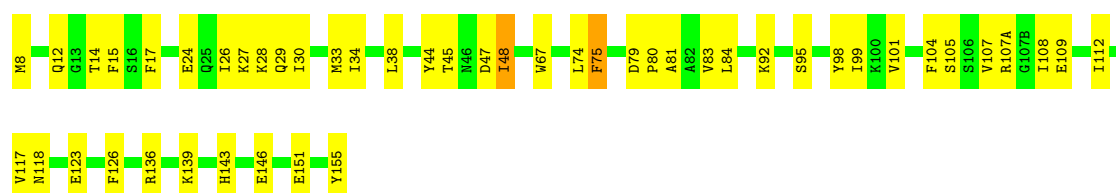
- Molecule 2: ribulose-1,5-bisphosphate carboxylase/oxygenase small subunit

Chain D:  63% 33%



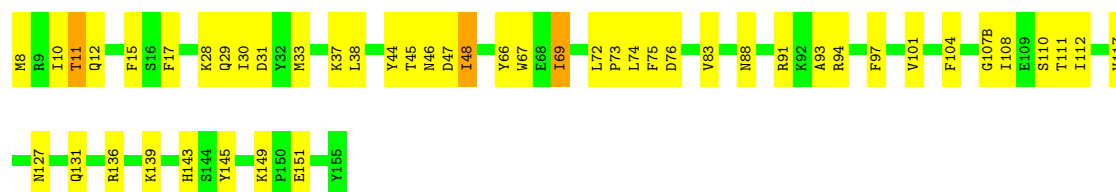
- Molecule 2: ribulose-1,5-bisphosphate carboxylase/oxygenase small subunit

Chain F:  65% 33%



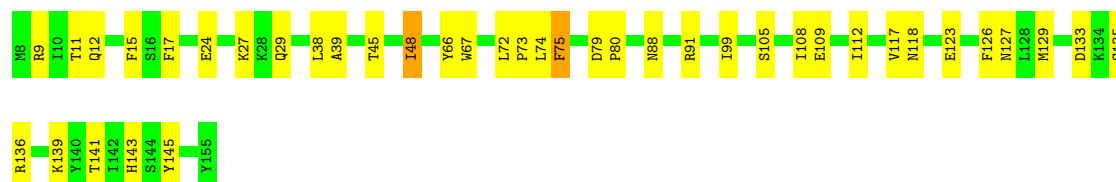
- Molecule 2: ribulose-1,5-bisphosphate carboxylase/oxygenase small subunit

Chain H:  65% 33%



- Molecule 2: ribulose-1,5-bisphosphate carboxylase/oxygenase small subunit

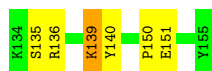
Chain J:  71% 28%



- Molecule 2: ribulose-1,5-bisphosphate carboxylase/oxygenase small subunit

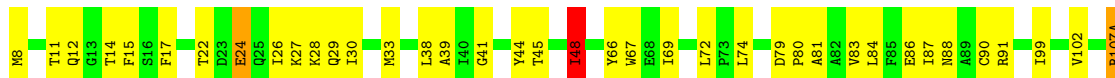
Chain L:  69% 28%





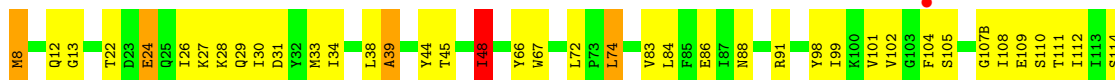
- Molecule 2: ribulose-1,5-bisphosphate carboxylase/oxygenase small subunit

Chain N: 63% 35% ..



- Molecule 2: ribulose-1,5-bisphosphate carboxylase/oxygenase small subunit

Chain P: % 62% 33% ..



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	201.33Å 146.99Å 197.23Å 90.00° 99.79° 90.00°	Depositor
Resolution (Å)	25.65 – 2.60 25.65 – 2.60	Depositor EDS
% Data completeness (in resolution range)	98.9 (25.65-2.60) 98.9 (25.65-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.26 (at 2.60Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.172 , 0.235 0.172 , 0.236	Depositor DCC
R_{free} test set	8610 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	24.6	Xtriage
Anisotropy	0.021	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 74.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	42000	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 2.72% 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: SO4

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	A	0.39	0/3793	0.96	18/5138 (0.4%)
1	C	0.41	0/3793	0.97	14/5138 (0.3%)
1	E	0.43	1/3793 (0.0%)	0.96	14/5138 (0.3%)
1	G	0.39	0/3793	0.93	14/5138 (0.3%)
1	I	0.38	0/3793	0.95	17/5138 (0.3%)
1	K	0.38	0/3793	0.91	13/5138 (0.3%)
1	M	0.41	0/3793	0.96	14/5138 (0.3%)
1	O	0.40	0/3793	0.94	20/5138 (0.4%)
2	B	0.37	0/1173	0.94	3/1583 (0.2%)
2	D	0.36	0/1173	0.99	7/1583 (0.4%)
2	F	0.37	0/1173	0.99	7/1583 (0.4%)
2	H	0.40	0/1173	0.94	2/1583 (0.1%)
2	J	0.39	0/1173	1.00	6/1583 (0.4%)
2	L	0.40	0/1173	1.05	7/1583 (0.4%)
2	N	0.38	0/1173	0.95	2/1583 (0.1%)
2	P	0.37	0/1173	1.00	5/1583 (0.3%)
All	All	0.39	1/39728 (0.0%)	0.96	163/53768 (0.3%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	138	MET	SD-CE	-9.94	1.54	1.79

All (163) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	12	GLN	N-CA-C	-9.44	98.35	110.53
1	E	214	TRP	N-CA-C	9.06	121.16	111.28
1	C	214	TRP	N-CA-C	8.72	120.87	111.36
2	F	12	GLN	N-CA-C	-8.63	98.89	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	365	ASP	N-CA-C	-8.57	97.79	110.48
2	P	12	GLN	N-CA-C	-8.52	99.54	110.53
1	O	329	GLY	N-CA-C	8.50	122.77	112.48
2	D	12	GLN	N-CA-C	-8.31	99.32	110.55
1	A	385	GLY	N-CA-C	-8.15	104.86	113.58
1	K	214	TRP	N-CA-C	8.12	119.75	111.07
2	J	12	GLN	N-CA-C	-8.11	100.07	110.53
2	N	12	GLN	N-CA-C	-8.10	99.62	110.55
1	M	330	THR	N-CA-C	-7.98	96.95	109.72
1	M	365	ASP	N-CA-C	-7.92	97.69	110.20
1	A	429	LEU	N-CA-C	-7.88	102.64	111.07
2	H	12	GLN	N-CA-C	-7.81	100.01	110.55
1	I	365	ASP	N-CA-C	-7.78	98.97	110.48
2	L	75	PHE	N-CA-C	7.77	123.23	112.04
1	A	214	TRP	N-CA-C	7.74	119.72	111.28
2	D	123	GLU	CA-C-N	7.68	127.57	119.05
2	D	123	GLU	C-N-CA	7.68	127.57	119.05
1	O	214	TRP	N-CA-C	7.62	119.58	111.28
1	K	365	ASP	N-CA-C	-7.38	97.57	109.96
1	M	214	TRP	N-CA-C	7.37	119.31	111.28
1	K	385	GLY	N-CA-C	-7.36	105.10	114.37
2	F	123	GLU	CA-C-N	7.32	127.17	119.05
2	F	123	GLU	C-N-CA	7.32	127.17	119.05
1	E	64	ALA	N-CA-C	7.26	119.90	110.53
1	I	214	TRP	N-CA-C	7.26	119.19	111.28
2	D	75	PHE	N-CA-C	7.19	122.32	112.90
1	C	330	THR	N-CA-C	-6.89	100.03	109.95
1	I	386	GLN	N-CA-C	-6.83	104.15	113.30
1	C	365	ASP	N-CA-C	-6.82	99.42	110.20
1	M	120	ILE	N-CA-C	6.80	117.56	110.62
1	C	429	LEU	N-CA-C	-6.77	103.97	111.82
1	G	214	TRP	N-CA-C	6.75	118.64	111.28
1	C	84	ALA	N-CA-C	-6.74	98.93	109.25
1	A	365	ASP	N-CA-C	-6.73	99.06	109.76
1	O	319	ARG	N-CA-C	-6.71	104.04	111.36
1	G	386	GLN	N-CA-C	-6.62	104.77	112.92
1	G	36	VAL	N-CA-C	-6.61	98.90	108.36
1	O	108	PHE	N-CA-C	6.60	120.22	109.59
1	E	202	ASP	N-CA-C	-6.60	101.82	110.53
1	K	202	ASP	N-CA-C	-6.58	101.66	110.55
1	C	386	GLN	N-CA-C	-6.52	104.56	113.30
1	E	386	GLN	N-CA-C	-6.51	104.58	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	385	GLY	N-CA-C	-6.46	105.60	114.64
1	M	329	GLY	N-CA-C	6.45	119.52	112.29
1	E	200	VAL	N-CA-C	-6.42	98.24	108.90
1	C	200	VAL	N-CA-C	-6.41	98.42	108.81
2	B	12	GLN	N-CA-C	-6.40	102.08	110.53
2	L	123	GLU	CA-C-N	6.37	126.28	119.28
2	L	123	GLU	C-N-CA	6.37	126.28	119.28
1	G	120	ILE	N-CA-C	6.34	116.49	110.53
1	O	365	ASP	N-CA-C	-6.30	99.37	109.96
1	K	386	GLN	N-CA-C	-6.27	105.57	113.72
2	J	133	ASP	N-CA-C	6.24	113.90	108.78
1	E	84	ALA	N-CA-C	-6.21	99.75	109.25
1	G	365	ASP	N-CA-C	-6.18	99.57	109.96
1	M	386	GLN	N-CA-C	-6.17	104.35	113.61
2	F	75	PHE	N-CA-C	6.14	120.79	113.12
1	I	202	ASP	N-CA-C	-6.09	102.49	110.53
1	A	404	GLY	N-CA-C	-6.00	108.07	114.67
1	O	386	GLN	N-CA-C	-6.00	105.26	113.30
1	I	385	GLY	N-CA-C	-5.99	107.35	114.48
1	I	200	VAL	N-CA-C	-5.98	99.12	108.81
1	I	366	MET	N-CA-C	5.97	117.79	107.93
1	K	200	VAL	N-CA-C	-5.97	98.99	108.90
1	C	36	VAL	N-CA-C	-5.96	99.84	108.36
1	A	202	ASP	N-CA-C	-5.93	102.70	110.53
1	O	350	LEU	N-CA-C	5.88	120.51	112.04
1	E	108	PHE	N-CA-C	5.88	119.30	109.95
1	K	223	GLU	N-CA-C	-5.87	104.96	111.36
2	L	151	GLU	N-CA-C	5.87	118.15	111.11
1	A	386	GLN	N-CA-C	-5.86	105.79	113.17
1	G	351	LEU	N-CA-C	5.84	117.06	109.64
2	P	123	GLU	CA-C-N	5.82	125.68	119.28
2	P	123	GLU	C-N-CA	5.82	125.68	119.28
1	O	330	THR	N-CA-C	-5.81	99.71	109.07
1	M	351	LEU	N-CA-C	5.79	116.99	109.64
1	K	155	VAL	N-CA-C	5.78	116.42	110.36
1	C	120	ILE	N-CA-C	5.76	116.41	110.36
1	K	429	LEU	N-CA-C	-5.71	105.05	111.28
1	G	429	LEU	N-CA-C	-5.71	104.96	111.07
1	A	200	VAL	N-CA-C	-5.70	99.54	108.95
1	I	329	GLY	N-CA-C	5.67	119.83	112.68
2	J	39	ALA	N-CA-C	-5.67	101.25	110.20
2	D	151	GLU	N-CA-C	5.67	118.19	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	14	THR	N-CA-C	5.65	118.38	111.82
1	K	319	ARG	N-CA-C	-5.64	105.28	111.82
1	E	385	GLY	N-CA-C	-5.61	107.81	114.48
1	K	351	LEU	N-CA-C	5.61	117.82	110.08
1	O	84	ALA	N-CA-C	-5.60	100.68	109.25
1	G	202	ASP	N-CA-C	-5.59	103.01	110.55
1	A	36	VAL	N-CA-C	-5.53	100.45	108.36
1	O	41	ARG	N-CA-C	-5.53	98.75	108.20
1	G	200	VAL	N-CA-C	-5.51	100.54	108.42
1	M	384	ALA	N-CA-C	-5.51	102.24	110.23
1	E	120	ILE	N-CA-C	5.50	116.23	110.62
2	F	151	GLU	N-CA-C	5.49	117.97	111.33
1	C	343	ARG	N-CA-C	-5.47	105.31	111.28
1	I	64	ALA	N-CA-C	5.47	117.14	110.41
1	M	209	GLN	N-CA-C	5.46	114.42	108.14
1	I	90	VAL	CA-C-N	5.44	126.64	119.84
1	I	90	VAL	C-N-CA	5.44	126.64	119.84
1	M	122	GLY	N-CA-C	5.43	118.80	112.50
1	C	202	ASP	N-CA-C	-5.42	102.45	110.48
1	A	384	ALA	N-CA-C	-5.39	102.41	110.23
1	E	41	ARG	N-CA-C	-5.37	99.02	108.20
1	M	200	VAL	N-CA-C	-5.37	99.99	108.90
1	C	350	LEU	N-CA-C	5.36	120.31	113.55
2	D	49	HIS	N-CA-C	-5.36	102.84	109.64
2	B	98	TYR	N-CA-C	-5.34	101.75	110.20
1	A	319	ARG	N-CA-C	-5.34	105.54	111.36
1	I	41	ARG	N-CA-C	-5.33	99.09	108.20
2	H	151	GLU	N-CA-C	5.32	117.77	111.33
2	P	66	TYR	N-CA-C	5.32	117.88	107.57
1	I	328	ALA	N-CA-C	-5.31	106.81	113.72
1	E	264	ILE	N-CA-C	5.31	115.28	107.75
1	O	36	VAL	N-CA-C	-5.30	100.78	108.36
2	F	95	SER	N-CA-C	5.29	116.73	111.07
1	A	7	ARG	N-CA-C	-5.29	105.53	113.89
1	I	351	LEU	N-CA-C	5.29	117.19	109.84
1	I	42	VAL	N-CA-C	5.28	115.91	108.36
1	I	120	ILE	N-CA-C	5.28	115.91	110.36
1	O	223	GLU	N-CA-C	-5.28	105.61	111.36
1	O	42	VAL	N-CA-C	5.27	116.17	108.53
1	O	200	VAL	N-CA-C	-5.27	100.15	108.90
1	A	90	VAL	CA-C-N	5.26	126.41	119.84
1	A	90	VAL	C-N-CA	5.26	126.41	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	42	VAL	N-CA-C	5.25	115.53	108.17
1	C	201	LYS	N-CA-C	5.25	117.17	109.24
1	M	201	LYS	N-CA-C	5.24	117.03	109.07
1	G	396	GLU	N-CA-C	5.23	116.79	111.14
1	O	72	ASP	N-CA-C	-5.23	105.76	111.82
1	O	140	LEU	CA-C-N	5.22	125.13	119.85
1	O	140	LEU	C-N-CA	5.22	125.13	119.85
1	O	351	LEU	N-CA-C	5.22	117.10	109.84
1	A	64	ALA	N-CA-C	5.19	116.79	110.41
1	K	68	VAL	N-CA-C	5.19	115.94	108.93
1	O	201	LYS	N-CA-C	5.18	116.94	109.07
1	C	273	GLY	N-CA-C	5.17	116.86	111.95
1	K	83	LYS	N-CA-C	5.17	116.81	108.34
2	D	39	ALA	N-CA-C	-5.15	100.90	109.46
1	G	274	TYR	N-CA-C	5.15	117.57	111.33
2	P	39	ALA	N-CA-C	-5.15	101.57	109.76
1	E	319	ARG	N-CA-C	-5.13	105.77	111.36
1	A	366	MET	N-CA-C	5.13	116.77	108.26
1	O	366	MET	N-CA-C	5.12	116.94	108.13
1	G	201	LYS	N-CA-C	5.11	116.84	109.07
2	J	123	GLU	CA-C-N	5.10	124.72	119.05
2	J	123	GLU	C-N-CA	5.10	124.72	119.05
2	J	126	PHE	N-CA-C	5.09	117.86	109.72
1	A	201	LYS	N-CA-C	5.08	116.97	108.99
2	F	126	PHE	N-CA-C	5.07	117.84	109.72
2	L	133	ASP	N-CA-C	5.07	113.61	108.75
1	E	112	SER	N-CA-C	5.05	116.86	108.02
1	A	394	LEU	N-CA-C	5.05	116.86	111.36
1	I	264	ILE	N-CA-C	5.05	116.26	108.44
1	G	41	ARG	N-CA-C	-5.04	99.58	108.20
1	M	264	ILE	N-CA-C	5.01	114.80	107.88
2	B	148	TYR	N-CA-C	-5.00	106.95	113.16
2	N	39	ALA	N-CA-C	-5.00	101.16	109.46

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	3712	0	3694	161	0
1	C	3712	0	3694	129	0
1	E	3712	0	3694	144	0
1	G	3712	0	3694	187	0
1	I	3712	0	3694	152	0
1	K	3712	0	3694	211	0
1	M	3712	0	3694	136	0
1	O	3712	0	3694	159	0
2	B	1144	0	1131	37	0
2	D	1144	0	1131	46	0
2	F	1144	0	1131	44	0
2	H	1144	0	1131	46	0
2	J	1144	0	1131	38	0
2	L	1144	0	1131	39	0
2	N	1144	0	1131	48	0
2	P	1144	0	1131	49	0
3	A	5	0	0	0	0
3	C	5	0	0	1	0
3	E	5	0	0	0	0
3	G	5	0	0	0	0
3	I	5	0	0	1	0
3	K	5	0	0	0	0
3	M	5	0	0	0	0
3	O	5	0	0	0	0
4	A	282	0	0	11	0
4	B	102	0	0	2	0
4	C	313	0	0	10	0
4	D	117	0	0	3	0
4	E	281	0	0	8	0
4	F	113	0	0	5	0
4	G	191	0	0	9	0
4	H	120	0	0	5	0
4	I	275	0	0	14	0
4	J	145	0	0	1	0
4	K	196	0	0	10	0
4	L	143	0	0	3	0
4	M	284	0	0	10	0
4	N	134	0	0	5	0
4	O	283	0	0	13	0
4	P	133	0	0	5	0
All	All	42000	0	38600	1480	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 19.

All (1480) 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)
2:H:72:LEU:H	1:M:7:ARG:HG2	1.20	1.05
2:B:8:MET:HE1	2:B:10:ILE:HD13	1.35	1.05
1:G:273:GLY:HA3	1:K:273:GLY:HA3	1.42	1.01
2:L:139:LYS:HE2	2:L:139:LYS:HA	1.42	1.01
1:O:159:ARG:HD3	1:O:164:LYS:O	1.62	0.99
1:E:273:GLY:HA3	1:M:273:GLY:HA3	1.44	0.97
1:C:161:ARG:HD3	4:C:4099:HOH:O	1.66	0.96
1:M:295:ARG:HG2	1:M:327:HIS:HB2	1.49	0.94
1:K:474:THR:HG22	1:K:475:SER:H	1.32	0.94
1:G:63:THR:HA	1:K:177:LYS:HD3	1.50	0.94
1:O:295:ARG:HG2	1:O:327:HIS:HB2	1.49	0.93
2:H:139:LYS:HA	2:H:139:LYS:HE2	1.48	0.93
2:F:139:LYS:HA	2:F:139:LYS:HE2	1.52	0.91
2:N:139:LYS:HE2	2:N:139:LYS:HA	1.49	0.91
1:I:319:ARG:HG3	1:I:374:VAL:HG23	1.50	0.91
1:A:19:PRO:HG2	1:A:22:LYS:HD3	1.51	0.91
1:A:273:GLY:HA3	1:I:273:GLY:HA3	1.53	0.91
1:E:6:THR:HA	4:E:4121:HOH:O	1.73	0.88
1:O:340:ILE:HD12	1:O:340:ILE:H	1.36	0.88
1:G:135:LEU:HD21	1:G:138:MET:HE2	1.56	0.88
1:G:330:THR:HG22	1:G:378:ALA:HB1	1.52	0.88
1:G:300:THR:HG21	1:K:309:MET:HE2	1.53	0.88
1:M:138:MET:CE	1:M:317:TRP:HE1	1.86	0.88
1:M:358:LEU:H	1:M:358:LEU:HD22	1.40	0.87
1:A:20:TYR:HA	1:A:22(A):MET:HE3	1.55	0.87
1:K:135:LEU:HD21	1:K:138:MET:HE2	1.57	0.86
1:O:330:THR:HG22	1:O:378:ALA:HB1	1.56	0.86
1:C:10:ASN:HB2	4:C:4041:HOH:O	1.74	0.86
1:A:300:THR:HG21	1:I:309:MET:HE2	1.58	0.85
1:I:330:THR:HG22	1:I:378:ALA:HB1	1.57	0.85
1:G:69:VAL:HG23	1:G:72:ASP:OD1	1.76	0.85
1:G:7:ARG:HB3	2:P:72:LEU:HB2	1.59	0.85
2:N:139:LYS:HE3	4:N:2342:HOH:O	1.77	0.84
1:I:8:ILE:HG22	1:I:9:LYS:H	1.42	0.84
1:A:295:ARG:HD2	1:A:327:HIS:HB2	1.60	0.84
1:K:359:GLN:HE22	1:K:478:VAL:HA	1.43	0.84
1:G:155:VAL:O	1:G:159:ARG:HG3	1.78	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:139:LYS:HE2	2:D:139:LYS:HA	1.58	0.83
1:K:192:ALA:HB1	1:K:197:LEU:HD12	1.59	0.83
2:L:139:LYS:HE3	4:L:212:HOH:O	1.78	0.83
1:M:213:ARG:HB2	1:M:216:GLU:OE2	1.80	0.82
1:I:459:LEU:O	1:I:463:LYS:HB2	1.81	0.81
1:E:7:ARG:HD3	1:E:7:ARG:N	1.96	0.80
1:E:192:ALA:HB1	1:E:197:LEU:HD12	1.64	0.80
1:E:140:LEU:HD13	1:E:320:MET:SD	2.21	0.79
1:G:192:ALA:HB1	1:G:197:LEU:HD12	1.64	0.79
1:A:330:THR:HG22	1:A:378:ALA:HB1	1.64	0.79
1:K:7:ARG:HA	1:K:7:ARG:NE	1.98	0.78
1:E:319:ARG:HG2	1:E:374:VAL:HG23	1.65	0.78
1:C:385:GLY:HA2	1:C:445:LEU:HD13	1.65	0.78
1:M:330:THR:HG22	1:M:378:ALA:HB1	1.66	0.78
1:M:334:LYS:HG3	1:M:335:LEU:HD13	1.64	0.78
1:K:319:ARG:HG3	1:K:374:VAL:HG23	1.66	0.78
1:I:201:LYS:HE3	4:I:4147:HOH:O	1.82	0.77
1:G:295:ARG:HG2	1:G:327:HIS:HB2	1.66	0.77
1:K:19:PRO:HG2	1:K:22:LYS:HB2	1.64	0.77
1:M:24:TYR:CZ	1:M:64:ALA:HB2	2.19	0.77
1:C:330:THR:HG22	1:C:378:ALA:HB1	1.66	0.77
1:G:7:ARG:HD3	2:P:74:LEU:HD11	1.66	0.77
1:A:24:TYR:CZ	1:A:64:ALA:HB2	2.21	0.76
1:O:8:ILE:HG22	1:O:9:LYS:H	1.51	0.76
1:C:273:GLY:HA3	1:O:273:GLY:HA3	1.65	0.75
1:A:86:LYS:HE2	1:A:88:ASP:OD1	1.85	0.75
1:C:24:TYR:CZ	1:C:64:ALA:HB2	2.21	0.75
1:G:300:THR:HG22	1:K:301:TYR:HB2	1.66	0.75
1:E:309:MET:HE2	1:M:300:THR:HG21	1.69	0.75
2:F:28:LYS:HD3	1:I:433:GLU:HG2	1.67	0.75
1:M:340:ILE:H	1:M:340:ILE:HD12	1.52	0.75
1:G:20:TYR:HE1	1:G:64:ALA:HB1	1.52	0.75
1:G:140:LEU:HD13	1:G:320:MET:SD	2.26	0.75
1:I:161:ARG:HD3	4:I:4084:HOH:O	1.86	0.74
1:C:177:LYS:HB2	1:O:63:THR:HA	1.68	0.74
1:K:142:LEU:HD12	1:K:369:ALA:HB2	1.69	0.74
1:I:19:PRO:HG2	1:I:22:LYS:HD3	1.70	0.74
1:A:24:TYR:CE2	1:A:64:ALA:HB2	2.23	0.74
2:F:38:LEU:HD11	2:F:112:ILE:HD11	1.70	0.74
1:I:295:ARG:HG2	1:I:327:HIS:HB2	1.68	0.74
1:C:358:LEU:HD12	1:C:477:PHE:CZ	2.23	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:161:ARG:HD3	4:M:4089:HOH:O	1.87	0.74
1:O:161:ARG:HD3	4:O:4071:HOH:O	1.86	0.73
1:C:7:ARG:HA	1:C:7:ARG:NE	2.02	0.73
2:P:30:ILE:HD13	2:P:83:VAL:HB	1.70	0.73
1:E:358:LEU:HD22	1:E:358:LEU:H	1.51	0.73
1:M:319:ARG:HG2	1:M:374:VAL:HG23	1.71	0.73
1:G:138:MET:HE1	1:G:317:TRP:HZ2	1.53	0.72
1:K:185:TYR:HB2	4:K:4124:HOH:O	1.88	0.72
1:G:9:LYS:HB3	1:G:14:GLU:HA	1.70	0.72
1:E:295:ARG:HG2	1:E:327:HIS:HB2	1.72	0.72
1:E:330:THR:HG22	1:E:378:ALA:HB1	1.72	0.72
2:F:79:ASP:OD2	2:F:81:ALA:HB3	1.89	0.72
1:M:297:GLY:O	1:M:300:THR:HB	1.89	0.72
1:A:319:ARG:HG3	1:A:374:VAL:HG23	1.70	0.72
1:C:60:GLU:HG3	1:C:127:PHE:CE1	2.25	0.72
1:E:213:ARG:HB2	1:E:216:GLU:OE2	1.89	0.72
1:K:161:ARG:HD3	4:K:4045:HOH:O	1.90	0.71
1:K:356:ARG:NH1	1:K:358:LEU:HD21	2.06	0.71
1:M:138:MET:HE2	1:M:317:TRP:HE1	1.53	0.71
1:K:213:ARG:HB2	1:K:216:GLU:OE2	1.90	0.71
1:K:475:SER:HB3	1:K:478:VAL:HG13	1.72	0.71
1:M:155:VAL:O	1:M:159:ARG:HG3	1.91	0.71
1:M:221:THR:HG21	1:M:238:HIS:CD2	2.25	0.71
2:D:72:LEU:N	1:K:7:ARG:HG2	2.06	0.71
1:I:142:LEU:HD12	1:I:369:ALA:HB2	1.73	0.70
1:G:134:ARG:HD3	1:G:136:GLU:OE2	1.91	0.70
1:I:7:ARG:HA	1:I:7:ARG:NE	2.06	0.70
1:K:358:LEU:H	1:K:358:LEU:HD22	1.55	0.70
1:C:155:VAL:O	1:C:159:ARG:HG3	1.91	0.70
1:M:347:LYS:HB3	1:M:351:LEU:HD22	1.72	0.70
1:O:8:ILE:HG22	1:O:9:LYS:N	2.07	0.70
1:K:140:LEU:HD13	1:K:320:MET:SD	2.31	0.70
1:K:187:ARG:HH11	1:K:187:ARG:HG2	1.55	0.70
1:G:18:ILE:HD12	4:G:4118:HOH:O	1.92	0.70
2:H:72:LEU:HG	2:H:73:PRO:HD2	1.73	0.70
1:A:213:ARG:HB2	1:A:216:GLU:OE2	1.91	0.70
1:E:319:ARG:HG2	1:E:374:VAL:CG2	2.22	0.70
1:G:39:LEU:HD22	1:G:363:PHE:CG	2.27	0.70
1:C:297:GLY:O	1:C:300:THR:HB	1.92	0.70
1:O:463:LYS:NZ	1:O:463:LYS:HB3	2.06	0.70
1:I:8:ILE:HG22	1:I:9:LYS:N	2.06	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:7:ARG:HG3	2:L:72:LEU:H	1.56	0.69
1:G:172:CYS:HB3	1:G:197:LEU:HD13	1.74	0.69
1:M:140:LEU:HD13	1:M:320:MET:SD	2.32	0.69
1:O:241:ASN:ND2	1:O:243:THR:H	1.90	0.69
1:A:140:LEU:HD13	1:A:320:MET:SD	2.33	0.69
1:K:474:THR:HG22	1:K:475:SER:N	2.07	0.69
1:A:8:ILE:HG22	1:A:9:LYS:H	1.58	0.69
1:E:155:VAL:O	1:E:159:ARG:HG3	1.93	0.69
1:E:463:LYS:NZ	1:E:463:LYS:HB3	2.08	0.69
2:F:74:LEU:HD11	1:O:7:ARG:HD3	1.75	0.69
1:G:319:ARG:HG3	1:G:374:VAL:HG23	1.74	0.69
2:N:38:LEU:HD11	2:N:112:ILE:HD11	1.74	0.69
1:O:213:ARG:HB2	1:O:216:GLU:OE2	1.93	0.69
1:K:295:ARG:HG2	1:K:327:HIS:HB2	1.75	0.69
1:E:185:TYR:OH	1:E:202:ASP:HA	1.93	0.69
1:G:15:SER:HB3	1:K:461:LEU:HD11	1.75	0.69
1:E:19:PRO:HG2	1:E:22:LYS:HB2	1.75	0.68
2:P:104:PHE:HB2	4:P:214:HOH:O	1.93	0.68
2:H:11:THR:HG21	2:H:17:PHE:CE2	2.28	0.68
1:O:135:LEU:HD21	1:O:138:MET:HE2	1.76	0.68
1:C:213:ARG:HB2	1:C:216:GLU:OE2	1.94	0.68
1:G:74:LEU:HA	2:P:104:PHE:CE2	2.29	0.68
1:E:150:GLY:C	1:E:322:GLY:HA2	2.18	0.68
1:I:135:LEU:HD21	1:I:138:MET:CE	2.24	0.68
1:A:39:LEU:HD23	1:A:136:GLU:HB2	1.74	0.68
1:C:310:ASN:OD1	1:C:312:ARG:HG2	1.93	0.68
1:I:140:LEU:HD13	1:I:320:MET:SD	2.34	0.68
1:A:13:TYR:CG	1:A:73:LEU:HD21	2.29	0.68
1:C:466:THR:HG21	1:C:468:ASN:ND2	2.08	0.68
2:J:72:LEU:HG	2:J:73:PRO:HD2	1.77	0.67
1:A:463:LYS:HA	4:A:4260:HOH:O	1.94	0.67
2:F:139:LYS:HE3	4:F:190:HOH:O	1.93	0.67
1:C:461:LEU:HD11	1:O:15:SER:HB3	1.77	0.67
1:E:222:MET:HE3	1:E:240:LEU:HD11	1.76	0.67
1:E:142:LEU:HD13	1:E:367:GLU:HB2	1.75	0.67
1:I:18:ILE:HD11	1:I:22(A):MET:HG2	1.77	0.67
1:K:86:LYS:HE2	1:K:88:ASP:OD1	1.95	0.67
1:K:463:LYS:HB3	1:K:463:LYS:NZ	2.10	0.67
1:M:138:MET:HE1	1:M:317:TRP:HE1	1.60	0.67
1:E:24:TYR:CZ	1:E:64:ALA:HB2	2.29	0.66
1:I:329:GLY:HA2	4:I:4054:HOH:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:19:PRO:HG2	1:O:22:LYS:HB2	1.78	0.66
1:G:177:LYS:HG2	1:G:203:ASP:OD1	1.96	0.66
1:I:222:MET:HE2	1:I:222:MET:HA	1.77	0.66
1:K:293:LEU:HB2	1:K:323:VAL:HG21	1.77	0.66
2:J:38:LEU:HD11	2:J:112:ILE:HD11	1.78	0.66
1:K:356:ARG:HH12	1:K:358:LEU:HD21	1.60	0.66
1:I:221:THR:HG21	1:I:238:HIS:CD2	2.31	0.66
1:A:135:LEU:HD21	1:A:138:MET:HE2	1.76	0.66
1:E:37:LEU:HB2	1:E:139:ARG:HB3	1.75	0.66
1:M:86:LYS:HE2	1:M:88:ASP:OD1	1.96	0.66
1:E:15:SER:HB3	1:M:461:LEU:HD11	1.78	0.66
1:K:177:LYS:HG2	1:K:203:ASP:OD1	1.96	0.66
1:I:159:ARG:NH1	1:I:375:MET:HE1	2.10	0.65
1:A:161:ARG:HD3	4:A:4049:HOH:O	1.96	0.65
1:C:24:TYR:OH	1:C:64:ALA:HB2	1.96	0.65
4:C:4077:HOH:O	2:H:107(B):GLY:HA3	1.96	0.65
2:D:38:LEU:HD11	2:D:112:ILE:HD11	1.78	0.65
2:H:38:LEU:HD21	2:H:112:ILE:HD11	1.79	0.65
1:I:177:LYS:HG2	1:I:203:ASP:OD1	1.96	0.65
2:N:27:LYS:HE2	2:N:80:PRO:HG3	1.77	0.65
1:O:204:GLU:HB3	1:O:294:HIS:CD2	2.32	0.65
1:E:20:TYR:HA	1:E:22(A):MET:HE3	1.79	0.65
1:A:459:LEU:O	1:A:463:LYS:HB2	1.96	0.65
1:O:159:ARG:NH1	1:O:397:ASP:OD1	2.24	0.65
1:A:8:ILE:HG22	1:A:9:LYS:N	2.11	0.64
1:E:172:CYS:HB3	1:E:197:LEU:HD13	1.78	0.64
1:E:241:ASN:ND2	1:E:243:THR:H	1.95	0.64
1:G:168:PRO:HD2	1:G:424:LEU:HD11	1.78	0.64
1:K:221:THR:O	1:K:225:VAL:HG23	1.97	0.64
2:J:129:MET:HB2	2:J:141:THR:HB	1.79	0.64
1:C:168:PRO:HD2	1:C:424:LEU:HD11	1.80	0.64
2:J:45:THR:CG2	2:J:67:TRP:HA	2.28	0.64
1:C:18:ILE:O	1:C:22(A):MET:HE2	1.97	0.64
1:I:24:TYR:CZ	1:I:64:ALA:HB2	2.32	0.64
1:K:7:ARG:HA	1:K:7:ARG:CZ	2.27	0.64
1:E:474:THR:HG22	1:E:475:SER:N	2.12	0.64
2:H:139:LYS:HE3	4:H:246:HOH:O	1.97	0.64
2:D:72:LEU:H	1:K:7:ARG:HG2	1.63	0.64
1:M:222:MET:HE3	1:M:240:LEU:HD11	1.79	0.64
2:F:108:ILE:HD12	2:F:108:ILE:N	2.12	0.64
1:K:177:LYS:HE3	1:K:203:ASP:OD1	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:138:MET:HE1	1:K:317:TRP:CZ2	2.32	0.63
1:K:212:MET:HE3	1:K:217:ARG:HH21	1.62	0.63
1:C:159:ARG:NH2	1:C:167:ARG:O	2.32	0.63
1:M:356:ARG:NH1	1:M:358:LEU:HD21	2.13	0.63
1:A:295:ARG:HD2	1:A:327:HIS:CB	2.27	0.63
1:G:213:ARG:HB2	1:G:216:GLU:OE2	1.99	0.63
1:G:358:LEU:HB3	1:G:477:PHE:CG	2.33	0.63
2:H:88:ASN:HD21	2:H:91:ARG:HH11	1.46	0.63
1:O:24:TYR:CZ	1:O:64:ALA:HB2	2.33	0.63
1:K:9:LYS:HB3	1:K:14:GLU:HA	1.79	0.63
2:D:139:LYS:HE3	4:D:183:HOH:O	1.99	0.63
1:E:25:TRP:CE2	1:E:27:PRO:HD3	2.33	0.63
1:C:128:LYS:HE3	1:O:335:LEU:O	1.99	0.63
1:E:475:SER:HB3	1:E:478:VAL:HG13	1.79	0.63
1:G:141:PRO:HG2	1:G:144:TYR:HB2	1.81	0.63
1:K:221:THR:HG21	1:K:238:HIS:CD2	2.34	0.63
1:I:86:LYS:HE2	1:I:88:ASP:OD1	1.99	0.63
1:A:185:TYR:OH	1:A:202:ASP:HA	1.98	0.62
1:I:134:ARG:HD3	1:I:136:GLU:OE2	1.98	0.62
1:E:175:LYS:HA	1:E:176:PRO:C	2.24	0.62
1:G:424:LEU:O	1:G:428:ILE:HG23	1.99	0.62
2:L:38:LEU:HD11	2:L:112:ILE:HD11	1.81	0.62
1:M:7:ARG:HA	1:M:7:ARG:NE	2.13	0.62
1:O:319:ARG:HG2	1:O:374:VAL:HG23	1.81	0.62
1:A:109:GLU:HB2	1:I:208:SER:O	1.98	0.62
1:K:227:LYS:HD2	4:P:185:HOH:O	1.99	0.62
1:M:312:ARG:NE	4:M:4091:HOH:O	2.32	0.62
1:M:19:PRO:HG2	1:M:22:LYS:HB2	1.82	0.62
1:C:359:GLN:NE2	1:C:478:VAL:HG12	2.14	0.62
1:G:17:VAL:HG13	1:G:66:TRP:O	2.00	0.62
1:E:359:GLN:HG2	1:E:477:PHE:O	1.99	0.62
1:K:24:TYR:CZ	1:K:64:ALA:HB2	2.35	0.62
1:A:221:THR:HG22	1:A:222:MET:HE2	1.81	0.62
1:C:7:ARG:HG2	2:J:72:LEU:H	1.63	0.62
1:C:150:GLY:C	1:C:322:GLY:HA2	2.25	0.62
1:K:172:CYS:HB3	1:K:197:LEU:HD13	1.81	0.62
1:C:43:THR:HB	1:C:132:ALA:HB3	1.81	0.62
1:M:150:GLY:C	1:M:322:GLY:HA2	2.25	0.62
1:K:79:LEU:CD1	1:K:104:GLU:HG2	2.30	0.61
2:N:107(B):GLY:HA3	4:O:4058:HOH:O	1.99	0.61
1:G:139:ARG:HD2	1:G:139:ARG:C	2.25	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:88:ASN:HA	2:P:91:ARG:HB2	1.82	0.61
2:D:108:ILE:HD12	2:D:108:ILE:N	2.14	0.61
1:G:138:MET:HE1	1:G:317:TRP:CZ2	2.33	0.61
1:K:310:ASN:OD1	1:K:312:ARG:HG2	2.00	0.61
1:A:19:PRO:CG	1:A:22:LYS:HD3	2.27	0.61
2:H:44:TYR:O	2:H:45:THR:HG23	2.01	0.61
1:O:139:ARG:HD2	1:O:139:ARG:C	2.26	0.61
2:P:45:THR:CG2	2:P:67:TRP:HA	2.30	0.61
1:A:13:TYR:CD1	1:A:73:LEU:HD21	2.36	0.61
1:G:474:THR:HG22	1:G:475:SER:H	1.63	0.61
1:E:297:GLY:O	1:E:300:THR:HB	2.01	0.61
1:K:178:LEU:HB3	1:K:211:PHE:CZ	2.34	0.61
1:A:177:LYS:HG2	1:A:203:ASP:OD1	2.00	0.61
1:A:474:THR:HG22	1:A:475:SER:H	1.66	0.61
1:G:18:ILE:O	1:G:22(A):MET:HE2	2.01	0.61
1:G:227:LYS:HD2	4:G:4098:HOH:O	2.01	0.61
1:I:334:LYS:HG3	1:I:335:LEU:HD22	1.82	0.61
1:I:357:ASN:OD1	1:I:359:GLN:HB2	2.00	0.61
1:C:206:ILE:C	1:C:207:ASN:HD22	2.09	0.61
1:G:161:ARG:HD3	4:G:4049:HOH:O	2.01	0.61
1:M:358:LEU:HD22	1:M:358:LEU:N	2.12	0.61
1:C:142:LEU:HD13	1:C:367:GLU:HB2	1.83	0.60
1:K:175:LYS:HA	1:K:176:PRO:C	2.25	0.60
2:N:26:ILE:O	2:N:30:ILE:HG13	2.00	0.60
2:N:28:LYS:HD3	1:O:433:GLU:HG2	1.81	0.60
1:E:388:HIS:CD2	1:E:388:HIS:H	2.19	0.60
1:G:221:THR:HG21	1:G:238:HIS:CD2	2.36	0.60
1:K:168:PRO:HD2	1:K:424:LEU:HD11	1.82	0.60
1:A:159:ARG:NH2	1:A:167:ARG:O	2.34	0.60
2:B:108:ILE:HD12	2:B:108:ILE:N	2.16	0.60
1:C:7:ARG:HG2	2:J:72:LEU:N	2.16	0.60
1:E:81:ARG:NH1	4:E:4072:HOH:O	2.34	0.60
1:G:80:TYR:HA	1:G:107:LEU:HD21	1.84	0.60
1:I:140:LEU:HD13	1:I:320:MET:CE	2.32	0.60
1:O:221:THR:HG22	1:O:222:MET:HE2	1.81	0.60
1:A:168:PRO:HD2	1:A:424:LEU:HD11	1.83	0.60
1:G:24:TYR:CZ	1:G:64:ALA:HB2	2.37	0.60
1:I:319:ARG:HG3	1:I:374:VAL:CG2	2.29	0.60
1:K:335:LEU:HD23	1:K:380:GLY:HA3	1.82	0.60
1:O:134:ARG:HA	1:O:308:GLY:O	2.00	0.60
1:E:204:GLU:HG2	1:E:205:ASN:N	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:138:MET:HE2	1:M:317:TRP:NE1	2.16	0.60
1:O:217:ARG:O	1:O:221:THR:HB	2.01	0.60
1:C:335:LEU:O	1:O:128:LYS:HE3	2.02	0.60
1:E:168:PRO:HD2	1:E:424:LEU:HD11	1.83	0.60
1:G:8:ILE:HG22	1:G:9:LYS:H	1.65	0.60
1:I:60:GLU:HG3	1:I:127:PHE:CE1	2.37	0.60
2:L:139:LYS:HA	2:L:139:LYS:CE	2.27	0.59
1:M:451:THR:HG22	1:M:451:THR:O	2.02	0.59
1:K:13:TYR:CE2	1:K:72:ASP:HB2	2.37	0.59
1:E:86:LYS:HE2	1:E:88:ASP:OD1	2.02	0.59
1:M:139:ARG:HD2	1:M:139:ARG:C	2.28	0.59
1:O:37:LEU:HB2	1:O:139:ARG:HB3	1.84	0.59
1:O:142:LEU:HD11	1:O:367:GLU:HB2	1.85	0.59
2:P:30:ILE:HA	2:P:33:MET:HE3	1.84	0.59
2:P:38:LEU:HD11	2:P:112:ILE:HD11	1.83	0.59
1:O:6:THR:HA	4:O:4178:HOH:O	2.02	0.59
1:C:379:SER:HB2	1:C:401:GLN:HB2	1.82	0.59
1:E:356:ARG:NH1	1:E:358:LEU:HD21	2.17	0.59
1:G:7:ARG:HG2	2:P:72:LEU:O	2.02	0.59
2:H:76:ASP:N	4:H:209:HOH:O	2.35	0.59
1:M:65:THR:HG23	1:M:67:THR:O	2.02	0.59
1:C:24:TYR:CE2	1:C:64:ALA:HB2	2.38	0.59
1:C:216:GLU:HG2	1:I:157:LEU:HD22	1.83	0.59
1:O:297:GLY:O	1:O:300:THR:HB	2.03	0.59
2:P:105:SER:HB3	2:P:108:ILE:HG21	1.84	0.59
1:G:379:SER:HB2	1:G:401:GLN:HB2	1.85	0.59
1:I:175:LYS:HA	1:I:176:PRO:C	2.28	0.59
1:O:138:MET:CE	1:O:317:TRP:HZ2	2.15	0.59
1:A:187:ARG:NH2	2:N:67:TRP:O	2.36	0.59
4:A:4134:HOH:O	2:P:107(B):GLY:HA3	2.02	0.59
1:C:139:ARG:HD2	1:C:139:ARG:C	2.28	0.59
1:O:140:LEU:HD13	1:O:320:MET:SD	2.42	0.59
1:E:18:ILE:O	1:E:22(A):MET:HE2	2.02	0.59
1:E:459:LEU:O	1:E:463:LYS:HB2	2.02	0.59
1:O:388:HIS:CD2	1:O:388:HIS:H	2.21	0.59
1:A:359:GLN:HG2	1:A:477:PHE:O	2.03	0.59
1:G:271:VAL:HG21	1:K:117:THR:OG1	2.02	0.59
1:I:213:ARG:HB2	1:I:216:GLU:OE2	2.02	0.59
2:N:108:ILE:HD12	2:N:108:ILE:N	2.18	0.59
1:O:463:LYS:HB3	1:O:463:LYS:HZ3	1.68	0.58
1:A:310:ASN:OD1	1:A:312:ARG:HG2	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:LYS:HE2	2:J:75:PHE:HD2	1.68	0.58
2:L:107(B):GLY:HA3	4:L:197:HOH:O	2.02	0.58
1:K:255:ASN:HD21	1:K:283:TRP:HE1	1.51	0.58
2:H:88:ASN:ND2	2:H:91:ARG:HH11	2.01	0.58
2:D:30:ILE:HD13	2:D:83:VAL:HB	1.86	0.58
1:E:141:PRO:HG2	1:E:144:TYR:HB2	1.86	0.58
1:G:8:ILE:HG22	1:G:9:LYS:N	2.18	0.58
2:H:108:ILE:N	2:H:108:ILE:HD12	2.19	0.58
1:K:43:THR:HB	1:K:132:ALA:HB3	1.85	0.58
1:G:13:TYR:CG	1:G:73:LEU:HD21	2.38	0.58
1:K:89:GLN:CD	1:K:94:PRO:HA	2.28	0.58
1:O:134:ARG:HD3	1:O:136:GLU:OE2	2.02	0.58
2:B:74:LEU:HB3	2:B:77:VAL:CG2	2.34	0.58
2:F:44:TYR:O	2:F:45:THR:HG23	2.02	0.58
1:K:20:TYR:HA	1:K:22(A):MET:HE3	1.85	0.58
1:M:358:LEU:H	1:M:358:LEU:CD2	2.14	0.58
2:P:24:GLU:OE1	2:P:24:GLU:HA	2.03	0.58
1:A:463:LYS:NZ	1:A:463:LYS:HB3	2.19	0.58
1:O:177:LYS:HG2	1:O:203:ASP:OD1	2.04	0.58
1:E:24:TYR:CE2	1:E:64:ALA:HB2	2.39	0.58
1:E:358:LEU:HD22	1:E:358:LEU:N	2.19	0.58
1:I:13:TYR:CG	1:I:73:LEU:HD21	2.38	0.58
2:N:88:ASN:HD21	2:N:91:ARG:HH11	1.50	0.58
1:O:358:LEU:HD23	4:O:4229:HOH:O	2.03	0.58
1:A:39:LEU:HD22	1:A:363:PHE:CG	2.39	0.58
1:A:186:GLY:HA3	2:N:66:TYR:OH	2.03	0.58
1:E:221:THR:HG22	1:E:222:MET:HE2	1.85	0.58
2:F:75:PHE:CE1	1:O:73:LEU:HB3	2.39	0.58
1:G:20:TYR:CD2	1:G:56:ALA:HA	2.39	0.58
1:K:264:ILE:HG13	1:K:290:ILE:HB	1.86	0.58
1:K:424:LEU:O	1:K:428:ILE:HG23	2.04	0.57
2:L:30:ILE:HD13	2:L:83:VAL:HB	1.84	0.57
2:N:127:ASN:HB2	2:N:145:TYR:CE2	2.38	0.57
1:A:9:LYS:HB3	1:A:14:GLU:HA	1.85	0.57
1:A:128:LYS:HE3	1:I:335:LEU:O	2.04	0.57
2:B:30:ILE:HD13	2:B:83:VAL:HB	1.87	0.57
1:C:37:LEU:HB2	1:C:139:ARG:HB3	1.86	0.57
1:G:12:ARG:HH21	1:G:68:VAL:HG21	1.68	0.57
1:M:11:SER:O	1:M:14:GLU:HG2	2.03	0.57
1:O:70:TRP:O	1:O:73:LEU:HB2	2.04	0.57
1:A:37:LEU:HB2	1:A:139:ARG:HB3	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:334:LYS:HG3	1:G:335:LEU:HD22	1.87	0.57
1:I:53:ALA:O	1:I:57:VAL:HG23	2.04	0.57
1:E:177:LYS:HG2	1:E:203:ASP:OD1	2.04	0.57
1:G:334:LYS:CG	1:G:335:LEU:HD22	2.34	0.57
1:K:39:LEU:HD13	1:K:363:PHE:CG	2.40	0.57
1:K:89:GLN:NE2	1:K:94:PRO:HA	2.19	0.57
1:M:175:LYS:HA	1:M:176:PRO:C	2.30	0.57
1:A:89:GLN:NE2	1:A:94:PRO:HA	2.19	0.57
1:C:187:ARG:HH11	1:C:187:ARG:CG	2.18	0.57
1:K:359:GLN:NE2	1:K:478:VAL:HA	2.16	0.57
1:E:159:ARG:NH2	1:E:167:ARG:O	2.37	0.57
1:G:20:TYR:CE1	1:G:64:ALA:HB1	2.37	0.57
1:I:221:THR:HG21	1:I:238:HIS:HD2	1.69	0.57
2:N:22:THR:O	2:N:26:ILE:HG13	2.04	0.57
1:O:446:ARG:HB2	1:O:446:ARG:NH1	2.19	0.57
2:D:127:ASN:HB2	2:D:145:TYR:CE2	2.39	0.57
2:H:45:THR:CG2	2:H:67:TRP:HA	2.34	0.57
1:K:13:TYR:HE2	1:K:72:ASP:HB2	1.70	0.57
1:K:155:VAL:O	1:K:159:ARG:HG3	2.04	0.57
1:A:461:LEU:HD11	1:I:15:SER:HB3	1.87	0.57
1:G:359:GLN:NE2	1:G:478:VAL:HG12	2.20	0.57
2:J:88:ASN:ND2	2:J:91:ARG:HH11	2.02	0.57
1:O:340:ILE:HD12	1:O:340:ILE:N	2.15	0.57
2:P:129:MET:HB2	2:P:141:THR:HB	1.86	0.56
1:A:16:GLY:HA2	1:I:461:LEU:HD21	1.87	0.56
2:B:17:PHE:HB2	1:G:425:GLU:OE2	2.04	0.56
2:B:45:THR:CG2	2:B:67:TRP:HA	2.35	0.56
1:E:63:THR:HA	1:M:177:LYS:HB2	1.87	0.56
1:M:356:ARG:HH12	1:M:358:LEU:HD21	1.69	0.56
1:E:343:ARG:HD3	1:E:347:LYS:HE3	1.87	0.56
1:I:8:ILE:CG2	1:I:9:LYS:H	2.18	0.56
1:A:155:VAL:O	1:A:159:ARG:HG3	2.06	0.56
1:G:157:LEU:O	1:G:161:ARG:HG3	2.04	0.56
1:A:15:SER:HB3	1:I:461:LEU:HD11	1.88	0.56
1:A:195:GLY:HA3	1:A:417:ALA:HB3	1.88	0.56
2:B:22:THR:OG1	2:B:25:GLN:HG3	2.06	0.56
1:C:216:GLU:HG2	1:I:157:LEU:CD2	2.36	0.56
1:G:135:LEU:HD21	1:G:138:MET:CE	2.34	0.56
1:G:309:MET:HE2	1:K:300:THR:HG21	1.87	0.56
1:M:319:ARG:CG	1:M:374:VAL:HG23	2.35	0.56
2:N:74:LEU:HD12	2:N:74:LEU:N	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:424:LEU:O	1:E:428:ILE:HG23	2.06	0.56
1:G:159:ARG:NH2	1:G:167:ARG:O	2.37	0.56
1:A:330:THR:O	1:A:332:VAL:N	2.39	0.56
1:E:221:THR:O	1:E:225:VAL:HG23	2.06	0.56
1:E:358:LEU:H	1:E:358:LEU:CD2	2.18	0.56
1:G:12:ARG:HH21	1:G:68:VAL:CG2	2.18	0.56
1:K:159:ARG:NH2	1:K:167:ARG:O	2.39	0.56
2:N:79:ASP:OD2	2:N:81:ALA:HB3	2.06	0.56
2:B:29:GLN:NE2	1:G:429:LEU:HD22	2.20	0.56
1:G:19:PRO:HG2	1:G:22:LYS:HB2	1.88	0.56
1:G:39:LEU:HD22	1:G:363:PHE:CD2	2.41	0.56
1:G:459:LEU:O	1:G:463:LYS:HB2	2.05	0.56
1:I:168:PRO:HD2	1:I:424:LEU:HD11	1.87	0.56
1:K:319:ARG:CG	1:K:374:VAL:HG23	2.35	0.56
1:K:343:ARG:HD2	1:K:360:GLU:OE1	2.05	0.56
2:D:30:ILE:HA	2:D:33:MET:HE2	1.87	0.55
2:J:88:ASN:HD21	2:J:91:ARG:HH11	1.52	0.55
1:M:39:LEU:HD22	1:M:363:PHE:CG	2.41	0.55
1:O:241:ASN:HD22	1:O:242:VAL:N	2.04	0.55
2:P:45:THR:HG21	2:P:67:TRP:HA	1.87	0.55
1:C:6:THR:N	4:C:4126:HOH:O	2.39	0.55
1:C:343:ARG:HD2	1:C:360:GLU:OE1	2.07	0.55
1:G:400:LEU:HB3	1:G:402:PHE:CE1	2.41	0.55
1:I:293:LEU:HD22	1:I:323:VAL:HG21	1.88	0.55
1:K:172:CYS:HB3	1:K:197:LEU:CD1	2.37	0.55
1:E:241:ASN:HD22	1:E:242:VAL:N	2.04	0.55
1:K:18:ILE:O	1:K:22(A):MET:HE2	2.06	0.55
1:K:70:TRP:O	1:K:73:LEU:HD23	2.07	0.55
1:K:158:GLU:CD	1:K:325:HIS:HE2	2.14	0.55
1:M:377:VAL:HG22	1:M:399:VAL:HB	1.89	0.55
1:A:343:ARG:HD3	1:A:347:LYS:HE3	1.88	0.55
1:C:180:LEU:HA	4:C:4074:HOH:O	2.06	0.55
1:I:37:LEU:HB2	1:I:139:ARG:HB3	1.89	0.55
1:K:81:ARG:O	1:K:83:LYS:HD3	2.07	0.55
1:A:381:GLY:HA2	1:I:66:TRP:CD1	2.42	0.55
2:H:38:LEU:HD11	2:H:112:ILE:HD11	1.87	0.55
2:P:86:GLU:OE2	2:P:86:GLU:HA	2.07	0.55
1:A:141:PRO:HG2	1:A:144:TYR:HB2	1.87	0.55
1:C:20:TYR:HA	1:C:22(A):MET:HE3	1.88	0.55
1:O:8:ILE:CG2	1:O:9:LYS:H	2.20	0.55
2:H:72:LEU:N	1:M:7:ARG:HG2	2.05	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:M:385:GLY:HA2	1:M:445:LEU:HD13	1.88	0.55
1:C:39:LEU:HD22	1:C:363:PHE:CG	2.42	0.55
1:O:358:LEU:N	1:O:358:LEU:HD22	2.22	0.55
1:A:159:ARG:NH1	1:A:397:ASP:OD1	2.40	0.55
1:C:176:PRO:HD2	1:C:180:LEU:HD11	1.89	0.55
1:G:59:GLY:C	1:G:64:ALA:HB3	2.32	0.55
1:I:79:LEU:CD1	1:I:104:GLU:HG2	2.37	0.55
1:K:45:GLN:HB2	1:K:48:VAL:CG2	2.37	0.55
1:K:255:ASN:O	1:K:259:GLU:HG3	2.07	0.55
1:A:139:ARG:C	1:A:139:ARG:HD2	2.32	0.54
1:C:7:ARG:HH11	2:J:74:LEU:HD12	1.70	0.54
1:E:159:ARG:NH1	1:E:397:ASP:OD1	2.40	0.54
1:G:293:LEU:HB3	1:G:323:VAL:HG11	1.90	0.54
1:K:187:ARG:O	1:K:187:ARG:HD3	2.07	0.54
1:M:168:PRO:HD2	1:M:424:LEU:HD11	1.89	0.54
2:D:30:ILE:O	2:D:34:ILE:HG13	2.08	0.54
1:K:474:THR:CG2	1:K:475:SER:H	2.14	0.54
2:N:90:CYS:SG	2:N:99:ILE:HD13	2.47	0.54
1:A:191:GLU:OE1	1:A:414:GLN:HG3	2.07	0.54
1:A:334:LYS:HG3	1:A:335:LEU:HD22	1.89	0.54
1:C:177:LYS:HG2	1:C:203:ASP:OD1	2.07	0.54
1:E:335:LEU:O	1:M:128:LYS:HE3	2.07	0.54
1:G:117:THR:O	1:G:121:ILE:HG12	2.07	0.54
1:K:45:GLN:HB2	1:K:48:VAL:HG21	1.88	0.54
1:O:475:SER:HB3	1:O:478:VAL:HG13	1.89	0.54
1:A:18:ILE:O	1:A:22(A):MET:HE2	2.07	0.54
1:K:25:TRP:CE2	1:K:27:PRO:HD3	2.42	0.54
1:K:25:TRP:NE1	1:K:27:PRO:HD3	2.21	0.54
1:O:79:LEU:HD11	1:O:104:GLU:HG2	1.90	0.54
2:P:8:MET:HG2	2:P:125:GLY:HA2	1.87	0.54
1:A:297:GLY:O	1:A:300:THR:HB	2.07	0.54
1:C:19:PRO:HG2	1:C:22:LYS:HB2	1.88	0.54
1:M:343:ARG:HD2	1:M:360:GLU:OE1	2.07	0.54
1:A:273:GLY:HA3	1:I:273:GLY:CA	2.31	0.54
2:B:24:GLU:HB2	4:B:196:HOH:O	2.08	0.54
2:F:47:ASP:HA	4:F:205:HOH:O	2.06	0.54
1:I:89:GLN:CD	1:I:94:PRO:HA	2.33	0.54
2:L:108:ILE:N	2:L:108:ILE:HD12	2.23	0.54
1:E:61:SER:HB3	1:E:124:VAL:HG11	1.89	0.54
1:G:359:GLN:HE21	1:G:478:VAL:HG12	1.73	0.54
1:I:141:PRO:HG2	1:I:144:TYR:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:335:LEU:N	1:K:335:LEU:HD22	2.22	0.54
1:M:89:GLN:NE2	1:M:94:PRO:HA	2.22	0.54
1:M:312:ARG:NH1	4:M:4090:HOH:O	2.41	0.54
1:E:141:PRO:HG2	1:E:144:TYR:CB	2.38	0.54
1:G:295:ARG:HD3	1:G:298:ASN:HB3	1.89	0.54
1:C:9:LYS:HE2	2:J:75:PHE:CD2	2.43	0.54
1:E:474:THR:CG2	1:E:475:SER:N	2.71	0.54
1:C:15:SER:HB3	1:O:461:LEU:HD11	1.90	0.54
1:C:39:LEU:HD23	1:C:136:GLU:HB2	1.89	0.54
1:E:43:THR:HB	1:E:132:ALA:HB3	1.89	0.54
2:F:139:LYS:HA	2:F:139:LYS:CE	2.30	0.54
1:G:7:ARG:HD3	2:P:74:LEU:CD1	2.35	0.54
1:A:150:GLY:C	1:A:322:GLY:HA2	2.34	0.53
2:B:67:TRP:O	1:I:187:ARG:NH2	2.40	0.53
1:C:175:LYS:HE3	3:C:4002:SO4:O1	2.08	0.53
1:M:264:ILE:HG13	1:M:290:ILE:HB	1.89	0.53
1:A:175:LYS:HA	1:A:176:PRO:C	2.32	0.53
1:K:212:MET:CE	1:K:217:ARG:HD3	2.38	0.53
2:B:42:ILE:HB	2:B:70:TRP:HB3	1.90	0.53
2:F:15:PHE:HE1	1:I:428:ILE:HG13	1.73	0.53
2:L:69:ILE:HD11	1:M:187:ARG:HD2	1.89	0.53
1:K:358:LEU:HD22	1:K:358:LEU:N	2.22	0.53
1:M:59:GLY:C	1:M:64:ALA:HB3	2.33	0.53
1:A:138:MET:CE	1:A:317:TRP:HE1	2.22	0.53
1:C:140:LEU:HD13	1:C:320:MET:SD	2.47	0.53
1:E:388:HIS:CD2	1:E:388:HIS:N	2.76	0.53
1:O:142:LEU:HD12	4:O:4236:HOH:O	2.09	0.53
1:E:431:ARG:HG3	1:E:437:TYR:CE2	2.43	0.53
2:F:27:LYS:HE2	2:F:80:PRO:HG3	1.88	0.53
1:I:385:GLY:HA2	1:I:445:LEU:HD13	1.91	0.53
1:K:181:SER:O	1:K:182:GLY:C	2.51	0.53
2:N:88:ASN:ND2	2:N:91:ARG:HH11	2.07	0.53
1:A:192:ALA:HB1	1:A:197:LEU:HD12	1.89	0.53
1:C:424:LEU:O	1:C:428:ILE:HG23	2.09	0.53
1:E:241:ASN:HD22	1:E:241:ASN:C	2.15	0.53
2:H:72:LEU:HD11	1:M:70:TRP:CE2	2.44	0.53
1:A:158:GLU:CD	1:A:325:HIS:HE2	2.17	0.53
1:C:271:VAL:HG21	1:O:117:THR:OG1	2.08	0.53
1:C:293:LEU:HB2	1:C:323:VAL:HG21	1.89	0.53
1:E:358:LEU:HD23	4:E:4260:HOH:O	2.08	0.53
1:O:18:ILE:HD11	1:O:22(A):MET:HG2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:25:TRP:CE2	1:A:27:PRO:HD3	2.42	0.53
1:C:385:GLY:HA2	1:C:445:LEU:CD1	2.35	0.53
1:I:135:LEU:HD21	1:I:138:MET:HE1	1.91	0.53
1:I:139:ARG:HD2	1:I:139:ARG:C	2.34	0.53
2:L:73:PRO:HD3	4:L:262:HOH:O	2.08	0.53
1:A:7:ARG:CD	1:A:7:ARG:N	2.72	0.53
1:E:9:LYS:HD3	1:E:9:LYS:N	2.24	0.53
1:K:338:ASP:OD1	1:K:339:PRO:HD2	2.09	0.53
1:K:383:HIS:HA	1:K:402:PHE:CD2	2.44	0.53
1:C:187:ARG:NH2	2:F:67:TRP:O	2.41	0.52
2:D:45:THR:CG2	2:D:67:TRP:HA	2.39	0.52
1:G:12:ARG:HE	1:G:18:ILE:HD11	1.73	0.52
1:G:141:PRO:HG2	1:G:144:TYR:CB	2.38	0.52
1:M:93:ASN:OD1	1:M:95:GLU:HB2	2.10	0.52
1:O:300:THR:HG22	1:O:301:TYR:CD2	2.44	0.52
1:E:295:ARG:HD3	1:E:298:ASN:HB3	1.90	0.52
2:F:29:GLN:O	2:F:33:MET:HG3	2.08	0.52
1:O:378:ALA:HB2	1:O:394:LEU:HD13	1.91	0.52
1:E:475:SER:CB	1:E:478:VAL:HG13	2.39	0.52
1:G:62:SER:HB3	1:G:82:ALA:HB2	1.90	0.52
1:G:129:ALA:HA	1:K:469:TYR:CE2	2.44	0.52
2:N:45:THR:CG2	2:N:67:TRP:HA	2.39	0.52
1:O:171:GLY:HA2	1:O:199:PHE:O	2.09	0.52
1:C:151:PRO:HD3	1:C:319:ARG:O	2.09	0.52
1:G:300:THR:HG22	1:K:301:TYR:CB	2.37	0.52
2:J:66:TYR:OH	1:O:186:GLY:HA3	2.09	0.52
1:M:158:GLU:CD	1:M:325:HIS:HE2	2.17	0.52
2:N:8:MET:HG2	2:N:125:GLY:HA2	1.92	0.52
1:O:241:ASN:HD22	1:O:241:ASN:C	2.17	0.52
1:C:11:SER:H	1:C:14:GLU:HB3	1.75	0.52
1:E:135:LEU:HD21	1:E:138:MET:HE2	1.90	0.52
1:E:221:THR:HG21	1:E:238:HIS:CD2	2.45	0.52
1:I:388:HIS:H	1:I:388:HIS:CD2	2.27	0.52
1:K:79:LEU:HD13	1:K:104:GLU:HG2	1.92	0.52
1:K:343:ARG:O	1:K:347:LYS:HG3	2.10	0.52
2:N:139:LYS:HA	2:N:139:LYS:CE	2.32	0.52
1:O:81:ARG:O	1:O:83:LYS:HD3	2.10	0.52
1:C:187:ARG:HG2	1:C:187:ARG:NH1	2.24	0.52
1:E:243:THR:HA	1:E:250:MET:HE3	1.91	0.52
1:G:362:LEU:N	1:G:362:LEU:HD12	2.25	0.52
1:A:63:THR:HA	1:I:177:LYS:HB2	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:62:SER:HB3	1:G:82:ALA:CB	2.40	0.52
1:K:79:LEU:HD11	1:K:104:GLU:HG2	1.91	0.52
1:M:142:LEU:HD12	1:M:369:ALA:HB2	1.92	0.52
1:M:312:ARG:CZ	4:M:4091:HOH:O	2.57	0.52
1:O:158:GLU:HG3	1:O:290:ILE:HD13	1.91	0.52
1:O:388:HIS:HE1	4:O:4266:HOH:O	1.93	0.52
1:A:318:MET:HE2	1:A:318:MET:HA	1.92	0.52
2:F:30:ILE:O	2:F:34:ILE:HG13	2.10	0.52
1:G:335:LEU:HD23	1:G:380:GLY:HA3	1.92	0.52
2:J:135:SER:C	2:J:136:ARG:HD2	2.35	0.52
1:K:429:LEU:HD22	2:L:29:GLN:NE2	2.24	0.52
1:M:37:LEU:HB2	1:M:139:ARG:HB3	1.91	0.52
1:M:159:ARG:NH2	1:M:167:ARG:O	2.39	0.52
1:G:292:HIS:HA	1:G:325:HIS:HB2	1.92	0.52
1:G:343:ARG:HD2	1:G:360:GLU:OE1	2.10	0.52
1:G:431:ARG:HG3	1:G:437:TYR:CE2	2.45	0.52
1:I:24:TYR:CE2	1:I:64:ALA:HB2	2.44	0.52
1:K:350:LEU:HD21	1:K:376:PRO:HG3	1.91	0.52
1:K:464:ASP:O	1:K:465:ILE:C	2.53	0.52
1:O:138:MET:HE3	1:O:317:TRP:CZ2	2.45	0.52
2:B:143:HIS:HD2	4:F:202:HOH:O	1.93	0.52
1:E:455:LEU:O	1:E:459:LEU:HG	2.10	0.52
1:G:39:LEU:HD11	1:G:98:PHE:HB3	1.91	0.52
1:G:150:GLY:C	1:G:322:GLY:HA2	2.34	0.52
2:H:136:ARG:HD2	4:I:4053:HOH:O	2.09	0.52
1:I:187:ARG:CG	1:I:187:ARG:HH11	2.23	0.52
1:I:273:GLY:O	1:I:277:ILE:HG13	2.10	0.52
1:M:24:TYR:CE2	1:M:64:ALA:HB2	2.45	0.52
1:M:69:VAL:HG23	1:M:72:ASP:OD1	2.10	0.52
1:O:330:THR:OG1	1:O:333:GLY:HA3	2.10	0.52
1:A:138:MET:HE1	1:A:317:TRP:HE1	1.75	0.51
1:A:473:ASP:HB2	4:A:4266:HOH:O	2.09	0.51
1:C:9:LYS:HB2	1:C:9:LYS:NZ	2.24	0.51
1:E:191:GLU:O	1:E:414:GLN:HG2	2.10	0.51
1:C:300:THR:HG21	1:O:309:MET:HE2	1.91	0.51
1:I:70:TRP:O	1:I:73:LEU:HD23	2.09	0.51
1:K:206:ILE:C	1:K:207:ASN:HD22	2.18	0.51
1:M:293:LEU:HB3	1:M:323:VAL:HG11	1.92	0.51
1:E:294:HIS:HA	1:E:327:HIS:CD2	2.46	0.51
1:G:79:LEU:CD2	1:G:104:GLU:HG2	2.41	0.51
1:M:39:LEU:HD23	1:M:136:GLU:HB2	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:59:GLY:C	1:K:64:ALA:HB3	2.35	0.51
1:M:89:GLN:CD	1:M:94:PRO:HA	2.35	0.51
2:B:38:LEU:HD11	2:B:112:ILE:HD11	1.93	0.51
2:F:107:VAL:HB	2:F:108:ILE:HD13	1.90	0.51
1:G:438:LEU:HB2	4:G:4139:HOH:O	2.10	0.51
1:I:13:TYR:HA	1:I:68:VAL:HG11	1.93	0.51
1:K:42:VAL:HG22	1:K:133:LEU:CD1	2.41	0.51
1:K:138:MET:HE1	1:K:317:TRP:HE1	1.76	0.51
2:L:67:TRP:O	1:M:187:ARG:NH2	2.44	0.51
2:L:135:SER:C	2:L:136:ARG:HD2	2.36	0.51
1:O:358:LEU:HD22	1:O:358:LEU:H	1.75	0.51
1:O:474:THR:HG22	1:O:475:SER:N	2.26	0.51
1:C:292:HIS:HA	1:C:325:HIS:HB2	1.92	0.51
2:H:38:LEU:HD21	2:H:112:ILE:CD1	2.40	0.51
1:I:200:VAL:O	1:I:238:HIS:HA	2.11	0.51
1:K:347:LYS:HB3	1:K:351:LEU:HD22	1.92	0.51
1:O:138:MET:CE	1:O:317:TRP:CZ2	2.94	0.51
1:A:238:HIS:HD2	1:A:240:LEU:HD23	1.76	0.51
1:E:164:LYS:NZ	1:E:198:ASP:OD1	2.42	0.51
1:I:292:HIS:HA	1:I:325:HIS:HB2	1.93	0.51
1:I:386:GLN:HA	1:I:389:GLN:HE21	1.76	0.51
2:B:139:LYS:HE3	4:B:169:HOH:O	2.11	0.51
1:C:319:ARG:CG	1:C:374:VAL:HG23	2.40	0.51
1:G:209:GLN:HB3	1:G:210:PRO:HD2	1.93	0.51
1:M:53:ALA:O	1:M:57:VAL:HG23	2.11	0.51
1:M:293:LEU:HD23	1:M:326:ILE:HD12	1.91	0.51
2:N:30:ILE:HA	2:N:33:MET:HE3	1.93	0.51
1:I:39:LEU:HD22	1:I:363:PHE:CG	2.46	0.51
1:K:36:VAL:HA	1:K:141:PRO:HD3	1.92	0.51
2:N:27:LYS:HE2	2:N:80:PRO:CG	2.41	0.51
2:P:8:MET:HG2	2:P:125:GLY:CA	2.41	0.51
1:A:89:GLN:CD	1:A:94:PRO:HA	2.36	0.50
1:E:8:ILE:HG22	1:E:9:LYS:N	2.26	0.50
1:I:138:MET:HE1	1:I:317:TRP:HZ2	1.75	0.50
1:A:440:GLU:O	1:A:444:ILE:HG13	2.11	0.50
2:H:88:ASN:HD22	2:H:91:ARG:HD2	1.77	0.50
1:K:327:HIS:HB3	4:K:4135:HOH:O	2.10	0.50
1:O:212:MET:HE3	1:O:217:ARG:HH21	1.76	0.50
1:C:9:LYS:O	1:C:14:GLU:HB2	2.11	0.50
1:G:463:LYS:NZ	1:G:463:LYS:HB3	2.26	0.50
1:K:138:MET:HE1	1:K:317:TRP:HZ2	1.73	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:83:VAL:O	2:N:87:ILE:HG13	2.11	0.50
2:P:104:PHE:HB2	4:P:174:HOH:O	2.11	0.50
1:C:79:LEU:HD13	1:C:104:GLU:HG2	1.93	0.50
1:G:138:MET:CE	1:G:317:TRP:HZ2	2.22	0.50
1:K:212:MET:HE3	1:K:217:ARG:NH2	2.26	0.50
1:K:407:ILE:HG23	1:K:413:ILE:HD11	1.93	0.50
1:M:61:SER:HB3	1:M:124:VAL:HG11	1.93	0.50
1:O:292:HIS:HA	1:O:325:HIS:HB2	1.93	0.50
1:A:323:VAL:CG1	1:A:325:HIS:O	2.59	0.50
1:G:164:LYS:NZ	1:G:198:ASP:OD1	2.43	0.50
1:G:221:THR:O	1:G:225:VAL:HG23	2.11	0.50
1:O:79:LEU:CD1	1:O:104:GLU:HG2	2.41	0.50
1:O:319:ARG:CG	1:O:374:VAL:HG23	2.41	0.50
1:A:122:GLY:HA3	4:A:4128:HOH:O	2.11	0.50
2:F:45:THR:CG2	2:F:67:TRP:HA	2.42	0.50
2:N:30:ILE:HD13	2:N:83:VAL:HB	1.93	0.50
2:N:44:TYR:O	2:N:45:THR:HG23	2.12	0.50
2:N:88:ASN:HD22	2:N:91:ARG:HD2	1.74	0.50
1:O:7:ARG:HA	1:O:7:ARG:NE	2.26	0.50
1:O:300:THR:HG21	4:O:4218:HOH:O	2.11	0.50
1:A:79:LEU:CD1	1:A:104:GLU:HG2	2.42	0.50
1:A:293:LEU:HD22	1:A:323:VAL:HG21	1.93	0.50
1:A:330:THR:HG22	1:A:378:ALA:CB	2.40	0.50
1:E:138:MET:CE	1:E:317:TRP:HZ2	2.24	0.50
1:E:185:TYR:O	1:E:189:VAL:HG23	2.11	0.50
2:P:45:THR:HG23	2:P:67:TRP:CB	2.42	0.50
2:B:129:MET:HB2	2:B:141:THR:HB	1.93	0.50
1:E:85:TYR:CZ	1:E:100:TYR:HB3	2.47	0.50
1:G:330:THR:OG1	1:G:333:GLY:HA3	2.11	0.50
1:O:39:LEU:HD13	1:O:363:PHE:CG	2.47	0.50
2:P:13:GLY:HA2	2:P:114:SER:O	2.12	0.50
1:A:327:HIS:HA	1:A:377:VAL:HB	1.94	0.50
2:B:17:PHE:HB2	1:G:425:GLU:CD	2.37	0.50
1:C:358:LEU:HD12	1:C:477:PHE:CE1	2.47	0.50
2:D:136:ARG:HD2	2:D:136:ARG:N	2.26	0.50
1:E:157:LEU:O	1:E:161:ARG:HG3	2.11	0.50
1:K:334:LYS:HG3	1:K:335:LEU:HD22	1.93	0.50
2:L:73:PRO:HG2	2:L:75:PHE:CZ	2.46	0.50
1:M:110:GLU:HB3	1:M:147:THR:HB	1.93	0.50
1:O:86:LYS:HE2	1:O:88:ASP:OD1	2.12	0.50
1:O:398:VAL:HG22	1:O:399:VAL:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:15:SER:HB3	1:K:461:LEU:CD1	2.41	0.49
1:I:204:GLU:HB3	1:I:294:HIS:CD2	2.48	0.49
2:J:88:ASN:HD22	2:J:91:ARG:HD2	1.76	0.49
1:K:463:LYS:HB3	1:K:463:LYS:HZ2	1.76	0.49
1:E:134:ARG:HD3	1:E:136:GLU:OE2	2.12	0.49
1:G:117:THR:OG1	1:K:271:VAL:HG21	2.12	0.49
1:I:187:ARG:NH1	1:I:187:ARG:HG2	2.28	0.49
1:I:379:SER:HB2	1:I:401:GLN:HB2	1.94	0.49
1:M:187:ARG:HH11	1:M:187:ARG:CG	2.25	0.49
2:N:102:VAL:HG13	2:N:111:THR:HG23	1.94	0.49
2:B:15:PHE:CZ	1:G:428:ILE:HD11	2.47	0.49
1:C:77:ALA:O	1:C:81:ARG:HG3	2.13	0.49
1:C:141:PRO:HG2	1:C:144:TYR:HB3	1.95	0.49
1:E:172:CYS:HB3	1:E:197:LEU:CD1	2.41	0.49
1:E:227:LYS:HD2	4:E:4112:HOH:O	2.11	0.49
1:G:427:MET:HE2	1:G:445:LEU:HD21	1.94	0.49
2:H:127:ASN:HB2	2:H:145:TYR:CE2	2.47	0.49
1:I:79:LEU:HD11	1:I:104:GLU:HG2	1.94	0.49
1:O:43:THR:HB	1:O:132:ALA:HB3	1.95	0.49
1:O:466:THR:HG22	4:O:4199:HOH:O	2.11	0.49
1:E:385:GLY:HA2	1:E:445:LEU:HD13	1.93	0.49
1:G:63:THR:CA	1:K:177:LYS:HD3	2.32	0.49
1:G:319:ARG:CG	1:G:374:VAL:HG23	2.41	0.49
2:J:17:PHE:HB2	1:M:425:GLU:OE2	2.11	0.49
1:K:13:TYR:CG	1:K:73:LEU:HD21	2.47	0.49
1:K:447:GLU:O	1:K:450:LYS:HB2	2.11	0.49
1:O:8:ILE:CG2	1:O:9:LYS:N	2.75	0.49
1:A:301:TYR:OH	1:A:314:ILE:HG12	2.12	0.49
2:D:73:PRO:HG2	2:D:75:PHE:CZ	2.47	0.49
4:E:4240:HOH:O	2:H:45:THR:HG22	2.13	0.49
1:G:209:GLN:HB3	1:G:210:PRO:CD	2.43	0.49
1:I:34:THR:HG21	1:O:142:LEU:HD23	1.94	0.49
1:I:358:LEU:HD12	1:I:477:PHE:CE1	2.47	0.49
2:L:45:THR:CG2	2:L:67:TRP:HA	2.43	0.49
1:O:209:GLN:HB3	1:O:210:PRO:CD	2.42	0.49
1:A:39:LEU:HD11	1:A:98:PHE:HB3	1.93	0.49
2:D:72:LEU:HD13	4:G:4056:HOH:O	2.11	0.49
1:E:7:ARG:H	1:E:7:ARG:HH11	1.61	0.49
1:G:388:HIS:H	1:G:388:HIS:CD2	2.29	0.49
2:J:15:PHE:HA	1:M:425:GLU:OE1	2.12	0.49
1:K:171:GLY:O	1:K:401:GLN:HA	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:335:LEU:N	1:O:335:LEU:HD22	2.28	0.49
1:A:343:ARG:HD2	1:A:360:GLU:OE1	2.12	0.49
1:A:410:PRO:HD3	1:A:461:LEU:HD11	1.95	0.49
1:I:446:ARG:HG2	4:I:4178:HOH:O	2.12	0.49
1:K:209:GLN:HB3	1:K:210:PRO:CD	2.42	0.49
1:K:359:GLN:HE22	1:K:478:VAL:CA	2.21	0.49
2:P:108:ILE:HG22	2:P:110:SER:H	1.78	0.49
1:A:39:LEU:HD22	1:A:363:PHE:CD1	2.48	0.49
1:C:134:ARG:HD3	1:C:136:GLU:OE2	2.13	0.49
1:G:175:LYS:HA	1:G:176:PRO:C	2.38	0.49
2:B:91:ARG:HG2	2:B:118:ASN:HD22	1.77	0.49
1:E:428:ILE:HD12	1:E:428:ILE:O	2.13	0.49
1:E:463:LYS:HB3	1:E:463:LYS:HZ2	1.78	0.49
1:G:18:ILE:HB	1:G:19:PRO:HD2	1.94	0.49
1:K:178:LEU:HD23	1:K:206:ILE:HG12	1.94	0.49
2:N:8:MET:HG2	2:N:125:GLY:CA	2.43	0.49
2:N:24:GLU:OE2	2:N:28:LYS:NZ	2.46	0.49
1:O:409:HIS:CE1	1:O:411:ASP:HB2	2.48	0.49
1:C:295:ARG:CG	1:C:327:HIS:HB2	2.42	0.48
2:D:105:SER:O	2:D:109:GLU:HA	2.13	0.48
1:K:25:TRP:HZ3	1:K:87:VAL:HG23	1.78	0.48
1:M:312:ARG:NH2	4:M:4091:HOH:O	2.46	0.48
1:O:293:LEU:HD22	1:O:323:VAL:HG21	1.95	0.48
1:A:93:ASN:OD1	1:A:95:GLU:HB2	2.13	0.48
1:I:19:PRO:CG	1:I:22:LYS:HD3	2.42	0.48
1:A:8:ILE:CG2	1:A:9:LYS:H	2.25	0.48
1:C:327:HIS:HB3	4:C:4124:HOH:O	2.12	0.48
1:G:187:ARG:NH1	1:G:187:ARG:HG2	2.29	0.48
1:I:319:ARG:CG	1:I:374:VAL:HG23	2.34	0.48
2:L:83:VAL:O	2:L:87:ILE:HG13	2.13	0.48
1:M:475:SER:HB3	1:M:478:VAL:HG13	1.95	0.48
2:N:41:GLY:HA2	4:N:1103:HOH:O	2.12	0.48
1:O:89:GLN:CD	1:O:94:PRO:HA	2.38	0.48
2:P:108:ILE:HG22	2:P:109:GLU:N	2.28	0.48
1:A:204:GLU:HB3	1:A:294:HIS:CD2	2.49	0.48
2:B:15:PHE:HE1	1:G:428:ILE:HG13	1.79	0.48
2:D:49:HIS:CE1	2:D:51:ARG:HB2	2.48	0.48
1:I:77:ALA:O	1:I:81:ARG:HG3	2.13	0.48
2:J:15:PHE:HE1	1:M:428:ILE:HG13	1.78	0.48
2:H:74:LEU:N	2:H:74:LEU:HD12	2.28	0.48
2:H:75:PHE:CE1	1:M:73:LEU:HB3	2.49	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:H:104:PHE:CE1	2:H:110:SER:HA	2.48	0.48
1:I:69:VAL:HA	4:I:4212:HOH:O	2.12	0.48
1:I:141:PRO:HG2	1:I:144:TYR:CB	2.44	0.48
1:O:241:ASN:HD22	1:O:243:THR:H	1.61	0.48
1:O:356:ARG:NH1	1:O:358:LEU:HD21	2.28	0.48
1:G:159:ARG:NH1	1:G:397:ASP:OD1	2.47	0.48
2:J:45:THR:HG21	2:J:67:TRP:HA	1.93	0.48
1:K:138:MET:HE1	1:K:317:TRP:NE1	2.28	0.48
1:K:187:ARG:HD3	1:K:191:GLU:HG2	1.95	0.48
1:M:104:GLU:HB2	4:M:4059:HOH:O	2.13	0.48
2:B:105:SER:OG	2:B:107:VAL:HG23	2.14	0.48
1:C:39:LEU:HD22	1:C:363:PHE:CD1	2.49	0.48
1:G:68:VAL:HG12	1:G:69:VAL:N	2.29	0.48
1:I:310:ASN:OD1	1:I:312:ARG:HG2	2.13	0.48
1:K:407:ILE:HG23	1:K:413:ILE:CD1	2.43	0.48
1:M:177:LYS:HG2	1:M:203:ASP:OD1	2.14	0.48
1:M:388:HIS:CD2	1:M:388:HIS:H	2.30	0.48
2:J:127:ASN:HB2	2:J:145:TYR:CE2	2.49	0.48
2:N:127:ASN:HB2	2:N:145:TYR:CZ	2.49	0.48
1:A:214:TRP:CE3	1:A:253:ARG:HG2	2.49	0.48
1:A:358:LEU:N	1:A:358:LEU:HD22	2.29	0.48
1:E:177:LYS:HB2	1:M:63:THR:HA	1.95	0.48
1:E:231:ALA:HA	4:E:4147:HOH:O	2.14	0.48
2:L:74:LEU:HB3	2:L:77:VAL:CG2	2.43	0.48
1:E:234:GLU:HB2	1:E:236:LYS:HE2	1.94	0.48
1:G:125:PHE:HB2	4:G:4140:HOH:O	2.13	0.48
1:K:170:LEU:HD11	1:K:421:ARG:HA	1.95	0.48
1:K:209:GLN:HB3	1:K:210:PRO:HD2	1.95	0.48
1:M:451:THR:O	1:M:451:THR:CG2	2.62	0.48
2:B:79:ASP:OD2	2:B:81:ALA:HB3	2.14	0.47
1:G:181:SER:O	1:G:185:TYR:HB2	2.13	0.47
1:K:187:ARG:O	1:K:191:GLU:HG2	2.13	0.47
1:M:8:ILE:HG22	1:M:9:LYS:N	2.29	0.47
1:M:43:THR:HB	1:M:132:ALA:HB3	1.96	0.47
1:A:350:LEU:HD21	1:A:376:PRO:HG3	1.96	0.47
2:D:11:THR:HG21	2:D:17:PHE:CE2	2.48	0.47
2:H:45:THR:HG21	2:H:67:TRP:HA	1.96	0.47
1:I:334:LYS:HG2	1:I:380:GLY:C	2.39	0.47
1:K:117:THR:HG22	1:K:317:TRP:CH2	2.49	0.47
1:C:175:LYS:HA	1:C:176:PRO:C	2.39	0.47
4:C:4060:HOH:O	2:F:45:THR:HG22	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:444:ILE:HG23	4:E:4204:HOH:O	2.14	0.47
1:G:187:ARG:CG	1:G:187:ARG:HH11	2.27	0.47
1:I:159:ARG:NH1	1:I:397:ASP:OD1	2.47	0.47
1:M:134:ARG:HA	1:M:308:GLY:O	2.14	0.47
1:A:134:ARG:HD3	1:A:136:GLU:OE2	2.14	0.47
1:A:200:VAL:O	1:A:238:HIS:HA	2.15	0.47
1:A:362:LEU:N	1:A:362:LEU:HD12	2.30	0.47
1:C:171:GLY:HA2	1:C:199:PHE:O	2.13	0.47
1:C:466:THR:HG23	1:C:467:PHE:N	2.29	0.47
2:F:26:ILE:O	2:F:30:ILE:HG13	2.14	0.47
1:K:138:MET:CE	1:K:317:TRP:HE1	2.26	0.47
1:K:139:ARG:C	1:K:139:ARG:HD2	2.39	0.47
1:M:206:ILE:C	1:M:207:ASN:HD22	2.22	0.47
1:O:61:SER:HB3	1:O:124:VAL:HG11	1.96	0.47
1:O:432:ASN:C	1:O:434:ASN:H	2.21	0.47
2:P:45:THR:HG23	2:P:67:TRP:HB3	1.95	0.47
1:A:70:TRP:O	1:A:73:LEU:HD23	2.14	0.47
1:C:187:ARG:CG	1:C:187:ARG:NH1	2.77	0.47
1:C:241:ASN:ND2	1:C:243:THR:H	2.13	0.47
2:D:44:TYR:O	2:D:45:THR:HG23	2.14	0.47
1:E:170:LEU:HD11	1:E:421:ARG:HA	1.96	0.47
1:I:81:ARG:NH1	4:I:4024:HOH:O	2.46	0.47
1:K:264:ILE:HG13	1:K:290:ILE:O	2.15	0.47
1:O:192:ALA:HB1	1:O:197:LEU:HD12	1.95	0.47
1:O:310:ASN:OD1	1:O:312:ARG:HG2	2.15	0.47
2:P:27:LYS:HD3	2:P:27:LYS:C	2.39	0.47
1:A:18:ILE:HD11	1:A:22(A):MET:HG2	1.97	0.47
1:C:318:MET:HE2	1:C:318:MET:HA	1.95	0.47
1:E:161:ARG:HD3	4:E:4116:HOH:O	2.15	0.47
2:F:14:THR:O	1:I:425:GLU:HG2	2.15	0.47
1:G:239:TYR:CE1	1:G:264:ILE:HD13	2.49	0.47
1:I:78:ASP:O	1:I:83:LYS:NZ	2.47	0.47
1:I:85:TYR:CZ	1:I:100:TYR:HB3	2.49	0.47
1:K:414:GLN:HB2	4:K:4196:HOH:O	2.13	0.47
1:M:141:PRO:HG2	1:M:144:TYR:CB	2.45	0.47
1:M:424:LEU:O	1:M:428:ILE:HG23	2.15	0.47
2:N:17:PHE:HB2	1:O:425:GLU:OE2	2.14	0.47
1:C:221:THR:HG21	1:C:238:HIS:CD2	2.50	0.47
1:E:9:LYS:HZ1	1:E:70:TRP:HB3	1.79	0.47
2:F:74:LEU:CD1	1:O:7:ARG:HD3	2.44	0.47
1:G:77:ALA:HB1	1:G:81:ARG:NH1	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:247:MET:HG2	1:K:247:MET:HG2	1.96	0.47
1:G:474:THR:HG22	1:G:475:SER:N	2.29	0.47
1:I:241:ASN:ND2	1:I:243:THR:H	2.13	0.47
1:I:474:THR:HG22	1:I:475:SER:N	2.29	0.47
2:J:88:ASN:HD21	2:J:91:ARG:NH1	2.12	0.47
2:J:145:TYR:CE1	2:L:150:PRO:HA	2.49	0.47
1:K:170:LEU:HD21	1:K:424:LEU:HD22	1.97	0.47
1:K:255:ASN:ND2	1:K:283:TRP:HE1	2.13	0.47
1:M:9:LYS:HB3	1:M:14:GLU:HA	1.96	0.47
1:M:93:ASN:C	1:M:95:GLU:H	2.22	0.47
1:O:59:GLY:C	1:O:64:ALA:HB3	2.39	0.47
1:O:343:ARG:O	1:O:347:LYS:HG3	2.15	0.47
2:P:48:ILE:HD13	2:P:126:PHE:CZ	2.49	0.47
1:C:187:ARG:HH11	1:C:187:ARG:HG2	1.78	0.47
1:G:388:HIS:HB3	1:G:427:MET:HE3	1.97	0.47
2:J:143:HIS:HD2	4:N:558:HOH:O	1.96	0.47
1:K:8:ILE:HG22	1:K:9:LYS:N	2.29	0.47
1:K:428:ILE:HG13	2:L:15:PHE:HE1	1.79	0.47
2:N:29:GLN:NE2	1:O:429:LEU:HD22	2.30	0.47
1:O:69:VAL:HG23	1:O:72:ASP:OD1	2.15	0.47
1:O:455:LEU:O	1:O:459:LEU:HG	2.15	0.47
1:A:398:VAL:HG22	1:A:399:VAL:N	2.30	0.47
1:C:295:ARG:HG2	1:C:327:HIS:HB2	1.97	0.47
1:C:319:ARG:HG3	1:C:374:VAL:HG23	1.96	0.47
1:G:172:CYS:HB3	1:G:197:LEU:CD1	2.43	0.47
1:K:141:PRO:HG2	1:K:144:TYR:CB	2.45	0.47
2:N:48:ILE:HD13	2:N:126:PHE:CZ	2.50	0.47
1:G:85:TYR:CZ	1:G:100:TYR:HB3	2.50	0.47
1:A:66:TRP:CD1	1:I:381:GLY:HA2	2.50	0.46
1:A:212:MET:HE3	1:A:217:ARG:HH21	1.79	0.46
1:C:141:PRO:HG2	1:C:144:TYR:CB	2.45	0.46
1:E:139:ARG:HD2	1:E:139:ARG:C	2.40	0.46
1:E:388:HIS:H	1:E:388:HIS:HD2	1.61	0.46
1:G:74:LEU:O	2:P:104:PHE:CZ	2.68	0.46
2:L:49:HIS:CE1	2:L:51:ARG:HB2	2.49	0.46
1:M:241:ASN:ND2	1:M:243:THR:H	2.13	0.46
1:E:66:TRP:CD1	1:M:381:GLY:HA2	2.51	0.46
1:I:185:TYR:OH	1:I:202:ASP:HA	2.15	0.46
1:K:295:ARG:HE	1:K:298:ASN:ND2	2.13	0.46
1:K:407:ILE:HA	1:K:413:ILE:HG12	1.96	0.46
1:E:6:THR:C	1:E:7:ARG:HD3	2.40	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:221:THR:HG22	1:G:222:MET:HE2	1.98	0.46
1:K:39:LEU:HD12	1:K:100:TYR:CE2	2.50	0.46
2:L:107:VAL:HB	2:L:108:ILE:HD13	1.97	0.46
1:M:70:TRP:O	1:M:73:LEU:HB2	2.14	0.46
1:M:193:LEU:HD22	1:M:236:LYS:HD2	1.98	0.46
2:P:39:ALA:HB3	2:P:104:PHE:HB3	1.96	0.46
1:A:127:PHE:HE1	1:I:334:LYS:HD2	1.79	0.46
2:D:72:LEU:N	2:D:72:LEU:HD12	2.31	0.46
1:E:435:ARG:O	1:E:437:TYR:N	2.49	0.46
2:F:74:LEU:CD1	2:F:74:LEU:N	2.78	0.46
1:K:9:LYS:NZ	1:K:70:TRP:HB2	2.30	0.46
1:A:212:MET:SD	1:A:217:ARG:HD3	2.55	0.46
1:A:239:TYR:CE1	1:A:264:ILE:HD13	2.50	0.46
2:F:33:MET:HE1	2:F:101:VAL:HG11	1.98	0.46
2:F:107(A):ARG:HB3	4:F:200:HOH:O	2.15	0.46
1:K:39:LEU:HD13	1:K:363:PHE:CD2	2.51	0.46
1:K:357:ASN:OD1	1:K:359:GLN:HB2	2.15	0.46
1:M:339:PRO:HG2	1:M:340:ILE:HD12	1.98	0.46
1:O:13:TYR:HA	1:O:68:VAL:HG11	1.97	0.46
2:P:26:ILE:O	2:P:30:ILE:HG13	2.14	0.46
2:B:145:TYR:CE1	2:D:150:PRO:HA	2.51	0.46
1:C:25:TRP:CE2	1:C:27:PRO:HD3	2.51	0.46
1:C:221:THR:O	1:C:225:VAL:HG23	2.15	0.46
1:E:90:VAL:HG13	1:E:91:PRO:HD2	1.98	0.46
1:G:17:VAL:HG22	1:G:67:THR:HB	1.97	0.46
2:J:117:VAL:O	2:J:118:ASN:HB2	2.16	0.46
1:M:18:ILE:O	1:M:22(A):MET:HE2	2.16	0.46
1:O:228:ALA:O	1:O:232:THR:HG23	2.16	0.46
1:O:463:LYS:NZ	1:O:463:LYS:CB	2.77	0.46
2:D:27:LYS:HD3	2:D:27:LYS:C	2.41	0.46
1:G:264:ILE:HG12	1:G:265:ILE:N	2.29	0.46
1:K:7:ARG:HG3	1:K:7:ARG:HH11	1.80	0.46
1:K:24:TYR:CE2	1:K:64:ALA:HB2	2.50	0.46
1:K:188:VAL:HG13	1:K:413:ILE:HD13	1.97	0.46
1:M:430:ALA:CB	1:M:444:ILE:HD13	2.46	0.46
2:N:28:LYS:HD3	1:O:433:GLU:CG	2.46	0.46
2:P:102:VAL:HG13	2:P:111:THR:HG23	1.98	0.46
2:P:136:ARG:HD2	2:P:136:ARG:N	2.30	0.46
1:A:127:PHE:CE1	1:I:334:LYS:HD2	2.50	0.46
1:A:221:THR:HG21	1:A:238:HIS:CD2	2.51	0.46
1:C:7:ARG:CG	2:J:72:LEU:H	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:105:LEU:HD21	1:C:144:TYR:HB2	1.98	0.46
1:C:428:ILE:HD11	2:H:15:PHE:CZ	2.51	0.46
1:E:117:THR:OG1	1:M:271:VAL:HG21	2.15	0.46
1:G:142:LEU:CD1	1:G:369:ALA:HB2	2.46	0.46
1:G:176:PRO:HB3	1:K:72:ASP:OD1	2.15	0.46
1:I:90:VAL:HG21	1:I:96:GLN:HB2	1.98	0.46
1:K:62:SER:HB3	1:K:82:ALA:HB2	1.98	0.46
1:K:138:MET:HE1	1:K:317:TRP:CE2	2.51	0.46
2:L:74:LEU:CD1	2:L:74:LEU:N	2.79	0.46
1:O:243:THR:HA	1:O:250:MET:HE3	1.96	0.46
4:C:4074:HOH:O	1:O:75:THR:HG22	2.14	0.46
1:E:208:SER:O	1:M:109:GLU:HB2	2.16	0.46
1:G:300:THR:HG21	1:K:309:MET:CE	2.36	0.46
1:A:142:LEU:HD12	1:A:369:ALA:HB2	1.97	0.46
1:C:18:ILE:HD11	1:C:22(A):MET:HG2	1.98	0.46
2:H:149:LYS:HD2	4:H:234:HOH:O	2.16	0.46
1:I:209:GLN:HB3	1:I:210:PRO:CD	2.45	0.46
1:K:398:VAL:HG22	1:K:399:VAL:N	2.31	0.46
1:K:461:LEU:HD22	1:K:462:TRP:CD1	2.51	0.46
1:M:209:GLN:HB3	1:M:210:PRO:HD2	1.98	0.46
1:I:214:TRP:CZ3	1:I:253:ARG:HA	2.52	0.45
2:L:105:SER:HB3	2:L:108:ILE:HG21	1.97	0.45
1:A:7:ARG:N	1:A:7:ARG:HD2	2.31	0.45
2:B:108:ILE:O	2:B:109:GLU:C	2.58	0.45
1:C:461:LEU:HD22	1:C:462:TRP:CD1	2.52	0.45
1:E:187:ARG:HD2	2:H:69:ILE:CD1	2.45	0.45
1:G:201:LYS:CB	1:G:239:TYR:HB2	2.45	0.45
1:G:410:PRO:O	1:K:8:ILE:HG12	2.17	0.45
1:A:13:TYR:HE2	1:A:81:ARG:HH22	1.64	0.45
1:A:222:MET:HE2	1:A:222:MET:HA	1.97	0.45
1:A:358:LEU:HB3	1:A:477:PHE:CG	2.52	0.45
1:C:13:TYR:HA	1:C:68:VAL:HG11	1.98	0.45
2:D:143:HIS:HD2	4:D:217:HOH:O	1.98	0.45
1:E:334:LYS:HG2	1:E:380:GLY:C	2.41	0.45
1:E:398:VAL:HG22	1:E:399:VAL:N	2.31	0.45
1:I:18:ILE:O	1:I:22(A):MET:HE2	2.16	0.45
2:J:136:ARG:HD2	2:J:136:ARG:N	2.31	0.45
1:K:18:ILE:HB	1:K:19:PRO:HD2	1.98	0.45
1:K:461:LEU:C	1:K:461:LEU:HD23	2.41	0.45
1:O:387:MET:O	1:O:391:ILE:HG12	2.17	0.45
1:O:451:THR:O	1:O:451:THR:HG22	2.15	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:P:135:SER:C	2:P:136:ARG:HD2	2.41	0.45
1:C:7:ARG:NH2	4:C:4281:HOH:O	2.49	0.45
2:D:28:LYS:HD3	1:E:433:GLU:HG2	1.99	0.45
1:E:292:HIS:HA	1:E:325:HIS:HB2	1.97	0.45
1:G:36:VAL:HA	1:G:141:PRO:HD3	1.98	0.45
1:G:201:LYS:HB2	1:G:239:TYR:HB2	1.98	0.45
1:G:400:LEU:HB3	1:G:402:PHE:HE1	1.81	0.45
1:G:466:THR:HG22	4:G:4133:HOH:O	2.17	0.45
1:I:158:GLU:HG3	1:I:290:ILE:HD13	1.99	0.45
1:K:256:PHE:O	1:K:260:LEU:HG	2.16	0.45
2:L:74:LEU:HD23	2:L:83:VAL:HG22	1.97	0.45
1:A:214:TRP:CZ3	1:A:253:ARG:HA	2.51	0.45
1:E:209:GLN:HB3	1:E:210:PRO:HD2	1.99	0.45
1:G:297:GLY:HA2	1:K:121:ILE:O	2.16	0.45
1:G:410:PRO:HD3	1:G:461:LEU:HD12	1.97	0.45
4:K:4047:HOH:O	2:L:16:SER:HB2	2.17	0.45
1:M:386:GLN:O	1:M:389:GLN:HG3	2.17	0.45
1:O:60:GLU:HG3	1:O:127:PHE:CE1	2.52	0.45
2:P:28:LYS:O	2:P:31:ASP:HB2	2.15	0.45
1:A:141:PRO:HG2	1:A:144:TYR:CB	2.47	0.45
1:C:79:LEU:CD1	1:C:104:GLU:HG2	2.46	0.45
1:C:428:ILE:HD12	1:C:428:ILE:O	2.16	0.45
4:N:1233:HOH:O	2:P:122:HIS:HE1	1.99	0.45
1:O:117:THR:O	1:O:121:ILE:HG12	2.17	0.45
1:O:209:GLN:HB3	1:O:210:PRO:HD2	1.99	0.45
1:A:8:ILE:CG2	1:A:9:LYS:N	2.78	0.45
1:A:343:ARG:CD	1:A:347:LYS:HE3	2.47	0.45
2:F:105:SER:O	2:F:109:GLU:HA	2.17	0.45
1:G:63:THR:O	1:G:64:ALA:C	2.60	0.45
1:G:193:LEU:HD22	1:G:236:LYS:HD2	1.98	0.45
1:A:330:THR:O	1:A:331:VAL:C	2.59	0.45
1:G:61:SER:HB3	1:G:124:VAL:CG1	2.47	0.45
1:I:331:VAL:HG13	1:I:337:GLY:O	2.16	0.45
1:K:204:GLU:CD	1:K:204:GLU:H	2.25	0.45
1:K:227:LYS:HE3	4:P:179:HOH:O	2.16	0.45
1:M:79:LEU:HD13	1:M:79:LEU:C	2.41	0.45
1:M:443:GLU:HG2	1:M:446:ARG:HH21	1.82	0.45
1:E:116:LEU:O	1:E:120:ILE:HG12	2.17	0.45
1:E:461:LEU:HD13	1:E:462:TRP:CZ2	2.52	0.45
2:F:108:ILE:HD12	2:F:108:ILE:H	1.81	0.45
1:G:206:ILE:O	1:G:206:ILE:HG22	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:440:GLU:O	1:G:444:ILE:HG13	2.17	0.45
2:H:136:ARG:CD	4:I:4053:HOH:O	2.62	0.45
1:I:382:ILE:HG12	4:I:4014:HOH:O	2.17	0.45
4:J:560:HOH:O	1:O:227:LYS:HD2	2.17	0.45
1:M:36:VAL:HA	1:M:141:PRO:HD3	1.98	0.45
1:M:68:VAL:HG13	4:M:4055:HOH:O	2.16	0.45
1:O:150:GLY:C	1:O:322:GLY:HA2	2.42	0.45
1:A:264:ILE:HG12	1:A:265:ILE:N	2.32	0.45
2:J:45:THR:HG23	2:J:67:TRP:CB	2.47	0.45
1:M:141:PRO:HG2	1:M:144:TYR:HB2	1.99	0.45
1:M:466:THR:HG23	4:M:4041:HOH:O	2.16	0.45
1:O:12:ARG:HD2	1:O:12:ARG:O	2.17	0.45
1:O:18:ILE:HB	1:O:19:PRO:HD2	1.98	0.45
1:A:273:GLY:O	1:A:277:ILE:HG13	2.17	0.44
2:B:108:ILE:HG22	2:B:110:SER:H	1.83	0.44
1:C:115:ASN:HD22	1:O:207:ASN:CG	2.25	0.44
2:D:74:LEU:CD1	2:D:74:LEU:N	2.80	0.44
2:F:146:GLU:HG3	2:F:155:TYR:CE2	2.51	0.44
1:G:73:LEU:HD22	1:G:73:LEU:N	2.32	0.44
1:G:138:MET:CE	1:G:317:TRP:CZ2	2.98	0.44
1:G:158:GLU:CD	1:G:325:HIS:HE2	2.24	0.44
2:H:37:LYS:HD2	2:H:37:LYS:N	2.32	0.44
2:J:74:LEU:CD1	2:J:74:LEU:N	2.80	0.44
1:O:158:GLU:HG3	1:O:290:ILE:CD1	2.47	0.44
1:A:431:ARG:HG3	1:A:437:TYR:CE2	2.52	0.44
1:E:142:LEU:HD12	1:E:369:ALA:HB2	1.99	0.44
2:H:30:ILE:HD13	2:H:83:VAL:HB	1.99	0.44
2:H:46:ASN:ND2	2:H:97:PHE:CE2	2.86	0.44
1:I:25:TRP:CE2	1:I:27:PRO:HD3	2.53	0.44
1:I:185:TYR:O	1:I:189:VAL:HG23	2.18	0.44
1:I:295:ARG:HD2	4:I:4150:HOH:O	2.17	0.44
2:J:27:LYS:C	2:J:27:LYS:HD3	2.42	0.44
2:J:108:ILE:N	2:J:108:ILE:HD12	2.32	0.44
2:J:139:LYS:HE2	2:J:139:LYS:HA	1.98	0.44
1:K:39:LEU:HD13	1:K:363:PHE:CB	2.47	0.44
1:K:150:GLY:C	1:K:322:GLY:HA2	2.42	0.44
2:P:22:THR:O	2:P:26:ILE:HG13	2.18	0.44
1:A:293:LEU:HB3	1:A:323:VAL:HG11	1.98	0.44
1:A:466:THR:HG23	4:A:4181:HOH:O	2.18	0.44
2:H:28:LYS:O	2:H:31:ASP:HB2	2.18	0.44
1:I:242:VAL:HG11	1:I:254:ALA:HA	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:392:HIS:HD2	4:I:4238:HOH:O	1.99	0.44
1:K:157:LEU:O	1:K:161:ARG:HG3	2.17	0.44
1:K:453:GLY:O	1:K:456:ARG:HB3	2.17	0.44
1:O:335:LEU:CD2	1:O:380:GLY:HA3	2.48	0.44
1:M:255:ASN:HD22	1:M:258:LYS:HE3	1.82	0.44
2:N:99:ILE:HB	2:N:118:ASN:HB3	1.98	0.44
1:O:175:LYS:HA	1:O:176:PRO:C	2.42	0.44
1:C:7:ARG:NH1	2:J:74:LEU:HD12	2.32	0.44
1:M:20:TYR:HA	1:M:22(A):MET:HE3	1.98	0.44
1:M:359:GLN:HG2	1:M:477:PHE:O	2.17	0.44
1:O:18:ILE:O	1:O:22(A):MET:HE2	2.17	0.44
1:G:334:LYS:HG2	1:G:335:LEU:HD22	2.00	0.44
1:K:206:ILE:O	1:K:206:ILE:HG22	2.17	0.44
1:K:255:ASN:HB3	4:K:4167:HOH:O	2.18	0.44
1:M:157:LEU:O	1:M:161:ARG:HG3	2.18	0.44
1:O:168:PRO:HD2	1:O:424:LEU:HD11	2.00	0.44
1:O:185:TYR:OH	1:O:202:ASP:HA	2.17	0.44
1:A:293:LEU:HD23	1:A:326:ILE:HD12	2.00	0.44
2:B:74:LEU:HB3	2:B:77:VAL:HG21	1.98	0.44
1:E:434:ASN:OD1	1:E:434:ASN:O	2.35	0.44
1:G:170:LEU:HG	1:G:424:LEU:HD22	1.98	0.44
1:K:318:MET:HE2	1:K:318:MET:HA	1.99	0.44
1:M:241:ASN:HD22	1:M:242:VAL:N	2.15	0.44
2:N:11:THR:HG21	2:N:17:PHE:CE2	2.53	0.44
2:N:143:HIS:HD2	4:P:212:HOH:O	2.00	0.44
4:A:4046:HOH:O	2:L:136:ARG:HD3	2.17	0.44
1:C:387:MET:O	1:C:391:ILE:HG12	2.18	0.44
1:G:311:PHE:CE2	1:G:315:CYS:SG	3.11	0.44
1:O:385:GLY:HA2	1:O:445:LEU:CD1	2.48	0.44
2:P:117:VAL:O	2:P:118:ASN:HB2	2.17	0.44
1:A:432:ASN:C	1:A:434:ASN:H	2.25	0.44
1:A:451:THR:O	1:A:451:THR:HG22	2.18	0.44
2:B:136:ARG:N	2:B:136:ARG:HD2	2.33	0.44
1:E:170:LEU:CD1	1:E:421:ARG:HA	2.48	0.44
2:F:27:LYS:HD3	2:F:27:LYS:C	2.43	0.44
1:I:26:ASN:OD1	1:I:29:TYR:N	2.51	0.44
2:J:9:ARG:HG3	2:J:9:ARG:HH11	1.83	0.44
2:L:11:THR:HG21	2:L:17:PHE:CE2	2.53	0.44
1:M:187:ARG:NH1	1:M:187:ARG:HG2	2.33	0.44
1:C:65:THR:HG23	1:C:67:THR:H	1.83	0.43
1:G:145:LEU:HD13	1:G:320:MET:HE3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:185:TYR:OH	1:G:202:ASP:HA	2.18	0.43
1:G:204:GLU:HB3	1:G:294:HIS:CD2	2.53	0.43
1:G:358:LEU:HD22	1:G:358:LEU:H	1.82	0.43
1:K:358:LEU:H	1:K:358:LEU:CD2	2.26	0.43
2:B:105:SER:O	2:B:109:GLU:HA	2.18	0.43
1:C:293:LEU:HB2	1:C:323:VAL:CG2	2.49	0.43
2:D:44:TYR:HA	2:D:98:TYR:O	2.17	0.43
1:E:241:ASN:HD22	1:E:243:THR:H	1.66	0.43
2:F:30:ILE:HD13	2:F:83:VAL:HB	2.00	0.43
2:F:38:LEU:HD21	2:F:112:ILE:CD1	2.48	0.43
1:G:255:ASN:HD21	1:G:283:TRP:HE1	1.66	0.43
1:I:93:ASN:OD1	1:I:95:GLU:HB2	2.18	0.43
1:M:292:HIS:HA	1:M:325:HIS:HB2	1.99	0.43
1:M:358:LEU:HB3	1:M:477:PHE:CD1	2.53	0.43
2:N:86:GLU:OE2	2:N:86:GLU:HA	2.19	0.43
2:D:74:LEU:HB3	2:D:77:VAL:CG2	2.48	0.43
1:G:72:ASP:C	1:G:74:LEU:H	2.26	0.43
1:G:388:HIS:HB3	1:G:427:MET:CE	2.48	0.43
2:H:93:ALA:O	2:H:94:ARG:HD3	2.18	0.43
1:I:90:VAL:HG13	1:I:91:PRO:HD2	2.01	0.43
1:I:165:PHE:CD1	1:I:165:PHE:N	2.84	0.43
1:K:175:LYS:HB2	1:K:407:ILE:HD12	2.00	0.43
1:A:157:LEU:CD2	1:K:216:GLU:HG2	2.48	0.43
1:A:169:LEU:HB2	1:A:399:VAL:HG22	2.01	0.43
2:B:108:ILE:N	2:B:108:ILE:CD1	2.81	0.43
1:C:142:LEU:CD1	1:C:367:GLU:HB2	2.49	0.43
2:D:123:GLU:OE1	2:D:124:PRO:HD2	2.18	0.43
1:E:356:ARG:HH12	1:E:358:LEU:HD21	1.82	0.43
1:G:153:THR:O	1:G:372:ARG:HD3	2.18	0.43
1:G:255:ASN:HD22	1:G:258:LYS:HE3	1.83	0.43
1:I:212:MET:HE3	1:I:217:ARG:HH21	1.84	0.43
1:O:170:LEU:HD23	1:O:400:LEU:HB2	2.01	0.43
1:C:222:MET:HA	1:C:222:MET:HE2	2.00	0.43
1:C:359:GLN:HE21	1:C:478:VAL:HG12	1.83	0.43
1:C:474:THR:HG22	1:C:475:SER:N	2.33	0.43
1:G:268:ASP:O	1:G:272:ILE:HG12	2.18	0.43
1:K:226:ASN:ND2	2:L:140:TYR:CD1	2.86	0.43
1:K:268:ASP:O	1:K:272:ILE:HG12	2.18	0.43
1:M:13:TYR:HA	1:M:68:VAL:HG11	2.01	0.43
2:N:17:PHE:HB2	1:O:425:GLU:CD	2.44	0.43
1:A:157:LEU:CD1	1:K:216:GLU:HG2	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:26:ILE:O	2:B:30:ILE:HG13	2.18	0.43
1:E:7:ARG:HG2	4:M:4021:HOH:O	2.17	0.43
2:F:74:LEU:N	2:F:74:LEU:HD12	2.34	0.43
1:K:358:LEU:HB3	1:K:477:PHE:CG	2.53	0.43
1:A:36:VAL:HA	1:A:141:PRO:HD3	1.99	0.43
1:A:50:PRO:HG2	4:A:4061:HOH:O	2.18	0.43
1:A:187:ARG:HH11	1:A:187:ARG:CG	2.32	0.43
1:A:338:ASP:OD1	1:A:339:PRO:HD2	2.19	0.43
1:C:145:LEU:HD12	1:C:145:LEU:HA	1.86	0.43
2:F:44:TYR:HA	2:F:98:TYR:O	2.18	0.43
2:F:143:HIS:HD2	4:H:162:HOH:O	2.02	0.43
1:I:39:LEU:HD22	1:I:363:PHE:CD2	2.54	0.43
1:K:174:THR:O	1:K:175:LYS:HD3	2.18	0.43
1:K:421:ARG:HG2	2:L:17:PHE:CD2	2.53	0.43
1:M:428:ILE:O	1:M:428:ILE:HD12	2.19	0.43
1:A:334:LYS:HG2	1:A:380:GLY:C	2.43	0.43
2:B:102:VAL:HG13	2:B:111:THR:HG23	2.00	0.43
2:D:88:ASN:HA	2:D:91:ARG:HB2	2.01	0.43
2:D:104:PHE:CE1	2:D:110:SER:HA	2.53	0.43
2:D:134:LYS:HE3	2:D:134:LYS:HB2	1.84	0.43
1:E:37:LEU:HB2	1:E:139:ARG:CB	2.44	0.43
1:E:39:LEU:HD12	1:E:136:GLU:HB2	2.01	0.43
1:E:186:GLY:HA3	2:H:66:TYR:OH	2.19	0.43
1:E:319:ARG:NH2	1:E:351:LEU:O	2.52	0.43
2:J:105:SER:O	2:J:109:GLU:HA	2.18	0.43
2:L:74:LEU:HB3	2:L:77:VAL:HG23	2.00	0.43
2:N:74:LEU:HD12	2:N:74:LEU:H	1.83	0.43
2:N:107(A):ARG:HB3	4:N:232:HOH:O	2.18	0.43
2:B:69:ILE:HG12	4:I:4060:HOH:O	2.19	0.43
4:C:4266:HOH:O	1:O:128:LYS:HG2	2.19	0.43
1:O:24:TYR:CE1	1:O:59:GLY:HA2	2.54	0.43
1:A:181:SER:O	1:A:185:TYR:HB2	2.18	0.43
1:A:214:TRP:CD2	1:A:253:ARG:HG2	2.54	0.43
1:A:221:THR:HG22	1:A:222:MET:CE	2.48	0.43
1:A:268:ASP:O	1:A:272:ILE:HG12	2.18	0.43
1:A:388:HIS:H	1:A:388:HIS:CD2	2.36	0.43
4:D:180:HOH:O	2:H:143:HIS:HD2	2.00	0.43
1:E:348:THR:HA	1:E:354:LEU:HD11	2.01	0.43
1:G:37:LEU:HB2	1:G:139:ARG:HB3	2.01	0.43
1:G:242:VAL:HG11	1:G:254:ALA:HA	2.01	0.43
1:I:398:VAL:HG22	1:I:399:VAL:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:J:29:GLN:NE2	1:M:429:LEU:HD22	2.34	0.43
2:L:8:MET:HE1	2:L:10:ILE:HD13	2.01	0.43
2:P:44:TYR:HA	2:P:98:TYR:O	2.19	0.43
2:D:30:ILE:HA	2:D:33:MET:CE	2.49	0.42
2:D:74:LEU:N	2:D:74:LEU:HD12	2.34	0.42
1:E:178:LEU:HD12	1:M:107:LEU:HD22	2.00	0.42
2:H:88:ASN:HD22	2:H:88:ASN:HA	1.70	0.42
1:I:214:TRP:CE3	1:I:253:ARG:HG2	2.54	0.42
1:K:65:THR:HG23	1:K:67:THR:O	2.19	0.42
1:K:134:ARG:HD3	1:K:136:GLU:OE2	2.19	0.42
1:K:181:SER:C	4:K:4124:HOH:O	2.62	0.42
1:M:312:ARG:NH2	1:M:361:GLY:HA3	2.34	0.42
1:O:49:ASP:O	1:O:50:PRO:C	2.62	0.42
1:O:340:ILE:H	1:O:340:ILE:CD1	2.14	0.42
1:C:78:ASP:O	1:C:83:LYS:NZ	2.52	0.42
1:C:398:VAL:HG22	1:C:399:VAL:N	2.34	0.42
2:D:22:THR:C	2:D:24:GLU:N	2.76	0.42
1:E:297:GLY:HA2	1:M:121:ILE:O	2.19	0.42
1:I:159:ARG:NH2	1:I:167:ARG:O	2.52	0.42
1:I:191:GLU:OE1	1:I:414:GLN:HG3	2.19	0.42
1:I:453:GLY:HA2	1:I:456:ARG:NH1	2.33	0.42
1:K:359:GLN:HG2	4:K:4177:HOH:O	2.18	0.42
2:L:30:ILE:HA	2:L:33:MET:HE3	2.01	0.42
1:M:293:LEU:CB	1:M:323:VAL:HG11	2.49	0.42
1:O:20:TYR:CD1	1:O:22(A):MET:HE3	2.53	0.42
1:O:201:LYS:HD2	1:O:239:TYR:CE2	2.54	0.42
1:E:134:ARG:HA	1:E:308:GLY:O	2.19	0.42
1:E:475:SER:HB3	1:E:478:VAL:CG1	2.48	0.42
1:G:90:VAL:HG21	1:G:96:GLN:HB2	2.01	0.42
1:I:463:LYS:NZ	1:I:463:LYS:HB3	2.33	0.42
1:K:60:GLU:HG3	1:K:127:PHE:CZ	2.54	0.42
1:K:157:LEU:HD22	1:M:216:GLU:HG2	2.00	0.42
1:K:206:ILE:HD12	1:K:212:MET:CE	2.50	0.42
1:M:61:SER:HB3	1:M:124:VAL:CG1	2.50	0.42
1:O:362:LEU:HD12	1:O:362:LEU:N	2.34	0.42
2:P:99:ILE:HB	2:P:118:ASN:HB3	2.01	0.42
1:E:10:ASN:OD1	1:E:10:ASN:O	2.38	0.42
1:G:293:LEU:HD22	1:G:323:VAL:HG21	2.02	0.42
1:I:8:ILE:HG23	4:I:4064:HOH:O	2.19	0.42
1:I:187:ARG:CG	1:I:187:ARG:NH1	2.81	0.42
1:K:222:MET:HE3	1:K:240:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:9:LYS:HB3	1:O:14:GLU:HA	2.00	0.42
1:O:68:VAL:HG13	4:O:4188:HOH:O	2.18	0.42
1:O:221:THR:HG21	1:O:240:LEU:HD21	2.01	0.42
2:P:8:MET:HE2	2:P:8:MET:HB2	1.69	0.42
2:P:107(B):GLY:C	2:P:108:ILE:HD12	2.44	0.42
1:A:79:LEU:HD13	1:A:104:GLU:HG2	1.99	0.42
1:A:134:ARG:NH1	1:A:136:GLU:OE2	2.51	0.42
2:B:86:GLU:OE2	2:B:86:GLU:HA	2.19	0.42
2:D:8:MET:O	2:D:8:MET:HG3	2.12	0.42
1:E:201:LYS:HB3	1:E:239:TYR:CD2	2.55	0.42
1:E:463:LYS:HB3	1:E:463:LYS:HZ3	1.84	0.42
1:G:80:TYR:CZ	1:K:179:GLY:HA2	2.54	0.42
1:G:222:MET:HE2	1:G:222:MET:HA	2.00	0.42
1:I:157:LEU:O	1:I:161:ARG:HG3	2.19	0.42
1:I:209:GLN:HB3	1:I:210:PRO:HD2	2.01	0.42
1:I:474:THR:CG2	1:I:475:SER:N	2.83	0.42
1:O:234:GLU:HB2	1:O:236:LYS:HE2	2.00	0.42
1:O:358:LEU:H	1:O:358:LEU:CD2	2.33	0.42
1:O:446:ARG:NH1	4:O:4177:HOH:O	2.48	0.42
1:A:301:TYR:CD1	1:A:301:TYR:C	2.97	0.42
1:C:90:VAL:O	1:C:91:PRO:C	2.62	0.42
2:D:38:LEU:HD21	2:D:112:ILE:CD1	2.49	0.42
2:D:72:LEU:O	1:K:7:ARG:HD3	2.19	0.42
1:G:222:MET:HE1	4:G:4039:HOH:O	2.19	0.42
1:K:141:PRO:HG2	1:K:144:TYR:HB2	2.02	0.42
1:K:430:ALA:CB	1:K:444:ILE:HD13	2.50	0.42
1:O:263:VAL:HG12	4:O:4132:HOH:O	2.19	0.42
1:A:116:LEU:O	1:A:120:ILE:HG12	2.19	0.42
1:A:117:THR:HG22	1:A:317:TRP:CH2	2.55	0.42
1:A:335:LEU:O	1:I:128:LYS:HE3	2.19	0.42
2:B:30:ILE:O	2:B:34:ILE:HG13	2.20	0.42
2:D:79:ASP:HA	2:D:80:PRO:HD2	1.91	0.42
1:E:474:THR:CG2	1:E:475:SER:H	2.33	0.42
1:G:241:ASN:ND2	1:G:243:THR:H	2.17	0.42
1:G:318:MET:HE2	1:G:318:MET:HA	2.01	0.42
1:G:385:GLY:HA2	1:G:445:LEU:CD1	2.49	0.42
1:G:386:GLN:O	1:G:389:GLN:HG2	2.20	0.42
1:I:170:LEU:HD23	1:I:400:LEU:HB2	2.02	0.42
1:I:178:LEU:HD23	1:I:206:ILE:CD1	2.50	0.42
1:K:300:THR:HG22	1:K:301:TYR:CD2	2.55	0.42
1:O:221:THR:HG22	1:O:222:MET:CE	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:VAL:O	1:A:96:GLN:HA	2.19	0.42
1:C:170:LEU:HD21	1:C:424:LEU:HD22	2.02	0.42
1:C:388:HIS:CD2	1:C:388:HIS:H	2.36	0.42
2:D:15:PHE:HE1	1:E:428:ILE:HG13	1.84	0.42
2:D:108:ILE:N	2:D:108:ILE:CD1	2.83	0.42
1:E:39:LEU:C	1:E:39:LEU:HD13	2.45	0.42
1:G:22:LYS:C	1:G:23:GLY:H	2.27	0.42
1:G:49:ASP:OD2	1:G:50:PRO:HD2	2.19	0.42
1:G:74:LEU:CA	2:P:104:PHE:CE2	3.01	0.42
2:H:47:ASP:HA	4:H:207:HOH:O	2.19	0.42
1:I:153:THR:O	1:I:372:ARG:HD3	2.20	0.42
1:I:418:THR:O	1:I:422:VAL:HG23	2.18	0.42
2:J:11:THR:HG21	2:J:17:PHE:CE2	2.54	0.42
1:M:474:THR:HG22	1:M:475:SER:N	2.34	0.42
2:B:91:ARG:HG2	2:B:118:ASN:ND2	2.34	0.42
1:C:60:GLU:OE2	1:O:334:LYS:NZ	2.52	0.42
1:G:12:ARG:NE	1:G:18:ILE:HD11	2.35	0.42
1:I:150:GLY:C	1:I:322:GLY:HA2	2.45	0.42
1:K:195:GLY:HA3	1:K:417:ALA:HB3	2.02	0.42
1:A:312:ARG:O	1:A:316:LYS:HG3	2.20	0.42
2:B:124:PRO:HB3	2:D:150:PRO:HB3	2.02	0.42
1:C:9:LYS:HB3	1:C:14:GLU:HA	2.00	0.42
1:C:369:ALA:O	1:C:370:SER:HB2	2.20	0.42
2:F:99:ILE:HB	2:F:118:ASN:HB3	2.02	0.42
1:G:388:HIS:CD2	1:G:388:HIS:N	2.88	0.42
1:I:212:MET:HE3	1:I:217:ARG:NH2	2.34	0.42
1:K:432:ASN:C	1:K:434:ASN:H	2.26	0.42
2:L:37:LYS:HD2	2:L:37:LYS:N	2.34	0.42
1:M:150:GLY:O	1:M:322:GLY:HA2	2.19	0.42
2:N:15:PHE:HA	1:O:425:GLU:OE1	2.20	0.42
1:O:335:LEU:HD21	1:O:380:GLY:HA3	2.02	0.42
1:E:271:VAL:HG11	1:M:114:ALA:O	2.20	0.41
2:H:8:MET:HE1	2:H:10:ILE:HD13	2.02	0.41
1:I:90:VAL:CG2	1:I:96:GLN:HB2	2.50	0.41
1:I:223:GLU:O	1:I:227:LYS:HG3	2.20	0.41
1:I:388:HIS:N	1:I:427:MET:HE3	2.35	0.41
1:M:157:LEU:CD1	1:O:216:GLU:HG2	2.50	0.41
1:A:216:GLU:HG2	1:O:157:LEU:HD13	2.02	0.41
4:A:4002:HOH:O	2:N:69:ILE:HG12	2.19	0.41
1:C:217:ARG:O	1:C:221:THR:HB	2.20	0.41
1:E:65:THR:HG23	1:E:67:THR:O	2.19	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:79:LEU:HD21	1:G:104:GLU:HG2	2.01	0.41
1:G:381:GLY:HA2	1:K:66:TRP:CD1	2.55	0.41
1:I:59:GLY:C	1:I:64:ALA:HB3	2.45	0.41
1:I:140:LEU:HA	1:I:141:PRO:HD2	1.94	0.41
1:I:217:ARG:O	1:I:221:THR:HB	2.20	0.41
2:J:79:ASP:HA	2:J:80:PRO:HD2	1.95	0.41
1:K:440:GLU:O	1:K:444:ILE:HG13	2.20	0.41
2:L:24:GLU:O	2:L:27:LYS:HB3	2.20	0.41
1:M:447:GLU:O	1:M:450:LYS:HB2	2.20	0.41
2:N:136:ARG:N	2:N:136:ARG:HD2	2.35	0.41
1:O:382:ILE:HG13	1:O:402:PHE:CD2	2.55	0.41
1:A:45:GLN:HG3	1:A:128:LYS:O	2.19	0.41
1:A:429:LEU:HD22	2:P:29:GLN:NE2	2.35	0.41
1:E:157:LEU:HD13	1:G:216:GLU:HG2	2.00	0.41
1:E:316:LYS:O	1:E:320:MET:HG3	2.20	0.41
1:I:178:LEU:HG	1:I:205:ASN:HD21	1.84	0.41
1:O:446:ARG:HB2	1:O:446:ARG:HH11	1.84	0.41
1:A:330:THR:OG1	1:A:333:GLY:HA3	2.20	0.41
2:B:45:THR:HG21	2:B:67:TRP:HA	2.01	0.41
1:C:181:SER:O	1:C:185:TYR:HB2	2.20	0.41
1:C:463:LYS:NZ	1:C:463:LYS:CB	2.84	0.41
1:E:77:ALA:O	1:E:81:ARG:HG3	2.20	0.41
1:G:387:MET:O	1:G:391:ILE:HG12	2.20	0.41
2:H:101:VAL:HG23	2:H:117:VAL:HG11	2.03	0.41
1:I:13:TYR:CD1	1:I:73:LEU:HD21	2.56	0.41
1:I:77:ALA:O	1:I:78:ASP:C	2.64	0.41
1:O:239:TYR:CE1	1:O:264:ILE:HD13	2.56	0.41
2:P:33:MET:HE1	2:P:101:VAL:HG11	2.01	0.41
1:A:463:LYS:HB3	1:A:463:LYS:HZ3	1.85	0.41
1:A:474:THR:HG22	1:A:475:SER:N	2.33	0.41
4:A:4046:HOH:O	2:L:136:ARG:CD	2.68	0.41
1:C:212:MET:SD	1:C:217:ARG:HD3	2.61	0.41
1:C:241:ASN:HD22	1:C:242:VAL:N	2.17	0.41
1:C:275:THR:HG23	1:O:245:ALA:O	2.21	0.41
1:C:466:THR:CG2	1:C:468:ASN:ND2	2.81	0.41
2:F:28:LYS:HD3	1:I:433:GLU:CG	2.43	0.41
2:F:104:PHE:CE2	1:O:74:LEU:HA	2.55	0.41
2:F:117:VAL:O	2:F:118:ASN:HB2	2.21	0.41
1:I:135:LEU:HD11	1:I:138:MET:HE2	2.01	0.41
1:I:327:HIS:NE2	4:I:4147:HOH:O	2.23	0.41
2:L:27:LYS:HD3	2:L:27:LYS:C	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:N:14:THR:O	1:O:425:GLU:HG2	2.20	0.41
1:C:177:LYS:HE3	1:C:205:ASN:HD21	1.85	0.41
1:C:301:TYR:CD1	1:C:301:TYR:C	2.98	0.41
1:C:466:THR:CG2	1:C:467:PHE:N	2.82	0.41
1:E:138:MET:CE	1:E:317:TRP:CZ2	3.03	0.41
1:E:214:TRP:CZ3	1:E:253:ARG:HA	2.56	0.41
1:G:63:THR:HG23	1:G:80:TYR:O	2.21	0.41
1:K:170:LEU:HD22	1:K:402:PHE:HE1	1.84	0.41
1:K:369:ALA:O	1:K:370:SER:HB2	2.21	0.41
1:M:117:THR:HG22	1:M:317:TRP:CH2	2.56	0.41
1:M:474:THR:HG22	1:M:475:SER:H	1.86	0.41
1:O:201:LYS:CB	1:O:239:TYR:HB2	2.51	0.41
1:C:429:LEU:HD22	2:H:29:GLN:NE2	2.36	0.41
2:D:33:MET:HE3	2:D:40:ILE:HD13	2.03	0.41
1:E:158:GLU:CD	1:E:325:HIS:HE2	2.26	0.41
1:E:191:GLU:OE1	1:E:414:GLN:HG3	2.20	0.41
2:F:29:GLN:NE2	1:I:429:LEU:HD22	2.35	0.41
2:F:136:ARG:HD2	4:G:4011:HOH:O	2.20	0.41
1:G:96:GLN:C	1:G:97:TYR:CD1	2.99	0.41
1:G:206:ILE:HD12	1:G:212:MET:CE	2.51	0.41
1:G:319:ARG:HD3	1:G:372:ARG:O	2.21	0.41
1:I:188:VAL:HG13	1:I:413:ILE:HD13	2.02	0.41
1:K:28:ASP:O	1:K:29:TYR:C	2.62	0.41
1:K:421:ARG:O	1:K:425:GLU:HG3	2.21	0.41
1:M:295:ARG:O	1:M:296:ALA:C	2.63	0.41
1:M:362:LEU:HD12	1:M:362:LEU:N	2.36	0.41
1:O:201:LYS:HB2	1:O:239:TYR:HB2	2.02	0.41
4:O:4014:HOH:O	2:P:136:ARG:HD3	2.20	0.41
1:A:85:TYR:CZ	1:A:100:TYR:HB3	2.55	0.41
1:C:86:LYS:HE2	1:C:88:ASP:OD1	2.20	0.41
1:G:187:ARG:O	1:G:191:GLU:HG2	2.21	0.41
1:I:193:LEU:CD2	1:I:200:VAL:HG23	2.51	0.41
1:I:378:ALA:HB2	1:I:394:LEU:HD13	2.03	0.41
1:K:396:GLU:HB2	1:K:431:ARG:HH12	1.85	0.41
1:O:474:THR:CG2	1:O:475:SER:N	2.84	0.41
1:A:17:VAL:HG11	4:A:4165:HOH:O	2.20	0.41
1:A:133:LEU:O	1:A:307:HIS:HA	2.21	0.41
1:A:138:MET:CE	1:A:317:TRP:NE1	2.84	0.41
1:A:216:GLU:HG2	1:O:157:LEU:CD1	2.51	0.41
1:A:295:ARG:O	1:A:296:ALA:C	2.63	0.41
1:C:221:THR:HG22	1:C:222:MET:HE2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:45:THR:HG21	2:D:67:TRP:HA	2.03	0.41
1:E:157:LEU:CD1	1:G:216:GLU:HG2	2.51	0.41
1:G:69:VAL:HG12	1:K:408:GLY:CA	2.50	0.41
1:G:81:ARG:O	1:G:83:LYS:HD3	2.21	0.41
1:G:223:GLU:O	1:G:227:LYS:HG3	2.20	0.41
1:G:243:THR:HA	1:G:250:MET:HE3	2.02	0.41
1:G:469:TYR:HB3	1:K:45:GLN:HE21	1.85	0.41
1:I:281:ALA:HB1	1:I:322:GLY:HA3	2.02	0.41
1:I:475:SER:HB3	1:I:478:VAL:HG13	2.02	0.41
2:J:99:ILE:HB	2:J:118:ASN:HB3	2.03	0.41
1:K:24:TYR:CD1	1:K:59:GLY:HA2	2.56	0.41
1:K:335:LEU:CD2	1:K:380:GLY:HA3	2.49	0.41
1:K:428:ILE:HG13	1:K:429:LEU:N	2.36	0.41
1:M:208:SER:O	1:M:209:GLN:HG3	2.21	0.41
2:P:147:SER:HA	2:P:154:ARG:CZ	2.51	0.41
1:A:34:THR:HG21	1:G:142:LEU:HD21	2.03	0.41
1:E:181:SER:O	1:E:185:TYR:HB2	2.21	0.41
2:F:8:MET:HE2	2:F:8:MET:HB2	1.80	0.41
2:F:17:PHE:HB2	1:I:425:GLU:OE1	2.21	0.41
1:I:319:ARG:HD2	1:I:368:TRP:CZ3	2.56	0.41
1:K:14:GLU:O	1:K:15:SER:C	2.64	0.41
1:K:297:GLY:O	1:K:300:THR:HB	2.21	0.41
2:N:27:LYS:HD3	2:N:27:LYS:C	2.46	0.41
1:O:61:SER:HB3	1:O:124:VAL:CG1	2.51	0.41
1:O:301:TYR:C	1:O:301:TYR:CD1	2.99	0.41
1:A:264:ILE:HG13	1:A:290:ILE:HB	2.03	0.40
2:B:10:ILE:HG13	2:B:98:TYR:CZ	2.57	0.40
1:C:204:GLU:OE1	1:C:294:HIS:NE2	2.54	0.40
1:C:222:MET:O	1:C:226:ASN:ND2	2.54	0.40
1:E:9:LYS:HE2	2:L:72:LEU:CD2	2.51	0.40
1:G:74:LEU:O	2:P:104:PHE:HZ	2.04	0.40
1:G:264:ILE:HG13	1:G:290:ILE:HB	2.02	0.40
1:G:348:THR:HA	1:G:354:LEU:HD21	2.03	0.40
2:H:72:LEU:H	1:M:7:ARG:CG	2.09	0.40
2:J:74:LEU:HD12	2:J:74:LEU:N	2.36	0.40
1:K:149:GLN:HG2	1:K:150:GLY:O	2.21	0.40
1:K:293:LEU:HB2	1:K:323:VAL:CG2	2.45	0.40
1:M:39:LEU:HD22	1:M:363:PHE:CD2	2.55	0.40
1:O:255:ASN:O	1:O:259:GLU:HG3	2.20	0.40
1:O:398:VAL:HG13	1:O:400:LEU:CD1	2.51	0.40
2:P:30:ILE:O	2:P:34:ILE:HG13	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:37:LEU:HB2	1:A:139:ARG:CB	2.51	0.40
1:A:90:VAL:HG13	1:A:91:PRO:HD2	2.02	0.40
1:A:316:LYS:HD3	1:A:366:MET:HE1	2.02	0.40
1:C:428:ILE:HG13	2:H:15:PHE:HE1	1.85	0.40
1:E:36:VAL:HA	1:E:141:PRO:HD3	2.03	0.40
1:G:140:LEU:HB2	1:G:145:LEU:HD21	2.02	0.40
2:H:33:MET:HE1	2:H:101:VAL:HG11	2.03	0.40
1:I:175:LYS:HE3	3:I:4005:SO4:O3	2.21	0.40
1:K:223:GLU:O	1:K:227:LYS:HG3	2.22	0.40
1:K:291:LEU:O	1:K:324:ASP:HB2	2.20	0.40
1:K:306:ASN:HB3	4:K:4086:HOH:O	2.21	0.40
1:K:388:HIS:ND1	1:K:441:GLY:HA3	2.36	0.40
2:L:108:ILE:HG22	2:L:110:SER:H	1.86	0.40
1:M:81:ARG:O	1:M:83:LYS:HD3	2.20	0.40
1:A:164:LYS:NZ	1:A:198:ASP:OD1	2.55	0.40
2:D:29:GLN:O	2:D:33:MET:HG3	2.20	0.40
1:K:178:LEU:CD2	1:K:206:ILE:HG12	2.52	0.40
1:K:388:HIS:H	1:K:388:HIS:CD2	2.39	0.40
1:M:344:GLY:HA3	4:M:4090:HOH:O	2.20	0.40
1:O:214:TRP:CZ3	1:O:253:ARG:HA	2.55	0.40
1:O:437:TYR:O	1:O:441:GLY:N	2.54	0.40
4:O:4014:HOH:O	2:P:136:ARG:CD	2.69	0.40
1:A:209:GLN:HB3	1:A:210:PRO:CD	2.50	0.40
1:A:209:GLN:HB3	1:A:210:PRO:HD2	2.02	0.40
1:A:356:ARG:NH1	1:A:358:LEU:HD21	2.36	0.40
1:C:206:ILE:O	1:C:206:ILE:HG22	2.20	0.40
1:E:187:ARG:HD2	2:H:69:ILE:HD11	2.03	0.40
1:E:187:ARG:CG	1:E:187:ARG:HH11	2.34	0.40
1:I:187:ARG:HH11	1:I:187:ARG:HG2	1.85	0.40
1:K:24:TYR:CE1	1:K:59:GLY:HA2	2.57	0.40
1:K:174:THR:HG21	1:K:185:TYR:CE1	2.57	0.40
1:K:185:TYR:OH	1:K:202:ASP:HA	2.21	0.40
1:K:358:LEU:HD23	4:K:4176:HOH:O	2.22	0.40
1:K:388:HIS:CD2	1:K:388:HIS:N	2.90	0.40
1:O:85:TYR:CZ	1:O:100:TYR:HB3	2.57	0.40
1:A:410:PRO:HD3	1:A:461:LEU:CD1	2.52	0.40
2:D:29:GLN:NE2	1:E:429:LEU:HD22	2.37	0.40
2:D:72:LEU:N	1:K:7:ARG:CG	2.81	0.40
2:D:127:ASN:HB2	2:D:145:TYR:CZ	2.57	0.40
2:F:107:VAL:O	2:F:107(A):ARG:C	2.63	0.40
2:F:136:ARG:NH2	4:F:160:HOH:O	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:187:ARG:NH1	1:G:187:ARG:CG	2.84	0.40
2:H:44:TYR:O	2:H:45:THR:CG2	2.69	0.40
1:I:241:ASN:HD22	1:I:242:VAL:N	2.19	0.40
1:K:138:MET:CE	1:K:317:TRP:CZ2	3.04	0.40
1:K:151:PRO:HA	1:K:322:GLY:O	2.22	0.40
2:L:136:ARG:HD2	2:L:136:ARG:N	2.36	0.40
2:N:134:LYS:HE3	2:N:134:LYS:HB2	1.89	0.40
1:O:227:LYS:HE2	1:O:227:LYS:HB3	1.79	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	471/493 (96%)	436 (93%)	26 (6%)	9 (2%)	6	13
1	C	471/493 (96%)	440 (93%)	27 (6%)	4 (1%)	16	34
1	E	471/493 (96%)	441 (94%)	27 (6%)	3 (1%)	21	42
1	G	471/493 (96%)	425 (90%)	39 (8%)	7 (2%)	8	18
1	I	471/493 (96%)	443 (94%)	24 (5%)	4 (1%)	16	34
1	K	471/493 (96%)	423 (90%)	45 (10%)	3 (1%)	21	42
1	M	471/493 (96%)	438 (93%)	27 (6%)	6 (1%)	9	21
1	O	471/493 (96%)	438 (93%)	27 (6%)	6 (1%)	9	21
2	B	136/138 (99%)	123 (90%)	11 (8%)	2 (2%)	8	18
2	D	136/138 (99%)	124 (91%)	11 (8%)	1 (1%)	18	38
2	F	136/138 (99%)	125 (92%)	10 (7%)	1 (1%)	18	38
2	H	136/138 (99%)	124 (91%)	11 (8%)	1 (1%)	18	38
2	J	136/138 (99%)	122 (90%)	12 (9%)	2 (2%)	8	18

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	L	136/138 (99%)	125 (92%)	10 (7%)	1 (1%)	18	38
2	N	136/138 (99%)	125 (92%)	9 (7%)	2 (2%)	8	18
2	P	136/138 (99%)	122 (90%)	12 (9%)	2 (2%)	8	18
All	All	4856/5048 (96%)	4474 (92%)	328 (7%)	54 (1%)	11	25

All (54) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	331	VAL
1	C	91	PRO
1	K	465	ILE
1	O	11	SER
1	A	295	ARG
1	E	11	SER
1	E	91	PRO
1	G	64	ALA
1	G	124	VAL
2	H	48	ILE
1	M	463	LYS
1	O	295	ARG
1	A	11	SER
1	A	15	SER
1	A	91	PRO
1	A	296	ALA
2	B	75	PHE
1	C	11	SER
2	J	75	PHE
1	M	295	ARG
1	O	91	PRO
1	G	11	SER
1	G	91	PRO
1	G	461	LEU
1	I	91	PRO
1	K	91	PRO
1	K	295	ARG
2	N	107(A)	ARG
1	O	15	SER
1	A	8	ILE
2	B	48	ILE
1	I	11	SER
2	J	48	ILE

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Mol	Chain	Res	Type
1	M	11	SER
2	P	48	ILE
2	P	118	ASN
1	C	177	LYS
2	D	48	ILE
1	G	15	SER
1	G	337	GLY
1	I	10	ASN
2	L	48	ILE
1	M	91	PRO
1	O	8	ILE
1	A	124	VAL
1	C	337	GLY
1	E	337	GLY
2	F	48	ILE
1	I	337	GLY
1	M	337	GLY
2	N	48	ILE
1	O	337	GLY
1	A	337	GLY
1	M	94	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	384/403 (95%)	367 (96%)	17 (4%)	25	50
1	C	384/403 (95%)	359 (94%)	25 (6%)	15	35
1	E	384/403 (95%)	351 (91%)	33 (9%)	10	22
1	G	384/403 (95%)	363 (94%)	21 (6%)	19	41
1	I	384/403 (95%)	363 (94%)	21 (6%)	19	41
1	K	384/403 (95%)	362 (94%)	22 (6%)	18	40
1	M	384/403 (95%)	360 (94%)	24 (6%)	16	36
1	O	384/403 (95%)	363 (94%)	21 (6%)	19	41

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	126/126 (100%)	122 (97%)	4 (3%)	34	62
2	D	126/126 (100%)	121 (96%)	5 (4%)	28	55
2	F	126/126 (100%)	122 (97%)	4 (3%)	34	62
2	H	126/126 (100%)	121 (96%)	5 (4%)	28	55
2	J	126/126 (100%)	124 (98%)	2 (2%)	55	79
2	L	126/126 (100%)	121 (96%)	5 (4%)	28	55
2	N	126/126 (100%)	122 (97%)	4 (3%)	34	62
2	P	126/126 (100%)	121 (96%)	5 (4%)	28	55
All	All	4080/4232 (96%)	3862 (95%)	218 (5%)	20	43

All (218) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	ARG
1	A	12	ARG
1	A	39	LEU
1	A	83	LYS
1	A	91	PRO
1	A	105	LEU
1	A	145	LEU
1	A	187	ARG
1	A	216	GLU
1	A	219	LEU
1	A	271	VAL
1	A	300	THR
1	A	354	LEU
1	A	389	GLN
1	A	400	LEU
1	A	438	LEU
1	A	463	LYS
2	B	24	GLU
2	B	48	ILE
2	B	84	LEU
2	B	136	ARG
1	C	7	ARG
1	C	39	LEU
1	C	73	LEU
1	C	91	PRO
1	C	105	LEU

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Mol	Chain	Res	Type
1	C	127	PHE
1	C	142	LEU
1	C	145	LEU
1	C	187	ARG
1	C	216	GLU
1	C	219	LEU
1	C	271	VAL
1	C	295	ARG
1	C	300	THR
1	C	319	ARG
1	C	323	VAL
1	C	350	LEU
1	C	351	LEU
1	C	358	LEU
1	C	400	LEU
1	C	428	ILE
1	C	438	LEU
1	C	446	ARG
1	C	463	LYS
1	C	466	THR
2	D	8	MET
2	D	24	GLU
2	D	48	ILE
2	D	84	LEU
2	D	92	LYS
1	E	7	ARG
1	E	9	LYS
1	E	73	LEU
1	E	78	ASP
1	E	79	LEU
1	E	83	LYS
1	E	91	PRO
1	E	105	LEU
1	E	138	MET
1	E	145	LEU
1	E	172	CYS
1	E	187	ARG
1	E	216	GLU
1	E	219	LEU
1	E	271	VAL
1	E	295	ARG
1	E	300	THR

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Mol	Chain	Res	Type
1	E	319	ARG
1	E	323	VAL
1	E	335	LEU
1	E	350	LEU
1	E	351	LEU
1	E	354	LEU
1	E	355	GLU
1	E	388	HIS
1	E	400	LEU
1	E	428	ILE
1	E	429	LEU
1	E	438	LEU
1	E	446	ARG
1	E	461	LEU
1	E	463	LYS
1	E	478	VAL
2	F	24	GLU
2	F	48	ILE
2	F	84	LEU
2	F	92	LYS
1	G	18	ILE
1	G	83	LYS
1	G	91	PRO
1	G	105	LEU
1	G	142	LEU
1	G	145	LEU
1	G	172	CYS
1	G	187	ARG
1	G	206	ILE
1	G	219	LEU
1	G	221	THR
1	G	271	VAL
1	G	288	ASP
1	G	295	ARG
1	G	319	ARG
1	G	350	LEU
1	G	354	LEU
1	G	388	HIS
1	G	428	ILE
1	G	438	LEU
1	G	463	LYS
2	H	11	THR

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Mol	Chain	Res	Type
2	H	48	ILE
2	H	69	ILE
2	H	111	THR
2	H	131	GLN
1	I	7	ARG
1	I	9	LYS
1	I	83	LYS
1	I	91	PRO
1	I	105	LEU
1	I	142	LEU
1	I	145	LEU
1	I	165	PHE
1	I	172	CYS
1	I	187	ARG
1	I	219	LEU
1	I	239	TYR
1	I	271	VAL
1	I	295	ARG
1	I	323	VAL
1	I	350	LEU
1	I	351	LEU
1	I	400	LEU
1	I	438	LEU
1	I	461	LEU
1	I	463	LYS
2	J	24	GLU
2	J	48	ILE
1	K	7	ARG
1	K	83	LYS
1	K	105	LEU
1	K	127	PHE
1	K	145	LEU
1	K	205	ASN
1	K	206	ILE
1	K	216	GLU
1	K	219	LEU
1	K	271	VAL
1	K	295	ARG
1	K	300	THR
1	K	319	ARG
1	K	323	VAL
1	K	350	LEU

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Mol	Chain	Res	Type
1	K	351	LEU
1	K	354	LEU
1	K	400	LEU
1	K	428	ILE
1	K	438	LEU
1	K	446	ARG
1	K	463	LYS
2	L	24	GLU
2	L	48	ILE
2	L	74	LEU
2	L	84	LEU
2	L	139	LYS
1	M	7	ARG
1	M	73	LEU
1	M	83	LYS
1	M	91	PRO
1	M	105	LEU
1	M	145	LEU
1	M	187	ARG
1	M	216	GLU
1	M	219	LEU
1	M	239	TYR
1	M	271	VAL
1	M	288	ASP
1	M	295	ARG
1	M	300	THR
1	M	319	ARG
1	M	335	LEU
1	M	350	LEU
1	M	351	LEU
1	M	354	LEU
1	M	358	LEU
1	M	400	LEU
1	M	428	ILE
1	M	461	LEU
1	M	463	LYS
2	N	24	GLU
2	N	48	ILE
2	N	72	LEU
2	N	84	LEU
1	O	73	LEU
1	O	83	LYS

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Mol	Chain	Res	Type
1	O	91	PRO
1	O	105	LEU
1	O	145	LEU
1	O	187	ARG
1	O	219	LEU
1	O	221	THR
1	O	271	VAL
1	O	295	ARG
1	O	300	THR
1	O	319	ARG
1	O	323	VAL
1	O	335	LEU
1	O	340	ILE
1	O	350	LEU
1	O	351	LEU
1	O	354	LEU
1	O	438	LEU
1	O	461	LEU
1	O	463	LYS
2	P	8	MET
2	P	24	GLU
2	P	48	ILE
2	P	74	LEU
2	P	84	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (115) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	92	ASN
1	A	241	ASN
1	A	255	ASN
1	A	359	GLN
1	A	388	HIS
1	A	389	GLN
1	A	401	GLN
2	B	118	ASN
2	B	122	HIS
2	B	143	HIS
1	C	10	ASN
1	C	115	ASN
1	C	207	ASN
1	C	226	ASN

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Mol	Chain	Res	Type
1	C	241	ASN
1	C	255	ASN
1	C	359	GLN
1	C	388	HIS
1	C	401	GLN
1	C	468	ASN
2	D	88	ASN
2	D	143	HIS
1	E	92	ASN
1	E	123	ASN
1	E	207	ASN
1	E	241	ASN
1	E	255	ASN
1	E	298	ASN
1	E	359	GLN
1	E	389	GLN
1	E	401	GLN
1	E	434	ASN
2	F	88	ASN
2	F	122	HIS
2	F	143	HIS
1	G	10	ASN
1	G	92	ASN
1	G	123	ASN
1	G	184	ASN
1	G	241	ASN
1	G	255	ASN
1	G	298	ASN
1	G	359	GLN
1	G	383	HIS
1	G	388	HIS
1	G	401	GLN
1	G	434	ASN
2	H	88	ASN
2	H	118	ASN
2	H	122	HIS
2	H	143	HIS
1	I	10	ASN
1	I	89	GLN
1	I	92	ASN
1	I	205	ASN
1	I	226	ASN

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Mol	Chain	Res	Type
1	I	241	ASN
1	I	255	ASN
1	I	388	HIS
1	I	389	GLN
1	I	392	HIS
1	I	434	ASN
2	J	88	ASN
2	J	118	ASN
2	J	143	HIS
1	K	10	ASN
1	K	92	ASN
1	K	96	GLN
1	K	184	ASN
1	K	207	ASN
1	K	241	ASN
1	K	255	ASN
1	K	298	ASN
1	K	359	GLN
1	K	388	HIS
1	K	401	GLN
1	K	414	GLN
1	K	434	ASN
2	L	12	GLN
2	L	88	ASN
2	L	118	ASN
2	L	143	HIS
1	M	89	GLN
1	M	92	ASN
1	M	115	ASN
1	M	123	ASN
1	M	226	ASN
1	M	241	ASN
1	M	255	ASN
1	M	388	HIS
1	M	392	HIS
1	M	401	GLN
1	M	414	GLN
1	M	434	ASN
1	M	468	ASN
2	N	12	GLN
2	N	88	ASN
2	N	118	ASN

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Mol	Chain	Res	Type
2	N	122	HIS
2	N	143	HIS
1	O	89	GLN
1	O	96	GLN
1	O	207	ASN
1	O	241	ASN
1	O	255	ASN
1	O	298	ASN
1	O	359	GLN
1	O	388	HIS
1	O	392	HIS
1	O	401	GLN
2	P	12	GLN
2	P	88	ASN
2	P	118	ASN
2	P	122	HIS
2	P	143	HIS

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](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SO4	C	4002	-	4,4,4	0.36	0	6,6,6	0.10	0
3	SO4	K	4008	-	4,4,4	0.36	0	6,6,6	0.08	0
3	SO4	O	4007	-	4,4,4	0.34	0	6,6,6	0.10	0
3	SO4	I	4005	-	4,4,4	0.38	0	6,6,6	0.07	0
3	SO4	E	4003	-	4,4,4	0.36	0	6,6,6	0.09	0
3	SO4	M	4006	-	4,4,4	0.34	0	6,6,6	0.08	0
3	SO4	G	4004	-	4,4,4	0.37	0	6,6,6	0.08	0
3	SO4	A	4001	-	4,4,4	0.38	0	6,6,6	0.08	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	4002	SO4	1	0
3	I	4005	SO4	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	473/493 (95%)	-0.42	7 (1%) 72 68	9, 27, 56, 77	0
1	C	473/493 (95%)	-0.54	4 (0%) 82 80	7, 21, 48, 70	0
1	E	473/493 (95%)	-0.55	3 (0%) 85 83	8, 21, 48, 75	0
1	G	473/493 (95%)	-0.09	24 (5%) 33 28	8, 31, 83, 101	0
1	I	473/493 (95%)	-0.44	6 (1%) 75 71	8, 25, 54, 87	0
1	K	473/493 (95%)	-0.11	19 (4%) 42 37	7, 29, 83, 98	0
1	M	473/493 (95%)	-0.61	9 (1%) 66 61	7, 19, 47, 95	0
1	O	473/493 (95%)	-0.51	6 (1%) 75 71	6, 22, 53, 96	0
2	B	138/138 (100%)	-0.29	0 100 100	14, 30, 46, 51	0
2	D	138/138 (100%)	-0.39	0 100 100	11, 28, 46, 54	0
2	F	138/138 (100%)	-0.47	0 100 100	15, 27, 42, 49	0
2	H	138/138 (100%)	-0.57	0 100 100	10, 22, 39, 48	0
2	J	138/138 (100%)	-0.62	0 100 100	9, 21, 37, 41	0
2	L	138/138 (100%)	-0.64	0 100 100	11, 22, 36, 44	0
2	N	138/138 (100%)	-0.54	0 100 100	9, 24, 41, 54	0
2	P	138/138 (100%)	-0.54	1 (0%) 84 82	10, 23, 41, 48	0
All	All	4888/5048 (96%)	-0.43	79 (1%) 70 66	6, 24, 56, 101	0

All (79) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	8	ILE	5.5
1	I	6	THR	5.0
1	O	7	ARG	4.8
1	M	6	THR	4.8
1	O	6	THR	4.7

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Mol	Chain	Res	Type	RSRZ
1	M	7	ARG	4.4
1	K	10	ASN	3.8
1	G	6	THR	3.7
1	I	8	ILE	3.7
1	G	69	VAL	3.7
1	K	8	ILE	3.6
1	G	64	ALA	3.6
1	K	7	ARG	3.5
1	G	68	VAL	3.5
1	K	478	VAL	3.5
1	G	8	ILE	3.5
1	A	6	THR	3.4
1	K	462	TRP	3.4
1	A	10	ASN	3.4
1	G	70	TRP	3.4
1	I	478	VAL	3.3
1	I	7	ARG	3.2
1	E	478	VAL	3.2
1	K	6	THR	3.1
1	K	474	THR	3.1
1	G	18	ILE	3.1
1	C	7	ARG	3.1
1	C	10	ASN	3.1
1	G	13	TYR	3.1
1	E	10	ASN	3.1
1	K	469	TYR	3.0
1	G	65	THR	3.0
1	K	13	TYR	3.0
1	K	473	ASP	3.0
1	K	330	THR	3.0
1	G	478	VAL	3.0
1	K	461	LEU	2.9
1	E	6	THR	2.9
1	O	8	ILE	2.9
1	G	461	LEU	2.8
1	A	478	VAL	2.8
1	M	12	ARG	2.8
1	G	330	THR	2.8
1	G	7	ARG	2.7
1	K	472	THR	2.7
1	O	478	VAL	2.6
2	P	104	PHE	2.6

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Mol	Chain	Res	Type	RSRZ
1	M	478	VAL	2.6
1	I	10	ASN	2.6
1	G	67	THR	2.5
1	C	8	ILE	2.5
1	M	9	LYS	2.5
1	G	66	TRP	2.5
1	A	7	ARG	2.4
1	A	477	PHE	2.4
1	O	10	ASN	2.4
1	K	465	ILE	2.4
1	K	467	PHE	2.4
1	G	12	ARG	2.3
1	K	9	LYS	2.3
1	M	10	ASN	2.3
1	C	474	THR	2.3
1	G	63	THR	2.3
1	I	11	SER	2.2
1	K	335	LEU	2.2
1	G	465	ILE	2.2
1	G	469	TYR	2.2
1	G	11	SER	2.1
1	G	477	PHE	2.1
1	G	17	VAL	2.1
1	A	11	SER	2.1
1	O	9	LYS	2.1
1	A	8	ILE	2.1
1	K	471	SER	2.1
1	M	64	ALA	2.0
1	G	474	THR	2.0
1	G	20	TYR	2.0
1	M	11	SER	2.0
1	K	466	THR	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	SO4	G	4004	5/5	0.81	0.18	91,91,91,92	0
3	SO4	K	4008	5/5	0.83	0.16	100,100,101,101	0
3	SO4	A	4001	5/5	0.93	0.10	51,52,53,53	0
3	SO4	C	4002	5/5	0.95	0.10	60,61,61,61	0
3	SO4	E	4003	5/5	0.95	0.09	59,60,60,60	0
3	SO4	I	4005	5/5	0.97	0.07	40,41,42,43	0
3	SO4	O	4007	5/5	0.98	0.06	41,41,41,43	0
3	SO4	M	4006	5/5	1.00	0.03	21,22,23,24	0

6.5 Other polymers [i](#)

There are no such residues in this entry.