



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:35 PM UTC

PDB ID : 6P4X / pdb_00006p4x
Title : Crystal Structure of the *S. cerevisiae* glucokinase, Glk1
Authors : Stoddard, P.R.; Garner, E.C.; Murray, A.W.
Deposited on : 2019-05-28
Resolution : 3.59 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

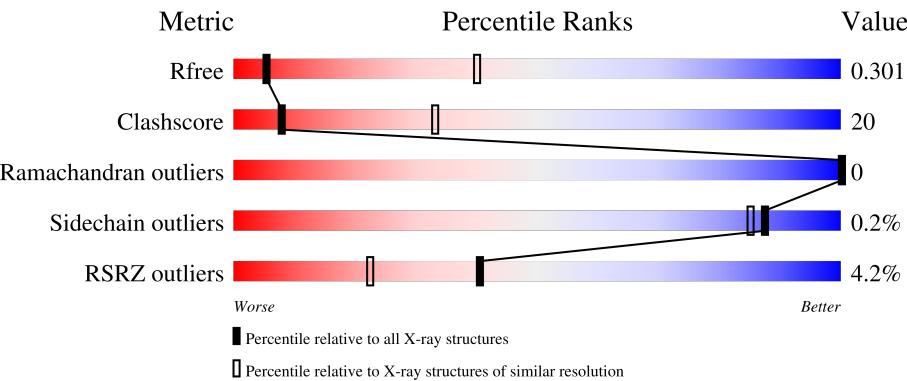
1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.59 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	1747 (3.70-3.50)
Clashscore	190562	1827 (3.70-3.50)
Ramachandran outliers	187476	1773 (3.70-3.50)
Sidechain outliers	187428	1772 (3.70-3.50)
RSRZ outliers	180081	1745 (3.70-3.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	500	5% 65% 30% ..
1	B	500	3% 64% 31% ..
1	C	500	5% 59% 36% ..
1	D	500	3% 60% 34% ..
1	E	500	3% 62% 33% ..

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Mol	Chain	Length	Quality of chain
1	F	500	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PO4	A	602	-	X	X	-
2	PO4	A	603	-	X	X	-
2	PO4	B	601	-	-	X	-

2 Entry composition [i](#)

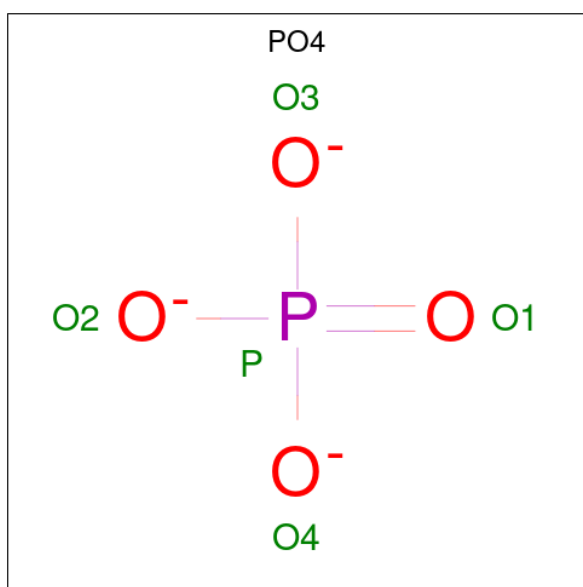
There are 2 unique types of molecules in this entry. The entry contains 22953 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glucokinase-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	491	Total	C	N	O	S	0	0	0
			3817	2414	651	731	21			
1	B	490	Total	C	N	O	S	0	0	0
			3815	2413	651	731	20			
1	C	493	Total	C	N	O	S	0	0	0
			3828	2421	654	732	21			
1	D	488	Total	C	N	O	S	0	0	0
			3786	2393	648	727	18			
1	E	489	Total	C	N	O	S	0	0	0
			3807	2409	650	728	20			
1	F	493	Total	C	N	O	S	0	0	0
			3835	2424	654	736	21			

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O₄P).

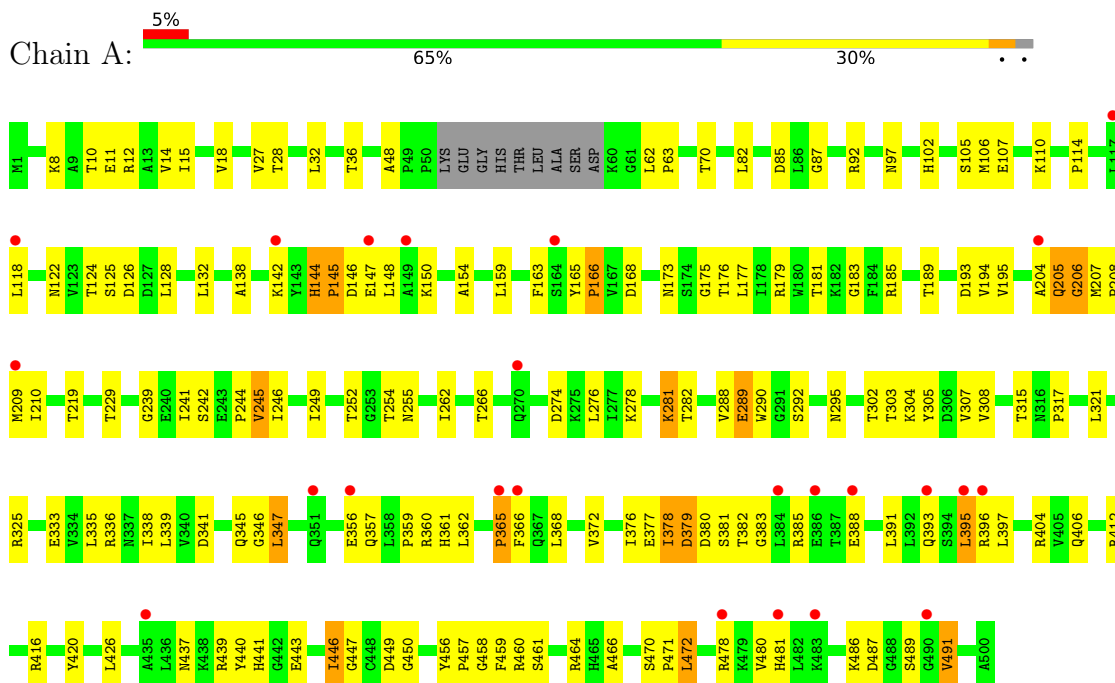


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	A	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	B	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	C	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	D	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	E	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		
2	F	1	Total	O	P	0	0
			5	4	1		

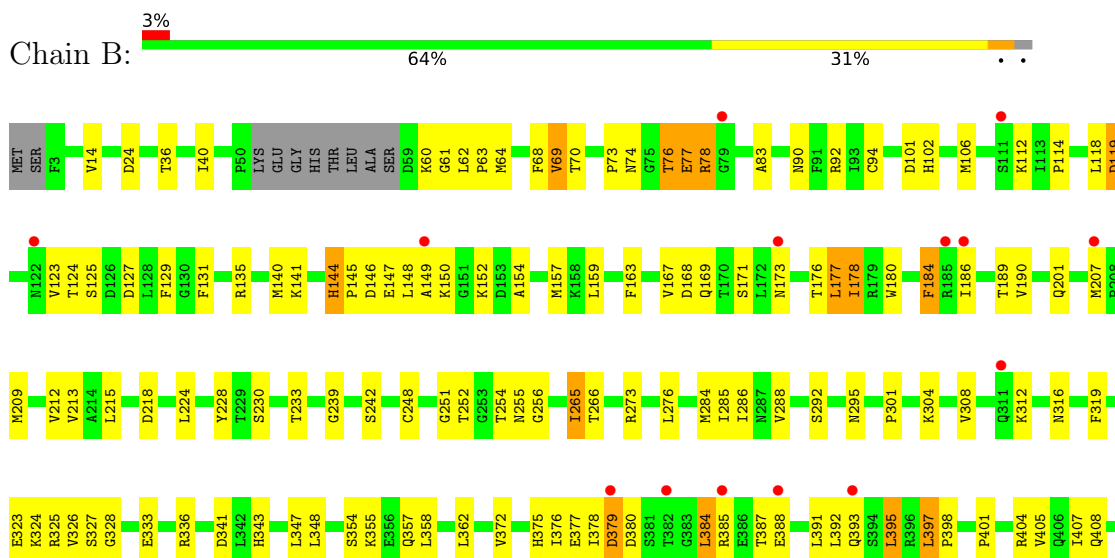
3 Residue-property plots

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: Glucokinase-1

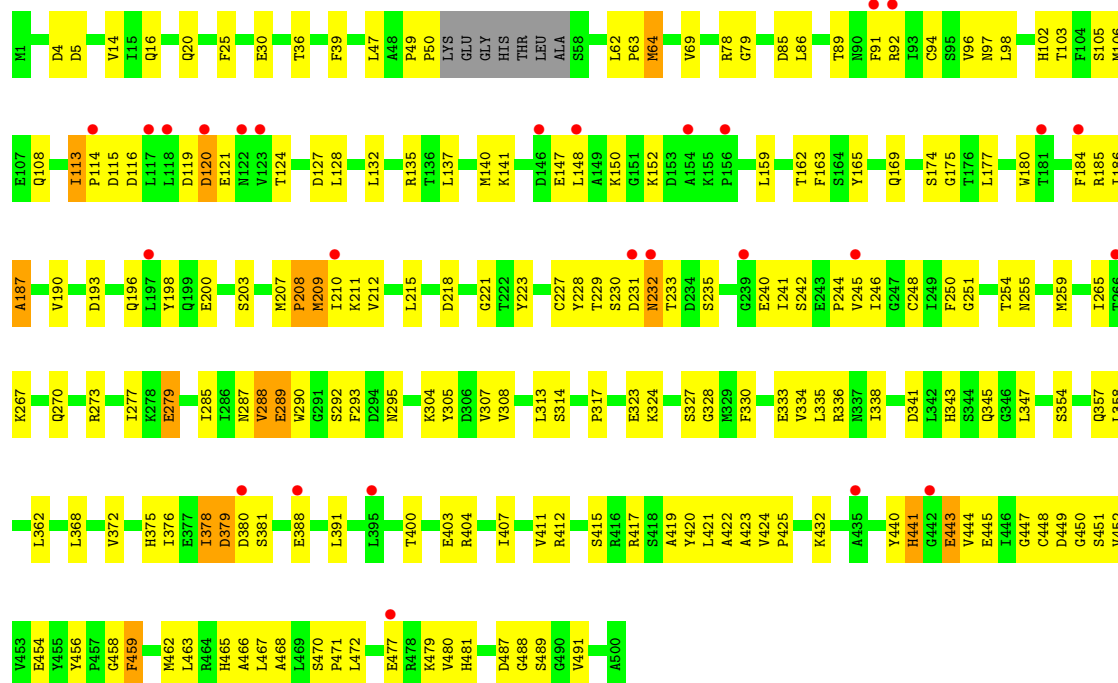


• Molecule 1: Glucokinase-1

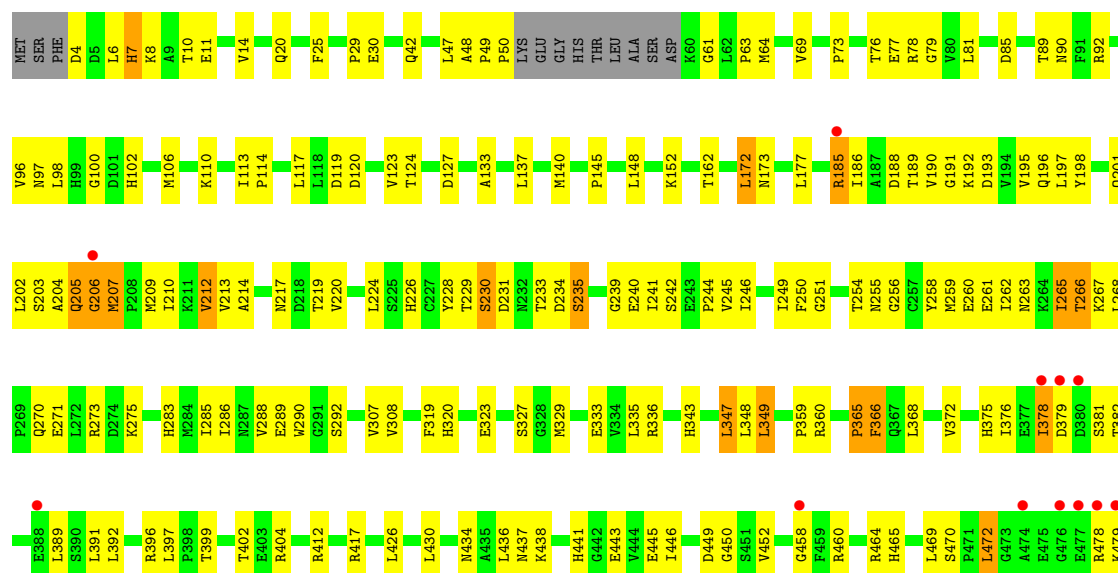


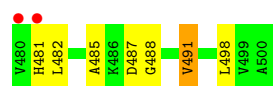


• Molecule 1: Glucokinase-1

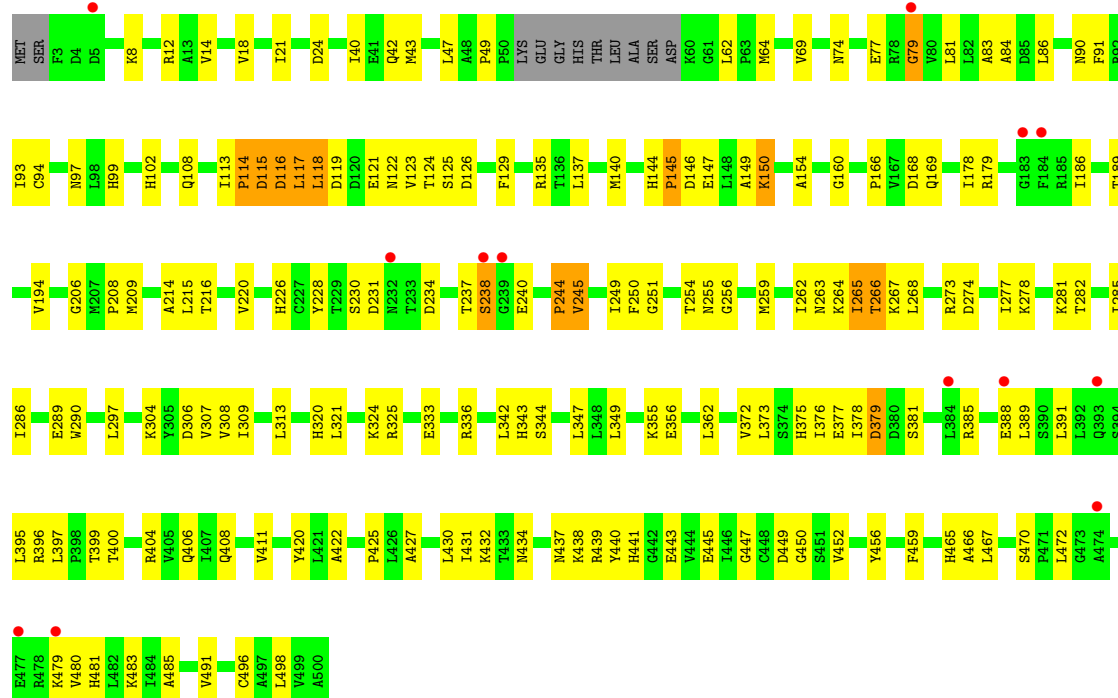


• Molecule 1: Glucokinase-1

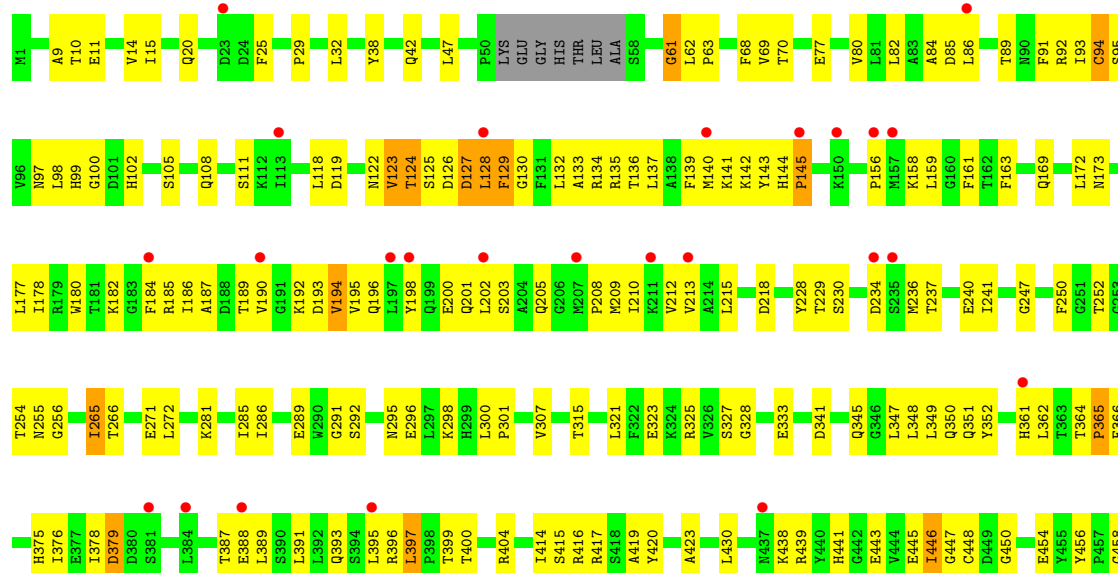




• Molecule 1: Glucokinase-1



• Molecule 1: Glucokinase-1





4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	177.75Å 177.75Å 323.95Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	155.83 – 3.59 155.83 – 3.59	Depositor EDS
% Data completeness (in resolution range)	100.0 (155.83-3.59) 92.4 (155.83-3.59)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.33 (at 3.58Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.267 , 0.300 0.271 , 0.301	Depositor DCC
R_{free} test set	3105 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	81.1	Xtriage
Anisotropy	0.229	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 74.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	22953	wwPDB-VP
Average B, all atoms (Å ²)	85.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.74% 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: PO4

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.34	3/3887 (0.1%)	1.04	45/5257 (0.9%)
1	B	0.21	1/3885 (0.0%)	0.96	32/5254 (0.6%)
1	C	0.31	3/3898 (0.1%)	1.00	44/5271 (0.8%)
1	D	0.22	0/3855	1.03	47/5217 (0.9%)
1	E	0.27	2/3877 (0.1%)	0.94	32/5243 (0.6%)
1	F	0.31	2/3905 (0.1%)	0.92	30/5280 (0.6%)
All	All	0.28	11/23307 (0.0%)	0.98	230/31522 (0.7%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	447	GLY	C-N	11.90	1.51	1.33
1	C	459	PHE	C-N	10.28	1.48	1.34
1	E	447	GLY	C-N	10.23	1.49	1.33
1	F	145	PRO	N-CD	9.86	1.61	1.47
1	A	145	PRO	N-CD	9.75	1.61	1.47
1	F	459	PHE	C-N	9.46	1.47	1.34
1	E	459	PHE	C-N	-8.04	1.22	1.33
1	C	120	ASP	CA-C	7.11	1.62	1.52
1	B	447	GLY	C-N	-6.66	1.24	1.33
1	A	459	PHE	C-N	6.32	1.43	1.33
1	C	115	ASP	CA-C	5.62	1.60	1.52

All (230) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	78	ARG	N-CA-C	33.03	152.68	112.38
1	E	117	LEU	N-CA-C	-29.84	78.70	112.72
1	A	205	GLN	N-CA-C	-26.11	74.32	110.35
1	D	207	MET	N-CA-C	22.05	156.30	108.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	124	THR	N-CA-C	22.01	137.03	111.71
1	D	379	ASP	N-CA-C	-21.01	71.50	108.69
1	A	206	GLY	N-CA-C	17.53	143.61	115.73
1	D	207	MET	CB-CA-C	-17.23	92.73	110.65
1	C	379	ASP	N-CA-C	-16.52	81.97	108.90
1	F	123	VAL	N-CA-C	16.14	128.99	111.88
1	C	120	ASP	N-CA-C	15.93	133.09	113.50
1	E	379	ASP	N-CA-C	-15.49	84.14	109.40
1	B	178	ILE	N-CA-C	15.03	124.66	110.53
1	E	116	ASP	N-CA-C	15.00	143.29	113.29
1	D	378	ILE	N-CA-C	-14.13	86.45	107.37
1	D	381	SER	N-CA-C	-13.51	89.69	109.15
1	F	128	LEU	N-CA-C	-13.45	96.92	113.20
1	C	378	ILE	N-CA-C	-13.38	86.00	107.28
1	C	443	GLU	N-CA-C	-13.33	86.98	109.24
1	C	447	GLY	O-C-N	-12.10	112.67	123.80
1	D	382	THR	N-CA-C	12.08	132.93	107.67
1	A	281	LYS	N-CA-C	11.92	128.74	108.23
1	E	378	ILE	N-CA-C	-11.72	89.44	107.73
1	C	79	GLY	N-CA-C	11.65	126.59	112.49
1	C	231	ASP	N-CA-C	11.53	128.01	112.68
1	B	395	LEU	N-CA-C	-11.47	93.95	110.59
1	F	379	ASP	N-CA-C	-11.23	88.03	108.02
1	A	472	LEU	N-CA-C	-11.04	93.94	110.28
1	D	365	PRO	N-CA-C	10.95	128.75	113.53
1	F	365	PRO	N-CA-C	10.91	129.07	113.47
1	F	129	PHE	N-CA-C	-10.81	99.28	111.82
1	A	379	ASP	N-CA-C	-10.78	91.71	109.07
1	A	491	VAL	N-CA-C	-10.77	102.55	111.81
1	B	473	GLY	N-CA-C	10.61	130.57	115.30
1	A	447	GLY	CA-C-N	10.52	139.77	122.73
1	A	447	GLY	C-N-CA	10.52	139.77	122.73
1	A	365	PRO	N-CA-C	10.46	130.73	113.78
1	B	459	PHE	O-C-N	10.28	133.01	122.12
1	B	379	ASP	N-CA-C	-10.26	99.07	111.69
1	A	381	SER	N-CA-C	-10.18	90.81	108.52
1	E	244	PRO	CB-CA-C	-10.18	102.14	111.40
1	C	210	ILE	N-CA-C	-10.00	93.58	108.17
1	C	444	VAL	N-CA-C	-9.98	93.74	108.12
1	D	491	VAL	N-CA-C	-9.90	103.06	112.96
1	B	119	ASP	N-CA-C	9.77	124.74	113.01
1	E	115	ASP	N-CA-C	-9.68	95.21	109.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	209	MET	N-CA-C	-9.62	94.53	109.25
1	E	378	ILE	CB-CA-C	9.51	123.32	111.25
1	D	206	GLY	CA-C-N	-9.43	106.86	123.08
1	D	206	GLY	C-N-CA	-9.43	106.86	123.08
1	C	279	GLU	N-CA-C	-9.26	98.29	110.43
1	C	232	ASN	N-CA-C	-9.12	101.17	114.39
1	B	78	ARG	N-CA-CB	-9.08	94.88	110.32
1	B	77	GLU	N-CA-C	9.07	123.92	109.86
1	A	244	PRO	CB-CA-C	-8.94	103.27	111.40
1	C	174	SER	N-CA-C	8.93	123.95	109.40
1	B	326	VAL	N-CA-C	8.90	120.70	111.00
1	D	438	LYS	N-CA-C	8.88	123.37	112.54
1	C	208	PRO	N-CA-C	-8.83	98.71	111.33
1	A	378	ILE	N-CA-C	-8.78	93.54	106.88
1	B	397	LEU	N-CA-C	8.75	122.36	109.42
1	B	459	PHE	CA-C-N	-8.71	107.91	120.29
1	B	459	PHE	C-N-CA	-8.71	107.91	120.29
1	E	238	SER	N-CA-C	8.71	125.66	113.56
1	F	193	ASP	N-CA-C	-8.64	93.91	108.26
1	D	379	ASP	N-CA-CB	8.54	125.16	110.81
1	F	94	CYS	N-CA-C	8.47	121.01	108.14
1	B	177	LEU	N-CA-C	8.46	122.20	109.25
1	C	120	ASP	CA-C-O	8.44	128.43	119.14
1	A	289	GLU	N-CA-C	-8.36	94.94	108.41
1	C	288	VAL	N-CA-C	-8.36	98.84	109.30
1	A	357	GLN	N-CA-C	-8.32	103.33	113.97
1	F	378	ILE	N-CA-C	-8.29	95.78	107.80
1	A	346	GLY	N-CA-C	8.24	127.59	114.90
1	C	121	GLU	N-CA-C	8.22	123.81	107.62
1	F	194	VAL	N-CA-C	-8.17	100.83	112.35
1	A	437	ASN	N-CA-C	8.12	122.46	112.23
1	E	119	ASP	N-CA-C	-8.02	103.30	113.72
1	B	387	THR	N-CA-C	-8.00	102.42	112.90
1	D	348	LEU	N-CA-C	7.98	123.10	113.12
1	D	381	SER	CB-CA-C	7.97	122.79	110.67
1	D	191	GLY	N-CA-C	7.91	131.93	113.18
1	F	127	ASP	N-CA-C	7.91	123.26	112.90
1	C	231	ASP	CB-CA-C	-7.90	97.04	110.24
1	E	116	ASP	N-CA-CB	-7.89	101.33	114.27
1	E	381	SER	N-CA-C	-7.71	98.47	109.96
1	C	447	GLY	CA-C-N	7.69	134.47	122.94
1	C	447	GLY	C-N-CA	7.69	134.47	122.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	208	PRO	CB-CA-C	7.66	123.20	111.40
1	D	235	SER	N-CA-C	-7.66	102.49	112.68
1	B	326	VAL	CB-CA-C	-7.64	102.00	112.24
1	C	289	GLU	N-CA-C	-7.64	92.57	107.62
1	C	381	SER	N-CA-C	-7.64	98.15	109.15
1	E	79	GLY	N-CA-C	7.62	131.23	113.18
1	F	265	ILE	N-CA-C	-7.60	95.87	107.73
1	D	487	ASP	N-CA-C	7.55	121.67	111.24
1	D	349	LEU	N-CA-C	-7.54	92.54	107.69
1	A	290	TRP	N-CA-C	-7.51	104.62	114.31
1	F	61	GLY	N-CA-C	7.45	121.66	112.64
1	E	282	THR	N-CA-C	7.33	122.35	113.41
1	D	7	HIS	N-CA-C	-7.31	104.49	113.41
1	D	229	THR	N-CA-C	-7.30	93.24	107.62
1	D	185	ARG	N-CA-C	-7.29	94.93	107.61
1	B	144	HIS	N-CA-C	7.27	125.89	109.81
1	A	245	VAL	N-CA-CB	-7.26	103.69	112.33
1	E	245	VAL	N-CA-CB	-7.22	103.74	112.33
1	E	114	PRO	CB-CA-C	7.19	120.59	111.39
1	A	144	HIS	N-CA-C	7.18	125.67	109.81
1	C	459	PHE	CA-C-N	-7.18	109.40	120.31
1	C	459	PHE	C-N-CA	-7.18	109.40	120.31
1	D	204	ALA	N-CA-C	-7.13	103.55	112.90
1	A	395	LEU	N-CA-C	-7.10	101.38	110.53
1	F	480	VAL	N-CA-C	-7.09	96.66	107.73
1	D	347	LEU	N-CA-C	7.09	121.98	113.12
1	F	193	ASP	CB-CA-C	7.05	120.99	110.14
1	C	64	MET	N-CA-C	-7.04	93.53	107.69
1	A	480	VAL	CB-CA-C	6.90	118.94	110.73
1	C	187	ALA	N-CA-C	6.90	118.49	110.97
1	A	27	VAL	N-CA-C	-6.86	97.62	107.77
1	B	69	VAL	N-CA-C	-6.81	96.45	107.28
1	F	145	PRO	N-CA-CB	6.81	107.19	102.35
1	D	382	THR	CB-CA-C	-6.79	102.38	112.09
1	D	203	SER	N-CA-C	-6.78	104.83	113.23
1	E	265	ILE	N-CA-C	-6.77	97.17	107.73
1	C	380	ASP	N-CA-C	-6.72	101.08	110.35
1	B	77	GLU	CA-C-N	-6.71	109.86	120.60
1	B	77	GLU	C-N-CA	-6.71	109.86	120.60
1	A	282	THR	N-CA-C	6.70	121.68	112.90
1	F	266	THR	N-CA-C	-6.69	104.93	113.23
1	D	241	ILE	N-CA-C	-6.57	97.72	107.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	378	ILE	CB-CA-C	6.57	120.55	110.96
1	D	265	ILE	N-CA-C	-6.55	98.06	107.37
1	C	288	VAL	CB-CA-C	6.55	121.09	111.33
1	D	213	VAL	N-CA-CB	-6.54	103.86	112.36
1	A	205	GLN	N-CA-CB	6.54	119.41	110.38
1	A	288	VAL	CB-CA-C	6.53	118.72	111.08
1	E	281	LYS	N-CA-C	6.50	119.15	109.59
1	F	349	LEU	N-CA-C	-6.50	94.12	107.70
1	A	381	SER	CB-CA-C	6.39	122.06	111.83
1	E	114	PRO	N-CA-C	-6.39	100.95	111.11
1	D	266	THR	N-CA-C	-6.36	104.56	112.90
1	F	145	PRO	CB-CA-C	-6.29	104.54	113.09
1	A	145	PRO	N-CA-CB	6.27	106.98	102.28
1	C	116	ASP	N-CA-C	6.25	119.30	110.23
1	B	266	THR	N-CA-C	-6.25	105.70	113.38
1	B	438	LYS	N-CA-C	6.24	117.88	111.14
1	A	447	GLY	O-C-N	-6.19	117.04	123.48
1	D	230	SER	N-CA-C	-6.17	99.75	109.50
1	F	365	PRO	CB-CA-C	-6.17	103.25	113.06
1	B	395	LEU	CB-CA-C	6.16	122.15	110.51
1	D	366	PHE	N-CA-C	-6.15	103.20	111.87
1	C	241	ILE	N-CA-C	-6.13	98.37	107.51
1	E	118	LEU	N-CA-C	6.12	120.95	112.45
1	D	189	THR	N-CA-C	-6.11	105.47	113.17
1	D	207	MET	N-CA-CB	-6.11	100.18	110.38
1	D	205	GLN	CB-CG-CD	-6.10	102.23	112.60
1	D	348	LEU	CB-CA-C	-6.07	99.55	109.56
1	F	348	LEU	N-CA-C	6.00	120.79	112.45
1	D	365	PRO	CB-CA-C	-5.95	102.80	112.62
1	D	209	MET	N-CA-C	-5.95	104.92	111.82
1	A	379	ASP	CB-CA-C	5.95	120.01	109.72
1	C	116	ASP	N-CA-CB	-5.94	100.86	109.83
1	A	481	HIS	N-CA-C	-5.90	100.53	109.85
1	C	152	LYS	N-CA-C	-5.89	106.25	113.50
1	C	211	LYS	CB-CA-C	5.87	119.87	109.72
1	D	347	LEU	N-CA-CB	-5.86	101.46	110.42
1	A	288	VAL	N-CA-C	-5.84	99.90	108.54
1	E	209	MET	N-CA-C	5.83	119.60	111.74
1	B	76	THR	N-CA-C	5.80	119.64	111.52
1	B	178	ILE	N-CA-CB	-5.75	103.20	110.57
1	E	150	LYS	N-CA-C	5.71	118.86	107.62
1	D	472	LEU	N-CA-C	-5.69	101.62	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	350	GLN	N-CA-C	-5.66	105.68	112.59
1	C	190	VAL	CB-CA-C	-5.64	104.43	112.22
1	A	347	LEU	N-CA-C	5.64	121.19	113.97
1	A	446	ILE	CA-C-N	-5.61	116.92	122.36
1	A	446	ILE	C-N-CA	-5.61	116.92	122.36
1	E	481	HIS	N-CA-C	5.57	117.04	110.97
1	C	113	ILE	N-CA-C	-5.56	102.84	108.96
1	C	211	LYS	N-CA-C	-5.56	100.12	109.07
1	E	381	SER	CB-CA-C	5.55	118.15	110.16
1	D	212	VAL	N-CA-C	5.55	116.75	108.54
1	D	212	VAL	CB-CA-C	-5.51	104.63	111.08
1	C	459	PHE	O-C-N	5.50	127.95	122.12
1	C	379	ASP	CB-CA-C	5.48	119.74	109.71
1	A	378	ILE	CB-CA-C	5.45	119.27	111.81
1	B	384	LEU	CB-CA-C	5.44	119.66	110.79
1	B	498	LEU	N-CA-C	5.44	116.89	111.07
1	E	117	LEU	N-CA-CB	5.42	118.78	110.70
1	E	118	LEU	CB-CA-C	-5.42	99.86	110.11
1	C	4	ASP	N-CA-C	5.39	117.24	111.36
1	D	488	GLY	N-CA-C	5.39	119.19	112.73
1	A	27	VAL	CB-CA-C	5.38	117.68	110.42
1	B	384	LEU	N-CA-C	-5.38	98.48	107.99
1	F	265	ILE	CB-CA-C	5.38	118.08	111.25
1	B	70	THR	N-CA-C	-5.36	106.58	113.23
1	E	244	PRO	N-CA-C	5.36	118.99	110.21
1	E	266	THR	N-CA-C	-5.35	106.60	113.23
1	B	184	PHE	CB-CA-C	-5.34	103.87	112.09
1	A	366	PHE	N-CA-C	-5.34	105.41	112.94
1	A	489	SER	N-CA-C	-5.33	105.52	112.23
1	E	263	ASN	N-CA-C	-5.33	106.63	113.02
1	D	185	ARG	CB-CA-C	5.32	118.18	110.79
1	E	145	PRO	N-CA-C	5.31	120.98	114.35
1	F	482	LEU	N-CA-CB	-5.31	102.00	111.08
1	A	145	PRO	N-CA-C	-5.28	104.66	112.26
1	D	366	PHE	N-CA-CB	5.26	119.60	111.39
1	C	5	ASP	N-CA-C	-5.25	106.02	112.90
1	A	347	LEU	N-CA-CB	-5.22	103.41	110.67
1	A	395	LEU	CB-CA-C	5.21	121.19	110.40
1	F	366	PHE	N-CA-C	-5.21	104.52	111.87
1	A	166	PRO	N-CA-C	-5.21	102.94	110.80
1	F	247	GLY	N-CA-C	-5.21	102.74	110.71
1	B	265	ILE	N-CA-C	-5.20	99.67	107.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	279	GLU	CB-CA-C	5.18	120.37	109.65
1	A	28	THR	N-CA-C	-5.18	103.42	110.36
1	A	472	LEU	CB-CA-C	5.17	118.49	109.65
1	E	117	LEU	CB-CA-C	5.14	119.42	110.94
1	E	149	ALA	N-CA-C	-5.14	106.96	113.18
1	C	190	VAL	N-CA-C	5.14	115.91	110.72
1	E	491	VAL	N-CA-C	-5.13	104.56	111.44
1	F	123	VAL	N-CA-CB	-5.12	105.29	111.94
1	F	397	LEU	N-CA-CB	-5.10	103.69	110.17
1	D	186	ILE	N-CA-CB	5.10	119.54	111.99
1	D	203	SER	N-CA-CB	5.09	118.38	110.44
1	A	447	GLY	CA-C-O	-5.07	116.31	120.92
1	B	152	LYS	N-CA-C	-5.07	106.51	113.30
1	D	172	LEU	CB-CA-C	-5.04	101.01	109.53
1	F	124	THR	N-CA-CB	-5.04	102.47	110.22
1	C	313	LEU	N-CA-CB	-5.03	103.26	110.65

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	3817	0	3838	161	0
1	B	3815	0	3836	153	0
1	C	3828	0	3852	158	0
1	D	3786	0	3798	163	0
1	E	3807	0	3832	138	0
1	F	3835	0	3858	202	0
2	A	15	0	0	15	0
2	B	10	0	0	2	0
2	C	10	0	0	1	0
2	D	10	0	0	0	0
2	E	10	0	0	1	0
2	F	10	0	0	1	0
All	All	22953	0	23014	906	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 20.

All (906) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:207:MET:SD	1:A:210:ILE:HD12	1.51	1.50
1:F:129:PHE:O	1:F:201:GLN:HG2	1.22	1.36
1:A:207:MET:SD	1:A:210:ILE:CD1	2.17	1.32
1:A:396:ARG:CD	2:A:602:PO4:O4	1.81	1.27
1:A:478:ARG:HD2	1:C:477:GLU:OE2	1.37	1.23
1:F:446:ILE:HD13	1:F:479:LYS:CE	1.72	1.20
1:A:396:ARG:HD2	2:A:602:PO4:O4	0.92	1.09
1:A:360:ARG:HG3	2:A:602:PO4:O2	1.51	1.08
1:A:378:ILE:CD1	1:A:457:PRO:HB2	1.84	1.08
1:B:77:GLU:OE1	1:B:228:TYR:HE1	1.35	1.07
1:D:133:ALA:HB1	1:D:202:LEU:HD23	1.38	1.05
1:E:124:THR:HG22	1:E:126:ASP:H	1.16	1.04
1:F:446:ILE:CD1	1:F:479:LYS:CE	2.36	1.04
1:D:333:GLU:OE2	1:D:365:PRO:O	1.76	1.03
1:D:172:LEU:O	1:D:173:ASN:CG	2.02	1.02
1:B:378:ILE:HG22	1:E:440:TYR:HB3	1.39	1.01
1:F:446:ILE:HD13	1:F:479:LYS:HE3	1.02	1.01
1:F:446:ILE:CD1	1:F:479:LYS:HE3	1.91	1.00
1:A:333:GLU:OE2	1:A:365:PRO:O	1.79	0.99
1:A:262:ILE:HD12	1:A:281:LYS:O	1.63	0.99
1:F:123:VAL:HG12	1:F:123:VAL:O	1.61	0.98
1:E:124:THR:HG22	1:E:126:ASP:N	1.80	0.95
1:F:129:PHE:O	1:F:201:GLN:CG	2.13	0.95
1:A:449:ASP:OD2	1:A:486:LYS:O	1.83	0.95
1:A:378:ILE:HD13	1:A:457:PRO:CB	1.96	0.95
1:F:161:PHE:HE2	1:F:194:VAL:HG13	1.28	0.95
1:F:126:ASP:C	1:F:129:PHE:HB3	1.92	0.94
1:E:116:ASP:C	1:E:118:LEU:H	1.51	0.94
1:D:133:ALA:CB	1:D:202:LEU:HD23	1.97	0.93
1:B:83:ALA:HB3	1:B:94:CYS:SG	2.07	0.93
1:F:454:GLU:OE1	1:F:484:ILE:HG12	1.68	0.92
1:A:359:PRO:HB3	1:A:396:ARG:HB3	1.50	0.92
1:A:378:ILE:HD12	1:A:457:PRO:HB2	1.50	0.91
1:C:242:SER:HA	1:C:443:GLU:O	1.69	0.91
1:F:333:GLU:OE1	1:F:365:PRO:O	1.89	0.90
1:C:119:ASP:OD1	1:C:120:ASP:N	2.04	0.90
1:D:412:ARG:HH12	1:F:439:ARG:HH21	1.18	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:ALA:C	1:A:205:GLN:O	1.96	0.90
1:E:116:ASP:C	1:E:118:LEU:N	2.21	0.90
1:A:70:THR:OG1	1:A:281:LYS:CE	2.20	0.90
1:D:479:LYS:HG3	1:F:479:LYS:O	1.72	0.89
1:A:360:ARG:CG	2:A:602:PO4:O2	2.21	0.89
1:A:464:ARG:NH1	1:C:443:GLU:OE2	2.05	0.89
1:B:77:GLU:OE1	1:B:228:TYR:CE1	2.24	0.88
1:A:70:THR:CB	1:A:281:LYS:HD2	2.04	0.88
1:A:207:MET:SD	1:A:210:ILE:HD11	2.11	0.88
1:F:128:LEU:HB2	1:F:132:LEU:HD13	1.53	0.88
1:A:377:GLU:OE1	1:A:456:TYR:OH	1.92	0.87
1:F:178:ILE:HG22	1:F:180:TRP:CD1	2.10	0.87
1:F:123:VAL:O	1:F:123:VAL:CG1	2.23	0.86
1:A:478:ARG:CD	1:C:477:GLU:OE2	2.24	0.86
1:A:70:THR:HB	1:A:281:LYS:HD2	1.57	0.85
1:A:464:ARG:NH1	1:C:443:GLU:CD	2.35	0.85
1:A:378:ILE:CD1	1:A:457:PRO:CB	2.53	0.85
1:E:83:ALA:HB3	1:E:94:CYS:SG	2.16	0.84
1:B:60:LYS:HG3	1:B:61:GLY:H	1.41	0.84
1:B:74:ASN:O	1:B:77:GLU:OE2	1.95	0.84
1:F:454:GLU:HB2	1:F:484:ILE:HG21	1.56	0.84
1:B:378:ILE:CG2	1:E:440:TYR:HB3	2.06	0.84
1:D:219:THR:HG21	1:D:255:ASN:HD22	1.43	0.84
1:B:125:SER:O	1:B:129:PHE:HD1	1.61	0.83
1:B:119:ASP:OD1	1:B:119:ASP:O	1.97	0.83
1:A:378:ILE:HD13	1:A:457:PRO:HB3	1.59	0.82
1:F:161:PHE:CE2	1:F:194:VAL:HG13	2.14	0.81
1:A:146:ASP:O	1:A:150:LYS:NZ	2.14	0.80
1:B:372:VAL:HA	1:B:391:LEU:HD21	1.62	0.80
1:F:129:PHE:CE1	1:F:201:GLN:HB2	2.16	0.80
1:A:460:ARG:HH12	1:C:232:ASN:HD22	1.29	0.79
1:A:360:ARG:HB2	2:A:602:PO4:O3	1.83	0.79
1:E:376:ILE:HG12	1:E:388:GLU:HG2	1.62	0.79
1:F:126:ASP:O	1:F:129:PHE:HB3	1.81	0.79
1:B:265:ILE:O	1:B:273:ARG:HD3	1.83	0.79
1:C:184:PHE:CE2	1:C:186:ILE:HD11	2.18	0.79
1:B:458:GLY:HA3	1:E:441:HIS:ND1	1.99	0.77
1:A:360:ARG:HD2	2:A:602:PO4:P	2.24	0.77
1:C:175:GLY:O	1:C:193:ASP:HA	1.83	0.77
1:D:239:GLY:HA3	1:F:454:GLU:O	1.84	0.77
1:D:172:LEU:O	1:D:173:ASN:OD1	2.03	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:144:HIS:CG	1:B:144:HIS:O	2.37	0.77
1:B:144:HIS:CD2	1:B:146:ASP:OD1	2.37	0.77
1:A:360:ARG:CD	2:A:602:PO4:O2	2.33	0.76
1:E:399:THR:O	1:E:404:ARG:NH1	2.18	0.76
1:A:464:ARG:NH1	1:C:443:GLU:OE1	2.19	0.76
1:A:70:THR:OG1	1:A:281:LYS:HE3	1.86	0.75
1:E:121:GLU:O	1:E:122:ASN:OD1	2.04	0.75
1:D:479:LYS:HB3	1:F:480:VAL:HA	1.69	0.75
1:E:117:LEU:O	1:E:117:LEU:HD12	1.87	0.75
1:B:24:ASP:HA	1:C:20:GLN:NE2	2.01	0.74
1:C:113:ILE:CG2	1:C:114:PRO:HD2	2.17	0.74
1:A:478:ARG:HH21	1:C:465:HIS:HD2	1.34	0.74
1:A:460:ARG:HH12	1:C:232:ASN:ND2	1.83	0.74
1:C:207:MET:HE3	1:C:209:MET:HA	1.70	0.74
1:C:287:ASN:ND2	1:C:289:GLU:OE2	2.20	0.74
1:E:40:ILE:HD11	1:E:431:ILE:HG23	1.70	0.74
1:F:133:ALA:HB2	1:F:201:GLN:HG3	1.69	0.74
1:C:207:MET:HG2	1:C:208:PRO:O	1.87	0.74
1:A:70:THR:OG1	1:A:281:LYS:HD2	1.88	0.73
1:E:124:THR:HG21	1:E:126:ASP:HB2	1.71	0.73
1:B:118:LEU:HD22	1:B:123:VAL:HG11	1.69	0.73
1:D:254:THR:HG22	1:D:323:GLU:HG3	1.70	0.73
1:A:252:THR:HB	2:A:603:PO4:O2	1.89	0.73
1:A:150:LYS:HB2	1:A:154:ALA:HB2	1.72	0.72
1:B:83:ALA:HB3	1:B:94:CYS:HG	1.54	0.72
1:F:161:PHE:HE2	1:F:194:VAL:CG1	1.99	0.72
1:C:85:ASP:HA	1:C:162:THR:HB	1.70	0.72
1:C:229:THR:HG22	1:C:229:THR:O	1.88	0.72
1:B:144:HIS:O	1:B:144:HIS:CD2	2.43	0.71
1:C:203:SER:HA	1:C:207:MET:HB2	1.72	0.71
1:A:14:VAL:HG22	1:A:347:LEU:HB3	1.73	0.71
1:E:268:LEU:O	1:E:273:ARG:NH2	2.24	0.71
1:C:292:SER:HB3	1:C:295:ASN:HD21	1.56	0.71
1:D:120:ASP:HB3	1:D:123:VAL:HG23	1.72	0.71
1:A:464:ARG:HH12	1:C:443:GLU:CD	1.95	0.71
1:B:375:HIS:HB2	1:B:391:LEU:HD22	1.72	0.71
1:C:372:VAL:HA	1:C:391:LEU:HD23	1.73	0.71
1:C:451:SER:N	2:C:602:PO4:O2	2.23	0.71
1:F:178:ILE:HG21	1:F:180:TRP:HE1	1.55	0.71
1:C:36:THR:HG21	1:C:471:PRO:HG3	1.73	0.70
1:F:230:SER:OG	1:F:234:ASP:OD2	2.08	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:GLU:O	1:A:356:GLU:HG3	1.91	0.70
1:B:177:LEU:O	1:B:190:VAL:O	2.09	0.70
1:B:385:ARG:HB3	1:B:404:ARG:HE	1.57	0.70
1:E:169:GLN:NE2	1:E:215:LEU:O	2.24	0.70
1:E:121:GLU:O	1:E:122:ASN:CG	2.35	0.70
1:E:160:GLY:HA2	1:E:214:ALA:HB3	1.74	0.69
1:C:169:GLN:NE2	1:C:215:LEU:O	2.25	0.69
1:D:412:ARG:NH1	1:F:439:ARG:HH21	1.90	0.69
1:E:443:GLU:HG2	1:E:480:VAL:HG11	1.74	0.69
1:B:378:ILE:HG22	1:E:440:TYR:CB	2.22	0.69
1:D:201:GLN:O	1:D:205:GLN:HG2	1.92	0.69
1:A:92:ARG:HG2	1:A:110:LYS:HG3	1.73	0.69
1:C:254:THR:HG22	1:C:323:GLU:HG3	1.73	0.69
1:F:111:SER:HB2	1:F:139:PHE:HE2	1.57	0.69
1:F:178:ILE:CG2	1:F:180:TRP:HE1	2.06	0.69
1:A:122:ASN:OD1	1:A:185:ARG:NH1	2.26	0.69
1:B:415:SER:HB3	1:B:462:MET:HE1	1.74	0.69
1:D:198:TYR:CE1	1:D:202:LEU:HD11	2.27	0.69
1:C:245:VAL:HG12	1:C:246:ILE:HG13	1.72	0.69
1:E:124:THR:CG2	1:E:126:ASP:HB2	2.23	0.69
1:C:47:LEU:HA	1:C:267:LYS:HE3	1.76	0.68
1:E:90:ASN:HA	1:E:113:ILE:HG23	1.76	0.68
1:C:336:ARG:HB3	1:C:368:LEU:HD12	1.74	0.68
1:C:85:ASP:OD1	1:C:162:THR:CG2	2.42	0.68
1:E:434:ASN:OD1	1:E:437:ASN:ND2	2.26	0.68
1:A:70:THR:OG1	1:A:281:LYS:CD	2.41	0.67
1:A:372:VAL:HA	1:A:391:LEU:HD11	1.74	0.67
1:F:94:CYS:HB3	1:F:108:GLN:CB	2.24	0.67
1:E:237:THR:O	1:E:238:SER:OG	2.11	0.67
1:E:47:LEU:HD13	1:E:264:LYS:O	1.94	0.67
1:B:76:THR:HG22	1:B:101:ASP:HA	1.77	0.67
1:A:241:ILE:HD13	1:C:378:ILE:HD13	1.76	0.67
1:C:376:ILE:HG22	1:C:376:ILE:O	1.93	0.67
1:D:464:ARG:NH1	1:F:240:GLU:OE2	2.27	0.67
1:E:79:GLY:O	1:E:97:ASN:HA	1.95	0.67
1:F:126:ASP:CA	1:F:129:PHE:HB3	2.24	0.67
1:D:173:ASN:O	1:D:195:VAL:HG21	1.95	0.66
1:D:133:ALA:CB	1:D:202:LEU:CD2	2.72	0.66
1:F:159:LEU:HD21	1:F:212:VAL:HG22	1.75	0.66
1:F:446:ILE:HD11	1:F:481:HIS:CD2	2.30	0.66
1:C:14:VAL:HG22	1:C:347:LEU:HB3	1.78	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:94:CYS:HB3	1:C:108:GLN:HG2	1.78	0.66
1:D:389:LEU:HB2	1:D:404:ARG:HD3	1.78	0.66
1:E:265:ILE:O	1:E:273:ARG:HD3	1.94	0.66
1:F:446:ILE:CD1	1:F:479:LYS:HE2	2.25	0.66
1:A:206:GLY:O	1:A:208:PRO:HD3	1.94	0.66
1:C:415:SER:HG	1:C:456:TYR:HH	1.42	0.66
1:F:446:ILE:HD11	1:F:481:HIS:HD2	1.60	0.66
1:F:126:ASP:HA	1:F:129:PHE:HB3	1.78	0.66
1:F:94:CYS:HB3	1:F:108:GLN:HB2	1.77	0.66
1:E:249:ILE:O	1:E:254:THR:HA	1.96	0.66
1:B:254:THR:HG22	1:B:323:GLU:HG3	1.78	0.66
1:D:6:LEU:HD13	1:D:6:LEU:O	1.96	0.66
1:E:18:VAL:HG21	1:E:406:GLN:HB3	1.76	0.66
1:A:63:PRO:HB2	1:A:289:GLU:HB2	1.78	0.66
1:B:416:ARG:NH1	2:B:601:PO4:O2	2.27	0.66
1:F:14:VAL:HG22	1:F:347:LEU:HB3	1.78	0.66
1:C:97:ASN:HB3	1:C:105:SER:HB3	1.76	0.65
1:F:178:ILE:CG2	1:F:180:TRP:NE1	2.59	0.65
1:C:251:GLY:O	1:C:327:SER:O	2.14	0.65
1:C:265:ILE:O	1:C:273:ARG:HD3	1.95	0.65
1:B:74:ASN:C	1:B:77:GLU:OE2	2.40	0.65
1:F:93:ILE:HD12	1:F:93:ILE:O	1.97	0.65
1:F:125:SER:O	1:F:129:PHE:HB2	1.97	0.65
1:C:85:ASP:OD1	1:C:162:THR:HG21	1.96	0.65
1:D:479:LYS:HD2	1:F:480:VAL:HG22	1.78	0.65
1:E:251:GLY:HA2	1:E:452:VAL:H	1.62	0.65
1:F:94:CYS:HB3	1:F:108:GLN:HA	1.79	0.65
1:B:73:PRO:HG3	1:B:224:LEU:HD23	1.80	0.64
1:D:268:LEU:O	1:D:273:ARG:NH2	2.30	0.64
1:F:93:ILE:O	1:F:93:ILE:CG1	2.44	0.64
1:B:159:LEU:HD23	1:B:212:VAL:HG22	1.79	0.64
1:C:255:ASN:HD21	1:C:289:GLU:CD	2.06	0.64
1:F:379:ASP:OD1	1:F:387:THR:OG1	2.16	0.64
1:A:219:THR:HG21	1:A:255:ASN:HB3	1.78	0.64
1:B:123:VAL:HB	1:B:186:ILE:HG21	1.80	0.64
1:C:184:PHE:CD2	1:C:186:ILE:HD11	2.32	0.64
1:E:144:HIS:CG	1:E:144:HIS:O	2.49	0.64
1:B:144:HIS:HE1	1:B:157:MET:HE1	1.63	0.64
1:F:97:ASN:H	1:F:105:SER:HB3	1.62	0.64
1:F:447:GLY:HA2	1:F:482:LEU:HD23	1.80	0.64
1:C:120:ASP:O	1:C:185:ARG:HB3	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:218:ASP:OD1	1:C:489:SER:HB3	1.97	0.64
1:D:85:ASP:HB3	1:D:162:THR:HB	1.80	0.64
1:D:434:ASN:ND2	1:D:437:ASN:HD21	1.96	0.64
1:A:82:LEU:HB2	1:A:159:LEU:HB3	1.81	0.63
1:D:212:VAL:O	1:D:212:VAL:HG13	1.97	0.63
1:D:240:GLU:OE1	1:F:464:ARG:NH2	2.30	0.63
1:B:92:ARG:NH2	1:B:487:ASP:OD1	2.31	0.63
1:A:360:ARG:CD	2:A:602:PO4:P	2.86	0.63
1:B:377:GLU:HG3	1:B:378:ILE:HG23	1.79	0.63
1:B:464:ARG:NH2	1:E:240:GLU:OE2	2.30	0.63
1:D:89:THR:O	1:D:113:ILE:HG22	1.98	0.63
1:F:446:ILE:HD12	1:F:479:LYS:HZ1	1.63	0.63
1:F:94:CYS:CB	1:F:108:GLN:HA	2.29	0.63
1:B:445:GLU:HB3	1:B:481:HIS:HB2	1.81	0.62
1:E:49:PRO:HD3	1:E:266:THR:HB	1.81	0.62
1:A:333:GLU:OE1	1:A:336:ARG:NH2	2.32	0.62
1:B:144:HIS:CE1	1:B:157:MET:HE1	2.35	0.62
1:A:470:SER:O	1:A:472:LEU:O	2.18	0.62
1:F:102:HIS:HB3	1:F:229:THR:HA	1.82	0.62
1:A:360:ARG:NE	2:A:602:PO4:O2	2.33	0.61
1:C:141:LYS:HB2	1:C:148:LEU:HD23	1.81	0.61
1:B:118:LEU:HA	1:B:123:VAL:HG21	1.82	0.61
1:A:18:VAL:HG21	1:A:406:GLN:HB3	1.83	0.61
1:C:184:PHE:HE2	1:C:186:ILE:HD11	1.63	0.61
1:F:163:PHE:HE2	1:F:178:ILE:HG12	1.66	0.61
1:C:62:LEU:HD21	1:C:293:PHE:HD1	1.66	0.61
1:E:144:HIS:O	1:E:144:HIS:ND1	2.33	0.61
1:D:434:ASN:HD21	1:D:437:ASN:HD21	1.49	0.61
1:A:166:PRO:HG3	1:A:181:THR:HG22	1.82	0.61
1:B:62:LEU:HD12	1:B:63:PRO:HD2	1.81	0.61
1:F:177:LEU:HA	1:F:190:VAL:HG13	1.81	0.61
1:F:178:ILE:CG2	1:F:180:TRP:CD1	2.84	0.60
1:A:262:ILE:CD1	1:A:281:LYS:O	2.42	0.60
1:B:393:GLN:C	1:B:395:LEU:O	2.44	0.60
1:E:333:GLU:OE2	1:E:336:ARG:NH2	2.34	0.60
1:D:260:GLU:HB3	1:D:286:ILE:HD12	1.83	0.60
1:C:113:ILE:HG23	1:C:114:PRO:HD2	1.82	0.60
1:D:478:ARG:HH11	1:F:477:GLU:HG3	1.66	0.60
1:A:378:ILE:HD11	1:C:441:HIS:HD2	1.67	0.60
1:C:113:ILE:HG22	1:C:114:PRO:HD2	1.84	0.60
1:F:178:ILE:HG21	1:F:180:TRP:NE1	2.17	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:378:ILE:O	1:D:378:ILE:CG1	2.50	0.60
1:F:93:ILE:O	1:F:93:ILE:HG13	2.01	0.60
1:F:445:GLU:HA	1:F:480:VAL:O	2.01	0.60
1:F:128:LEU:C	1:F:128:LEU:HD12	2.26	0.60
1:B:449:ASP:OD1	1:B:450:GLY:N	2.35	0.60
1:D:333:GLU:OE1	1:D:336:ARG:NH2	2.35	0.59
1:F:430:LEU:HD11	1:F:479:LYS:HD2	1.84	0.59
1:B:316:ASN:OD1	1:B:324:LYS:NZ	2.24	0.59
1:D:449:ASP:OD1	1:D:450:GLY:N	2.35	0.59
1:A:249:ILE:O	1:A:254:THR:HA	2.03	0.59
1:D:49:PRO:HA	1:D:267:LYS:HD3	1.84	0.59
1:B:102:HIS:ND1	1:B:230:SER:O	2.36	0.59
1:D:479:LYS:NZ	1:F:443:GLU:OE1	2.28	0.59
1:F:82:LEU:HA	1:F:95:SER:HA	1.85	0.59
1:F:82:LEU:HG	1:F:95:SER:HB2	1.85	0.59
1:F:126:ASP:HA	1:F:129:PHE:CB	2.33	0.59
1:C:449:ASP:OD1	1:C:450:GLY:N	2.35	0.59
1:E:255:ASN:HD21	1:E:289:GLU:HA	1.67	0.59
1:B:455:TYR:HA	1:E:238:SER:O	2.03	0.59
1:D:479:LYS:H	1:D:481:HIS:CE1	2.21	0.59
1:E:449:ASP:OD1	1:E:450:GLY:N	2.35	0.59
1:B:64:MET:HE2	1:B:286:ILE:HG21	1.85	0.58
1:F:296:GLU:HG3	1:F:298:LYS:HE3	1.85	0.58
1:A:449:ASP:OD1	1:A:450:GLY:N	2.35	0.58
1:A:478:ARG:HH21	1:C:465:HIS:CD2	2.19	0.58
1:C:25:PHE:HD1	1:C:417:ARG:HD3	1.68	0.58
1:D:4:ASP:O	1:D:8:LYS:HB2	2.03	0.58
1:B:146:ASP:OD1	1:B:147:GLU:N	2.37	0.58
1:B:252:THR:HA	1:B:328:GLY:HA2	1.86	0.58
1:F:94:CYS:SG	1:F:95:SER:N	2.76	0.58
1:A:441:HIS:CG	1:C:458:GLY:HA3	2.38	0.58
1:C:96:VAL:HG11	1:C:491:VAL:HG13	1.86	0.58
1:D:465:HIS:NE2	1:F:475:GLU:OE2	2.36	0.58
1:F:361:HIS:HB2	1:F:395:LEU:HD11	1.86	0.58
1:D:79:GLY:O	1:D:97:ASN:HA	2.03	0.58
1:E:250:PHE:O	1:E:450:GLY:HA3	2.03	0.58
1:F:124:THR:OG1	1:F:187:ALA:HB3	2.04	0.58
1:A:420:TYR:CD1	1:A:466:ALA:HB2	2.38	0.58
1:C:250:PHE:O	1:C:450:GLY:HA3	2.04	0.57
1:F:68:PHE:HE2	1:F:169:GLN:HB3	1.68	0.57
1:F:448:CYS:O	1:F:484:ILE:HA	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:145:PRO:HB2	1:B:148:LEU:HD23	1.86	0.57
1:F:178:ILE:HG22	1:F:180:TRP:HD1	1.66	0.57
1:F:84:ALA:HA	1:F:93:ILE:HG22	1.87	0.57
1:F:393:GLN:C	1:F:395:LEU:O	2.48	0.57
1:F:395:LEU:HD12	1:F:396:ARG:H	1.68	0.57
1:A:376:ILE:HG12	1:A:388:GLU:HG2	1.85	0.57
1:C:443:GLU:OE1	1:C:481:HIS:HE1	1.87	0.57
1:D:464:ARG:HG3	1:D:482:LEU:HD12	1.85	0.57
1:E:83:ALA:O	1:E:93:ILE:HD12	2.03	0.57
1:F:195:VAL:HG23	1:F:215:LEU:HD12	1.85	0.57
1:D:378:ILE:O	1:D:378:ILE:HG13	2.04	0.57
1:B:24:ASP:OD2	1:B:304:LYS:NZ	2.35	0.57
1:D:479:LYS:HE3	1:F:478:ARG:HA	1.86	0.57
1:D:202:LEU:O	1:D:207:MET:N	2.36	0.57
1:D:242:SER:HA	1:D:443:GLU:HA	1.87	0.56
1:C:470:SER:HB3	1:C:471:PRO:HD2	1.87	0.56
1:E:84:ALA:HB2	1:E:93:ILE:CD1	2.35	0.56
1:F:196:GLN:O	1:F:200:GLU:HG2	2.05	0.56
1:A:145:PRO:HA	1:A:148:LEU:HB3	1.88	0.56
1:D:378:ILE:O	1:D:378:ILE:HD12	2.06	0.56
1:F:361:HIS:HB2	1:F:395:LEU:CD1	2.36	0.56
1:C:185:ARG:HH12	1:C:187:ALA:HA	1.71	0.56
1:D:63:PRO:HG2	1:D:289:GLU:HB2	1.88	0.56
1:E:14:VAL:HG22	1:E:347:LEU:HB3	1.88	0.56
1:B:255:ASN:OD1	1:B:256:GLY:N	2.38	0.56
1:D:69:VAL:HB	1:D:285:ILE:HD12	1.86	0.56
1:E:115:ASP:O	1:E:116:ASP:HB2	2.04	0.56
1:E:150:LYS:HE2	1:E:154:ALA:HA	1.86	0.56
1:E:356:GLU:CD	1:E:356:GLU:O	2.48	0.56
1:F:136:THR:O	1:F:140:MET:HB2	2.05	0.56
1:F:161:PHE:CE2	1:F:194:VAL:CG1	2.84	0.56
1:A:359:PRO:HG2	1:A:397:LEU:HB3	1.87	0.56
1:B:336:ARG:HG3	1:B:362:LEU:HD12	1.88	0.56
1:F:93:ILE:O	1:F:93:ILE:CD1	2.53	0.56
1:C:102:HIS:NE2	1:C:235:SER:OG	2.34	0.56
1:D:192:LYS:HE2	1:D:197:LEU:HD11	1.88	0.56
1:D:244:PRO:HA	1:D:445:GLU:O	2.06	0.56
1:D:81:LEU:HD11	1:D:498:LEU:HB2	1.87	0.56
1:E:465:HIS:ND1	2:E:601:PO4:O2	2.39	0.56
1:B:316:ASN:HB2	1:B:319:PHE:HB2	1.87	0.56
1:C:124:THR:HB	1:C:127:ASP:HB3	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:PRO:HA	1:B:131:PHE:HE2	1.71	0.55
1:C:103:THR:O	1:C:228:TYR:OH	2.24	0.55
1:E:123:VAL:HB	1:E:186:ILE:HG22	1.88	0.55
1:E:168:ASP:HB2	1:E:178:ILE:HD11	1.88	0.55
1:F:178:ILE:HG22	1:F:180:TRP:NE1	2.20	0.55
1:F:415:SER:OG	1:F:456:TYR:OH	2.19	0.55
1:A:292:SER:HB2	1:A:295:ASN:HD21	1.71	0.55
1:F:124:THR:HG21	1:F:186:ILE:C	2.31	0.55
1:B:180:TRP:CD1	1:B:184:PHE:O	2.59	0.55
1:E:226:HIS:HB2	1:E:485:ALA:HB2	1.86	0.55
1:F:94:CYS:HB3	1:F:108:GLN:CA	2.37	0.55
1:F:144:HIS:CD2	1:F:145:PRO:CD	2.90	0.55
1:D:333:GLU:CD	1:D:365:PRO:O	2.49	0.55
1:E:121:GLU:HG3	1:E:122:ASN:N	2.21	0.55
1:C:85:ASP:OD1	1:C:489:SER:HB2	2.07	0.55
1:E:69:VAL:HG21	1:E:220:VAL:HG11	1.88	0.55
1:B:64:MET:HE3	1:B:288:VAL:HG22	1.88	0.55
1:D:271:GLU:O	1:D:275:LYS:HD3	2.07	0.54
1:F:202:LEU:HD11	1:F:210:ILE:HD11	1.89	0.54
1:D:479:LYS:H	1:D:481:HIS:HE1	1.55	0.54
1:F:68:PHE:HB2	1:F:172:LEU:HG	1.88	0.54
1:F:236:MET:HG3	1:F:237:THR:H	1.72	0.54
1:C:375:HIS:CG	1:C:391:LEU:HD22	2.42	0.54
1:D:458:GLY:HA3	1:F:441:HIS:CG	2.42	0.54
1:E:304:LYS:O	1:E:308:VAL:HG23	2.06	0.54
1:E:438:LYS:HG3	1:E:439:ARG:N	2.22	0.54
1:D:92:ARG:HB3	1:D:110:LYS:HG2	1.89	0.54
1:A:356:GLU:O	1:A:356:GLU:CG	2.55	0.54
1:E:166:PRO:CG	1:E:179:ARG:HB2	2.38	0.54
1:F:323:GLU:O	1:F:327:SER:N	2.41	0.54
1:A:304:LYS:H	1:A:304:LYS:HD2	1.73	0.54
1:D:251:GLY:HA2	1:D:452:VAL:HG23	1.89	0.54
1:C:207:MET:HE3	1:C:209:MET:CA	2.38	0.54
1:E:420:TYR:CD1	1:E:466:ALA:HB2	2.42	0.54
1:A:274:ASP:O	1:A:278:LYS:HG3	2.07	0.54
1:F:446:ILE:HD12	1:F:479:LYS:NZ	2.23	0.54
1:A:461:SER:OG	2:A:601:PO4:O3	2.26	0.54
1:D:201:GLN:O	1:D:205:GLN:CG	2.55	0.54
1:D:230:SER:OG	1:D:233:THR:O	2.26	0.54
1:F:129:PHE:CD1	1:F:201:GLN:HB2	2.43	0.54
1:B:449:ASP:OD2	1:B:486:LYS:HA	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:467:LEU:HD13	1:F:479:LYS:HD3	1.89	0.53
1:A:360:ARG:HD2	2:A:602:PO4:O3	2.07	0.53
1:C:196:GLN:NE2	1:C:200:GLU:OE2	2.41	0.53
1:D:133:ALA:HA	1:D:202:LEU:HD21	1.90	0.53
1:A:307:VAL:HG21	1:D:347:LEU:HD21	1.91	0.53
1:D:198:TYR:O	1:D:202:LEU:HG	2.09	0.53
1:B:239:GLY:HA2	1:E:456:TYR:O	2.08	0.53
1:F:250:PHE:O	1:F:450:GLY:HA3	2.09	0.53
1:B:251:GLY:HA2	1:B:452:VAL:HG23	1.89	0.53
1:F:416:ARG:NH1	2:F:601:PO4:O3	2.42	0.53
1:F:447:GLY:HA2	1:F:482:LEU:CD2	2.39	0.53
1:B:218:ASP:OD1	1:B:218:ASP:N	2.41	0.53
1:D:96:VAL:HG22	1:D:106:MET:HG3	1.91	0.53
1:F:127:ASP:C	1:F:129:PHE:N	2.66	0.53
1:B:333:GLU:OE1	1:B:336:ARG:NH2	2.42	0.53
1:C:102:HIS:HE2	1:C:235:SER:HG	1.54	0.52
1:F:63:PRO:HG2	1:F:289:GLU:HB2	1.90	0.52
1:F:69:VAL:HB	1:F:285:ILE:HD12	1.92	0.52
1:A:385:ARG:HB2	1:A:404:ARG:HE	1.74	0.52
1:C:159:LEU:HD12	1:C:212:VAL:HG22	1.91	0.52
1:D:47:LEU:HD21	1:D:286:ILE:HD13	1.92	0.52
1:A:372:VAL:HA	1:A:391:LEU:CD1	2.38	0.52
1:C:259:MET:HG2	1:C:285:ILE:HG12	1.91	0.52
1:F:173:ASN:HB3	1:F:213:VAL:HA	1.91	0.52
1:B:69:VAL:O	1:B:285:ILE:HG13	2.08	0.52
1:C:221:GLY:HA3	1:C:488:GLY:O	2.10	0.52
1:F:420:TYR:CD1	1:F:466:ALA:HB2	2.45	0.52
1:E:362:LEU:HD22	1:E:397:LEU:HD13	1.91	0.52
1:A:439:ARG:HH22	1:C:412:ARG:HH22	1.58	0.52
1:A:464:ARG:NH2	1:C:240:GLU:OE2	2.42	0.52
1:C:229:THR:O	1:C:229:THR:CG2	2.57	0.52
1:A:335:LEU:HD23	1:A:368:LEU:HD21	1.91	0.52
1:C:354:SER:HB3	1:C:357:GLN:HG3	1.92	0.52
1:E:309:ILE:HA	1:E:313:LEU:HB2	1.91	0.52
1:E:440:TYR:CG	1:E:441:HIS:HD2	2.27	0.52
1:F:416:ARG:HH11	1:F:462:MET:HG2	1.74	0.52
1:A:175:GLY:O	1:A:193:ASP:OD1	2.28	0.52
1:F:375:HIS:HB3	1:F:391:LEU:HD13	1.92	0.52
1:C:420:TYR:CD1	1:C:466:ALA:HB2	2.45	0.52
1:D:120:ASP:HB3	1:D:123:VAL:CG2	2.38	0.52
1:E:385:ARG:HH12	1:E:408:GLN:NE2	2.08	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:245:VAL:HG13	1:A:246:ILE:HG13	1.92	0.51
1:A:175:GLY:O	1:A:193:ASP:HA	2.10	0.51
1:A:380:ASP:O	1:A:382:THR:N	2.43	0.51
1:B:477:GLU:HA	1:B:480:VAL:HG22	1.91	0.51
1:D:234:ASP:CG	1:D:234:ASP:O	2.53	0.51
1:A:166:PRO:O	1:A:177:LEU:HD12	2.10	0.51
1:F:89:THR:HG21	1:F:92:ARG:HH21	1.74	0.51
1:F:295:ASN:HA	1:F:321:LEU:HD12	1.92	0.51
1:A:219:THR:HG21	1:A:255:ASN:HD22	1.76	0.51
1:C:89:THR:O	1:C:113:ILE:HG12	2.09	0.51
1:D:96:VAL:HG11	1:D:491:VAL:HG23	1.92	0.51
1:F:144:HIS:CD2	1:F:145:PRO:HD2	2.45	0.51
1:A:393:GLN:O	1:A:395:LEU:O	2.28	0.51
1:B:454:GLU:OE2	1:B:486:LYS:CE	2.58	0.51
1:D:188:ASP:O	1:D:192:LYS:NZ	2.33	0.51
1:B:462:MET:HE2	1:E:441:HIS:HE1	1.76	0.51
1:B:145:PRO:O	1:B:148:LEU:HG	2.09	0.51
1:C:277:ILE:O	1:C:279:GLU:O	2.28	0.51
1:C:333:GLU:HA	1:C:336:ARG:HG2	1.92	0.51
1:A:144:HIS:O	1:A:144:HIS:ND1	2.44	0.51
1:A:295:ASN:HA	1:A:321:LEU:HD12	1.93	0.51
1:C:196:GLN:O	1:C:200:GLU:HG3	2.11	0.51
1:E:47:LEU:CD1	1:E:264:LYS:O	2.58	0.51
1:A:242:SER:HB3	1:A:443:GLU:HB2	1.92	0.51
1:D:434:ASN:CG	1:D:437:ASN:HD21	2.19	0.51
1:D:11:GLU:HG3	1:D:402:THR:HG21	1.92	0.51
1:D:198:TYR:CZ	1:D:202:LEU:HD11	2.45	0.51
1:B:224:LEU:HD13	1:B:496:CYS:HB2	1.93	0.50
1:E:113:ILE:O	1:E:114:PRO:C	2.54	0.50
1:F:127:ASP:C	1:F:129:PHE:H	2.15	0.50
1:F:472:LEU:O	1:F:476:GLY:HA3	2.10	0.50
1:B:118:LEU:HD22	1:B:123:VAL:CG1	2.39	0.50
1:D:119:ASP:OD1	1:D:185:ARG:NH2	2.44	0.50
1:B:481:HIS:CG	1:E:479:LYS:HD3	2.47	0.50
1:F:130:GLY:O	1:F:134:ARG:HG3	2.12	0.50
1:E:81:LEU:HD11	1:E:498:LEU:HB2	1.93	0.50
1:E:262:ILE:O	1:E:262:ILE:HG22	2.11	0.50
1:F:186:ILE:HG21	1:F:190:VAL:HG23	1.94	0.50
1:E:166:PRO:HG3	1:E:179:ARG:HB2	1.94	0.50
1:E:216:THR:HG21	1:E:496:CYS:SG	2.52	0.50
1:C:30:GLU:H	1:C:30:GLU:CD	2.20	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:GLU:OE1	1:A:154:ALA:HB1	2.12	0.50
1:B:60:LYS:CG	1:B:61:GLY:H	2.19	0.50
1:B:385:ARG:CB	1:B:404:ARG:HE	2.24	0.50
1:C:85:ASP:CG	1:C:489:SER:HB2	2.37	0.50
1:C:177:LEU:HD13	1:C:180:TRP:NE1	2.27	0.50
1:C:207:MET:HE3	1:C:208:PRO:O	2.12	0.50
1:F:362:LEU:HD22	1:F:397:LEU:HD22	1.94	0.50
1:C:119:ASP:OD1	1:C:119:ASP:C	2.54	0.49
1:A:11:GLU:O	1:A:15:ILE:HG12	2.11	0.49
1:B:397:LEU:HD12	1:B:398:PRO:HD2	1.93	0.49
1:D:245:VAL:HG13	1:D:246:ILE:HG13	1.94	0.49
1:F:393:GLN:O	1:F:395:LEU:O	2.30	0.49
1:B:304:LYS:O	1:B:308:VAL:HG23	2.12	0.49
1:B:343:HIS:HE1	1:B:355:LYS:HA	1.76	0.49
1:D:441:HIS:CD2	1:F:458:GLY:HA3	2.47	0.49
1:E:385:ARG:HH12	1:E:408:GLN:CD	2.20	0.49
1:A:114:PRO:HG2	1:A:118:LEU:HD23	1.93	0.49
1:A:138:ALA:O	1:A:142:LYS:HG3	2.12	0.49
1:A:276:LEU:O	1:A:281:LYS:HB2	2.11	0.49
1:E:379:ASP:HB3	1:E:385:ARG:NH1	2.27	0.49
1:F:423:ALA:HB2	1:F:463:LEU:HD23	1.93	0.49
1:C:341:ASP:O	1:C:345:GLN:HG2	2.13	0.49
1:D:292:SER:HB3	1:D:320:HIS:HA	1.94	0.49
1:E:467:LEU:O	1:E:470:SER:OG	2.28	0.49
1:B:354:SER:HB2	1:B:357:GLN:HG2	1.94	0.49
1:C:419:ALA:HA	1:C:459:PHE:CZ	2.48	0.49
1:A:168:ASP:HB3	1:A:176:THR:HG1	1.77	0.49
1:B:140:MET:HG3	1:B:207:MET:HE2	1.94	0.49
1:B:474:ALA:HA	1:B:477:GLU:HB3	1.94	0.49
1:C:248:CYS:O	1:C:448:CYS:HA	2.12	0.49
1:D:360:ARG:HG3	1:D:396:ARG:NH2	2.28	0.49
1:E:438:LYS:HG3	1:E:439:ARG:H	1.76	0.49
1:F:446:ILE:CD1	1:F:479:LYS:NZ	2.74	0.49
1:B:69:VAL:HB	1:B:285:ILE:HD12	1.95	0.49
1:C:230:SER:OG	1:C:233:THR:OG1	2.30	0.49
1:A:377:GLU:OE1	1:A:456:TYR:CZ	2.66	0.49
1:F:399:THR:O	1:F:404:ARG:NH1	2.46	0.49
1:B:163:PHE:HE2	1:B:177:LEU:HD12	1.77	0.49
1:B:347:LEU:HD21	1:C:307:VAL:HG21	1.94	0.49
1:F:137:LEU:HA	1:F:140:MET:HE2	1.95	0.49
1:B:163:PHE:CE2	1:B:177:LEU:HD12	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:LEU:HA	1:C:140:MET:HB2	1.95	0.48
1:D:372:VAL:O	1:D:376:ILE:HG13	2.13	0.48
1:D:375:HIS:ND1	1:D:391:LEU:HD22	2.28	0.48
1:E:259:MET:HE3	1:E:285:ILE:HG13	1.94	0.48
1:E:349:LEU:HD11	1:E:397:LEU:HD12	1.94	0.48
1:A:97:ASN:HB3	1:A:105:SER:OG	2.13	0.48
1:C:336:ARG:NH1	1:C:362:LEU:O	2.39	0.48
1:C:477:GLU:HA	1:C:480:VAL:HG22	1.95	0.48
1:D:78:ARG:O	1:D:98:LEU:HB2	2.13	0.48
1:D:360:ARG:H	1:D:396:ARG:NH2	2.11	0.48
1:F:182:LYS:HE2	1:F:315:THR:HG21	1.95	0.48
1:F:203:SER:HA	1:F:208:PRO:HD2	1.96	0.48
1:A:92:ARG:HD2	1:A:110:LYS:HE3	1.95	0.48
1:B:112:LYS:HG2	1:B:135:ARG:HD2	1.95	0.48
1:B:168:ASP:HB2	1:B:178:ILE:HD11	1.95	0.48
1:C:64:MET:SD	1:C:288:VAL:HG12	2.53	0.48
1:E:83:ALA:HB3	1:E:94:CYS:HG	1.75	0.48
1:A:341:ASP:O	1:A:345:GLN:HG2	2.13	0.48
1:D:270:GLN:CD	1:D:273:ARG:HH11	2.22	0.48
1:D:399:THR:O	1:D:404:ARG:NH1	2.46	0.48
1:F:419:ALA:HA	1:F:459:PHE:CZ	2.48	0.48
1:B:92:ARG:HH21	1:B:489:SER:HB2	1.78	0.48
1:D:265:ILE:HG12	1:D:286:ILE:HD11	1.96	0.48
1:B:375:HIS:O	1:B:379:ASP:HB3	2.12	0.48
1:F:130:GLY:HA2	1:F:201:GLN:HE21	1.78	0.48
1:D:359:PRO:HG2	1:D:397:LEU:HD13	1.94	0.48
1:D:378:ILE:O	1:D:378:ILE:CD1	2.61	0.48
1:F:189:THR:HB	1:F:192:LYS:HE3	1.95	0.48
1:B:144:HIS:CD2	1:B:144:HIS:C	2.90	0.48
1:B:385:ARG:NH2	1:B:408:GLN:OE1	2.42	0.48
1:A:206:GLY:O	1:A:208:PRO:CD	2.60	0.48
1:B:150:LYS:O	1:B:154:ALA:HB2	2.13	0.48
1:B:248:CYS:HA	1:B:256:GLY:HA2	1.96	0.48
1:C:78:ARG:O	1:C:98:LEU:HB2	2.14	0.48
1:D:231:ASP:CG	1:F:483:LYS:HG3	2.39	0.48
1:A:10:THR:O	1:A:14:VAL:HG23	2.14	0.47
1:E:24:ASP:HA	1:F:20:GLN:HG3	1.95	0.47
1:C:135:ARG:HH11	1:C:135:ARG:HA	1.79	0.47
1:C:376:ILE:HG12	1:C:388:GLU:HG2	1.95	0.47
1:D:349:LEU:HD11	1:D:397:LEU:HD21	1.96	0.47
1:B:141:LYS:HA	1:B:145:PRO:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:ILE:O	1:C:376:ILE:CG2	2.62	0.47
1:D:64:MET:HE3	1:D:286:ILE:HG21	1.97	0.47
1:F:419:ALA:HB2	1:F:459:PHE:CE2	2.49	0.47
1:A:166:PRO:HG2	1:A:179:ARG:O	2.15	0.47
1:B:125:SER:O	1:B:129:PHE:CD1	2.53	0.47
1:B:265:ILE:HD13	1:B:286:ILE:HD11	1.96	0.47
1:D:77:GLU:HG2	1:D:498:LEU:HD21	1.97	0.47
1:D:137:LEU:HD13	1:D:206:GLY:CA	2.45	0.47
1:D:335:LEU:HD23	1:D:368:LEU:HD21	1.96	0.47
1:E:273:ARG:O	1:E:277:ILE:HG13	2.15	0.47
1:E:377:GLU:OE1	1:E:456:TYR:CE1	2.67	0.47
1:F:122:ASN:OD1	1:F:185:ARG:NH2	2.42	0.47
1:A:147:GLU:O	1:A:209:MET:SD	2.73	0.47
1:B:144:HIS:HD2	1:B:146:ASP:OD1	1.94	0.47
1:B:422:ALA:O	1:B:425:PRO:HD2	2.14	0.47
1:C:180:TRP:NE1	1:C:186:ILE:HB	2.30	0.47
1:D:360:ARG:H	1:D:396:ARG:HH21	1.62	0.47
1:D:372:VAL:HA	1:D:391:LEU:CD2	2.45	0.47
1:D:434:ASN:OD1	1:D:437:ASN:ND2	2.47	0.47
1:E:375:HIS:HB3	1:E:391:LEU:HD13	1.96	0.47
1:F:158:LYS:H	1:F:158:LYS:HD2	1.79	0.47
1:B:189:THR:O	1:B:189:THR:OG1	2.33	0.47
1:D:145:PRO:HA	1:D:148:LEU:HB3	1.97	0.47
1:D:389:LEU:HD22	1:D:404:ARG:NH1	2.30	0.47
1:F:376:ILE:HG12	1:F:388:GLU:HG2	1.96	0.47
1:A:125:SER:HB3	1:A:189:THR:HG22	1.96	0.47
1:C:147:GLU:HG2	1:C:150:LYS:HB3	1.96	0.47
1:C:415:SER:OG	1:C:456:TYR:OH	2.16	0.47
1:D:137:LEU:HD11	1:D:207:MET:N	2.30	0.47
1:F:292:SER:HB3	1:F:295:ASN:HD21	1.80	0.47
1:A:239:GLY:CA	1:C:454:GLU:O	2.63	0.47
1:B:308:VAL:O	1:B:312:LYS:HB2	2.14	0.47
1:C:132:LEU:HB3	1:C:198:TYR:HE1	1.80	0.47
1:E:86:LEU:HD13	1:E:91:PHE:HB2	1.97	0.47
1:A:361:HIS:ND1	1:A:395:LEU:HD22	2.30	0.46
1:A:393:GLN:C	1:A:395:LEU:O	2.57	0.46
1:B:129:PHE:C	1:B:201:GLN:HG2	2.40	0.46
1:F:128:LEU:HB2	1:F:132:LEU:CD1	2.35	0.46
1:A:345:GLN:OE1	1:D:308:VAL:HG21	2.15	0.46
1:D:392:LEU:HD23	1:D:399:THR:HG21	1.97	0.46
1:E:256:GLY:HA3	1:E:290:TRP:CH2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:259:MET:HG2	1:E:285:ILE:HG12	1.97	0.46
1:F:291:GLY:HA3	1:F:323:GLU:HG3	1.98	0.46
1:D:102:HIS:HE2	1:D:235:SER:HB3	1.81	0.46
1:D:137:LEU:HD21	1:D:207:MET:CB	2.46	0.46
1:D:458:GLY:HA3	1:F:441:HIS:ND1	2.31	0.46
1:A:102:HIS:O	1:A:229:THR:HG22	2.16	0.46
1:A:305:TYR:HA	1:A:308:VAL:HG12	1.98	0.46
1:B:148:LEU:C	1:B:148:LEU:HD12	2.40	0.46
1:C:163:PHE:HE1	1:C:177:LEU:HD21	1.81	0.46
1:C:270:GLN:CD	1:C:270:GLN:H	2.24	0.46
1:D:234:ASP:O	1:D:234:ASP:OD1	2.33	0.46
1:A:362:LEU:HD22	1:A:397:LEU:HD22	1.98	0.46
1:E:84:ALA:HB2	1:E:93:ILE:HD13	1.97	0.46
1:E:262:ILE:O	1:E:262:ILE:CG2	2.60	0.46
1:C:69:VAL:HB	1:C:285:ILE:HD12	1.98	0.46
1:D:10:THR:O	1:D:14:VAL:HG23	2.16	0.46
1:D:30:GLU:OE1	1:D:30:GLU:N	2.49	0.46
1:D:250:PHE:O	1:D:450:GLY:HA3	2.15	0.46
1:D:319:PHE:O	1:D:320:HIS:ND1	2.48	0.46
1:E:129:PHE:HZ	1:E:194:VAL:HG13	1.79	0.46
1:F:379:ASP:OD2	1:F:388:GLU:HB2	2.15	0.46
1:A:478:ARG:NE	1:C:468:ALA:CB	2.79	0.46
1:D:478:ARG:HD3	1:F:477:GLU:HG3	1.98	0.46
1:E:237:THR:C	1:E:238:SER:HG	2.16	0.46
1:F:136:THR:O	1:F:140:MET:CB	2.63	0.46
1:F:144:HIS:CG	1:F:145:PRO:CD	2.98	0.46
1:A:347:LEU:HD21	1:D:307:VAL:HG21	1.97	0.46
1:A:379:ASP:OD2	1:A:385:ARG:HD3	2.16	0.46
1:B:393:GLN:HA	1:B:395:LEU:O	2.16	0.46
1:B:464:ARG:NH1	1:E:443:GLU:OE2	2.49	0.46
1:C:180:TRP:HB3	1:C:185:ARG:HA	1.98	0.46
1:C:470:SER:HB2	1:C:472:LEU:HD23	1.98	0.46
1:D:113:ILE:HD12	1:D:114:PRO:HD2	1.98	0.46
1:F:47:LEU:HD21	1:F:286:ILE:HD13	1.98	0.46
1:A:336:ARG:HG3	1:A:362:LEU:HD12	1.98	0.46
1:B:68:PHE:CE2	1:B:171:SER:HA	2.51	0.46
1:D:42:GLN:NE2	1:D:61:GLY:HA2	2.31	0.46
1:D:137:LEU:CD1	1:D:207:MET:N	2.80	0.46
1:D:255:ASN:OD1	1:D:289:GLU:HA	2.15	0.46
1:F:255:ASN:OD1	1:F:256:GLY:N	2.45	0.46
1:F:271:GLU:HG2	1:F:272:LEU:N	2.31	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:302:THR:OG1	1:A:325:ARG:NH1	2.44	0.45
1:A:470:SER:HB2	1:A:471:PRO:HD2	1.96	0.45
1:C:207:MET:C	1:C:208:PRO:O	2.53	0.45
1:C:248:CYS:SG	1:C:448:CYS:SG	3.12	0.45
1:E:274:ASP:O	1:E:278:LYS:N	2.48	0.45
1:F:99:HIS:CG	1:F:100:GLY:H	2.33	0.45
1:A:181:THR:C	1:A:183:GLY:H	2.24	0.45
1:C:94:CYS:HB3	1:C:108:GLN:HE21	1.82	0.45
1:F:468:ALA:O	1:F:473:GLY:HA3	2.16	0.45
1:C:305:TYR:HA	1:C:308:VAL:HG12	1.99	0.45
1:D:25:PHE:CD1	1:D:417:ARG:HD3	2.52	0.45
1:E:343:HIS:HE1	1:E:355:LYS:HA	1.80	0.45
1:E:449:ASP:HB2	1:E:485:ALA:O	2.15	0.45
1:F:118:LEU:HB3	1:F:184:PHE:HD2	1.81	0.45
1:F:128:LEU:HD12	1:F:128:LEU:O	2.16	0.45
1:D:343:HIS:ND1	1:D:349:LEU:O	2.40	0.45
1:E:344:SER:HA	1:E:355:LYS:HD2	1.97	0.45
1:A:252:THR:CB	2:A:603:PO4:O2	2.62	0.45
1:B:118:LEU:HA	1:B:123:VAL:CG2	2.45	0.45
1:B:145:PRO:CB	1:B:148:LEU:HD23	2.47	0.45
1:D:137:LEU:HD13	1:D:206:GLY:N	2.31	0.45
1:A:377:GLU:OE1	1:A:456:TYR:CE1	2.70	0.45
1:B:147:GLU:OE1	1:B:150:LYS:HE3	2.16	0.45
1:B:327:SER:OG	1:B:452:VAL:HG21	2.16	0.45
1:B:388:GLU:CD	1:B:404:ARG:HB3	2.42	0.45
1:C:419:ALA:HB2	1:C:459:PHE:CE2	2.51	0.45
1:D:177:LEU:O	1:D:190:VAL:O	2.34	0.45
1:D:430:LEU:HD13	1:D:436:LEU:HD11	1.99	0.45
1:F:25:PHE:CD2	1:F:417:ARG:HD3	2.52	0.45
1:F:142:LYS:HE2	1:F:143:TYR:CE2	2.51	0.45
1:A:85:ASP:OD2	1:A:92:ARG:HB2	2.17	0.45
1:A:128:LEU:O	1:A:132:LEU:HG	2.16	0.45
1:A:441:HIS:HE1	1:C:462:MET:HE3	1.82	0.45
1:B:177:LEU:HD23	1:B:177:LEU:C	2.41	0.45
1:C:163:PHE:CE1	1:C:165:TYR:HB2	2.51	0.45
1:D:73:PRO:HD3	1:D:224:LEU:HD22	1.99	0.45
1:E:377:GLU:OE1	1:E:456:TYR:HE1	2.00	0.45
1:B:276:LEU:HD13	1:B:284:MET:HE1	1.98	0.45
1:C:443:GLU:HG2	1:C:479:LYS:HB3	1.99	0.45
1:E:306:ASP:HB3	1:E:325:ARG:CZ	2.46	0.45
1:E:389:LEU:HD13	1:E:404:ARG:HH11	1.82	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:29:PRO:HA	1:F:32:LEU:HB2	1.99	0.45
1:B:148:LEU:HD12	1:B:149:ALA:N	2.32	0.45
1:C:175:GLY:O	1:C:193:ASP:CA	2.60	0.45
1:D:124:THR:OG1	1:D:127:ASP:OD1	2.30	0.45
1:D:137:LEU:HD13	1:D:206:GLY:C	2.42	0.45
1:B:169:GLN:NE2	1:B:215:LEU:O	2.35	0.44
1:D:372:VAL:HA	1:D:391:LEU:HD23	1.98	0.44
1:F:144:HIS:CD2	1:F:145:PRO:HD3	2.52	0.44
1:F:454:GLU:OE1	1:F:484:ILE:CG1	2.53	0.44
1:B:308:VAL:HG22	1:C:345:GLN:O	2.18	0.44
1:B:416:ARG:HH12	2:B:601:PO4:P	2.40	0.44
1:C:290:TRP:C	1:C:290:TRP:CD1	2.95	0.44
1:E:74:ASN:HB3	1:E:77:GLU:OE2	2.17	0.44
1:A:321:LEU:HD23	1:A:321:LEU:HA	1.79	0.44
1:C:323:GLU:O	1:C:327:SER:N	2.50	0.44
1:D:288:VAL:HG12	1:D:290:TRP:HB3	1.98	0.44
1:E:244:PRO:HA	1:E:445:GLU:O	2.18	0.44
1:E:347:LEU:HD21	1:F:307:VAL:HG21	1.99	0.44
1:F:10:THR:O	1:F:14:VAL:HG23	2.17	0.44
1:B:301:PRO:HA	1:C:16:GLN:OE1	2.18	0.44
1:B:487:ASP:OD2	1:B:491:VAL:HG23	2.17	0.44
1:C:106:MET:HE2	1:C:487:ASP:OD2	2.18	0.44
1:E:124:THR:CG2	1:E:126:ASP:CB	2.95	0.44
1:A:449:ASP:OD2	1:A:486:LYS:C	2.58	0.44
1:F:77:GLU:HG2	1:F:498:LEU:HD11	1.99	0.44
1:A:163:PHE:CE2	1:A:194:VAL:HG11	2.53	0.44
1:B:348:LEU:HD12	1:B:348:LEU:HA	1.87	0.44
1:D:258:TYR:OH	1:D:260:GLU:OE1	2.20	0.44
1:D:481:HIS:CD2	1:D:482:LEU:HG	2.53	0.44
1:F:42:GLN:HB3	1:F:62:LEU:HG	1.98	0.44
1:D:90:ASN:OD1	1:D:90:ASN:N	2.51	0.44
1:E:146:ASP:OD1	1:E:147:GLU:N	2.50	0.44
1:A:36:THR:HG21	1:A:471:PRO:CG	2.48	0.44
1:D:226:HIS:HB2	1:D:485:ALA:HB2	1.99	0.44
1:E:8:LYS:O	1:E:12:ARG:HG3	2.17	0.44
1:E:230:SER:OG	1:E:234:ASP:HB2	2.17	0.44
1:F:137:LEU:HG	1:F:141:LYS:HE3	2.00	0.44
1:B:408:GLN:HA	1:B:411:VAL:HG12	2.00	0.44
1:C:86:LEU:HA	1:C:91:PHE:CB	2.48	0.44
1:D:98:LEU:HB3	1:D:228:TYR:OH	2.18	0.44
1:E:231:ASP:OD1	1:E:483:LYS:NZ	2.28	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:42:GLN:HB3	1:F:61:GLY:O	2.18	0.44
1:B:341:ASP:OD2	1:C:304:LYS:NZ	2.44	0.43
1:B:426:LEU:HD22	1:B:446:ILE:HD13	1.99	0.43
1:D:29:PRO:HG3	1:D:469:LEU:HD12	1.99	0.43
1:E:472:LEU:HD23	1:E:472:LEU:H	1.83	0.43
1:A:82:LEU:HB2	1:A:159:LEU:CB	2.47	0.43
1:A:321:LEU:O	1:A:325:ARG:HG2	2.17	0.43
1:B:62:LEU:O	1:B:64:MET:HG3	2.17	0.43
1:C:423:ALA:HB2	1:C:463:LEU:HD23	1.99	0.43
1:D:114:PRO:HG2	1:D:117:LEU:HD23	2.00	0.43
1:D:162:THR:HG23	1:D:217:ASN:HA	2.00	0.43
1:D:193:ASP:HB3	1:D:196:GLN:HB3	2.00	0.43
1:F:85:ASP:HB3	1:F:92:ARG:HG3	1.99	0.43
1:A:426:LEU:HD22	1:A:446:ILE:HD12	2.00	0.43
1:E:375:HIS:CG	1:E:391:LEU:HD13	2.53	0.43
1:F:80:VAL:HG22	1:F:97:ASN:HB2	2.00	0.43
1:A:70:THR:OG1	1:A:281:LYS:HE2	2.15	0.43
1:A:106:MET:O	1:A:107:GLU:HG3	2.18	0.43
1:A:305:TYR:CE2	1:A:338:ILE:HG12	2.53	0.43
1:C:424:VAL:HB	1:C:425:PRO:HD3	2.00	0.43
1:D:198:TYR:CE1	1:D:202:LEU:HD21	2.53	0.43
1:D:262:ILE:HG22	1:D:273:ARG:HG2	2.00	0.43
1:D:263:ASN:HA	1:D:273:ARG:HD2	1.99	0.43
1:F:173:ASN:HB2	1:F:195:VAL:HG11	1.99	0.43
1:A:8:LYS:O	1:A:12:ARG:HG2	2.19	0.43
1:A:207:MET:O	1:A:207:MET:HG3	2.18	0.43
1:C:400:THR:O	1:C:404:ARG:HG3	2.18	0.43
1:D:172:LEU:HG	1:D:214:ALA:HA	2.01	0.43
1:D:231:ASP:O	1:F:483:LYS:HE2	2.18	0.43
1:D:259:MET:HE2	1:D:283:HIS:HB3	2.01	0.43
1:E:400:THR:O	1:E:404:ARG:HG3	2.18	0.43
1:E:427:ALA:O	1:E:431:ILE:HG22	2.17	0.43
1:F:38:TYR:OH	1:F:298:LYS:HD2	2.19	0.43
1:A:487:ASP:OD2	1:A:491:VAL:HG23	2.18	0.43
1:B:124:THR:OG1	1:B:127:ASP:HB2	2.18	0.43
1:B:327:SER:OG	1:B:328:GLY:N	2.52	0.43
1:C:223:TYR:CZ	1:C:227:CYS:SG	3.11	0.43
1:D:4:ASP:CG	1:D:7:HIS:HB3	2.43	0.43
1:D:220:VAL:HG13	1:D:285:ILE:HG21	2.00	0.43
1:D:426:LEU:HD22	1:D:446:ILE:HD12	2.00	0.43
1:E:64:MET:HE3	1:E:286:ILE:HG21	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:137:LEU:HD13	1:E:206:GLY:HA3	2.01	0.43
1:E:166:PRO:HG2	1:E:179:ARG:HB2	2.01	0.43
1:F:93:ILE:HD11	1:F:136:THR:HA	2.01	0.43
1:F:301:PRO:O	1:F:325:ARG:NH1	2.52	0.43
1:A:32:LEU:O	1:A:36:THR:HG22	2.18	0.43
1:A:209:MET:HE3	1:A:209:MET:HB2	1.86	0.43
1:B:14:VAL:HG21	1:B:347:LEU:O	2.18	0.43
1:B:144:HIS:NE2	1:B:146:ASP:OD1	2.51	0.43
1:B:230:SER:OG	1:B:233:THR:OG1	2.20	0.43
1:D:251:GLY:HA2	1:D:452:VAL:H	1.82	0.43
1:F:351:GLN:HG3	1:F:352:TYR:CD2	2.54	0.43
1:A:144:HIS:HB2	1:A:146:ASP:CG	2.43	0.43
1:A:335:LEU:O	1:A:339:LEU:HG	2.19	0.43
1:B:384:LEU:HD23	1:B:384:LEU:HA	1.84	0.43
1:B:448:CYS:O	1:B:484:ILE:HA	2.18	0.43
1:E:422:ALA:O	1:E:425:PRO:HD2	2.19	0.43
1:A:255:ASN:OD1	1:A:289:GLU:HA	2.19	0.43
1:A:360:ARG:CG	2:A:602:PO4:P	3.06	0.43
1:C:36:THR:HG21	1:C:471:PRO:CG	2.45	0.43
1:C:124:THR:O	1:C:128:LEU:N	2.52	0.43
1:C:314:SER:O	1:C:317:PRO:HG3	2.18	0.43
1:E:42:GLN:HB3	1:E:62:LEU:HG	2.01	0.43
1:E:140:MET:O	1:E:145:PRO:HB3	2.19	0.43
1:F:11:GLU:O	1:F:15:ILE:HG12	2.18	0.43
1:F:218:ASP:OD2	1:F:489:SER:OG	2.29	0.43
1:F:446:ILE:O	1:F:446:ILE:HG12	2.18	0.43
1:A:85:ASP:OD2	1:A:92:ARG:NH1	2.52	0.43
1:A:303:THR:HG22	1:D:20:GLN:HE22	1.84	0.43
1:C:328:GLY:HA3	1:C:452:VAL:HG21	2.00	0.43
1:E:320:HIS:O	1:E:324:LYS:HG3	2.18	0.43
1:E:389:LEU:HD13	1:E:404:ARG:NH1	2.34	0.43
1:F:111:SER:HB2	1:F:139:PHE:CE2	2.46	0.43
1:F:159:LEU:HD11	1:F:198:TYR:HE2	1.83	0.43
1:D:173:ASN:C	1:D:195:VAL:HG21	2.43	0.42
1:F:400:THR:O	1:F:404:ARG:HG3	2.18	0.42
1:F:441:HIS:O	1:F:443:GLU:HG3	2.18	0.42
1:C:305:TYR:CZ	1:C:338:ILE:HG12	2.55	0.42
1:D:198:TYR:HE1	1:D:202:LEU:HD21	1.83	0.42
1:E:47:LEU:HA	1:E:267:LYS:HE3	2.01	0.42
1:E:307:VAL:HG11	1:F:347:LEU:HG	2.00	0.42
1:B:173:ASN:O	1:B:173:ASN:ND2	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:379:ASP:OD2	1:C:388:GLU:N	2.52	0.42
1:F:389:LEU:HD13	1:F:404:ARG:HH11	1.84	0.42
1:B:173:ASN:HB3	1:B:213:VAL:O	2.20	0.42
1:C:407:ILE:O	1:C:411:VAL:HG13	2.20	0.42
1:E:102:HIS:ND1	1:E:230:SER:O	2.51	0.42
1:E:430:LEU:HD23	1:E:430:LEU:HA	1.89	0.42
1:F:135:ARG:HA	1:F:135:ARG:HD3	1.85	0.42
1:F:159:LEU:HD22	1:F:210:ILE:HB	2.01	0.42
1:F:47:LEU:HD22	1:F:265:ILE:HG23	2.00	0.42
1:C:343:HIS:CD2	1:C:358:LEU:HD21	2.55	0.42
1:D:48:ALA:HA	1:D:266:THR:HB	2.02	0.42
1:D:260:GLU:HG3	1:D:261:GLU:N	2.33	0.42
1:E:290:TRP:CD1	1:E:290:TRP:C	2.98	0.42
1:A:173:ASN:ND2	1:A:173:ASN:O	2.53	0.42
1:A:458:GLY:HA3	1:C:441:HIS:CD2	2.54	0.42
1:B:292:SER:HB2	1:B:295:ASN:HB2	2.01	0.42
1:C:92:ARG:NH1	1:C:108:GLN:HE22	2.18	0.42
1:B:375:HIS:CB	1:B:391:LEU:HD22	2.46	0.42
1:C:47:LEU:HD21	1:C:432:LYS:NZ	2.35	0.42
1:D:464:ARG:HD3	1:D:479:LYS:HD3	2.02	0.42
1:F:62:LEU:HD23	1:F:62:LEU:HA	1.91	0.42
1:B:14:VAL:HG22	1:B:347:LEU:HB3	2.02	0.42
1:B:78:ARG:HD3	1:B:78:ARG:N	2.34	0.42
1:B:106:MET:HE1	1:B:487:ASP:OD2	2.20	0.42
1:C:49:PRO:HG3	1:C:267:LYS:HA	2.02	0.42
1:D:460:ARG:NH2	1:F:240:GLU:HB2	2.35	0.42
1:A:315:THR:O	1:A:317:PRO:HD3	2.20	0.42
1:B:148:LEU:HA	1:B:209:MET:HE1	2.01	0.42
1:C:422:ALA:O	1:C:425:PRO:HD2	2.19	0.42
1:E:231:ASP:OD1	1:E:231:ASP:N	2.50	0.42
1:E:372:VAL:HG21	1:E:395:LEU:HD11	2.02	0.42
1:F:25:PHE:CE2	1:F:414:ILE:HG12	2.55	0.42
1:B:325:ARG:HD3	1:B:417:ARG:NH2	2.34	0.41
1:C:467:LEU:HB2	1:C:477:GLU:HG3	2.02	0.41
1:D:479:LYS:CG	1:F:479:LYS:O	2.55	0.41
1:F:252:THR:HA	1:F:328:GLY:H	1.85	0.41
1:D:76:THR:HA	1:D:100:GLY:O	2.21	0.41
1:D:249:ILE:O	1:D:254:THR:HA	2.20	0.41
1:D:479:LYS:CB	1:F:480:VAL:HA	2.42	0.41
1:E:93:ILE:O	1:E:93:ILE:HG23	2.20	0.41
1:E:297:LEU:HD12	1:F:9:ALA:HB1	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:LEU:HD23	1:A:62:LEU:HA	1.98	0.41
1:B:90:ASN:HA	1:B:114:PRO:HD3	2.02	0.41
1:B:308:VAL:HG21	1:C:345:GLN:OE1	2.20	0.41
1:B:388:GLU:OE1	1:B:404:ARG:HB3	2.20	0.41
1:D:323:GLU:O	1:D:327:SER:N	2.48	0.41
1:E:21:ILE:HD11	1:E:342:LEU:HD21	2.02	0.41
1:E:99:HIS:O	1:E:228:TYR:OH	2.38	0.41
1:F:93:ILE:HD13	1:F:136:THR:HG22	2.02	0.41
1:B:173:ASN:HB3	1:B:213:VAL:C	2.44	0.41
1:B:392:LEU:HD21	1:B:407:ILE:HD12	2.02	0.41
1:B:473:GLY:O	1:B:474:ALA:HB3	2.19	0.41
1:E:396:ARG:HA	1:E:396:ARG:HD3	1.85	0.41
1:F:134:ARG:HG2	1:F:205:GLN:HE22	1.85	0.41
1:A:478:ARG:CZ	1:C:468:ALA:CB	2.98	0.41
1:B:78:ARG:H	1:B:78:ARG:HG2	1.20	0.41
1:D:85:ASP:CB	1:D:162:THR:HB	2.50	0.41
1:D:256:GLY:HA3	1:D:290:TRP:CH2	2.55	0.41
1:E:137:LEU:HD11	1:E:208:PRO:HG3	2.02	0.41
1:F:202:LEU:HD12	1:F:203:SER:N	2.35	0.41
1:F:300:LEU:HD12	1:F:301:PRO:HD2	2.02	0.41
1:F:482:LEU:HG	1:F:483:LYS:O	2.20	0.41
1:A:87:GLY:HA2	1:A:165:TYR:HE1	1.86	0.41
1:A:439:ARG:H	1:A:439:ARG:HG3	1.73	0.41
1:B:36:THR:O	1:B:40:ILE:HG12	2.21	0.41
1:B:242:SER:HA	1:B:443:GLU:O	2.20	0.41
1:B:380:ASP:OD2	1:B:385:ARG:HA	2.21	0.41
1:E:43:MET:HE2	1:E:432:LYS:HD3	2.03	0.41
1:E:321:LEU:O	1:E:325:ARG:HG2	2.21	0.41
1:F:446:ILE:HG21	1:F:479:LYS:NZ	2.36	0.41
1:B:154:ALA:HB3	1:B:209:MET:HB2	2.02	0.41
1:B:385:ARG:HB3	1:B:404:ARG:NE	2.28	0.41
1:C:49:PRO:HA	1:C:50:PRO:HD3	1.89	0.41
1:A:124:THR:HG22	1:A:126:ASP:H	1.85	0.41
1:A:380:ASP:O	1:A:382:THR:HG23	2.21	0.41
1:C:63:PRO:HB2	1:C:289:GLU:HB2	2.01	0.41
1:C:86:LEU:HA	1:C:91:PHE:HB3	2.02	0.41
1:C:330:PHE:O	1:C:334:VAL:HG23	2.21	0.41
1:D:25:PHE:HD1	1:D:417:ARG:HD3	1.86	0.41
1:A:147:GLU:HA	1:A:150:LYS:HG3	2.03	0.41
1:A:360:ARG:CB	2:A:602:PO4:O3	2.62	0.41
1:B:358:LEU:HD12	1:B:358:LEU:HA	1.97	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:455:TYR:CA	1:E:238:SER:O	2.68	0.41
1:C:324:LYS:HG2	1:C:330:PHE:CZ	2.55	0.41
1:C:391:LEU:HD12	1:C:391:LEU:HA	1.95	0.41
1:C:400:THR:HB	1:C:403:GLU:HG3	2.02	0.41
1:D:329:MET:HE2	1:D:366:PHE:CD1	2.56	0.41
1:E:135:ARG:HD2	1:E:135:ARG:HA	1.90	0.41
1:E:245:VAL:O	1:E:245:VAL:HG22	2.20	0.41
1:F:86:LEU:HB2	1:F:91:PHE:CD1	2.55	0.41
1:F:459:PHE:HA	1:F:462:MET:HE3	2.02	0.41
1:A:168:ASP:HB3	1:A:176:THR:OG1	2.21	0.41
1:F:98:LEU:HD22	1:F:228:TYR:CE2	2.56	0.41
1:F:241:ILE:HG22	1:F:241:ILE:O	2.21	0.41
1:F:438:LYS:HE2	1:F:438:LYS:HB2	1.94	0.41
1:A:193:ASP:OD1	1:A:195:VAL:HG22	2.21	0.40
1:A:382:THR:O	1:A:383:GLY:C	2.64	0.40
1:B:455:TYR:O	1:E:238:SER:C	2.64	0.40
1:B:498:LEU:HD23	1:B:498:LEU:O	2.21	0.40
1:C:244:PRO:HA	1:C:445:GLU:O	2.22	0.40
1:C:335:LEU:HD23	1:C:368:LEU:HD13	2.02	0.40
1:C:421:LEU:O	1:C:425:PRO:HD3	2.20	0.40
1:E:117:LEU:HD13	1:E:123:VAL:HG11	2.03	0.40
1:F:254:THR:HG22	1:F:323:GLU:HA	2.04	0.40
1:A:8:LYS:HD2	1:A:8:LYS:HA	1.94	0.40
1:A:378:ILE:HD11	1:C:441:HIS:CD2	2.51	0.40
1:A:464:ARG:HH22	1:C:240:GLU:CD	2.29	0.40
1:B:343:HIS:CE1	1:B:355:LYS:HA	2.56	0.40
1:B:372:VAL:O	1:B:376:ILE:HG13	2.21	0.40
1:B:401:PRO:O	1:B:405:VAL:HG23	2.21	0.40
1:D:152:LYS:HE3	1:D:152:LYS:HB2	1.92	0.40
1:D:193:ASP:OD1	1:D:195:VAL:HG22	2.21	0.40
1:F:341:ASP:O	1:F:345:GLN:HG2	2.21	0.40
1:D:49:PRO:HA	1:D:50:PRO:HD3	1.91	0.40
1:E:94:CYS:HA	1:E:108:GLN:HA	2.02	0.40
1:E:125:SER:HB3	1:E:189:THR:HG23	2.03	0.40
1:E:373:LEU:HD13	1:E:411:VAL:HG22	2.04	0.40
1:F:156:PRO:HA	1:F:209:MET:O	2.21	0.40
1:F:364:THR:HB	1:F:365:PRO:HD2	2.03	0.40
1:F:389:LEU:O	1:F:393:GLN:HG2	2.21	0.40
1:A:412:ARG:O	1:A:416:ARG:HG3	2.21	0.40
1:C:39:PHE:CZ	1:C:425:PRO:HB3	2.56	0.40
1:F:70:THR:OG1	1:F:281:LYS:HB3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:48:ALA:HA	1:A:266:THR:HB	2.03	0.40
1:B:167:VAL:HG13	1:B:176:THR:O	2.22	0.40
1:C:378:ILE:O	1:C:378:ILE:HG23	2.22	0.40
1:D:137:LEU:HD11	1:D:207:MET:H	1.86	0.40
1:D:140:MET:SD	1:D:210:ILE:HD11	2.62	0.40
1:D:470:SER:O	1:D:472:LEU:O	2.39	0.40
1:E:385:ARG:HE	1:E:385:ARG:HB3	1.49	0.40
1:F:119:ASP:OD1	1:F:119:ASP:N	2.47	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	487/500 (97%)	476 (98%)	11 (2%)	0	100	100
1	B	486/500 (97%)	479 (99%)	7 (1%)	0	100	100
1	C	489/500 (98%)	482 (99%)	7 (1%)	0	100	100
1	D	484/500 (97%)	478 (99%)	6 (1%)	0	100	100
1	E	485/500 (97%)	481 (99%)	4 (1%)	0	100	100
1	F	489/500 (98%)	487 (100%)	2 (0%)	0	100	100
All	All	2920/3000 (97%)	2883 (99%)	37 (1%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	423/431 (98%)	422 (100%)	1 (0%)	87	85
1	B	423/431 (98%)	423 (100%)	0	100	100
1	C	424/431 (98%)	422 (100%)	2 (0%)	81	80
1	D	418/431 (97%)	418 (100%)	0	100	100
1	E	422/431 (98%)	422 (100%)	0	100	100
1	F	426/431 (99%)	425 (100%)	1 (0%)	87	85
All	All	2536/2586 (98%)	2532 (100%)	4 (0%)	87	85

All (4) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	440	TYR
1	C	440	TYR
1	C	441	HIS
1	F	446	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	316	ASN
1	B	144	HIS
1	B	173	ASN
1	B	287	ASN
1	B	343	HIS
1	B	406	GLN
1	C	20	GLN
1	C	97	ASN
1	C	122	ASN
1	C	232	ASN
1	C	320	HIS
1	C	337	ASN
1	C	350	GLN
1	C	361	HIS
1	C	367	GLN
1	C	406	GLN
1	C	441	HIS
1	C	465	HIS

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Mol	Chain	Res	Type
1	C	481	HIS
1	D	20	GLN
1	D	42	GLN
1	D	169	GLN
1	D	437	ASN
1	E	255	ASN
1	E	337	ASN
1	E	408	GLN
1	F	232	ASN
1	F	295	ASN
1	F	345	GLN
1	F	351	GLN
1	F	367	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

13 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	$\# Z > 2$
2	PO4	A	603	-	4,4,4	3.06	4 (100%)	6,6,6	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	PO4	D	602	-	4,4,4	0.95	0	6,6,6	0.53	0
2	PO4	F	601	-	4,4,4	0.97	0	6,6,6	0.53	0
2	PO4	B	602	-	4,4,4	0.93	0	6,6,6	0.47	0
2	PO4	B	601	-	4,4,4	0.97	0	6,6,6	0.46	0
2	PO4	E	602	-	4,4,4	0.94	0	6,6,6	0.53	0
2	PO4	A	601	-	4,4,4	0.93	0	6,6,6	0.55	0
2	PO4	C	602	-	4,4,4	0.95	0	6,6,6	0.44	0
2	PO4	C	601	-	4,4,4	1.02	0	6,6,6	0.38	0
2	PO4	E	601	-	4,4,4	0.94	0	6,6,6	0.50	0
2	PO4	D	601	-	4,4,4	0.96	0	6,6,6	0.54	0
2	PO4	F	602	-	4,4,4	0.94	0	6,6,6	0.49	0
2	PO4	A	602	-	4,4,4	3.06	4 (100%)	6,6,6	0.46	0

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	602	PO4	P-O1	4.67	1.61	1.50
2	A	603	PO4	P-O1	4.67	1.61	1.50
2	A	602	PO4	P-O3	2.36	1.61	1.54
2	A	603	PO4	P-O3	2.36	1.61	1.54
2	A	602	PO4	P-O2	2.34	1.61	1.54
2	A	603	PO4	P-O2	2.34	1.61	1.54
2	A	602	PO4	P-O4	-2.13	1.48	1.54
2	A	603	PO4	P-O4	-2.13	1.48	1.54

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

7 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	603	PO4	2	0
2	F	601	PO4	1	0
2	B	601	PO4	2	0
2	A	601	PO4	1	0
2	C	602	PO4	1	0
2	E	601	PO4	1	0
2	A	602	PO4	12	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	491/500 (98%)	0.51	24 (4%)	35	20	46, 72, 116, 141	0
1	B	490/500 (98%)	0.49	14 (2%)	53	30	53, 78, 111, 134	0
1	C	493/500 (98%)	0.59	27 (5%)	30	18	53, 81, 160, 168	0
1	D	488/500 (97%)	0.36	14 (2%)	53	30	47, 73, 104, 130	0
1	E	489/500 (97%)	0.42	13 (2%)	56	32	53, 77, 109, 123	0
1	F	493/500 (98%)	0.71	31 (6%)	26	16	58, 84, 174, 185	0
All	All	2944/3000 (98%)	0.51	123 (4%)	40	22	46, 77, 150, 185	0

All (123) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	388	GLU	4.9
1	F	437	ASN	4.3
1	B	379	ASP	4.0
1	B	385	ARG	4.0
1	C	91	PHE	3.7
1	F	157	MET	3.6
1	D	477	GLU	3.5
1	C	388	GLU	3.4
1	F	481	HIS	3.3
1	B	185	ARG	3.2
1	B	111	SER	3.2
1	E	238	SER	3.2
1	C	118	LEU	3.2
1	A	356	GLU	3.2
1	D	479	LYS	3.2
1	A	478	ARG	3.2
1	E	5	ASP	3.1
1	F	197	LEU	3.1
1	B	207	MET	3.1

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Mol	Chain	Res	Type	RSRZ
1	A	149	ALA	3.0
1	F	484	ILE	3.0
1	B	149	ALA	3.0
1	E	474	ALA	3.0
1	D	478	ARG	3.0
1	E	479	LYS	2.9
1	A	481	HIS	2.9
1	F	140	MET	2.9
1	F	213	VAL	2.8
1	C	117	LEU	2.8
1	B	311	GLN	2.8
1	F	198	TYR	2.8
1	A	396	ARG	2.8
1	E	232	ASN	2.8
1	A	388	GLU	2.7
1	F	202	LEU	2.7
1	A	386	GLU	2.7
1	E	239	GLY	2.7
1	C	245	VAL	2.6
1	D	474	ALA	2.6
1	B	173	ASN	2.6
1	A	393	GLN	2.6
1	F	128	LEU	2.6
1	B	122	ASN	2.6
1	A	117	LEU	2.5
1	C	156	PRO	2.5
1	E	393	GLN	2.5
1	D	206	GLY	2.5
1	D	378	ILE	2.5
1	D	481	HIS	2.5
1	F	384	LEU	2.5
1	C	477	GLU	2.5
1	B	393	GLN	2.5
1	F	23	ASP	2.5
1	F	207	MET	2.4
1	A	435	ALA	2.4
1	F	474	ALA	2.4
1	C	395	LEU	2.4
1	F	477	GLU	2.4
1	D	476	GLY	2.4
1	F	490	GLY	2.4
1	B	382	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	186	ILE	2.4
1	F	388	GLU	2.4
1	D	388	GLU	2.4
1	F	479	LYS	2.4
1	C	184	PHE	2.3
1	C	442	GLY	2.3
1	A	384	LEU	2.3
1	A	118	LEU	2.3
1	C	114	PRO	2.3
1	F	235	SER	2.3
1	C	266	THR	2.3
1	A	395	LEU	2.3
1	A	365	PRO	2.3
1	C	181	THR	2.3
1	C	232	ASN	2.3
1	F	211	LYS	2.3
1	C	148	LEU	2.3
1	E	477	GLU	2.3
1	C	92	ARG	2.3
1	D	185	ARG	2.3
1	E	184	PHE	2.3
1	C	239	GLY	2.3
1	C	122	ASN	2.2
1	A	164	SER	2.2
1	F	381	SER	2.2
1	C	123	VAL	2.2
1	E	384	LEU	2.2
1	C	197	LEU	2.2
1	E	79	GLY	2.2
1	C	120	ASP	2.2
1	F	145	PRO	2.2
1	A	366	PHE	2.2
1	F	150	LYS	2.2
1	A	209	MET	2.2
1	F	361	HIS	2.2
1	A	270	GLN	2.2
1	F	113	ILE	2.2
1	A	490	GLY	2.1
1	A	204	ALA	2.1
1	C	231	ASP	2.1
1	F	184	PHE	2.1
1	B	79	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	E	183	GLY	2.1
1	D	380	ASP	2.1
1	C	435	ALA	2.1
1	C	380	ASP	2.1
1	D	379	ASP	2.1
1	F	234	ASP	2.1
1	E	388	GLU	2.1
1	F	190	VAL	2.1
1	A	147	GLU	2.1
1	A	142	LYS	2.1
1	C	146	ASP	2.0
1	A	483	LYS	2.0
1	C	154	ALA	2.0
1	A	351	GLN	2.0
1	F	395	LEU	2.0
1	C	210	ILE	2.0
1	F	86	LEU	2.0
1	D	458	GLY	2.0
1	F	156	PRO	2.0
1	D	480	VAL	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(Å ²)	Q<0.9
2	PO4	A	603	5/5	0.52	0.20	86,86,87,88	0
2	PO4	A	602	5/5	0.77	0.16	90,91,91,92	0
2	PO4	E	602	5/5	0.79	0.16	72,73,74,74	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	PO4	F	602	5/5	0.81	0.17	81,82,83,83	0
2	PO4	F	601	5/5	0.88	0.11	65,66,66,67	0
2	PO4	B	602	5/5	0.90	0.11	73,74,74,74	0
2	PO4	C	602	5/5	0.91	0.12	80,81,81,81	0
2	PO4	E	601	5/5	0.92	0.11	75,75,75,77	0
2	PO4	D	602	5/5	0.92	0.09	62,62,63,64	0
2	PO4	B	601	5/5	0.93	0.09	68,68,69,69	0
2	PO4	A	601	5/5	0.95	0.09	62,63,63,63	0
2	PO4	C	601	5/5	0.95	0.08	60,61,61,62	0
2	PO4	D	601	5/5	0.96	0.07	58,60,61,61	0

6.5 Other polymers [i](#)

There are no such residues in this entry.