



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 01:55 AM UTC

PDB ID : 3GR9 / pdb_00003gr9
Title : Crystal structure of ColD H188K S187N
Authors : Holden, H.M.; Cook, P.D.; Kubiak, R.L.; Toomey, D.P.
Deposited on : 2009-03-25
Resolution : 2.20 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

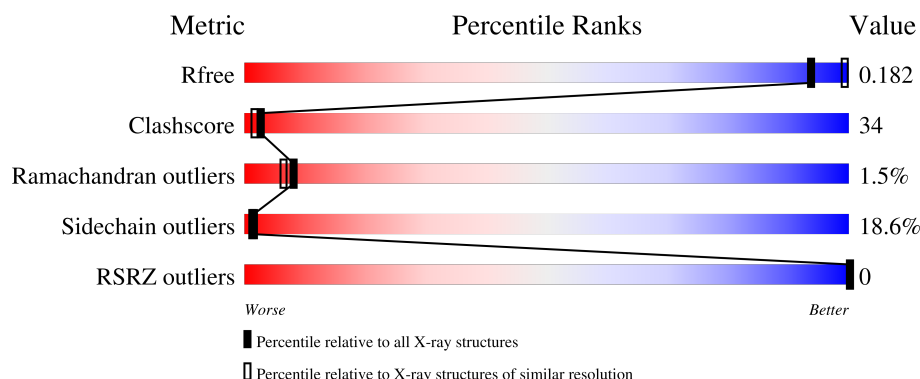
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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.



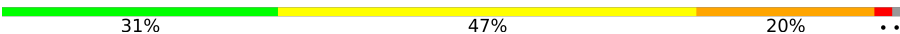
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	390	
1	B	390	
1	C	390	
1	D	390	
1	E	390	

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Mol	Chain	Length	Quality of chain
1	F	390	
1	G	390	
1	H	390	

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	AKG	B	402	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 25205 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 ColD.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	384	Total	C	N	O	P	S	0	1	0
			3092	1983	505	589	1	14			
1	B	385	Total	C	N	O	P	S	0	1	0
			3104	1992	506	591	1	14			
1	C	388	Total	C	N	O	P	S	0	1	0
			3128	2007	510	595	1	15			
1	D	381	Total	C	N	O	P	S	0	1	0
			3072	1969	502	586	1	14			
1	E	383	Total	C	N	O	P	S	0	1	0
			3082	1977	503	587	1	14			
1	F	386	Total	C	N	O	P	S	0	1	0
			3112	1996	508	593	1	14			
1	G	387	Total	C	N	O	P	S	0	1	0
			3120	2002	509	594	1	14			
1	H	381	Total	C	N	O	P	S	0	1	0
			3072	1969	502	586	1	14			

There are 32 discrepancies between the modelled and reference sequences:

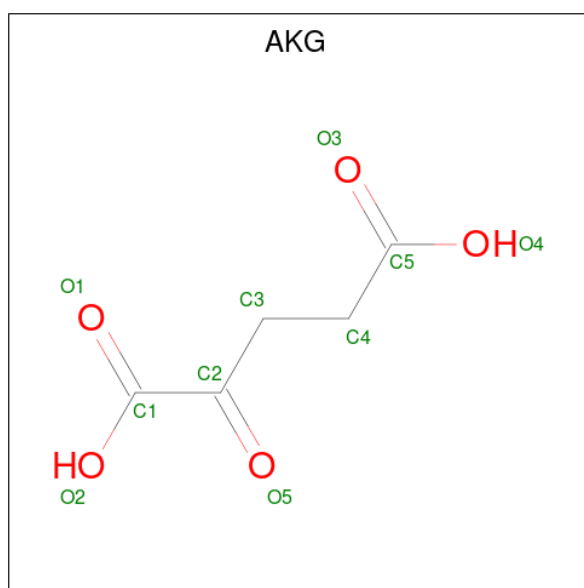
Chain	Residue	Modelled	Actual	Comment	Reference
A	-1	GLY	-	expression tag	UNP Q9F118
A	0	HIS	-	expression tag	UNP Q9F118
A	187	ASN	SER	engineered mutation	UNP Q9F118
A	188	LLP	HIS	engineered mutation	UNP Q9F118
B	-1	GLY	-	expression tag	UNP Q9F118
B	0	HIS	-	expression tag	UNP Q9F118
B	187	ASN	SER	engineered mutation	UNP Q9F118
B	188	LLP	HIS	engineered mutation	UNP Q9F118
C	-1	GLY	-	expression tag	UNP Q9F118
C	0	HIS	-	expression tag	UNP Q9F118
C	187	ASN	SER	engineered mutation	UNP Q9F118
C	188	LLP	HIS	engineered mutation	UNP Q9F118
D	-1	GLY	-	expression tag	UNP Q9F118

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Chain	Residue	Modelled	Actual	Comment	Reference
D	0	HIS	-	expression tag	UNP Q9F118
D	187	ASN	SER	engineered mutation	UNP Q9F118
D	188	LLP	HIS	engineered mutation	UNP Q9F118
E	-1	GLY	-	expression tag	UNP Q9F118
E	0	HIS	-	expression tag	UNP Q9F118
E	187	ASN	SER	engineered mutation	UNP Q9F118
E	188	LLP	HIS	engineered mutation	UNP Q9F118
F	-1	GLY	-	expression tag	UNP Q9F118
F	0	HIS	-	expression tag	UNP Q9F118
F	187	ASN	SER	engineered mutation	UNP Q9F118
F	188	LLP	HIS	engineered mutation	UNP Q9F118
G	-1	GLY	-	expression tag	UNP Q9F118
G	0	HIS	-	expression tag	UNP Q9F118
G	187	ASN	SER	engineered mutation	UNP Q9F118
G	188	LLP	HIS	engineered mutation	UNP Q9F118
H	-1	GLY	-	expression tag	UNP Q9F118
H	0	HIS	-	expression tag	UNP Q9F118
H	187	ASN	SER	engineered mutation	UNP Q9F118
H	188	LLP	HIS	engineered mutation	UNP Q9F118

- Molecule 2 is 2-OXOGLUTARIC ACID (CCD ID: AKG) (formula: C₅H₆O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	5	5		
2	B	1	Total	C	O	0	0
			10	5	5		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	C	1	Total	C	O	0	0
			10	5	5		
2	D	1	Total	C	O	0	0
			10	5	5		
2	F	1	Total	C	O	0	0
			10	5	5		
2	H	1	Total	C	O	0	0
			10	5	5		

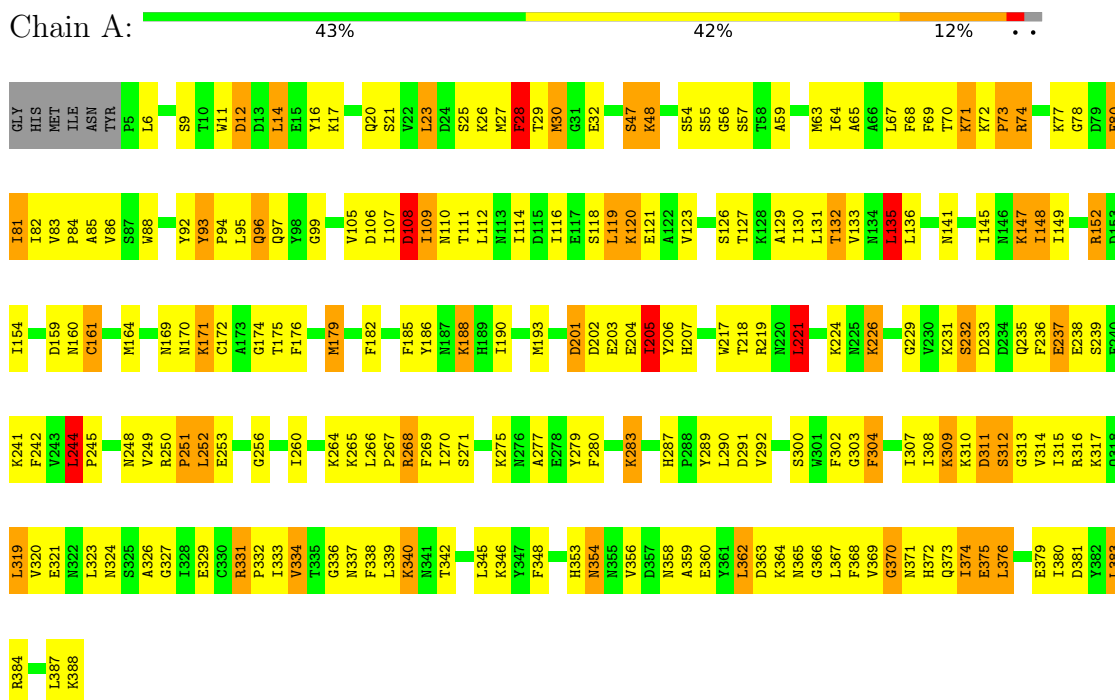
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	42	Total	O	0	0
			42	42		
3	B	52	Total	O	0	0
			52	52		
3	C	50	Total	O	0	0
			50	50		
3	D	55	Total	O	0	0
			55	55		
3	E	37	Total	O	0	0
			37	37		
3	F	43	Total	O	0	0
			43	43		
3	G	41	Total	O	0	0
			41	41		
3	H	43	Total	O	0	0
			43	43		

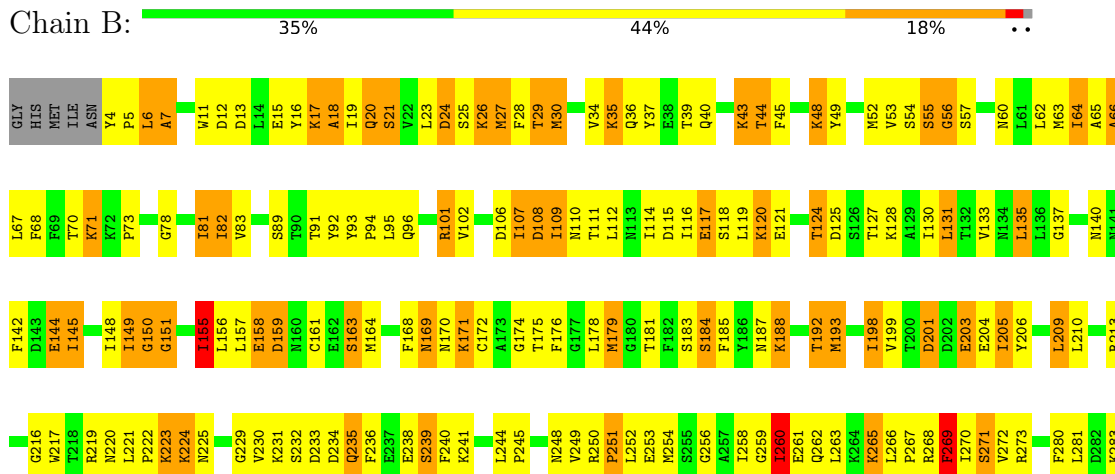
3 Residue-property plots

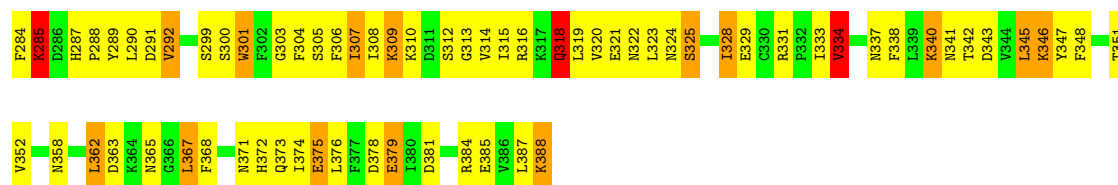
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Cold



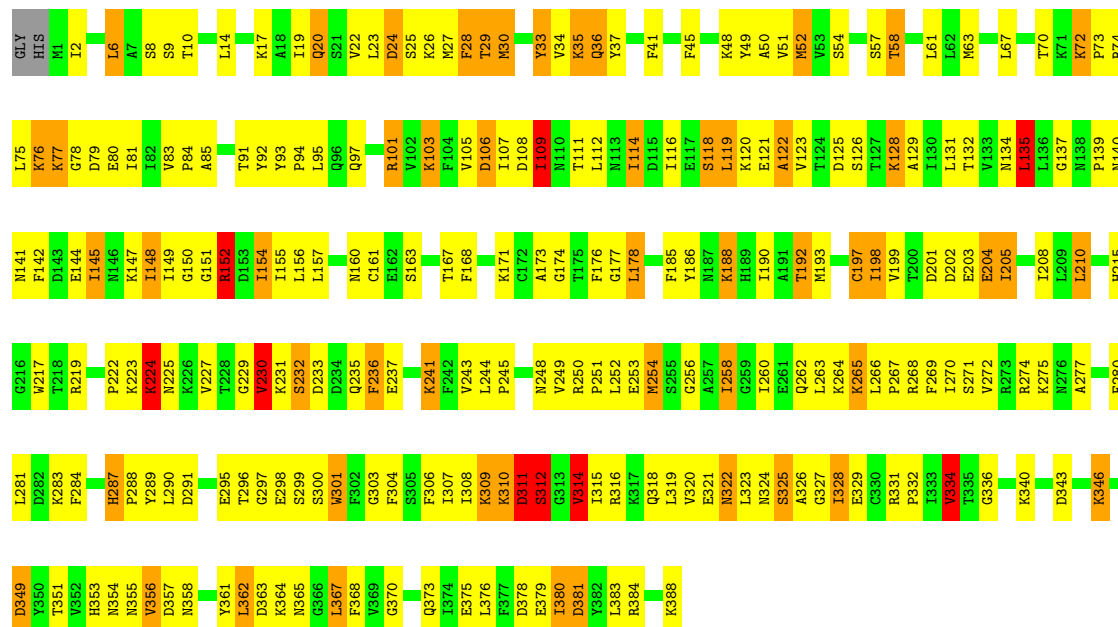
• Molecule 1: Cold





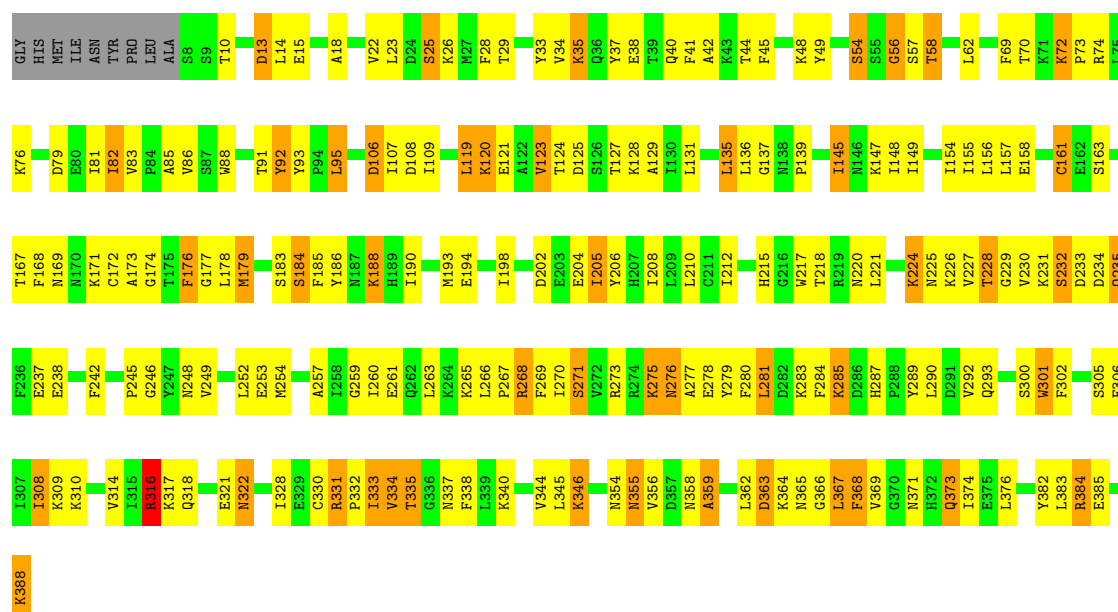
• Molecule 1: Cold

Chain C: 37% 46% 14% ..



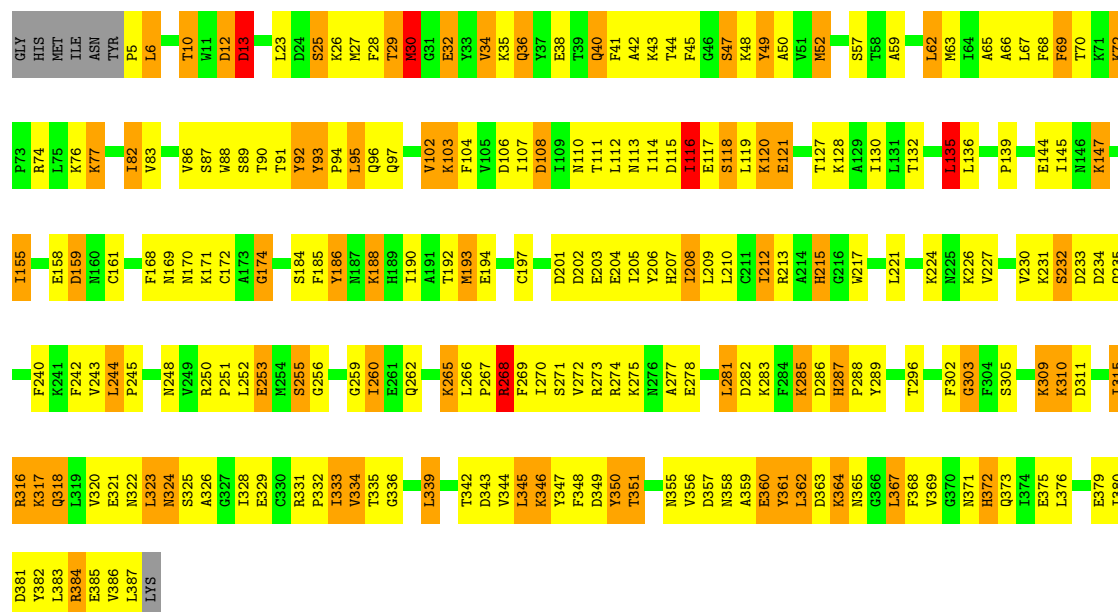
• Molecule 1: Cold

Chain D: 45% 40% 12% .



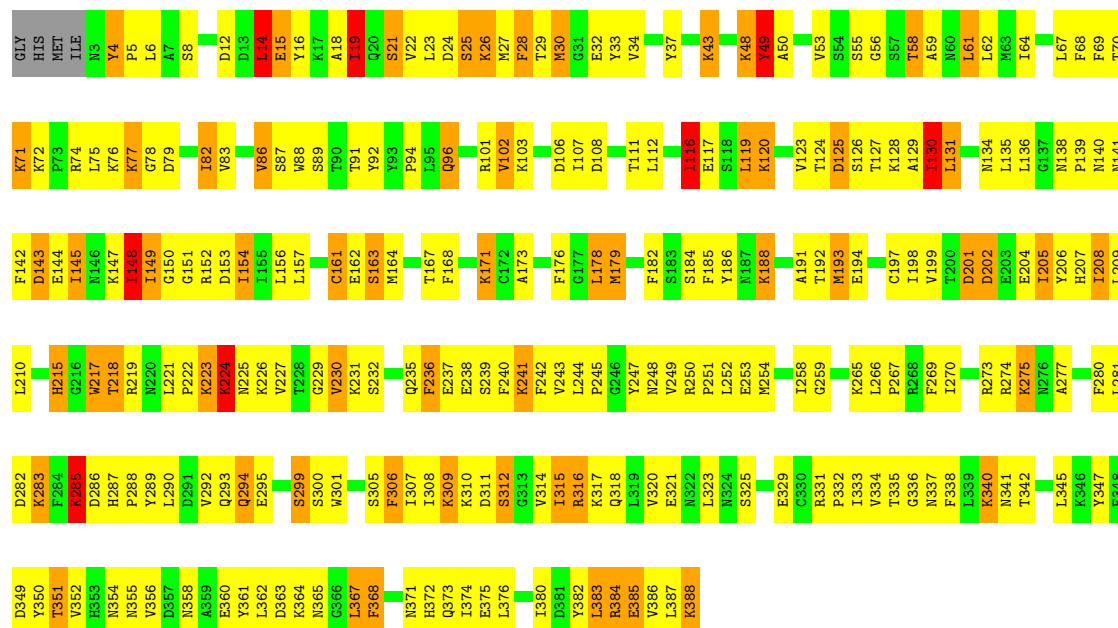
- Molecule 1: ColD

Chain E:  40% 40% 17% ..

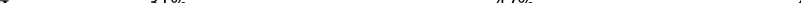


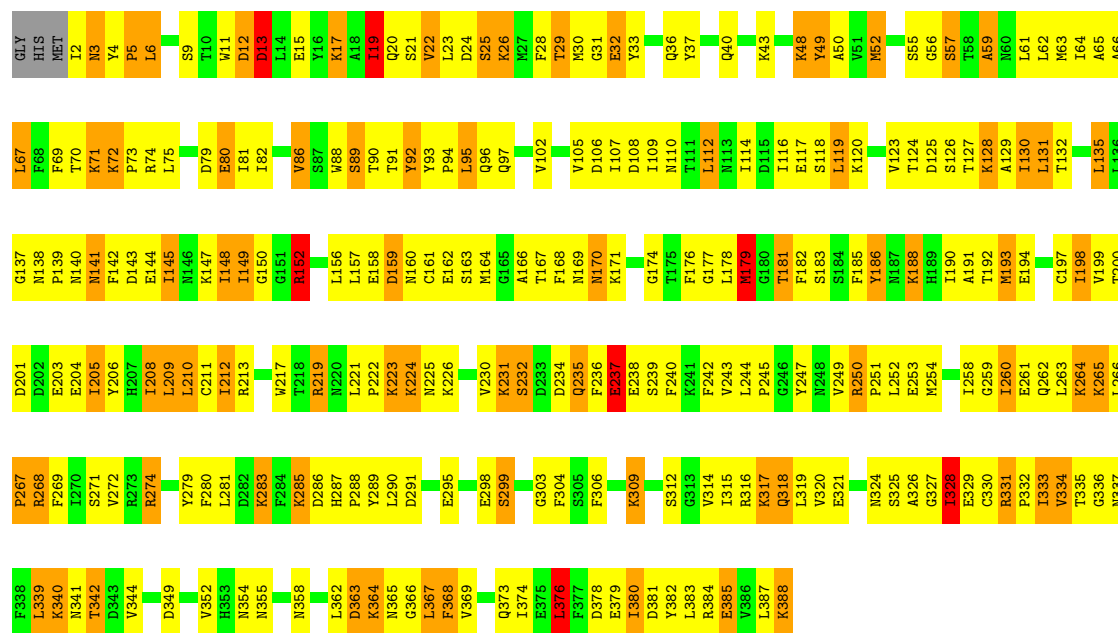
- Molecule 1: ColD

Chain F: 34% 48% 15% 3%

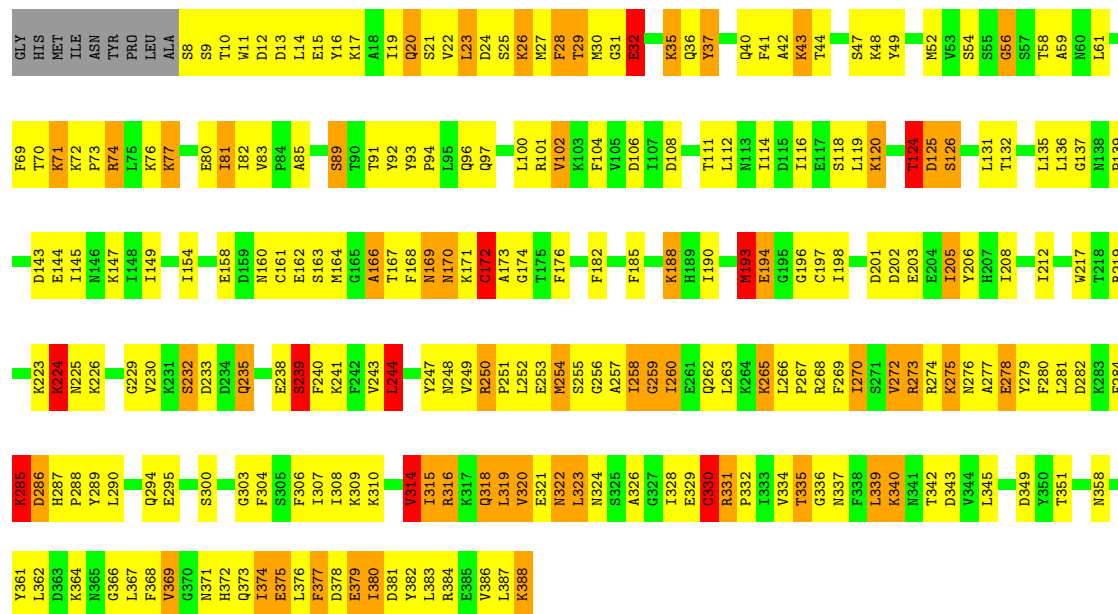


- Molecule 1: ColD

Chain G:  31% 47% 20% 2%



- Molecule 1: ColD



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	69.73Å 114.66Å 114.57Å 78.98° 76.23° 76.33°	Depositor
Resolution (Å)	50.00 – 2.20 50.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	90.8 (50.00-2.20) 90.7 (50.00-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.62 (at 2.20Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.177 , 0.272 0.182 , 0.182	Depositor DCC
R_{free} test set	15300 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å ²)	19.3	Xtriage
Anisotropy	0.172	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 54.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	0.289 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	25205	wwPDB-VP
Average B, all atoms (Å ²)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.91 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.4201e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: AKG, LLP

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	0.90	2/3134 (0.1%)	1.48	39/4230 (0.9%)
1	B	0.90	1/3147 (0.0%)	1.49	49/4249 (1.2%)
1	C	0.90	3/3171 (0.1%)	1.49	54/4281 (1.3%)
1	D	0.92	2/3113 (0.1%)	1.50	43/4201 (1.0%)
1	E	0.86	3/3124 (0.1%)	1.46	41/4219 (1.0%)
1	F	0.86	2/3155 (0.1%)	1.46	48/4260 (1.1%)
1	G	0.86	2/3163 (0.1%)	1.46	48/4271 (1.1%)
1	H	0.83	2/3113 (0.1%)	1.50	44/4201 (1.0%)
All	All	0.88	17/25120 (0.1%)	1.48	366/33912 (1.1%)

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	52	MET	SD-CE	9.59	2.03	1.79
1	F	164	MET	SD-CE	7.42	1.98	1.79
1	D	179	MET	SD-CE	6.99	1.97	1.79
1	A	164	MET	SD-CE	6.68	1.96	1.79
1	E	52	MET	SD-CE	6.63	1.96	1.79
1	E	30	MET	SD-CE	5.90	1.94	1.79
1	D	123	VAL	CA-CB	-5.78	1.47	1.54
1	E	116	ILE	CA-CB	-5.66	1.46	1.54
1	H	244	LEU	CA-C	-5.55	1.46	1.52
1	H	193	MET	SD-CE	5.52	1.93	1.79
1	G	231	LYS	CB-CG	5.50	1.69	1.52
1	G	179	MET	SD-CE	5.38	1.93	1.79
1	C	254	MET	SD-CE	5.37	1.93	1.79
1	C	123	VAL	CA-CB	-5.28	1.47	1.54
1	A	130	ILE	CA-CB	-5.18	1.47	1.54
1	F	30	MET	SD-CE	-5.14	1.66	1.79
1	B	95	LEU	CA-C	-5.04	1.46	1.52

All (366) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	25	SER	N-CA-C	-12.39	99.14	114.75
1	E	227	VAL	N-CA-C	11.34	121.99	111.45
1	B	178	LEU	N-CA-C	-11.12	98.98	112.54
1	G	13	ASP	N-CA-C	-10.95	100.66	114.56
1	B	249	VAL	N-CA-C	10.80	121.52	111.91
1	C	119	LEU	N-CA-C	-9.64	100.46	110.97
1	H	330	CYS	N-CA-C	9.52	123.94	108.99
1	B	155	ILE	N-CA-C	9.46	123.25	109.63
1	C	91	THR	N-CA-C	-9.45	100.07	111.69
1	H	322	ASN	N-CA-C	9.38	122.70	111.82
1	H	91	THR	N-CA-C	-9.31	101.34	112.89
1	H	205	ILE	CB-CA-C	-9.30	100.06	111.97
1	B	91	THR	N-CA-C	-9.23	100.33	111.69
1	D	316	ARG	N-CA-C	9.23	122.18	111.11
1	C	92	TYR	N-CA-C	8.93	122.30	111.40
1	H	379	GLU	N-CA-C	-8.93	101.55	111.28
1	G	25	SER	N-CA-C	-8.90	101.65	111.36
1	F	116	ILE	N-CA-C	8.90	118.93	110.30
1	F	28	PHE	N-CA-C	8.89	123.92	112.89
1	D	54	SER	N-CA-C	8.85	120.92	111.28
1	F	24	ASP	N-CA-C	-8.76	101.81	111.36
1	A	135	LEU	N-CA-C	8.67	122.52	109.25
1	D	279	TYR	N-CA-C	-8.44	102.08	111.28
1	A	54	SER	N-CA-C	8.44	120.48	111.28
1	H	147	LYS	N-CA-C	-8.39	102.08	111.14
1	G	198	ILE	N-CA-C	-8.37	95.99	108.46
1	D	302	PHE	N-CA-C	-8.27	101.33	111.33
1	G	178	LEU	N-CA-C	-8.25	102.22	111.71
1	A	108	ASP	N-CA-C	-8.19	95.89	109.07
1	D	276	ASN	N-CA-C	-8.14	101.47	111.40
1	E	371	ASN	N-CA-C	-8.09	96.29	108.99
1	F	224	LYS	N-CA-C	-8.06	96.55	109.76
1	E	135	LEU	N-CA-C	7.99	121.94	109.96
1	E	13	ASP	N-CA-C	7.94	122.81	113.20
1	B	269	PHE	N-CA-C	-7.88	102.28	111.03
1	H	194	GLU	N-CA-C	-7.86	95.81	108.55
1	F	201	ASP	N-CA-C	-7.83	103.24	114.12
1	G	129	ALA	N-CA-C	7.82	120.75	108.79
1	F	285	LYS	N-CA-C	7.78	120.51	111.02
1	C	205	ILE	CB-CA-C	-7.73	101.99	111.88
1	G	194	GLU	N-CA-C	-7.71	97.66	109.14
1	B	56	GLY	N-CA-C	-7.70	103.50	112.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	243	VAL	N-CA-C	7.69	121.81	113.43
1	B	6	LEU	N-CA-C	-7.69	102.90	111.82
1	A	119	LEU	N-CA-C	-7.62	103.05	111.36
1	H	320	VAL	N-CA-C	-7.61	102.92	110.30
1	C	287	HIS	N-CA-C	7.57	120.47	109.71
1	D	95	LEU	N-CA-C	-7.45	103.10	111.07
1	F	49	TYR	N-CA-C	7.44	121.60	109.85
1	G	95	LEU	N-CA-C	-7.38	103.32	111.36
1	H	201	ASP	N-CA-C	-7.36	104.54	113.97
1	H	300	SER	N-CA-C	-7.34	103.89	112.92
1	B	171	LYS	N-CA-C	-7.33	96.59	109.06
1	A	300	SER	N-CA-C	-7.33	103.91	112.92
1	C	78	GLY	N-CA-C	-7.33	104.34	114.67
1	G	210	LEU	N-CA-C	-7.30	103.32	111.71
1	D	13	ASP	N-CA-C	7.27	120.08	111.71
1	G	191	ALA	N-CA-C	7.27	120.26	108.41
1	C	28	PHE	N-CA-C	7.26	122.27	113.41
1	H	89	SER	N-CA-C	7.25	120.11	111.33
1	F	194	GLU	N-CA-C	-7.25	98.05	109.50
1	A	32	GLU	N-CA-C	7.24	119.25	111.36
1	H	92	TYR	N-CA-C	7.20	122.73	113.88
1	B	219	ARG	N-CA-C	7.18	121.67	112.34
1	F	375	GLU	N-CA-C	7.16	120.61	110.23
1	E	347	TYR	N-CA-C	7.14	122.25	112.90
1	G	59	ALA	N-CA-C	-7.13	103.59	111.36
1	C	256	GLY	N-CA-C	-7.09	104.06	112.64
1	A	9	SER	N-CA-C	7.09	119.36	109.15
1	C	125	ASP	N-CA-C	-7.09	104.10	112.89
1	F	161	CYS	N-CA-C	7.07	119.84	111.71
1	H	335	THR	N-CA-C	-7.06	102.50	113.02
1	G	92	TYR	N-CA-C	7.04	122.19	112.04
1	F	96	GLN	N-CA-C	-7.03	103.70	111.36
1	D	58	THR	N-CA-C	-7.00	104.00	112.54
1	E	91	THR	N-CA-C	-7.00	104.21	112.89
1	B	7	ALA	N-CA-C	6.97	119.52	109.14
1	B	289	TYR	N-CA-C	6.95	122.74	112.94
1	E	92	TYR	N-CA-C	6.95	121.81	113.12
1	B	161	CYS	N-CA-C	6.95	119.70	111.71
1	E	29	THR	CB-CA-C	-6.94	98.08	109.53
1	C	174	GLY	N-CA-C	-6.92	106.22	115.21
1	C	140	ASN	N-CA-C	-6.90	100.77	110.50
1	E	69	PHE	N-CA-C	6.90	121.87	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	102	VAL	N-CA-C	6.88	118.03	107.99
1	D	176	PHE	N-CA-C	6.79	118.77	111.36
1	F	231	LYS	N-CA-C	6.78	119.73	108.96
1	G	352	VAL	N-CA-C	6.77	117.60	107.51
1	B	201	ASP	N-CA-C	-6.77	103.45	113.61
1	D	91	THR	N-CA-C	-6.76	103.71	112.23
1	A	251	PRO	N-CA-C	-6.76	101.76	111.22
1	B	362	LEU	N-CA-C	-6.75	103.92	111.28
1	D	281	LEU	CA-C-O	6.74	127.72	120.10
1	E	365	ASN	CA-C-N	-6.74	117.53	122.18
1	E	365	ASN	C-N-CA	-6.74	117.53	122.18
1	D	135	LEU	N-CA-C	6.73	120.64	109.46
1	E	272	VAL	CB-CA-C	-6.73	103.05	112.14
1	D	293	GLN	N-CA-C	6.72	120.62	109.46
1	B	331	ARG	N-CA-C	6.71	114.04	108.07
1	D	290	LEU	N-CA-C	6.70	119.82	108.90
1	H	116	ILE	N-CA-C	6.67	117.46	110.72
1	F	102	VAL	N-CA-C	6.63	117.85	108.36
1	C	204	GLU	N-CA-C	-6.60	103.71	111.03
1	B	43	LYS	N-CA-C	-6.58	104.03	111.07
1	E	12	ASP	N-CA-C	-6.58	98.99	108.07
1	G	96	GLN	N-CA-C	-6.58	104.19	111.36
1	F	92	TYR	N-CA-C	6.58	119.73	111.24
1	F	227	VAL	N-CA-C	6.58	117.56	111.45
1	F	385	GLU	N-CA-C	-6.57	103.38	111.40
1	E	172	CYS	N-CA-C	6.54	120.16	109.76
1	B	174	GLY	N-CA-C	-6.53	106.92	114.69
1	F	295	GLU	N-CA-C	6.52	119.68	110.23
1	H	102	VAL	N-CA-C	6.51	117.67	108.36
1	C	295	GLU	N-CA-C	6.50	119.71	109.96
1	H	19	ILE	CB-CA-C	-6.50	103.25	112.22
1	E	104	PHE	N-CA-C	6.48	120.07	110.48
1	C	135	LEU	N-CA-C	6.47	120.05	109.76
1	H	343	ASP	N-CA-C	6.47	118.42	111.36
1	B	55	SER	N-CA-C	6.47	118.05	108.60
1	F	306	PHE	CB-CA-C	-6.47	100.17	110.14
1	F	130	ILE	CB-CA-C	-6.44	103.07	110.41
1	G	237	GLU	N-CA-C	6.42	121.15	113.12
1	G	204	GLU	N-CA-C	-6.42	103.97	110.97
1	B	124	THR	N-CA-C	6.41	116.91	108.07
1	D	85	ALA	N-CA-C	6.40	120.69	113.01
1	H	172	CYS	N-CA-C	6.40	120.31	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	174	GLY	N-CA-C	-6.39	106.31	114.37
1	B	343	ASP	N-CA-C	6.39	118.04	111.14
1	F	148	ILE	N-CA-C	-6.38	104.42	110.42
1	D	92	TYR	N-CA-C	6.38	121.25	112.90
1	C	154	ILE	N-CA-C	6.37	117.47	108.36
1	D	198	ILE	CB-CA-C	-6.35	101.23	110.63
1	A	116	ILE	CB-CA-C	-6.34	103.85	111.97
1	D	215	HIS	N-CA-C	6.34	120.80	113.38
1	H	198	ILE	CB-CA-C	-6.34	101.25	110.63
1	F	351	THR	N-CA-C	-6.31	99.09	108.99
1	C	270	ILE	N-CA-C	6.28	117.06	110.72
1	H	258	ILE	CB-CA-C	-6.24	101.06	111.29
1	F	270	ILE	CB-CA-C	-6.23	103.85	112.02
1	A	152	ARG	N-CA-C	6.23	119.28	110.50
1	E	72	LYS	N-CA-C	-6.23	98.75	109.15
1	E	102	VAL	N-CA-C	6.22	117.54	108.58
1	C	85	ALA	N-CA-C	6.20	120.31	112.87
1	A	370	GLY	N-CA-C	6.20	122.00	112.51
1	E	323	LEU	N-CA-C	6.19	118.11	111.36
1	B	198	ILE	CB-CA-C	-6.18	101.99	110.77
1	B	145	ILE	N-CA-C	-6.17	104.73	110.53
1	H	285	LYS	N-CA-C	6.17	118.00	111.28
1	C	101	ARG	CA-C-N	-6.16	115.55	123.19
1	C	101	ARG	C-N-CA	-6.16	115.55	123.19
1	F	173	ALA	N-CA-C	-6.16	101.98	110.35
1	H	386	VAL	N-CA-C	-6.14	104.35	110.62
1	F	91	THR	N-CA-C	-6.14	104.49	112.23
1	F	154	ILE	CB-CA-C	-6.14	102.19	111.33
1	A	72	LYS	N-CA-C	-6.13	97.39	109.10
1	H	37	TYR	N-CA-C	6.12	117.95	111.28
1	G	91	THR	N-CA-C	-6.12	104.16	111.69
1	G	19	ILE	N-CA-C	-6.10	105.19	110.74
1	E	42	ALA	N-CA-C	-6.08	104.76	111.82
1	A	364	LYS	N-CA-C	6.07	120.75	113.23
1	F	293	GLN	CA-C-N	-6.06	114.35	122.72
1	F	293	GLN	C-N-CA	-6.06	114.35	122.72
1	H	69	PHE	N-CA-C	6.06	120.38	112.92
1	D	363	ASP	N-CA-C	6.05	117.88	111.28
1	B	220	ASN	N-CA-C	-6.04	105.09	112.88
1	H	224	LYS	N-CA-C	-6.04	99.36	108.96
1	A	92	TYR	N-CA-C	5.99	120.77	112.45
1	H	56	GLY	N-CA-C	-5.99	105.55	112.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	109	ILE	N-CA-C	5.98	120.51	111.89
1	B	251	PRO	N-CA-C	-5.98	100.38	111.03
1	A	374	ILE	N-CA-C	-5.98	99.11	108.86
1	G	67	LEU	N-CA-C	5.97	119.67	112.38
1	A	161	CYS	N-CA-C	5.96	119.66	112.38
1	C	109	ILE	N-CA-C	5.96	117.42	110.62
1	G	152	ARG	N-CA-C	5.95	118.86	110.23
1	D	230	VAL	N-CA-C	5.95	116.74	107.28
1	E	32	GLU	N-CA-C	5.95	117.85	111.36
1	B	102	VAL	N-CA-C	5.95	117.15	108.58
1	E	174	GLY	N-CA-C	-5.95	107.86	115.42
1	C	35	LYS	N-CA-C	5.94	118.52	111.33
1	F	282	ASP	N-CA-C	-5.94	104.71	111.07
1	A	11	TRP	N-CA-C	5.93	119.15	109.59
1	G	224	LYS	N-CA-C	-5.91	99.60	109.24
1	H	108	ASP	N-CA-C	-5.88	99.65	109.24
1	F	226	LYS	N-CA-C	5.88	120.18	112.89
1	G	349	ASP	N-CA-C	-5.87	95.89	107.69
1	C	370	GLY	N-CA-C	5.87	120.05	112.54
1	E	159	ASP	N-CA-C	-5.87	97.60	107.99
1	G	330	CYS	N-CA-C	5.85	118.08	109.24
1	F	86	VAL	N-CA-C	5.85	116.71	108.17
1	B	331	ARG	N-CA-CB	-5.84	105.28	111.29
1	F	14	LEU	N-CA-C	5.81	119.19	111.75
1	A	201	ASP	N-CA-C	-5.81	105.52	113.30
1	D	335	THR	N-CA-C	-5.80	105.39	112.88
1	D	365	ASN	CA-C-N	-5.79	117.19	122.80
1	D	365	ASN	C-N-CA	-5.79	117.19	122.80
1	B	374	ILE	N-CA-C	-5.78	99.41	108.95
1	C	326	ALA	N-CA-C	5.77	120.16	113.18
1	G	159	ASP	N-CA-C	-5.76	99.14	108.41
1	B	66	ALA	N-CA-C	5.75	118.01	111.11
1	C	33	TYR	N-CA-C	-5.74	104.92	111.07
1	A	304	PHE	N-CA-C	5.74	118.06	108.02
1	G	86	VAL	N-CA-C	5.74	116.83	106.61
1	C	346	LYS	N-CA-C	-5.73	104.39	111.33
1	D	106	ASP	N-CA-C	5.72	118.57	110.50
1	C	173	ALA	N-CA-C	-5.72	102.43	110.50
1	F	218	THR	CB-CA-C	-5.72	100.54	110.09
1	G	57	SER	N-CA-C	5.72	117.51	111.28
1	F	164	MET	N-CA-C	-5.71	101.39	109.96
1	H	219	ARG	N-CA-C	5.71	119.06	111.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	13	ASP	N-CA-C	-5.70	106.67	113.97
1	B	318	GLN	N-CA-C	-5.69	103.84	112.04
1	B	371	ASN	N-CA-C	-5.69	100.51	109.50
1	C	327	GLY	N-CA-C	-5.69	106.89	115.32
1	F	202	ASP	N-CA-C	5.68	118.00	108.23
1	E	372	HIS	N-CA-C	5.68	115.78	108.34
1	G	127	THR	N-CA-C	5.67	117.92	109.59
1	C	309	LYS	N-CA-C	5.67	118.23	110.24
1	C	230	VAL	N-CA-C	5.65	116.14	107.77
1	G	107	ILE	CB-CA-C	-5.65	103.11	111.19
1	A	190	ILE	N-CA-C	-5.65	100.94	108.96
1	B	198	ILE	CA-C-N	-5.64	116.11	122.48
1	B	198	ILE	C-N-CA	-5.64	116.11	122.48
1	G	119	LEU	N-CA-C	-5.63	104.35	111.11
1	B	192	THR	N-CA-C	-5.62	103.26	111.30
1	E	255	SER	N-CA-C	-5.62	105.92	112.89
1	B	78	GLY	N-CA-C	-5.62	107.91	115.21
1	D	322	ASN	N-CA-C	5.61	117.07	111.07
1	D	174	GLY	N-CA-C	-5.61	106.76	114.67
1	H	124	THR	N-CA-CB	-5.61	102.53	111.62
1	D	158	GLU	N-CA-C	5.60	118.59	109.24
1	F	215	HIS	N-CA-C	5.60	122.72	110.80
1	F	342	THR	N-CA-C	5.59	118.10	111.33
1	E	303	GLY	N-CA-C	-5.58	103.09	111.19
1	H	270	ILE	N-CA-C	5.58	115.81	110.74
1	F	163	SER	N-CA-C	5.57	117.13	110.44
1	A	23	LEU	N-CA-C	-5.57	105.11	111.07
1	D	268	ARG	N-CA-C	5.55	117.33	111.28
1	E	272	VAL	N-CA-C	5.55	116.28	110.62
1	H	23	LEU	N-CA-C	-5.54	105.14	111.07
1	A	147	LYS	N-CA-C	-5.53	104.94	110.97
1	C	178	LEU	N-CA-C	-5.53	105.79	112.54
1	A	96	GLN	N-CA-C	-5.52	105.17	111.14
1	H	323	LEU	N-CA-C	-5.52	105.42	111.82
1	D	205	ILE	CB-CA-C	-5.51	104.83	111.88
1	D	359	ALA	N-CA-C	-5.50	105.44	111.82
1	H	166	ALA	N-CA-C	-5.50	102.34	110.48
1	E	95	LEU	N-CA-C	-5.50	104.98	110.97
1	G	376	LEU	N-CA-C	5.50	119.62	111.87
1	F	208	ILE	CB-CA-C	-5.49	104.65	112.22
1	F	82	ILE	N-CA-C	5.48	116.19	108.36
1	H	28	PHE	N-CA-C	5.47	119.94	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	268	ARG	N-CA-C	-5.46	104.19	111.24
1	B	44	THR	N-CA-C	5.46	117.66	111.11
1	C	122	ALA	N-CA-C	5.46	119.44	112.34
1	A	244	LEU	O-C-N	5.46	125.76	121.88
1	F	19	ILE	CB-CA-C	-5.46	104.69	112.22
1	E	25	SER	N-CA-C	-5.46	105.49	111.82
1	G	374	ILE	CB-CA-C	-5.45	103.29	110.98
1	C	349	ASP	N-CA-C	-5.45	96.89	107.62
1	E	93	TYR	CA-C-N	5.45	125.53	119.32
1	E	93	TYR	C-N-CA	5.45	125.53	119.32
1	D	139	PRO	N-CA-C	5.44	120.03	111.38
1	F	301	TRP	N-CA-C	5.44	118.84	111.17
1	F	251	PRO	N-CA-C	-5.43	103.04	111.13
1	D	173	ALA	N-CA-C	-5.43	103.37	110.53
1	E	361	TYR	N-CA-C	-5.43	104.40	111.02
1	D	25	SER	N-CA-C	-5.42	106.17	112.89
1	F	205	ILE	CB-CA-C	-5.41	102.42	111.29
1	B	301	TRP	N-CA-C	5.40	118.79	111.17
1	D	338	PHE	N-CA-C	5.40	118.09	111.82
1	F	143	ASP	N-CA-C	-5.40	104.94	112.45
1	G	328	ILE	CB-CA-C	-5.40	103.50	110.84
1	A	93	TYR	CA-C-O	5.40	123.29	118.33
1	D	161	CYS	N-CA-C	5.39	119.48	113.01
1	C	36	GLN	N-CA-C	-5.39	105.49	111.36
1	B	169	ASN	N-CA-C	-5.38	107.09	113.38
1	D	119	LEU	N-CA-C	5.37	116.81	111.07
1	G	139	PRO	N-CA-C	5.37	119.46	111.41
1	G	80	GLU	N-CA-C	5.36	117.48	108.96
1	F	275	LYS	N-CA-C	-5.35	105.34	111.07
1	C	192	THR	N-CA-C	-5.35	104.03	110.88
1	G	342	THR	N-CA-C	5.35	117.11	111.28
1	F	15	GLU	N-CA-C	-5.34	103.38	111.56
1	B	151	GLY	N-CA-C	-5.34	97.81	113.30
1	C	118	SER	N-CA-C	-5.32	105.94	112.90
1	E	194	GLU	N-CA-C	-5.32	100.64	108.99
1	G	363	ASP	N-CA-C	5.31	117.75	111.33
1	H	377	PHE	N-CA-C	5.31	117.48	111.11
1	B	18	ALA	N-CA-C	-5.30	105.58	111.36
1	A	221	LEU	CA-C-N	5.29	125.27	120.03
1	A	221	LEU	C-N-CA	5.29	125.27	120.03
1	B	163	SER	N-CA-C	5.29	118.86	111.30
1	G	89	SER	N-CA-C	5.28	117.72	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	56	GLY	N-CA-C	-5.27	106.33	113.24
1	C	54	SER	N-CA-C	5.26	117.77	111.71
1	A	256	GLY	N-CA-C	-5.26	106.12	112.49
1	H	32	GLU	N-CA-C	5.25	116.81	111.14
1	H	270	ILE	CB-CA-C	-5.24	105.02	111.94
1	A	205	ILE	CB-CA-C	-5.24	105.07	112.14
1	C	10	THR	N-CA-C	-5.24	106.48	112.92
1	B	101	ARG	CB-CA-C	5.23	118.66	110.19
1	G	135	LEU	N-CA-C	5.23	118.14	109.46
1	E	82	ILE	CB-CA-C	-5.22	102.87	110.81
1	C	227	VAL	N-CA-C	5.22	116.05	111.56
1	G	219	ARG	N-CA-C	5.21	119.12	112.87
1	D	49	TYR	N-CA-C	5.20	117.30	109.23
1	A	148	ILE	CB-CA-C	-5.20	105.13	112.14
1	C	315	ILE	N-CA-C	5.20	115.79	108.36
1	A	80	GLU	N-CA-C	5.19	117.22	108.96
1	E	248	ASN	N-CA-C	-5.19	98.93	108.02
1	G	69	PHE	N-CA-C	5.19	120.47	113.72
1	C	243	VAL	N-CA-C	5.19	118.71	113.47
1	A	326	ALA	N-CA-C	-5.19	106.54	112.92
1	E	49	TYR	N-CA-C	5.19	117.56	109.52
1	B	159	ASP	N-CA-C	-5.19	99.31	108.23
1	E	66	ALA	N-CA-C	5.19	117.61	111.33
1	C	129	ALA	N-CA-C	5.18	116.17	108.60
1	A	28	PHE	N-CA-C	5.18	119.75	113.38
1	E	349	ASP	N-CA-C	-5.17	96.85	107.67
1	C	289	TYR	N-CA-C	5.17	121.31	112.99
1	B	260	ILE	CB-CA-C	-5.16	105.28	112.04
1	G	181	THR	N-CA-C	5.16	118.15	109.95
1	A	309	LYS	N-CA-C	5.16	117.71	110.23
1	E	59	ALA	N-CA-C	-5.16	105.57	111.14
1	D	72	LYS	N-CA-C	-5.15	98.34	109.01
1	D	308	ILE	N-CA-C	-5.15	102.86	109.30
1	B	340	LYS	N-CA-C	-5.15	106.95	113.18
1	C	363	ASP	CA-C-N	-5.14	114.52	122.49
1	C	363	ASP	C-N-CA	-5.14	114.52	122.49
1	D	246	GLY	N-CA-C	5.14	121.72	112.77
1	H	314	VAL	CB-CA-C	-5.14	102.86	111.29
1	G	339	LEU	CA-CB-CG	-5.13	98.35	116.30
1	D	330	CYS	N-CA-C	5.12	116.08	108.86
1	C	134	ASN	N-CA-C	-5.12	100.17	108.41
1	C	208	ILE	N-CA-C	-5.11	105.00	110.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	331	ARG	CB-CA-C	-5.10	104.54	110.76
1	D	227	VAL	N-CA-C	5.10	116.19	111.45
1	A	25	SER	N-CA-C	-5.09	106.33	112.54
1	A	69	PHE	N-CA-C	5.09	119.58	113.17
1	C	312	SER	N-CA-C	5.08	116.51	111.07
1	B	54	SER	N-CA-C	5.08	117.55	111.71
1	A	73	PRO	N-CA-C	5.08	118.47	110.80
1	E	324	ASN	N-CA-C	-5.08	105.64	111.07
1	G	365	ASN	CA-C-N	-5.08	118.68	122.18
1	G	365	ASN	C-N-CA	-5.08	118.68	122.18
1	B	149	ILE	N-CA-C	5.08	115.74	110.82
1	C	381	ASP	N-CA-C	-5.07	105.20	111.33
1	C	30	MET	N-CA-C	5.07	118.14	110.64
1	H	143	ASP	N-CA-C	-5.07	105.46	111.69
1	C	168	PHE	N-CA-C	-5.06	99.42	108.13
1	C	328	ILE	N-CA-C	5.06	115.14	107.80
1	H	120	LYS	CA-C-N	5.06	127.48	120.29
1	H	120	LYS	C-N-CA	5.06	127.48	120.29
1	F	338	PHE	N-CA-C	5.05	116.79	111.28
1	E	212	ILE	N-CA-C	5.05	119.56	113.00
1	F	360	GLU	N-CA-C	-5.05	105.69	111.14
1	C	224	LYS	N-CA-C	-5.04	99.21	108.02
1	G	250	ARG	N-CA-C	5.04	116.17	109.93
1	A	376	LEU	N-CA-C	5.03	118.90	112.26
1	C	314	VAL	N-CA-C	5.03	115.83	108.53
1	H	380	ILE	N-CA-C	5.03	115.25	110.42
1	B	273	ARG	N-CA-C	5.02	116.44	111.07
1	G	333	ILE	N-CA-C	-5.02	101.12	108.54
1	H	114	ILE	N-CA-C	5.01	115.86	109.30
1	G	56	GLY	N-CA-C	-5.00	106.67	113.37

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	3092	0	3063	178	0
1	B	3104	0	3070	217	0
1	C	3128	0	3099	203	0
1	D	3072	0	3039	149	0
1	E	3082	0	3050	198	0
1	F	3112	0	3076	260	0
1	G	3120	0	3088	269	0
1	H	3072	0	3039	224	0
2	A	10	0	4	1	0
2	B	10	0	4	5	0
2	C	10	0	4	1	0
2	D	10	0	4	2	0
2	F	10	0	4	3	0
2	H	10	0	4	0	0
3	A	42	0	0	4	0
3	B	52	0	0	4	0
3	C	50	0	0	4	0
3	D	55	0	0	7	0
3	E	37	0	0	4	0
3	F	43	0	0	4	0
3	G	41	0	0	6	0
3	H	43	0	0	6	0
All	All	25205	0	24548	1660	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 34.

All (1660) 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:C:52:MET:SD	1:C:52:MET:CE	2.03	1.46
1:F:188:LLP:H4'1	2:F:405:AKG:O5	1.36	1.25
1:B:124:THR:HG22	1:B:125:ASP:H	1.11	1.15
1:C:152:ARG:CG	1:C:152:ARG:HH21	1.59	1.12
1:F:222:PRO:HG2	1:F:225:ASN:HB3	1.26	1.09
1:E:316:ARG:NH2	1:E:364:LYS:HA	1.70	1.06
1:F:26:LYS:HB3	1:F:27:MET:HE2	1.34	1.05
1:H:124:THR:HG22	1:H:126:SER:H	1.18	1.05
1:G:222:PRO:HD2	1:G:225:ASN:HB3	1.40	1.04
1:G:6:LEU:HD12	1:G:329:GLU:HG2	1.36	1.02
1:C:128:LYS:NZ	1:C:128:LYS:HB3	1.74	1.01
1:F:315:ILE:HD13	1:F:315:ILE:H	1.24	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:63:MET:HE3	1:G:157:LEU:HD13	1.43	1.00
1:E:6:LEU:HD13	1:E:329:GLU:HG2	1.41	1.00
1:H:266:LEU:HB3	1:H:267:PRO:HD3	1.46	0.97
1:H:335:THR:HB	3:H:400:HOH:O	1.64	0.97
1:F:383:LEU:HD11	1:F:387:LEU:HD12	1.47	0.97
1:G:314:VAL:HG11	1:G:319:LEU:HD11	1.47	0.96
1:C:152:ARG:HH21	1:C:152:ARG:HG3	1.29	0.95
1:H:288:PRO:HG2	1:H:289:TYR:CD1	2.01	0.95
1:G:266:LEU:HB3	1:G:267:PRO:HD3	1.49	0.94
1:G:142:PHE:HA	1:G:145:ILE:HG13	1.50	0.94
1:C:67:LEU:HD13	1:C:75:LEU:HD12	1.49	0.94
1:G:274:ARG:HH11	1:G:274:ARG:HG2	1.33	0.94
1:E:384:ARG:HH11	1:E:384:ARG:HG3	1.30	0.93
1:H:12:ASP:HB3	1:H:14:LEU:HD12	1.47	0.92
1:B:36:GLN:HE21	1:B:40:GLN:HG2	1.30	0.92
1:A:310:LYS:O	1:A:311:ASP:HB2	1.65	0.92
1:C:310:LYS:O	1:C:311:ASP:HB2	1.69	0.91
1:H:288:PRO:HG2	1:H:289:TYR:HD1	1.34	0.91
1:A:93:TYR:HB2	1:A:94:PRO:HD3	1.53	0.90
1:B:133:VAL:HG22	1:B:159:ASP:HB3	1.52	0.90
1:B:333:ILE:HG22	1:B:334:VAL:HG23	1.54	0.90
1:E:117:GLU:OE2	1:E:120:LYS:NZ	2.05	0.90
1:C:274:ARG:HG2	1:C:274:ARG:HH11	1.36	0.90
1:E:303:GLY:HA3	1:E:368:PHE:CZ	2.08	0.88
1:G:317:LYS:O	1:G:321:GLU:HG3	1.74	0.88
1:D:156:LEU:HD12	1:D:157:LEU:H	1.39	0.88
1:G:287:HIS:CG	1:G:288:PRO:HD2	2.09	0.88
1:C:67:LEU:CD1	1:C:75:LEU:HD12	2.04	0.87
1:B:48:LYS:HB2	1:B:201:ASP:HA	1.56	0.87
1:H:14:LEU:HD12	1:H:14:LEU:H	1.40	0.87
1:C:152:ARG:HH21	1:C:152:ARG:HG2	1.36	0.87
1:E:315:ILE:HD11	1:E:318:GLN:HB2	1.57	0.87
1:D:124:THR:HG22	1:D:125:ASP:H	1.37	0.86
1:D:306:PHE:HB2	1:D:367:LEU:HD13	1.57	0.86
1:F:384:ARG:HG3	1:F:384:ARG:HH11	1.39	0.86
1:G:287:HIS:CD2	1:G:288:PRO:HD2	2.10	0.85
1:B:269:PHE:CE1	1:B:373:GLN:HG3	2.11	0.85
1:H:303:GLY:HA3	1:H:368:PHE:CZ	2.11	0.85
1:B:124:THR:HG22	1:B:125:ASP:N	1.92	0.85
1:H:278:GLU:HA	1:H:281:LEU:HD12	1.57	0.84
1:F:289:TYR:O	1:F:290:LEU:HD23	1.75	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:111:THR:HG22	1:F:294:GLN:HE21	1.41	0.84
1:A:193:MET:HE3	1:B:252:LEU:HD13	1.60	0.84
1:G:124:THR:HG22	1:G:125:ASP:N	1.91	0.84
1:E:382:TYR:O	1:E:386:VAL:HG23	1.77	0.83
1:E:336:GLY:HA2	1:E:362:LEU:HD21	1.61	0.83
1:B:287:HIS:CG	1:B:288:PRO:HD2	2.13	0.83
1:E:253:GLU:OE1	1:E:253:GLU:HA	1.76	0.83
1:G:209:LEU:HA	1:G:212:ILE:HG12	1.60	0.83
1:C:6:LEU:CD1	1:C:329:GLU:HB3	2.10	0.82
1:C:144:GLU:HA	1:C:147:LYS:HD3	1.61	0.82
1:G:285:LYS:HD2	1:G:286:ASP:OD2	1.79	0.82
1:F:48:LYS:HE2	1:F:201:ASP:HB3	1.61	0.82
1:A:6:LEU:HG	1:A:329:GLU:HG2	1.61	0.82
1:A:332:PRO:HG2	1:B:240:PHE:CD1	2.15	0.82
1:H:208:ILE:O	1:H:212:ILE:HG12	1.80	0.81
1:B:36:GLN:NE2	1:B:40:GLN:HG2	1.95	0.81
1:F:26:LYS:HB3	1:F:27:MET:CE	2.08	0.81
1:H:255:SER:HA	1:H:258:ILE:HD12	1.60	0.81
1:D:156:LEU:HD12	1:D:157:LEU:N	1.95	0.81
1:G:62:LEU:HD11	1:G:249:VAL:HG21	1.63	0.81
1:B:124:THR:CG2	1:B:125:ASP:H	1.92	0.81
1:B:187:ASN:OD1	1:B:188:LLP:HG3	1.81	0.81
1:C:254:MET:O	1:C:258:ILE:HD12	1.80	0.81
1:C:322:ASN:N	1:C:322:ASN:HD22	1.77	0.81
1:F:309:LYS:O	1:F:312:SER:HB3	1.78	0.81
1:H:31:GLY:N	1:H:253:GLU:OE1	2.12	0.81
1:D:331:ARG:HB2	1:D:332:PRO:HD2	1.61	0.80
1:C:152:ARG:HG3	1:C:152:ARG:NH2	1.91	0.80
1:H:26:LYS:HA	1:H:28:PHE:CZ	2.16	0.80
1:A:71:LYS:HA	1:A:71:LYS:CE	2.12	0.80
1:G:120:LYS:HA	1:G:148:ILE:HD13	1.64	0.80
1:B:340:LYS:HE3	1:B:363:ASP:OD1	1.81	0.79
1:E:265:LYS:HG3	1:E:268:ARG:NH1	1.97	0.79
1:E:265:LYS:C	1:E:267:PRO:HD2	2.06	0.79
1:C:254:MET:HB2	3:C:419:HOH:O	1.82	0.79
1:C:312:SER:OG	1:C:314:VAL:HG13	1.82	0.79
1:H:81:ILE:HG13	1:H:82:ILE:N	1.95	0.79
1:G:287:HIS:CE1	1:G:288:PRO:HG2	2.18	0.79
1:C:328:ILE:HD13	1:C:383:LEU:HD12	1.64	0.79
1:D:124:THR:HG22	1:D:125:ASP:N	1.96	0.79
1:F:238:GLU:HA	1:F:241:LYS:HE2	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:284:PHE:HZ	1:H:387:LEU:HD12	1.45	0.79
1:G:236:PHE:CE1	1:H:332:PRO:HD3	2.18	0.78
1:B:341:ASN:O	1:B:345:LEU:HD22	1.82	0.78
1:A:119:LEU:O	1:A:123:VAL:HG23	1.84	0.78
1:B:303:GLY:HA3	1:B:368:PHE:CE2	2.19	0.78
1:E:268:ARG:HG2	1:E:268:ARG:HH21	1.47	0.78
1:B:269:PHE:CD1	1:B:373:GLN:HG3	2.19	0.77
1:G:135:LEU:HD11	1:G:334:VAL:HG21	1.67	0.77
1:C:139:PRO:HD2	1:C:296:THR:O	1.85	0.77
1:E:265:LYS:HG3	1:E:268:ARG:HH11	1.49	0.77
1:H:168:PHE:CD2	1:H:169:ASN:ND2	2.53	0.77
1:B:268:ARG:O	1:B:272:VAL:HG23	1.83	0.77
1:F:266:LEU:HB3	1:F:267:PRO:HD3	1.66	0.77
1:H:32:GLU:H	1:H:32:GLU:CD	1.93	0.77
1:C:120:LYS:HA	1:C:148:ILE:HD13	1.67	0.77
1:D:271:SER:O	1:D:275:LYS:HD3	1.84	0.77
1:F:111:THR:HG22	1:F:294:GLN:NE2	1.99	0.77
1:C:149:ILE:CG2	1:C:149:ILE:O	2.33	0.76
1:H:81:ILE:HD11	1:H:131:LEU:HB2	1.67	0.76
1:C:188:LLP:OP1	2:C:403:AKG:O4	2.03	0.76
1:A:332:PRO:HG2	1:B:240:PHE:CE1	2.20	0.76
1:E:168:PHE:CE2	1:E:169:ASN:ND2	2.54	0.76
1:G:112:LEU:HD23	1:G:112:LEU:N	2.01	0.76
1:D:281:LEU:O	1:D:285:LYS:HB3	1.86	0.76
1:F:161:CYS:HB2	1:F:188:LLP:C2	2.16	0.76
1:F:82:ILE:HD12	1:F:127:THR:HG21	1.68	0.75
1:B:337:ASN:O	1:B:340:LYS:HG2	1.86	0.75
1:H:83:VAL:HG12	1:H:131:LEU:HB3	1.66	0.75
1:B:319:LEU:O	1:B:323:LEU:HG	1.85	0.75
1:G:289:TYR:CD2	1:G:314:VAL:HG21	2.22	0.75
1:F:48:LYS:HB2	1:F:201:ASP:HA	1.69	0.75
1:H:315:ILE:HD13	1:H:315:ILE:H	1.50	0.75
1:B:316:ARG:O	1:B:320:VAL:HG23	1.87	0.75
1:C:152:ARG:HB2	1:C:154:ILE:HG13	1.69	0.75
1:E:384:ARG:HG3	1:E:384:ARG:NH1	1.95	0.75
1:C:210:LEU:N	1:C:210:LEU:HD23	2.02	0.74
1:D:70:THR:OG1	1:D:73:PRO:HA	1.87	0.74
1:G:203:GLU:HG2	1:G:226:LYS:HG3	1.67	0.74
1:G:274:ARG:HG2	1:G:274:ARG:NH1	1.94	0.74
1:A:376:LEU:O	1:A:380:ILE:HD12	1.85	0.74
1:B:188:LLP:OP3	2:B:402:AKG:H41	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:332:PRO:HG3	1:F:236:PHE:CE2	2.23	0.74
1:H:247:TYR:HB3	3:H:394:HOH:O	1.87	0.74
1:G:124:THR:HG22	1:G:125:ASP:H	1.52	0.74
1:B:30:MET:HG2	1:B:250:ARG:HD2	1.69	0.74
1:F:315:ILE:HD13	1:F:315:ILE:N	2.02	0.74
1:B:119:LEU:HD23	1:B:148:ILE:HD12	1.70	0.74
1:F:162:GLU:HG3	1:F:188:LLP:O3	1.88	0.73
1:B:256:GLY:O	1:B:260:ILE:HD12	1.87	0.73
1:C:152:ARG:HB2	1:C:154:ILE:CD1	2.18	0.73
1:G:314:VAL:CG1	1:G:319:LEU:HD11	2.16	0.73
1:D:322:ASN:HD22	1:D:322:ASN:N	1.87	0.73
1:F:111:THR:CG2	1:F:294:GLN:NE2	2.51	0.73
1:F:222:PRO:HG2	1:F:225:ASN:CB	2.12	0.73
1:E:265:LYS:HG2	1:E:269:PHE:CE1	2.24	0.73
1:F:207:HIS:CE1	1:F:222:PRO:HG3	2.23	0.73
1:G:376:LEU:O	1:G:380:ILE:HG13	1.89	0.73
1:A:63:MET:HG3	1:A:179:MET:HE3	1.71	0.73
1:B:268:ARG:HA	1:B:271:SER:OG	1.88	0.73
1:C:149:ILE:O	1:C:149:ILE:HG22	1.89	0.73
1:B:108:ASP:C	1:B:108:ASP:OD1	2.30	0.72
1:A:16:TYR:HE1	1:B:23:LEU:HD22	1.53	0.72
1:B:70:THR:OG1	1:B:73:PRO:HA	1.89	0.72
1:F:383:LEU:HD11	1:F:387:LEU:CD1	2.19	0.72
1:C:152:ARG:CG	1:C:152:ARG:NH2	2.32	0.72
1:G:161:CYS:HB2	1:G:188:LLP:C3	2.19	0.72
1:H:145:ILE:O	1:H:149:ILE:HD12	1.89	0.72
1:H:20:GLN:NE2	1:H:24:ASP:OD2	2.22	0.72
1:F:287:HIS:HE1	1:F:289:TYR:CZ	2.08	0.72
1:H:387:LEU:O	1:H:388:LYS:HD2	1.90	0.72
1:G:266:LEU:HB3	1:G:267:PRO:CD	2.19	0.72
1:H:266:LEU:HB3	1:H:267:PRO:CD	2.20	0.72
1:B:81:ILE:HD11	1:B:131:LEU:HB2	1.72	0.71
1:D:106:ASP:HB2	1:D:356:VAL:HA	1.72	0.71
1:F:362:LEU:HD23	1:F:362:LEU:O	1.89	0.71
1:C:84:PRO:CA	1:C:114:ILE:HD12	2.20	0.71
1:G:149:ILE:O	1:G:152:ARG:HG3	1.89	0.71
1:H:287:HIS:CG	1:H:288:PRO:HD2	2.26	0.71
1:A:308:ILE:HB	1:A:365:ASN:HB3	1.71	0.71
1:C:128:LYS:HB3	1:C:128:LYS:HZ3	1.51	0.71
1:B:115:ASP:HB3	1:B:118:SER:HB2	1.73	0.71
1:F:224:LYS:HA	1:F:229:GLY:O	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:340:LYS:NZ	3:F:396:HOH:O	2.22	0.71
1:A:289:TYR:HA	1:A:309:LYS:HD2	1.73	0.71
1:B:235:GLN:O	1:B:239:SER:HB2	1.91	0.71
1:C:280:PHE:CZ	1:C:304:PHE:HB3	2.26	0.71
1:D:54:SER:OG	1:D:58:THR:HG21	1.91	0.71
1:E:30:MET:HG3	1:E:34:VAL:HG11	1.72	0.71
1:F:101:ARG:NH1	1:F:349:ASP:OD1	2.22	0.71
1:H:287:HIS:NE2	1:H:290:LEU:HD12	2.05	0.71
1:B:53:VAL:CA	1:B:251:PRO:HG3	2.20	0.71
1:B:376:LEU:HB3	1:B:379:GLU:HG3	1.71	0.70
1:E:12:ASP:OD1	1:E:12:ASP:C	2.34	0.70
1:G:222:PRO:CD	1:G:225:ASN:HB3	2.18	0.70
1:H:326:ALA:HB1	1:H:382:TYR:OH	1.91	0.70
1:A:384:ARG:O	1:A:384:ARG:NH1	2.23	0.70
1:E:266:LEU:N	1:E:267:PRO:HD2	2.05	0.70
1:G:213:ARG:HD2	1:G:251:PRO:HD2	1.73	0.70
1:D:331:ARG:HB2	1:D:332:PRO:CD	2.21	0.70
1:E:385:GLU:OE1	1:E:385:GLU:HA	1.91	0.70
1:F:384:ARG:HG3	1:F:384:ARG:O	1.92	0.70
1:B:48:LYS:N	1:B:201:ASP:OD1	2.24	0.70
1:F:116:ILE:HG22	1:F:117:GLU:N	2.05	0.70
1:E:221:LEU:O	1:E:231:LYS:HE2	1.92	0.70
1:F:82:ILE:HD12	1:F:127:THR:CG2	2.22	0.70
1:F:83:VAL:HG12	1:F:131:LEU:HB3	1.74	0.70
1:H:266:LEU:O	1:H:270:ILE:HD12	1.92	0.70
1:B:303:GLY:HA3	1:B:368:PHE:CZ	2.27	0.70
1:E:48:LYS:HB2	1:E:201:ASP:HA	1.72	0.69
1:F:6:LEU:HD12	1:F:329:GLU:HG2	1.74	0.69
1:F:383:LEU:CD1	1:F:387:LEU:HD12	2.22	0.69
1:H:70:THR:HG21	1:H:74:ARG:HE	1.56	0.69
1:C:6:LEU:HD12	1:C:329:GLU:HB3	1.73	0.69
1:C:274:ARG:HG2	1:C:274:ARG:NH1	2.06	0.69
1:E:34:VAL:O	1:E:38:GLU:HG3	1.93	0.69
1:G:281:LEU:O	1:G:285:LYS:HB3	1.92	0.69
1:C:48:LYS:N	1:C:201:ASP:OD1	2.23	0.69
1:D:306:PHE:HB2	1:D:367:LEU:CD1	2.21	0.69
1:E:278:GLU:HA	1:E:281:LEU:HD12	1.74	0.69
1:D:284:PHE:CZ	1:D:384:ARG:HA	2.28	0.69
1:D:363:ASP:OD2	1:D:364:LYS:HE3	1.92	0.69
1:H:81:ILE:HD11	1:H:131:LEU:CB	2.23	0.69
1:H:318:GLN:O	1:H:322:ASN:ND2	2.26	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:41:PHE:O	1:C:45:PHE:HD1	1.76	0.69
1:G:33:TYR:HB2	1:G:253:GLU:OE2	1.91	0.69
1:E:331:ARG:HG3	1:E:332:PRO:O	1.92	0.69
1:H:272:VAL:HG11	1:H:373:GLN:O	1.92	0.69
1:B:83:VAL:HG12	1:B:131:LEU:HB3	1.75	0.69
1:C:80:GLU:HB3	1:C:126:SER:O	1.93	0.69
1:C:277:ALA:O	1:C:280:PHE:HB3	1.93	0.69
1:F:140:ASN:HB2	1:F:142:PHE:CE2	2.27	0.69
1:C:6:LEU:HD12	1:C:329:GLU:CG	2.23	0.69
1:E:269:PHE:O	1:E:273:ARG:HG3	1.93	0.69
1:A:362:LEU:HD23	1:A:363:ASP:N	2.08	0.68
1:F:383:LEU:HD12	1:F:383:LEU:O	1.93	0.68
1:H:20:GLN:HE22	1:H:24:ASP:CG	2.01	0.68
1:H:285:LYS:HB2	1:H:285:LYS:NZ	1.99	0.68
1:F:142:PHE:HA	1:F:145:ILE:HG13	1.75	0.68
1:F:384:ARG:HG3	1:F:384:ARG:NH1	2.05	0.68
1:C:266:LEU:HB3	1:C:267:PRO:HD3	1.74	0.68
1:D:355:ASN:C	1:D:355:ASN:HD22	2.01	0.68
1:G:62:LEU:HD11	1:G:249:VAL:CG2	2.23	0.68
1:E:28:PHE:HB2	1:F:193:MET:HG2	1.76	0.68
1:B:5:PRO:HA	1:B:329:GLU:OE1	1.93	0.68
1:C:48:LYS:HB2	1:C:201:ASP:HA	1.76	0.68
1:E:12:ASP:OD1	1:E:13:ASP:N	2.27	0.68
1:A:207:HIS:ND1	1:A:226:LYS:HB2	2.09	0.68
1:D:334:VAL:HG12	1:D:335:THR:HG23	1.75	0.68
1:G:88:TRP:CD1	1:G:90:THR:HG1	2.12	0.68
1:B:108:ASP:OD1	1:B:110:ASN:N	2.25	0.67
1:D:40:GLN:OE1	1:D:260:ILE:HG23	1.93	0.67
1:C:144:GLU:O	1:C:145:ILE:C	2.37	0.67
1:E:117:GLU:O	1:E:120:LYS:HB3	1.93	0.67
1:E:310:LYS:O	1:E:311:ASP:HB2	1.94	0.67
1:H:170:ASN:N	1:H:170:ASN:HD22	1.93	0.67
1:A:16:TYR:CE1	1:B:23:LEU:HD22	2.29	0.67
1:G:5:PRO:HA	1:G:329:GLU:HB2	1.76	0.67
1:B:30:MET:HE3	1:B:34:VAL:HG11	1.75	0.67
1:C:128:LYS:HB3	1:C:128:LYS:HZ2	1.58	0.67
1:C:379:GLU:CD	1:C:379:GLU:H	2.02	0.67
1:F:119:LEU:HD12	1:F:123:VAL:HG23	1.77	0.67
1:F:315:ILE:H	1:F:315:ILE:CD1	2.05	0.67
1:D:124:THR:CG2	1:D:125:ASP:H	2.07	0.67
1:D:276:ASN:ND2	1:D:376:LEU:HD12	2.09	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:30:MET:HE1	1:G:213:ARG:NH2	2.10	0.67
1:A:204:GLU:HB2	1:A:226:LYS:HG3	1.77	0.67
1:C:322:ASN:N	1:C:322:ASN:ND2	2.43	0.67
1:E:315:ILE:HD11	1:E:318:GLN:CB	2.25	0.67
1:G:6:LEU:HD12	1:G:329:GLU:CG	2.19	0.67
1:G:222:PRO:HD2	1:G:225:ASN:CB	2.20	0.67
1:G:124:THR:CG2	1:G:125:ASP:H	2.08	0.66
1:H:124:THR:HG22	1:H:126:SER:N	2.02	0.66
1:C:303:GLY:HA3	1:C:368:PHE:CE2	2.30	0.66
1:H:254:MET:O	1:H:257:ALA:N	2.25	0.66
1:F:18:ALA:O	1:F:22:VAL:HG23	1.95	0.66
1:B:291:ASP:HB2	1:B:307:ILE:HG22	1.77	0.66
1:E:23:LEU:HD21	1:F:19:ILE:HD12	1.76	0.66
1:F:289:TYR:C	1:F:309:LYS:HG3	2.20	0.66
1:C:57:SER:HB2	1:D:248:ASN:HB3	1.78	0.66
1:F:310:LYS:O	1:F:311:ASP:HB2	1.96	0.66
1:G:138:ASN:HA	1:G:299:SER:HB2	1.77	0.66
1:G:274:ARG:HH11	1:G:274:ARG:CG	2.07	0.66
1:E:303:GLY:HA3	1:E:368:PHE:CE1	2.30	0.66
1:E:360:GLU:HA	1:E:363:ASP:HB2	1.78	0.66
1:G:124:THR:CG2	1:G:125:ASP:N	2.57	0.66
1:G:380:ILE:O	1:G:383:LEU:HB3	1.96	0.66
1:E:108:ASP:OD1	1:E:110:ASN:N	2.28	0.66
1:F:124:THR:HG22	1:F:125:ASP:N	2.11	0.66
1:B:209:LEU:N	1:B:209:LEU:HD23	2.09	0.66
1:F:287:HIS:CD2	1:F:288:PRO:HD2	2.31	0.66
1:H:284:PHE:CZ	1:H:387:LEU:HD12	2.29	0.66
1:A:148:ILE:O	1:A:152:ARG:NH2	2.29	0.65
1:F:25:SER:O	1:F:27:MET:HG2	1.96	0.65
1:H:320:VAL:HG13	1:H:330:CYS:SG	2.36	0.65
1:D:202:ASP:OD1	1:D:205:ILE:HG12	1.96	0.65
1:A:193:MET:HE3	1:B:252:LEU:CD1	2.27	0.65
1:C:331:ARG:HD3	1:C:368:PHE:CD1	2.31	0.65
1:H:145:ILE:HG22	1:H:149:ILE:HD13	1.79	0.65
1:A:71:LYS:HA	1:A:71:LYS:HE3	1.77	0.65
1:B:280:PHE:HD2	1:B:281:LEU:HD23	1.61	0.65
1:F:23:LEU:HD23	1:F:28:PHE:HE1	1.61	0.65
1:F:26:LYS:CB	1:F:27:MET:HE2	2.19	0.65
1:F:129:ALA:HA	1:F:154:ILE:HG22	1.79	0.65
1:D:42:ALA:HB3	3:D:439:HOH:O	1.97	0.65
1:B:376:LEU:O	1:B:379:GLU:HG2	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:20:GLN:NE2	1:H:24:ASP:CG	2.55	0.65
1:D:217:TRP:HB2	3:D:427:HOH:O	1.97	0.65
1:H:287:HIS:ND1	1:H:288:PRO:HD2	2.12	0.65
1:C:67:LEU:HD13	1:C:75:LEU:CD1	2.24	0.64
1:F:149:ILE:O	1:F:152:ARG:HB2	1.97	0.64
1:E:281:LEU:O	1:E:282:ASP:C	2.40	0.64
1:A:171:LYS:HD3	1:A:175:THR:OG1	1.97	0.64
1:B:375:GLU:O	1:B:376:LEU:HD23	1.97	0.64
1:G:192:THR:O	1:G:193:MET:HB2	1.97	0.64
1:C:70:THR:HG21	1:C:74:ARG:HE	1.62	0.64
1:D:289:TYR:CG	1:D:314:VAL:HG21	2.32	0.64
1:F:285:LYS:HG3	1:F:286:ASP:N	2.12	0.64
1:A:319:LEU:O	1:A:323:LEU:HG	1.98	0.64
1:A:376:LEU:C	1:A:380:ILE:HD12	2.22	0.64
1:B:82:ILE:HD12	1:B:127:THR:HG23	1.78	0.64
1:E:106:ASP:OD1	1:E:358:ASN:HB2	1.97	0.64
1:G:164:MET:HE1	1:G:190:ILE:HG12	1.79	0.64
1:C:308:ILE:HD12	1:C:365:ASN:O	1.97	0.64
1:E:242:PHE:HE2	1:F:335:THR:HG21	1.63	0.64
1:F:281:LEU:CD2	1:F:292:VAL:HG21	2.28	0.64
1:H:224:LYS:HA	1:H:229:GLY:O	1.98	0.64
1:G:55:SER:HB2	3:G:420:HOH:O	1.98	0.64
1:G:266:LEU:O	1:G:269:PHE:HB2	1.96	0.64
1:H:255:SER:CA	1:H:258:ILE:HD12	2.26	0.64
1:B:24:ASP:N	1:B:24:ASP:OD1	2.28	0.64
1:B:378:ASP:O	1:B:381:ASP:HB2	1.98	0.64
1:C:152:ARG:HB2	1:C:154:ILE:CG1	2.27	0.64
1:E:333:ILE:HG21	1:E:362:LEU:HD11	1.79	0.64
1:F:76:LYS:N	1:F:79:ASP:OD2	2.27	0.64
1:F:130:ILE:HG13	1:F:154:ILE:HG21	1.79	0.64
1:F:383:LEU:HD12	1:F:383:LEU:C	2.21	0.64
1:H:12:ASP:HB3	1:H:14:LEU:CD1	2.24	0.64
1:B:248:ASN:OD1	1:B:248:ASN:C	2.42	0.63
1:B:379:GLU:H	1:B:379:GLU:CD	2.05	0.63
1:C:152:ARG:HG3	1:C:154:ILE:HD11	1.80	0.63
1:B:320:VAL:O	1:B:324:ASN:ND2	2.32	0.63
1:E:44:THR:HB	1:E:45:PHE:CD1	2.32	0.63
1:B:64:ILE:HG22	1:B:65:ALA:N	2.12	0.63
1:H:384:ARG:O	1:H:384:ARG:NH1	2.31	0.63
1:E:36:GLN:CG	1:E:260:ILE:HD11	2.28	0.63
1:G:168:PHE:O	1:G:169:ASN:C	2.40	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:VAL:HB	1:A:114:ILE:HD11	1.80	0.63
1:D:15:GLU:O	1:D:18:ALA:HB3	1.99	0.63
1:B:20:GLN:O	1:B:23:LEU:HB2	1.98	0.63
1:E:28:PHE:CB	1:F:193:MET:HG2	2.29	0.63
1:E:286:ASP:O	1:E:288:PRO:HD3	1.98	0.63
1:F:266:LEU:HB3	1:F:267:PRO:CD	2.29	0.63
1:G:161:CYS:HB2	1:G:188:LLP:C2	2.28	0.63
1:G:274:ARG:NH2	1:G:298:GLU:HG2	2.12	0.63
1:A:96:GLN:HB2	1:A:348:PHE:CE2	2.34	0.63
1:A:171:LYS:HD2	1:A:176:PHE:CE2	2.34	0.63
1:F:129:ALA:HA	1:F:154:ILE:CG2	2.28	0.63
1:F:254:MET:O	1:F:258:ILE:HG13	1.98	0.63
1:G:72:LYS:HD2	1:G:73:PRO:HD2	1.80	0.63
1:B:205:ILE:O	1:B:209:LEU:HG	1.99	0.63
1:D:287:HIS:HE1	1:D:289:TYR:CE1	2.16	0.63
1:F:362:LEU:HD23	1:F:362:LEU:C	2.23	0.63
1:H:41:PHE:O	1:H:44:THR:HB	1.98	0.63
1:D:193:MET:HA	3:D:444:HOH:O	1.99	0.62
1:F:26:LYS:C	1:F:27:MET:HE2	2.24	0.62
1:F:185:PHE:O	1:F:186:TYR:C	2.41	0.62
1:A:57:SER:HB2	1:B:248:ASN:HB3	1.81	0.62
1:H:145:ILE:HG22	1:H:149:ILE:CD1	2.29	0.62
1:H:203:GLU:OE1	1:H:226:LYS:HE2	1.98	0.62
1:C:135:LEU:HD11	1:C:334:VAL:HG21	1.80	0.62
1:F:161:CYS:HB2	1:F:188:LLP:H2'2	1.81	0.62
1:G:52:MET:HG2	1:G:251:PRO:HG3	1.81	0.62
1:G:143:ASP:OD2	1:G:168:PHE:HE2	1.83	0.62
1:H:11:TRP:HA	1:H:15:GLU:OE1	1.99	0.62
1:E:93:TYR:HB2	1:E:94:PRO:HD3	1.81	0.62
1:F:106:ASP:OD2	1:F:358:ASN:HB2	1.99	0.62
1:G:50:ALA:CB	1:G:199:VAL:HG12	2.29	0.62
1:G:376:LEU:HA	1:G:379:GLU:OE1	2.00	0.62
1:D:34:VAL:HG23	1:D:253:GLU:OE1	2.00	0.62
1:G:48:LYS:HB2	1:G:201:ASP:HA	1.82	0.62
1:E:332:PRO:HG3	1:F:236:PHE:CD2	2.34	0.62
1:H:124:THR:CG2	1:H:126:SER:H	2.04	0.62
1:H:287:HIS:CE1	1:H:290:LEU:HD12	2.34	0.62
1:D:70:THR:HG21	1:D:74:ARG:NE	2.15	0.62
1:D:266:LEU:HB3	1:D:267:PRO:HD3	1.81	0.62
1:E:360:GLU:O	1:E:363:ASP:HB3	2.00	0.62
1:G:158:GLU:OE2	1:G:174:GLY:N	2.32	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:179:MET:HG2	1:G:198:ILE:CG2	2.29	0.62
1:A:161:CYS:HB2	1:A:188:LLP:C2	2.30	0.62
1:F:192:THR:O	1:F:193:MET:HB2	1.99	0.62
1:G:334:VAL:HG12	1:G:335:THR:HG23	1.81	0.62
1:F:106:ASP:CG	1:F:358:ASN:HB2	2.25	0.62
1:F:285:LYS:HA	3:F:430:HOH:O	2.00	0.62
1:G:363:ASP:OD2	1:G:364:LYS:HE2	2.00	0.61
1:C:57:SER:OG	1:C:188:LLP:OP2	2.16	0.61
1:D:305:SER:HB2	1:D:333:ILE:HD11	1.82	0.61
1:E:242:PHE:CE2	1:F:335:THR:HG21	2.34	0.61
1:G:242:PHE:HE2	1:H:335:THR:HG21	1.64	0.61
1:G:279:TYR:CZ	1:G:283:LYS:HE2	2.35	0.61
1:A:265:LYS:C	1:A:267:PRO:HD2	2.25	0.61
1:F:34:VAL:HG23	1:F:253:GLU:OE1	2.01	0.61
1:C:83:VAL:HG12	1:C:131:LEU:HB3	1.82	0.61
1:G:266:LEU:O	1:G:269:PHE:N	2.34	0.61
1:A:106:ASP:OD2	1:A:356:VAL:HA	2.00	0.61
1:C:20:GLN:HA	1:C:23:LEU:HD12	1.83	0.61
1:H:171:LYS:HG2	1:H:176:PHE:CE1	2.36	0.61
1:F:223:LYS:O	1:F:230:VAL:HA	2.01	0.61
1:G:162:GLU:HG3	1:G:188:LLP:O3	2.00	0.61
1:F:70:THR:HG21	1:F:74:ARG:HE	1.66	0.61
1:G:116:ILE:O	1:G:120:LYS:HG3	2.01	0.61
1:A:71:LYS:HA	1:A:71:LYS:HE2	1.82	0.61
1:C:81:ILE:HD11	1:C:131:LEU:HB2	1.82	0.61
1:E:230:VAL:O	1:E:230:VAL:HG13	2.01	0.61
1:G:33:TYR:N	1:G:253:GLU:OE2	2.33	0.61
1:G:168:PHE:O	1:G:171:LYS:N	2.34	0.61
1:A:67:LEU:HD22	1:A:74:ARG:HG3	1.83	0.61
1:A:253:GLU:HA	1:A:253:GLU:OE1	2.01	0.61
1:B:119:LEU:HD23	1:B:148:ILE:CD1	2.30	0.61
1:C:202:ASP:HB3	1:C:205:ILE:HG13	1.82	0.61
1:B:131:LEU:C	1:B:131:LEU:HD12	2.26	0.60
1:B:265:LYS:O	1:B:268:ARG:HG3	2.01	0.60
1:F:23:LEU:O	1:F:26:LYS:NZ	2.31	0.60
1:A:331:ARG:HD3	1:A:368:PHE:CD1	2.36	0.60
1:E:204:GLU:O	1:E:208:ILE:HG13	1.99	0.60
1:F:222:PRO:CG	1:F:225:ASN:HB3	2.18	0.60
1:B:287:HIS:ND1	1:B:288:PRO:HD2	2.16	0.60
1:C:34:VAL:O	1:C:37:TYR:HB3	2.02	0.60
1:F:138:ASN:HA	1:F:299:SER:HB2	1.84	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:235:GLN:O	1:G:236:PHE:C	2.44	0.60
1:C:328:ILE:HD13	1:C:383:LEU:CD1	2.31	0.60
1:G:149:ILE:HG22	1:G:150:GLY:N	2.15	0.60
1:H:303:GLY:HA3	1:H:368:PHE:CE2	2.36	0.60
1:A:218:THR:O	1:A:221:LEU:HB2	2.01	0.60
1:H:287:HIS:CE1	1:H:290:LEU:HG	2.36	0.60
1:D:204:GLU:HG3	1:D:226:LYS:HB3	1.82	0.60
1:B:372:HIS:HD2	1:B:376:LEU:HD11	1.66	0.60
1:F:217:TRP:CD1	1:F:217:TRP:C	2.79	0.60
1:G:208:ILE:O	1:G:211:CYS:HB3	2.02	0.60
1:H:278:GLU:HA	1:H:281:LEU:CD1	2.29	0.60
1:A:367:LEU:C	1:A:367:LEU:HD12	2.26	0.60
1:B:26:LYS:HA	1:B:28:PHE:CZ	2.37	0.60
1:D:218:THR:O	1:D:221:LEU:HB2	2.02	0.60
1:A:6:LEU:HD21	1:A:329:GLU:O	2.03	0.59
1:E:360:GLU:O	1:E:361:TYR:C	2.42	0.59
1:G:12:ASP:HB2	1:G:265:LYS:NZ	2.17	0.59
1:H:93:TYR:O	1:H:96:GLN:N	2.35	0.59
1:B:266:LEU:O	1:B:269:PHE:HB2	2.03	0.59
1:G:324:ASN:C	1:G:326:ALA:H	2.10	0.59
1:H:203:GLU:O	1:H:206:TYR:HB3	2.01	0.59
1:C:24:ASP:OD1	1:C:24:ASP:N	2.33	0.59
1:D:382:TYR:O	1:D:385:GLU:HB2	2.02	0.59
1:B:140:ASN:HB2	1:B:142:PHE:CZ	2.37	0.59
1:B:158:GLU:OE2	1:B:176:PHE:HB2	2.01	0.59
1:D:333:ILE:HG21	1:D:362:LEU:HD11	1.84	0.59
1:F:204:GLU:O	1:F:208:ILE:HG13	2.03	0.59
1:G:156:LEU:HD23	1:G:177:GLY:HA2	1.83	0.59
1:H:287:HIS:CE1	1:H:289:TYR:CE1	2.90	0.59
1:A:217:TRP:CD1	1:A:217:TRP:C	2.80	0.59
1:A:319:LEU:N	1:A:319:LEU:HD23	2.17	0.59
1:D:283:LYS:O	1:D:384:ARG:HD3	2.02	0.59
1:F:156:LEU:HD12	1:F:157:LEU:H	1.67	0.59
1:F:204:GLU:O	1:F:205:ILE:C	2.43	0.59
1:F:315:ILE:HG12	1:F:315:ILE:O	2.02	0.59
1:G:159:ASP:O	3:G:392:HOH:O	2.17	0.59
1:D:124:THR:CG2	1:D:125:ASP:N	2.64	0.59
1:G:20:GLN:O	1:G:23:LEU:HB2	2.03	0.59
1:H:266:LEU:C	1:H:270:ILE:HD12	2.27	0.59
1:A:235:GLN:O	1:A:236:PHE:C	2.44	0.59
1:D:184:SER:HB3	1:D:190:ILE:HG13	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:362:LEU:C	1:G:362:LEU:HD23	2.27	0.59
1:D:70:THR:HG21	1:D:74:ARG:HE	1.68	0.59
1:H:266:LEU:O	1:H:269:PHE:HB2	2.01	0.59
1:F:363:ASP:C	1:F:364:LYS:HD3	2.28	0.59
1:G:37:TYR:CE1	1:G:259:GLY:HA3	2.38	0.59
1:H:272:VAL:O	1:H:276:ASN:ND2	2.36	0.59
1:G:140:ASN:HB3	1:G:145:ILE:HD11	1.85	0.59
1:H:279:TYR:CD2	1:H:380:ILE:HG21	2.38	0.59
1:A:6:LEU:O	1:A:372:HIS:NE2	2.36	0.58
1:C:19:ILE:O	1:C:23:LEU:HG	2.03	0.58
1:B:145:ILE:O	1:B:149:ILE:HD12	2.02	0.58
1:D:88:TRP:CZ2	2:D:404:AKG:H41	2.38	0.58
1:F:337:ASN:O	1:F:340:LYS:HG2	2.02	0.58
1:A:106:ASP:CG	1:A:356:VAL:HA	2.29	0.58
1:B:280:PHE:CD2	1:B:281:LEU:HD23	2.38	0.58
1:E:108:ASP:OD1	1:E:108:ASP:C	2.45	0.58
1:G:144:GLU:HA	1:G:144:GLU:OE1	2.03	0.58
1:D:74:ARG:HB3	1:D:155:ILE:HD11	1.84	0.58
1:G:379:GLU:H	1:G:379:GLU:CD	2.11	0.58
1:H:168:PHE:CE2	1:H:169:ASN:ND2	2.65	0.58
1:E:36:GLN:HG3	1:E:260:ILE:HD11	1.84	0.58
1:F:331:ARG:HB2	1:F:332:PRO:HD2	1.83	0.58
1:C:297:GLY:C	1:C:298:GLU:HG3	2.29	0.58
1:D:206:TYR:CZ	1:D:210:LEU:HD11	2.38	0.58
1:A:289:TYR:CA	1:A:309:LYS:HD2	2.33	0.58
1:E:40:GLN:O	1:E:44:THR:OG1	2.21	0.58
1:E:268:ARG:HH21	1:E:268:ARG:CG	2.17	0.58
1:H:124:THR:CG2	1:H:125:ASP:N	2.65	0.58
1:A:217:TRP:NE1	1:A:219:ARG:HB2	2.19	0.58
1:H:287:HIS:CE1	1:H:288:PRO:HD2	2.39	0.58
1:B:82:ILE:HD12	1:B:127:THR:CG2	2.33	0.57
1:C:215:HIS:HD1	1:D:88:TRP:HE1	1.51	0.57
1:F:156:LEU:HD12	1:F:157:LEU:N	2.18	0.57
1:A:6:LEU:HG	1:A:329:GLU:CG	2.30	0.57
1:D:92:TYR:O	1:D:95:LEU:HB2	2.04	0.57
1:G:2:ILE:HD13	1:G:329:GLU:OE2	2.05	0.57
1:H:243:VAL:O	1:H:244:LEU:HD13	2.05	0.57
1:B:224:LYS:HA	1:B:229:GLY:O	2.03	0.57
1:G:22:VAL:O	1:G:25:SER:OG	2.20	0.57
1:C:6:LEU:HD12	1:C:329:GLU:CB	2.34	0.57
1:F:53:VAL:HG23	1:F:55:SER:O	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:GLU:HB2	1:A:226:LYS:CG	2.33	0.57
1:B:109:ILE:HG13	1:B:109:ILE:O	2.04	0.57
1:B:287:HIS:CD2	1:B:288:PRO:HD2	2.39	0.57
1:F:23:LEU:HD23	1:F:28:PHE:CE1	2.38	0.57
1:G:11:TRP:HA	1:G:15:GLU:OE1	2.04	0.57
1:A:84:PRO:HA	1:A:105:VAL:O	2.04	0.57
1:E:372:HIS:H	1:E:376:LEU:HD11	1.68	0.57
1:B:375:GLU:C	1:B:376:LEU:HD23	2.29	0.57
1:C:76:LYS:O	1:C:79:ASP:HB2	2.04	0.57
1:C:308:ILE:HG21	1:C:314:VAL:HG22	1.86	0.57
1:F:161:CYS:HB2	1:F:188:LLP:C2'	2.34	0.57
1:F:337:ASN:HB2	1:F:363:ASP:HB2	1.87	0.57
1:H:56:GLY:O	1:H:59:ALA:HB3	2.03	0.57
1:B:17:LYS:O	1:B:21:SER:OG	2.23	0.57
1:F:382:TYR:O	1:F:386:VAL:HG23	2.05	0.57
1:G:160:ASN:HA	3:G:392:HOH:O	2.04	0.57
1:G:160:ASN:HB3	1:G:181:THR:O	2.05	0.57
1:G:261:GLU:O	1:G:264:LYS:HB2	2.05	0.57
1:H:111:THR:O	1:H:112:LEU:HB2	2.05	0.57
1:H:316:ARG:NH1	1:H:366:GLY:O	2.34	0.57
1:H:36:GLN:HB3	1:H:260:ILE:HD11	1.87	0.57
1:H:279:TYR:CE2	1:H:380:ILE:HG21	2.40	0.57
1:H:315:ILE:HD13	1:H:315:ILE:N	2.20	0.57
1:E:350:TYR:HD1	1:E:350:TYR:H	1.52	0.57
1:C:192:THR:O	1:C:193:MET:HB2	2.05	0.56
1:D:120:LYS:CA	1:D:148:ILE:HD13	2.34	0.56
1:F:96:GLN:HE21	1:F:347:TYR:HB3	1.70	0.56
1:F:108:ASP:OD1	1:F:108:ASP:C	2.48	0.56
1:F:336:GLY:HA3	1:F:363:ASP:OD1	2.05	0.56
1:G:32:GLU:O	1:G:36:GLN:N	2.34	0.56
1:G:50:ALA:HB2	1:G:199:VAL:HG12	1.86	0.56
1:C:107:ILE:HD12	1:C:107:ILE:C	2.30	0.56
1:D:292:VAL:HB	3:D:407:HOH:O	2.04	0.56
1:E:289:TYR:HA	1:E:309:LYS:HD2	1.87	0.56
1:F:188:LLP:OP3	2:F:405:AKG:O3	2.23	0.56
1:A:332:PRO:HD3	1:B:236:PHE:CE1	2.41	0.56
1:C:222:PRO:HD2	1:C:225:ASN:HB3	1.87	0.56
1:E:207:HIS:O	1:E:210:LEU:HB2	2.06	0.56
1:E:274:ARG:O	1:E:277:ALA:HB3	2.06	0.56
1:H:23:LEU:HA	1:H:28:PHE:HE1	1.70	0.56
1:H:235:GLN:HG3	1:H:239:SER:OG	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:36:GLN:HG2	1:C:260:ILE:HD11	1.86	0.56
1:H:284:PHE:CZ	1:H:384:ARG:HD2	2.40	0.56
1:D:322:ASN:N	1:D:322:ASN:ND2	2.50	0.56
1:H:119:LEU:HD21	1:H:145:ILE:HD13	1.87	0.56
1:H:131:LEU:C	1:H:131:LEU:HD12	2.30	0.56
1:H:190:ILE:HG22	1:H:262:GLN:HB3	1.87	0.56
1:D:280:PHE:HD2	1:D:281:LEU:HD12	1.70	0.56
1:G:141:ASN:C	1:G:141:ASN:OD1	2.48	0.56
1:G:268:ARG:O	1:G:272:VAL:HG23	2.06	0.56
1:H:288:PRO:HG2	1:H:289:TYR:CE1	2.39	0.56
1:A:70:THR:HG21	1:A:74:ARG:HE	1.71	0.56
1:B:93:TYR:HB2	1:B:94:PRO:HD3	1.86	0.56
1:E:88:TRP:CD1	1:E:90:THR:H	2.23	0.56
1:H:145:ILE:CG2	1:H:149:ILE:CD1	2.84	0.56
1:H:331:ARG:HD3	1:H:368:PHE:CD1	2.40	0.56
1:B:188:LLP:OP3	2:B:402:AKG:O3	2.24	0.56
1:G:88:TRP:HD1	1:G:90:THR:HG1	1.53	0.56
1:H:170:ASN:N	1:H:170:ASN:ND2	2.52	0.56
1:B:309:LYS:O	1:B:312:SER:HB3	2.06	0.56
1:F:243:VAL:HG23	1:F:244:LEU:HD12	1.88	0.56
1:B:96:GLN:HB2	1:B:348:PHE:CE2	2.41	0.56
1:B:232:SER:HB3	1:B:238:GLU:OE1	2.05	0.56
1:A:331:ARG:HD3	1:A:368:PHE:CE1	2.42	0.55
1:E:215:HIS:O	1:E:242:PHE:HD1	1.89	0.55
1:E:326:ALA:HB1	1:E:382:TYR:OH	2.06	0.55
1:F:29:THR:O	1:F:30:MET:C	2.48	0.55
1:G:2:ILE:HG23	1:G:327:GLY:O	2.07	0.55
1:A:111:THR:O	1:A:112:LEU:HB2	2.05	0.55
1:C:223:LYS:O	1:C:230:VAL:HA	2.06	0.55
1:C:322:ASN:ND2	1:C:322:ASN:H	2.03	0.55
1:H:284:PHE:HE1	1:H:287:HIS:CD2	2.24	0.55
1:D:259:GLY:O	1:D:260:ILE:C	2.45	0.55
1:G:19:ILE:O	1:G:20:GLN:C	2.49	0.55
1:H:202:ASP:HB3	1:H:205:ILE:HG12	1.87	0.55
1:A:65:ALA:O	1:A:68:PHE:HB2	2.06	0.55
1:A:337:ASN:O	1:A:340:LYS:HG2	2.06	0.55
1:C:161:CYS:HB2	1:C:188:LLP:C2	2.36	0.55
1:B:36:GLN:HE22	1:B:40:GLN:HE21	1.53	0.55
1:E:34:VAL:HG12	1:E:35:LYS:N	2.22	0.55
1:F:316:ARG:O	1:F:320:VAL:HG23	2.06	0.55
1:F:373:GLN:OE1	1:F:373:GLN:N	2.30	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:289:TYR:HA	1:G:309:LYS:HD3	1.89	0.55
1:A:141:ASN:O	1:A:145:ILE:HG13	2.07	0.55
1:E:355:ASN:C	1:E:355:ASN:OD1	2.49	0.55
1:G:382:TYR:O	1:G:385:GLU:N	2.40	0.55
1:H:164:MET:HE1	1:H:190:ILE:CD1	2.37	0.55
1:A:242:PHE:CE1	1:B:89:SER:HB3	2.42	0.55
1:B:155:ILE:HG22	1:B:156:LEU:N	2.22	0.55
1:C:79:ASP:HB3	1:C:128:LYS:HG3	1.88	0.55
1:C:103:LYS:HG3	1:C:351:THR:HG23	1.89	0.55
1:G:108:ASP:OD1	1:G:110:ASN:N	2.36	0.55
1:G:288:PRO:HG2	1:G:289:TYR:H	1.70	0.55
1:G:355:ASN:C	1:G:355:ASN:OD1	2.50	0.55
1:B:117:GLU:HA	1:B:117:GLU:OE1	2.07	0.55
1:C:217:TRP:CD2	1:C:219:ARG:HG3	2.42	0.55
1:F:6:LEU:CD1	1:F:329:GLU:HG2	2.37	0.55
1:A:362:LEU:HD23	1:A:362:LEU:C	2.32	0.54
1:B:37:TYR:CE1	1:B:263:LEU:HD11	2.42	0.54
1:B:45:PHE:O	1:B:175:THR:HG21	2.06	0.54
1:E:278:GLU:CA	1:E:281:LEU:HD12	2.36	0.54
1:F:15:GLU:O	1:F:16:TYR:C	2.49	0.54
1:F:82:ILE:CD1	1:F:127:THR:HG21	2.34	0.54
1:A:71:LYS:CE	1:A:71:LYS:CA	2.86	0.54
1:D:284:PHE:CE1	1:D:384:ARG:HB2	2.42	0.54
1:F:48:LYS:HB3	1:F:49:TYR:CD1	2.43	0.54
1:F:218:THR:O	1:F:221:LEU:HB2	2.08	0.54
1:G:262:GLN:NE2	1:G:262:GLN:HA	2.22	0.54
1:A:48:LYS:HB2	1:A:201:ASP:HA	1.89	0.54
1:A:303:GLY:HA3	1:A:368:PHE:CE2	2.43	0.54
1:A:331:ARG:HG3	1:A:368:PHE:HD1	1.72	0.54
1:B:11:TRP:HE3	1:B:16:TYR:CE1	2.25	0.54
1:C:120:LYS:CA	1:C:148:ILE:HD13	2.38	0.54
1:A:289:TYR:CD1	1:A:290:LEU:HG	2.43	0.54
1:B:254:MET:O	1:B:258:ILE:HG13	2.07	0.54
1:E:192:THR:O	1:E:193:MET:HB2	2.06	0.54
1:H:32:GLU:OE2	1:H:253:GLU:OE2	2.25	0.54
1:A:338:PHE:HB2	3:A:424:HOH:O	2.07	0.54
1:D:129:ALA:HA	1:D:155:ILE:O	2.08	0.54
1:H:320:VAL:O	1:H:321:GLU:C	2.49	0.54
1:C:167:THR:HA	1:C:171:LYS:O	2.07	0.54
1:D:253:GLU:OE1	1:D:253:GLU:HA	2.07	0.54
1:G:288:PRO:HB2	1:G:289:TYR:HD1	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:250:ARG:NH2	1:D:185:PHE:CE1	2.75	0.54
1:D:35:LYS:CB	1:D:35:LYS:NZ	2.70	0.54
1:D:265:LYS:C	1:D:267:PRO:HD2	2.32	0.54
1:A:47:SER:HB2	3:A:400:HOH:O	2.08	0.54
1:B:30:MET:HB3	1:B:251:PRO:O	2.07	0.54
1:C:119:LEU:O	1:C:120:LYS:C	2.50	0.54
1:C:132:THR:HB	3:C:410:HOH:O	2.07	0.54
1:D:56:GLY:HA3	1:D:183:SER:HB2	1.90	0.54
1:E:29:THR:O	1:E:30:MET:C	2.51	0.54
1:F:58:THR:HG21	1:F:249:VAL:CG1	2.38	0.54
1:F:96:GLN:NE2	1:F:347:TYR:HB3	2.22	0.54
1:F:205:ILE:HG22	1:F:209:LEU:CD1	2.38	0.54
1:H:70:THR:OG1	1:H:73:PRO:HA	2.08	0.54
1:H:106:ASP:OD1	1:H:358:ASN:HB2	2.08	0.54
1:B:111:THR:O	1:B:112:LEU:HB2	2.08	0.54
1:C:58:THR:HG21	1:C:249:VAL:CG1	2.38	0.54
1:C:303:GLY:HA3	1:C:368:PHE:CZ	2.42	0.54
1:D:355:ASN:C	1:D:355:ASN:ND2	2.65	0.54
1:F:37:TYR:CE1	1:F:259:GLY:HA3	2.43	0.54
1:F:103:LYS:HA	1:F:351:THR:O	2.07	0.54
1:F:219:ARG:NH2	1:F:240:PHE:CE1	2.76	0.54
1:G:28:PHE:O	1:G:253:GLU:HB2	2.08	0.54
1:G:59:ALA:HA	1:G:198:ILE:HD11	1.89	0.54
1:H:101:ARG:NH2	1:H:351:THR:HB	2.23	0.54
1:A:136:LEU:C	1:A:302:PHE:HB3	2.32	0.53
1:B:34:VAL:O	1:B:35:LYS:C	2.51	0.53
1:E:360:GLU:HA	1:E:363:ASP:CB	2.38	0.53
1:F:124:THR:HG22	1:F:125:ASP:H	1.72	0.53
1:F:277:ALA:O	1:F:280:PHE:HB3	2.08	0.53
1:F:306:PHE:HB2	1:F:367:LEU:HD13	1.89	0.53
1:G:217:TRP:CD1	1:G:217:TRP:C	2.86	0.53
1:H:164:MET:HE1	1:H:190:ILE:HG12	1.90	0.53
1:A:93:TYR:CB	1:A:94:PRO:HD3	2.31	0.53
1:B:188:LLP:C4'	2:B:402:AKG:O5	2.56	0.53
1:C:106:ASP:CG	1:C:358:ASN:HB2	2.33	0.53
1:F:305:SER:HB2	1:F:333:ILE:HD13	1.90	0.53
1:G:287:HIS:CG	1:G:288:PRO:CD	2.90	0.53
1:G:331:ARG:CB	1:G:332:PRO:CD	2.86	0.53
1:A:136:LEU:O	1:A:302:PHE:N	2.36	0.53
1:A:252:LEU:HD21	1:B:193:MET:HE3	1.90	0.53
1:B:362:LEU:C	1:B:362:LEU:HD23	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:144:GLU:HA	1:G:147:LYS:HD3	1.91	0.53
1:A:320:VAL:O	1:A:321:GLU:C	2.49	0.53
1:C:67:LEU:HD12	1:C:75:LEU:HD12	1.90	0.53
1:E:32:GLU:O	1:E:36:GLN:HB3	2.08	0.53
1:E:303:GLY:CA	1:E:368:PHE:CE1	2.92	0.53
1:F:315:ILE:N	1:F:315:ILE:CD1	2.69	0.53
1:G:217:TRP:HD1	1:G:217:TRP:O	1.91	0.53
1:H:119:LEU:CD2	1:H:145:ILE:HD13	2.37	0.53
1:H:164:MET:HE1	1:H:190:ILE:HD11	1.90	0.53
1:H:337:ASN:O	1:H:340:LYS:HD3	2.09	0.53
1:E:383:LEU:HG	1:E:387:LEU:HD12	1.90	0.53
1:F:289:TYR:HA	1:F:309:LYS:HD2	1.91	0.53
1:F:305:SER:HB2	1:F:333:ILE:CD1	2.38	0.53
1:F:388:LYS:HE3	1:F:388:LYS:HA	1.91	0.53
1:G:222:PRO:HG2	1:G:224:LYS:O	2.08	0.53
1:H:25:SER:O	1:H:26:LYS:HB2	2.09	0.53
1:H:277:ALA:O	1:H:281:LEU:HD12	2.08	0.53
1:B:315:ILE:O	1:B:318:GLN:HB2	2.08	0.53
1:C:94:PRO:O	1:C:95:LEU:C	2.49	0.53
1:F:308:ILE:HB	1:F:365:ASN:HB3	1.90	0.53
1:F:331:ARG:HB2	1:F:332:PRO:CD	2.38	0.53
1:H:93:TYR:N	1:H:94:PRO:CD	2.71	0.53
1:B:320:VAL:O	1:B:321:GLU:C	2.52	0.53
1:E:96:GLN:HB2	1:E:348:PHE:CE2	2.43	0.53
1:F:202:ASP:OD1	1:F:205:ILE:HG12	2.08	0.53
1:G:21:SER:O	1:G:22:VAL:C	2.51	0.53
3:G:395:HOH:O	1:H:93:TYR:HB2	2.09	0.53
1:H:287:HIS:ND1	1:H:290:LEU:HB2	2.23	0.53
1:C:50:ALA:HA	1:C:198:ILE:O	2.09	0.53
1:E:356:VAL:HG23	1:E:356:VAL:O	2.09	0.53
1:A:78:GLY:N	1:A:99:GLY:O	2.38	0.53
1:C:152:ARG:HG2	1:C:152:ARG:NH2	2.14	0.53
1:D:188:LLP:OP3	2:D:404:AKG:O3	2.27	0.53
1:D:333:ILE:O	1:D:333:ILE:HG22	2.06	0.53
1:A:315:ILE:H	1:A:315:ILE:HD12	1.73	0.53
1:C:67:LEU:CD1	1:C:75:LEU:CD1	2.83	0.53
1:F:32:GLU:N	1:F:253:GLU:OE2	2.42	0.53
1:F:167:THR:HG23	1:F:171:LYS:O	2.09	0.53
1:C:308:ILE:CG2	1:C:314:VAL:HG22	2.39	0.52
1:D:273:ARG:NH1	1:D:301:TRP:O	2.42	0.52
1:D:354:ASN:CG	1:D:355:ASN:N	2.66	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:159:ASP:OD1	1:E:188:LLP:H2'2	2.09	0.52
1:F:5:PRO:HA	1:F:329:GLU:HB2	1.91	0.52
1:F:167:THR:HG22	1:F:168:PHE:N	2.23	0.52
1:G:266:LEU:HA	1:G:269:PHE:HB2	1.91	0.52
1:C:122:ALA:HB2	1:C:353:HIS:CD2	2.44	0.52
1:D:161:CYS:HB3	1:D:183:SER:HB3	1.92	0.52
1:E:362:LEU:C	1:E:362:LEU:HD23	2.34	0.52
1:A:171:LYS:HG2	1:A:172:CYS:N	2.25	0.52
1:B:168:PHE:O	1:B:169:ASN:HB2	2.08	0.52
1:E:36:GLN:HG2	1:E:260:ILE:HD11	1.90	0.52
1:E:52:MET:HE1	1:E:255:SER:C	2.35	0.52
1:G:120:LYS:HA	1:G:148:ILE:CD1	2.37	0.52
1:A:171:LYS:HB3	1:A:176:PHE:CZ	2.45	0.52
1:C:141:ASN:O	1:C:145:ILE:HG12	2.10	0.52
1:G:382:TYR:O	1:G:383:LEU:C	2.52	0.52
1:A:93:TYR:N	1:A:94:PRO:CD	2.73	0.52
1:G:26:LYS:HE2	1:H:16:TYR:OH	2.09	0.52
1:C:224:LYS:HA	1:C:229:GLY:O	2.09	0.52
1:F:150:GLY:C	1:F:152:ARG:H	2.18	0.52
1:G:235:GLN:O	1:G:239:SER:HB2	2.10	0.52
1:G:285:LYS:HG3	1:G:286:ASP:N	2.23	0.52
1:H:254:MET:N	3:H:423:HOH:O	2.30	0.52
1:H:287:HIS:CE1	1:H:290:LEU:CG	2.92	0.52
1:A:26:LYS:HA	1:A:28:PHE:CZ	2.45	0.52
1:B:53:VAL:HA	1:B:251:PRO:HG3	1.90	0.52
1:B:60:ASN:OD1	1:B:181:THR:HG21	2.10	0.52
1:C:49:TYR:OH	1:C:203:GLU:HG3	2.10	0.52
1:G:217:TRP:CE2	1:G:219:ARG:HB2	2.45	0.52
1:H:158:GLU:OE2	1:H:174:GLY:N	2.30	0.52
1:H:284:PHE:CE1	1:H:287:HIS:CD2	2.97	0.52
1:A:55:SER:HB3	3:B:396:HOH:O	2.08	0.52
1:B:337:ASN:HB2	1:B:363:ASP:HB2	1.92	0.52
1:E:111:THR:O	1:E:112:LEU:HB2	2.10	0.52
1:A:289:TYR:HD1	1:A:290:LEU:CD2	2.23	0.52
1:C:111:THR:O	1:C:112:LEU:HB2	2.10	0.52
1:E:252:LEU:HB3	3:E:389:HOH:O	2.09	0.52
1:E:324:ASN:ND2	3:E:407:HOH:O	2.43	0.52
1:E:358:ASN:O	1:E:359:ALA:C	2.52	0.52
1:E:384:ARG:HH11	1:E:384:ARG:CG	2.11	0.52
1:G:70:THR:O	1:G:71:LYS:C	2.53	0.52
1:A:248:ASN:HB3	1:B:57:SER:HB2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:287:HIS:CG	1:B:288:PRO:CD	2.91	0.52
1:E:203:GLU:OE1	1:E:226:LYS:HE3	2.10	0.52
1:G:200:THR:HG21	1:G:205:ILE:HG22	1.92	0.52
1:H:255:SER:HA	1:H:258:ILE:CD1	2.37	0.52
1:A:221:LEU:O	1:A:231:LYS:NZ	2.31	0.51
1:B:216:GLY:HA3	1:B:244:LEU:O	2.10	0.51
1:B:376:LEU:C	1:B:379:GLU:HG2	2.35	0.51
1:G:106:ASP:OD2	1:G:358:ASN:HB2	2.10	0.51
1:A:56:GLY:O	1:A:59:ALA:HB3	2.10	0.51
1:A:362:LEU:HD23	1:A:363:ASP:CA	2.40	0.51
1:C:107:ILE:HD12	1:C:107:ILE:O	2.10	0.51
1:D:362:LEU:HD23	1:D:363:ASP:N	2.25	0.51
1:F:111:THR:O	1:F:112:LEU:HB2	2.09	0.51
1:F:373:GLN:H	1:F:373:GLN:CD	2.17	0.51
1:G:221:LEU:HB2	1:G:231:LYS:HD2	1.91	0.51
1:G:303:GLY:HA3	1:G:368:PHE:CE2	2.44	0.51
1:H:279:TYR:HE2	1:H:380:ILE:CG2	2.22	0.51
1:D:266:LEU:N	1:D:267:PRO:HD2	2.25	0.51
1:F:171:LYS:HB3	1:F:176:PHE:CZ	2.46	0.51
1:G:130:ILE:HG22	1:G:132:THR:HG23	1.91	0.51
1:H:253:GLU:N	3:H:423:HOH:O	2.43	0.51
1:B:30:MET:CE	1:B:34:VAL:HG11	2.40	0.51
1:C:152:ARG:CB	1:C:154:ILE:CD1	2.88	0.51
1:C:380:ILE:O	1:C:383:LEU:N	2.44	0.51
1:D:119:LEU:O	1:D:123:VAL:HG23	2.11	0.51
1:D:231:LYS:HB3	1:D:238:GLU:CD	2.35	0.51
1:F:119:LEU:HG	1:F:148:ILE:HD12	1.92	0.51
1:F:205:ILE:O	1:F:208:ILE:HB	2.10	0.51
1:F:224:LYS:HG3	1:F:225:ASN:N	2.25	0.51
1:H:284:PHE:CE1	1:H:384:ARG:HD2	2.45	0.51
1:A:93:TYR:O	1:A:97:GLN:HG3	2.10	0.51
1:C:106:ASP:OD2	1:C:358:ASN:HB2	2.11	0.51
1:E:324:ASN:C	1:E:326:ALA:H	2.18	0.51
1:F:88:TRP:O	1:F:89:SER:C	2.52	0.51
1:F:205:ILE:HA	1:F:208:ILE:HD12	1.93	0.51
1:F:287:HIS:CE1	1:F:289:TYR:CZ	2.96	0.51
1:H:331:ARG:CD	1:H:368:PHE:CD1	2.93	0.51
1:A:169:ASN:O	1:A:170:ASN:HB2	2.09	0.51
1:C:232:SER:OG	1:C:233:ASP:N	2.43	0.51
1:E:266:LEU:O	1:E:269:PHE:HB2	2.11	0.51
1:G:316:ARG:O	1:G:317:LYS:C	2.54	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:274:ARG:NH1	1:H:295:GLU:OE2	2.39	0.51
1:B:188:LLP:OP3	2:B:402:AKG:C4	2.57	0.51
1:D:231:LYS:HB3	1:D:238:GLU:OE2	2.10	0.51
1:F:141:ASN:O	1:F:145:ILE:HG12	2.09	0.51
1:G:12:ASP:N	1:G:15:GLU:OE1	2.39	0.51
1:H:308:ILE:O	1:H:361:TYR:OH	2.15	0.51
1:C:84:PRO:N	1:C:114:ILE:HD12	2.25	0.51
1:E:221:LEU:HG	3:E:398:HOH:O	2.11	0.51
1:F:58:THR:HG21	1:F:249:VAL:HG12	1.93	0.51
1:F:167:THR:HG23	1:F:171:LYS:C	2.36	0.51
1:G:135:LEU:HD12	1:G:162:GLU:OE1	2.10	0.51
1:H:384:ARG:O	1:H:387:LEU:O	2.28	0.51
1:A:353:HIS:O	1:A:354:ASN:HB3	2.11	0.51
1:C:343:ASP:O	1:C:346:LYS:HB2	2.11	0.51
1:G:37:TYR:CE1	1:G:259:GLY:C	2.89	0.51
1:G:205:ILE:O	1:G:206:TYR:C	2.51	0.51
1:G:235:GLN:HG2	1:G:236:PHE:N	2.26	0.51
1:A:324:ASN:O	1:A:327:GLY:N	2.40	0.50
1:E:82:ILE:HD13	1:E:127:THR:HG23	1.93	0.50
1:F:217:TRP:C	1:F:217:TRP:HD1	2.18	0.50
1:H:278:GLU:CA	1:H:281:LEU:HD12	2.35	0.50
1:A:86:VAL:HG22	1:A:336:GLY:O	2.10	0.50
1:A:277:ALA:O	1:A:280:PHE:HB3	2.11	0.50
1:C:45:PHE:CD1	1:C:45:PHE:N	2.79	0.50
1:C:70:THR:OG1	1:C:73:PRO:HA	2.11	0.50
1:E:262:GLN:HA	1:E:262:GLN:NE2	2.26	0.50
1:G:385:GLU:O	1:G:388:LYS:HD2	2.12	0.50
1:H:160:ASN:HA	3:H:391:HOH:O	2.11	0.50
1:H:287:HIS:ND1	1:H:290:LEU:N	2.60	0.50
1:A:57:SER:OG	1:A:188:LLP:OP2	2.25	0.50
1:A:266:LEU:O	1:A:267:PRO:C	2.55	0.50
1:B:29:THR:O	1:B:30:MET:C	2.54	0.50
1:E:320:VAL:HG22	1:E:367:LEU:HD12	1.94	0.50
1:E:362:LEU:HD23	1:E:363:ASP:N	2.27	0.50
1:F:111:THR:HG23	1:F:294:GLN:NE2	2.26	0.50
1:F:178:LEU:HD23	1:F:179:MET:HE2	1.93	0.50
1:H:37:TYR:HB2	1:H:260:ILE:CG1	2.41	0.50
1:A:289:TYR:CE1	1:A:290:LEU:HG	2.46	0.50
1:C:147:LYS:O	1:C:150:GLY:N	2.33	0.50
1:D:40:GLN:O	1:D:44:THR:N	2.39	0.50
1:E:315:ILE:H	1:E:315:ILE:HD13	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:376:LEU:HB2	1:F:380:ILE:HD12	1.91	0.50
1:G:331:ARG:HB2	1:G:332:PRO:HD2	1.94	0.50
1:G:331:ARG:HD3	1:G:368:PHE:CD1	2.46	0.50
1:A:171:LYS:HD2	1:A:176:PHE:CZ	2.46	0.50
1:F:235:GLN:C	1:F:237:GLU:N	2.68	0.50
1:F:235:GLN:C	1:F:237:GLU:H	2.18	0.50
1:G:49:TYR:CD2	1:G:206:TYR:CD2	3.00	0.50
1:G:217:TRP:NE1	1:G:219:ARG:HB2	2.26	0.50
1:B:20:GLN:OE1	1:B:20:GLN:HA	2.01	0.50
1:B:37:TYR:CE1	1:B:263:LEU:CD1	2.95	0.50
1:B:135:LEU:HD21	1:B:334:VAL:HG21	1.92	0.50
1:C:6:LEU:HD12	1:C:329:GLU:HG2	1.94	0.50
1:D:106:ASP:CB	1:D:356:VAL:HA	2.41	0.50
1:D:362:LEU:HD23	1:D:362:LEU:C	2.37	0.50
1:E:103:LYS:HA	1:E:351:THR:HG23	1.92	0.50
1:E:277:ALA:O	1:E:281:LEU:HG	2.12	0.50
1:F:253:GLU:OE1	1:F:253:GLU:HA	2.12	0.50
1:G:179:MET:HG2	1:G:198:ILE:HG23	1.94	0.50
1:G:304:PHE:HB2	1:G:369:VAL:HG23	1.92	0.50
1:A:171:LYS:HG2	1:A:172:CYS:H	1.76	0.50
1:B:320:VAL:HG12	1:B:324:ASN:HD21	1.75	0.50
1:D:149:ILE:HG23	1:D:154:ILE:HB	1.93	0.50
1:E:118:SER:O	1:E:121:GLU:N	2.38	0.50
1:A:63:MET:CG	1:A:179:MET:HE3	2.39	0.50
1:B:53:VAL:C	1:B:251:PRO:HG3	2.37	0.50
1:B:304:PHE:HA	3:B:424:HOH:O	2.11	0.50
1:D:109:ILE:HG13	1:D:109:ILE:O	2.11	0.50
1:F:269:PHE:O	1:F:273:ARG:HG3	2.12	0.50
1:F:341:ASN:O	1:F:345:LEU:HD12	2.12	0.50
1:H:287:HIS:CE1	1:H:289:TYR:CD1	2.99	0.50
1:A:12:ASP:C	1:A:12:ASP:OD1	2.54	0.50
1:C:161:CYS:HB2	1:C:188:LLP:C3	2.42	0.50
1:E:10:THR:HG22	1:E:373:GLN:NE2	2.27	0.50
1:E:343:ASP:O	1:E:346:LYS:HB2	2.12	0.50
1:G:213:ARG:O	1:G:213:ARG:HG2	2.12	0.50
1:G:331:ARG:HB2	1:G:332:PRO:CD	2.42	0.50
1:B:234:ASP:OD1	1:B:234:ASP:C	2.52	0.49
1:C:160:ASN:OD1	1:C:163:SER:HB2	2.11	0.49
1:F:111:THR:CG2	1:F:294:GLN:HE22	2.25	0.49
1:G:171:LYS:HB3	1:G:176:PHE:CZ	2.47	0.49
1:H:35:LYS:O	1:H:36:GLN:C	2.51	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:331:ARG:CD	1:H:368:PHE:HD1	2.25	0.49
1:B:281:LEU:HD23	1:B:281:LEU:N	2.26	0.49
1:C:265:LYS:HB2	1:C:269:PHE:CZ	2.47	0.49
1:C:361:TYR:CD1	1:C:361:TYR:C	2.91	0.49
1:E:333:ILE:O	1:E:333:ILE:HG22	2.12	0.49
1:F:33:TYR:HB2	1:F:253:GLU:HG3	1.93	0.49
1:F:235:GLN:O	1:F:237:GLU:N	2.45	0.49
1:F:287:HIS:HE1	1:F:289:TYR:CE1	2.30	0.49
1:G:108:ASP:OD1	1:G:108:ASP:C	2.56	0.49
1:G:225:ASN:ND2	1:G:231:LYS:HG3	2.27	0.49
1:G:333:ILE:HD13	1:G:366:GLY:HA3	1.94	0.49
1:B:25:SER:O	1:B:26:LYS:HB2	2.11	0.49
1:D:249:VAL:HG23	1:D:249:VAL:O	2.12	0.49
1:A:82:ILE:CG2	1:A:83:VAL:N	2.75	0.49
1:A:311:ASP:O	1:A:312:SER:C	2.55	0.49
1:D:208:ILE:O	1:D:212:ILE:HG23	2.12	0.49
1:G:13:ASP:O	1:G:17:LYS:HB2	2.12	0.49
1:B:206:TYR:O	1:B:209:LEU:HB2	2.13	0.49
1:G:30:MET:CE	1:G:213:ARG:NH2	2.75	0.49
1:G:182:PHE:N	1:G:182:PHE:CD1	2.80	0.49
1:G:288:PRO:HG2	1:G:289:TYR:CD1	2.47	0.49
1:H:167:THR:O	1:H:167:THR:HG22	2.10	0.49
1:C:297:GLY:O	1:C:298:GLU:HG3	2.13	0.49
1:D:224:LYS:HA	1:D:229:GLY:O	2.13	0.49
1:E:135:LEU:HD11	1:E:334:VAL:HG21	1.95	0.49
1:F:56:GLY:O	1:F:59:ALA:HB3	2.13	0.49
1:G:12:ASP:HB2	1:G:265:LYS:HZ3	1.76	0.49
1:A:71:LYS:HE3	1:A:71:LYS:CA	2.42	0.49
1:A:265:LYS:O	1:A:266:LEU:C	2.54	0.49
1:B:266:LEU:N	1:B:267:PRO:HD2	2.28	0.49
1:C:142:PHE:HA	1:C:145:ILE:HG13	1.94	0.49
1:C:190:ILE:HB	1:C:262:GLN:HB3	1.95	0.49
1:E:62:LEU:HG	1:E:212:ILE:HG13	1.95	0.49
1:F:43:LYS:HA	3:F:424:HOH:O	2.11	0.49
1:F:111:THR:HG23	1:F:294:GLN:HE22	1.77	0.49
1:E:118:SER:O	1:E:119:LEU:C	2.55	0.49
1:E:217:TRP:CD1	1:E:217:TRP:C	2.90	0.49
1:G:340:LYS:O	1:G:342:THR:N	2.43	0.49
1:B:19:ILE:HG23	1:B:254:MET:HE2	1.94	0.49
1:B:188:LLP:H4'1	2:B:402:AKG:H41	1.95	0.49
1:B:192:THR:O	1:B:193:MET:HB2	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:269:PHE:HA	1:B:373:GLN:HB2	1.95	0.49
1:D:176:PHE:CD1	1:D:176:PHE:N	2.80	0.49
1:D:289:TYR:CD2	1:D:314:VAL:HG21	2.48	0.49
1:E:106:ASP:OD2	1:E:357:ASP:N	2.46	0.49
1:H:258:ILE:O	1:H:259:GLY:C	2.55	0.49
1:H:275:LYS:HE2	1:H:275:LYS:HB3	1.36	0.49
1:H:303:GLY:HA3	1:H:368:PHE:HZ	1.74	0.49
1:H:388:LYS:HA	1:H:388:LYS:CE	2.42	0.49
1:A:80:GLU:OE1	1:A:127:THR:OG1	2.27	0.49
1:A:287:HIS:HE1	1:A:289:TYR:CE1	2.31	0.49
1:C:151:GLY:O	1:C:152:ARG:O	2.30	0.49
1:E:93:TYR:N	1:E:94:PRO:CD	2.76	0.49
1:E:282:ASP:O	1:E:285:LYS:HB2	2.12	0.49
1:H:266:LEU:HG	1:H:270:ILE:HD11	1.95	0.49
1:C:322:ASN:O	1:C:325:SER:OG	2.28	0.48
1:D:168:PHE:O	1:D:169:ASN:HB2	2.11	0.48
1:D:300:SER:O	1:D:301:TRP:C	2.56	0.48
1:E:380:ILE:O	1:E:381:ASP:C	2.55	0.48
1:F:67:LEU:HD12	1:F:75:LEU:HD12	1.94	0.48
1:G:235:GLN:CG	1:G:236:PHE:N	2.75	0.48
1:G:303:GLY:HA3	1:G:368:PHE:CZ	2.48	0.48
1:D:267:PRO:O	1:D:270:ILE:HB	2.13	0.48
1:E:169:ASN:C	1:E:171:LYS:N	2.71	0.48
1:A:291:ASP:HB2	1:A:307:ILE:O	2.13	0.48
1:C:215:HIS:NE2	1:C:250:ARG:NH1	2.61	0.48
1:C:322:ASN:C	1:C:325:SER:HG	2.21	0.48
1:H:279:TYR:CE2	1:H:380:ILE:CG2	2.96	0.48
1:H:289:TYR:HA	1:H:309:LYS:HD2	1.96	0.48
1:A:217:TRP:C	1:A:217:TRP:HD1	2.21	0.48
1:E:50:ALA:HB1	1:E:197[A]:CYS:SG	2.54	0.48
1:E:268:ARG:O	1:E:269:PHE:C	2.55	0.48
1:E:270:ILE:O	1:E:271:SER:C	2.55	0.48
1:F:315:ILE:HD11	1:F:318:GLN:HG2	1.94	0.48
1:F:356:VAL:HG23	1:F:356:VAL:O	2.13	0.48
1:H:315:ILE:O	1:H:319:LEU:HD12	2.13	0.48
1:A:6:LEU:HD22	1:A:370:GLY:H	1.79	0.48
1:B:4:TYR:O	1:B:329:GLU:HB2	2.12	0.48
1:C:58:THR:O	1:C:61:LEU:HB3	2.13	0.48
1:E:289:TYR:HA	1:E:309:LYS:CD	2.43	0.48
1:H:182:PHE:O	1:H:196:GLY:HA2	2.13	0.48
1:H:284:PHE:CZ	1:H:387:LEU:CD1	2.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:186:TYR:CD2	1:A:186:TYR:C	2.92	0.48
1:A:383:LEU:HD22	1:A:387:LEU:HD12	1.95	0.48
1:C:202:ASP:OD1	1:C:205:ILE:HG12	2.13	0.48
1:G:15:GLU:HG2	1:G:258:ILE:HG23	1.95	0.48
1:G:93:TYR:N	1:G:94:PRO:CD	2.75	0.48
1:G:287:HIS:ND1	1:G:290:LEU:HB2	2.28	0.48
1:G:316:ARG:O	1:G:320:VAL:HG23	2.14	0.48
1:H:131:LEU:HD12	1:H:132:THR:N	2.29	0.48
1:B:6:LEU:HG	1:B:329:GLU:HB3	1.96	0.48
1:B:280:PHE:HD2	1:B:281:LEU:CD2	2.25	0.48
1:C:217:TRP:CD1	1:C:217:TRP:C	2.92	0.48
1:C:241:LYS:HB2	1:C:241:LYS:HE2	1.44	0.48
1:D:15:GLU:OE2	1:D:261:GLU:HB3	2.13	0.48
1:D:354:ASN:CG	1:D:355:ASN:H	2.22	0.48
1:E:215:HIS:O	1:E:242:PHE:CD1	2.67	0.48
1:F:385:GLU:O	1:F:388:LYS:HG2	2.13	0.48
1:A:287:HIS:CE1	1:A:290:LEU:HG	2.49	0.48
1:D:204:GLU:HA	1:D:226:LYS:HG3	1.96	0.48
1:D:242:PHE:CD1	1:D:242:PHE:N	2.81	0.48
1:E:25:SER:O	1:E:26:LYS:HB2	2.14	0.48
1:E:161:CYS:HB2	1:E:188:LLP:C2	2.44	0.48
1:F:289:TYR:C	1:F:290:LEU:HD23	2.38	0.48
1:F:318:GLN:OE1	1:F:318:GLN:HA	2.12	0.48
1:G:337:ASN:HB2	1:G:363:ASP:HB2	1.96	0.48
1:A:108:ASP:OD1	1:A:110:ASN:N	2.40	0.48
1:A:311:ASP:O	1:A:313:GLY:N	2.47	0.48
1:B:321:GLU:O	1:B:325:SER:OG	2.32	0.48
1:D:82:ILE:HD12	1:D:127:THR:CG2	2.44	0.48
1:F:68:PHE:N	1:F:68:PHE:CD1	2.82	0.48
1:F:243:VAL:HG23	1:F:244:LEU:CD1	2.44	0.48
1:G:148:ILE:O	1:G:149:ILE:C	2.55	0.48
1:A:132:THR:HA	3:A:411:HOH:O	2.14	0.48
1:A:224:LYS:HA	1:A:229:GLY:O	2.14	0.48
1:B:24:ASP:HA	1:B:26:LYS:NZ	2.29	0.48
1:B:64:ILE:O	1:B:65:ALA:C	2.56	0.48
1:C:9:SER:O	1:C:373:GLN:NE2	2.47	0.48
1:D:14:LEU:HD12	1:D:265:LYS:HZ1	1.79	0.48
1:D:38:GLU:HB2	3:D:443:HOH:O	2.13	0.48
1:F:70:THR:O	1:F:71:LYS:C	2.57	0.48
1:F:86:VAL:O	1:F:87:SER:HB2	2.13	0.48
1:F:141:ASN:OD1	1:F:141:ASN:C	2.55	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:306:PHE:O	1:G:366:GLY:HA2	2.14	0.48
1:G:368:PHE:CD1	1:G:368:PHE:C	2.92	0.48
1:H:164:MET:HE1	1:H:190:ILE:CG1	2.44	0.48
1:H:377:PHE:O	1:H:380:ILE:HB	2.14	0.48
1:C:79:ASP:CB	1:C:128:LYS:HG3	2.44	0.47
1:D:23:LEU:HA	1:D:28:PHE:HE1	1.79	0.47
1:D:106:ASP:OD2	1:D:358:ASN:HB2	2.12	0.47
1:D:120:LYS:HA	1:D:148:ILE:HD13	1.96	0.47
1:E:115:ASP:OD2	1:E:118:SER:HB2	2.14	0.47
1:F:269:PHE:HA	1:F:373:GLN:HB2	1.96	0.47
1:G:3:ASN:OD1	1:G:3:ASN:N	2.47	0.47
1:G:52:MET:O	1:G:251:PRO:HG3	2.13	0.47
1:A:6:LEU:CG	1:A:329:GLU:HG2	2.40	0.47
1:B:292:VAL:HG12	3:B:399:HOH:O	2.12	0.47
1:C:34:VAL:HG23	1:C:253:GLU:OE1	2.14	0.47
1:C:84:PRO:HA	1:C:114:ILE:HD12	1.95	0.47
1:C:137:GLY:O	1:C:299:SER:HA	2.14	0.47
1:G:15:GLU:OE2	1:G:262:GLN:NE2	2.47	0.47
1:G:71:LYS:HA	1:G:71:LYS:HD3	1.43	0.47
1:G:280:PHE:HB2	1:G:380:ILE:HD13	1.95	0.47
1:D:266:LEU:N	1:D:267:PRO:CD	2.77	0.47
1:E:102:VAL:O	1:E:350:TYR:HA	2.14	0.47
1:E:168:PHE:CD2	1:E:169:ASN:ND2	2.81	0.47
1:F:58:THR:CG2	1:F:249:VAL:HG11	2.45	0.47
1:G:112:LEU:N	1:G:112:LEU:CD2	2.76	0.47
1:G:162:GLU:HG3	1:G:188:LLP:HO3	1.78	0.47
1:H:331:ARG:CG	1:H:368:PHE:HD1	2.27	0.47
1:B:376:LEU:HB3	1:B:379:GLU:CG	2.43	0.47
1:C:356:VAL:O	1:C:357:ASP:C	2.56	0.47
1:D:344:VAL:CG1	1:D:345:LEU:N	2.77	0.47
1:E:303:GLY:C	1:E:368:PHE:CE1	2.92	0.47
1:F:218:THR:HB	1:F:221:LEU:HD12	1.96	0.47
1:F:248:ASN:OD1	1:F:248:ASN:C	2.58	0.47
1:G:141:ASN:O	1:G:145:ILE:HG12	2.14	0.47
1:G:171:LYS:HB3	1:G:176:PHE:HZ	1.79	0.47
1:G:333:ILE:CD1	1:G:366:GLY:HA3	2.44	0.47
1:G:373:GLN:CD	1:G:373:GLN:H	2.22	0.47
1:B:30:MET:HE3	1:B:30:MET:HB2	1.69	0.47
1:B:55:SER:O	1:B:56:GLY:C	2.54	0.47
1:C:252:LEU:HD12	1:D:252:LEU:HD12	1.97	0.47
1:G:138:ASN:OD1	1:G:295:GLU:HA	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:71:LYS:HD3	1:H:71:LYS:HA	1.51	0.47
1:A:289:TYR:CD1	1:A:290:LEU:CD2	2.97	0.47
1:C:319:LEU:O	1:C:320:VAL:C	2.57	0.47
1:E:10:THR:CG2	1:E:373:GLN:NE2	2.78	0.47
1:E:265:LYS:HG2	1:E:269:PHE:CZ	2.48	0.47
1:F:144:GLU:OE1	1:F:144:GLU:HA	2.14	0.47
1:A:371:ASN:C	1:A:372:HIS:HD2	2.22	0.47
1:B:23:LEU:HD23	1:B:23:LEU:HA	1.54	0.47
1:B:342:THR:O	1:B:346:LYS:HG2	2.14	0.47
1:D:269:PHE:CG	1:D:373:GLN:HG3	2.50	0.47
1:D:273:ARG:HB3	1:D:371:ASN:HD21	1.79	0.47
1:E:158:GLU:CD	1:E:174:GLY:H	2.20	0.47
1:E:331:ARG:O	1:E:368:PHE:N	2.41	0.47
1:E:373:GLN:OE1	1:E:373:GLN:N	2.43	0.47
1:F:124:THR:CG2	1:F:125:ASP:N	2.78	0.47
1:F:217:TRP:HD1	1:F:217:TRP:O	1.98	0.47
1:F:273:ARG:NH1	1:F:371:ASN:O	2.48	0.47
1:G:167:THR:HA	1:G:171:LYS:O	2.14	0.47
1:G:217:TRP:CD1	1:G:219:ARG:HB2	2.50	0.47
1:H:345:LEU:HA	1:H:345:LEU:HD23	1.77	0.47
1:A:289:TYR:HD1	1:A:290:LEU:HD23	1.79	0.47
1:B:184:SER:HB2	1:B:192:THR:OG1	2.14	0.47
1:C:118:SER:O	1:C:122:ALA:N	2.37	0.47
1:D:232:SER:OG	1:D:233:ASP:N	2.48	0.47
1:D:269:PHE:HA	1:D:373:GLN:HB2	1.97	0.47
1:D:273:ARG:CB	1:D:371:ASN:HD21	2.27	0.47
1:E:62:LEU:O	1:E:63:MET:C	2.58	0.47
1:E:303:GLY:C	1:E:368:PHE:HE1	2.23	0.47
1:F:374:ILE:O	1:F:374:ILE:HG13	2.14	0.47
1:G:203:GLU:HA	1:G:206:TYR:HB3	1.97	0.47
1:H:304:PHE:HB2	1:H:369:VAL:HG22	1.97	0.47
1:H:320:VAL:HA	1:H:323:LEU:HD12	1.96	0.47
1:A:85:ALA:N	1:A:105:VAL:O	2.47	0.47
1:A:185:PHE:CG	1:A:186:TYR:N	2.83	0.47
1:B:222:PRO:HG2	1:B:225:ASN:HB3	1.96	0.47
1:B:341:ASN:C	1:B:345:LEU:HD22	2.40	0.47
1:C:101:ARG:NH1	1:C:349:ASP:OD1	2.42	0.47
1:D:367:LEU:CD1	1:D:367:LEU:N	2.78	0.47
1:E:303:GLY:HA3	1:E:368:PHE:HZ	1.75	0.47
1:H:185:PHE:HB3	1:H:188:LLP:HG2	1.97	0.47
1:B:53:VAL:N	1:B:251:PRO:HG3	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:243:VAL:O	1:E:244:LEU:HD13	2.15	0.47
1:F:67:LEU:HD12	1:F:75:LEU:CD1	2.45	0.47
1:G:206:TYR:O	1:G:209:LEU:HD12	2.14	0.47
1:G:235:GLN:O	1:G:237:GLU:N	2.48	0.47
1:G:315:ILE:HB	1:G:318:GLN:HB2	1.96	0.47
1:H:372:HIS:H	1:H:376:LEU:HD11	1.79	0.47
1:C:145:ILE:HG12	1:C:145:ILE:H	1.49	0.46
1:F:206:TYR:CD2	1:F:207:HIS:HD2	2.32	0.46
1:G:285:LYS:HD2	1:G:286:ASP:CG	2.39	0.46
1:G:333:ILE:HD11	1:G:367:LEU:N	2.30	0.46
1:H:318:GLN:O	1:H:321:GLU:HB3	2.15	0.46
1:B:168:PHE:C	1:B:170:ASN:N	2.73	0.46
1:C:70:THR:HG21	1:C:74:ARG:NE	2.30	0.46
1:C:355:ASN:OD1	3:C:423:HOH:O	2.19	0.46
1:E:184:SER:HG	1:E:192:THR:HG1	1.50	0.46
1:G:37:TYR:HE1	1:G:259:GLY:C	2.23	0.46
1:C:152:ARG:CG	1:C:154:ILE:HD11	2.45	0.46
1:F:134:ASN:OD1	1:F:140:ASN:ND2	2.32	0.46
1:G:61:LEU:HD21	1:G:247:TYR:CE1	2.49	0.46
1:G:182:PHE:HB3	3:G:409:HOH:O	2.15	0.46
1:G:309:LYS:O	1:G:312:SER:HB3	2.15	0.46
1:H:268:ARG:O	1:H:272:VAL:HB	2.15	0.46
1:H:272:VAL:HG11	1:H:373:GLN:C	2.40	0.46
1:H:287:HIS:CD2	1:H:288:PRO:HD2	2.51	0.46
1:A:70:THR:O	1:A:71:LYS:C	2.58	0.46
1:C:202:ASP:HB3	1:C:205:ILE:CG1	2.44	0.46
1:E:120:LYS:HB2	1:E:120:LYS:HE3	1.37	0.46
1:G:92:TYR:C	1:G:94:PRO:HD2	2.41	0.46
1:A:148:ILE:O	1:A:148:ILE:HG22	2.15	0.46
1:A:217:TRP:CE2	1:A:219:ARG:HB2	2.51	0.46
1:E:135:LEU:HG	1:E:136:LEU:HG	1.96	0.46
1:F:6:LEU:HD12	1:F:329:GLU:CG	2.43	0.46
1:A:136:LEU:HA	1:A:302:PHE:HB3	1.97	0.46
1:C:6:LEU:HD12	1:C:329:GLU:OE2	2.16	0.46
1:C:310:LYS:O	1:C:311:ASP:CB	2.50	0.46
1:D:337:ASN:HB2	1:D:359:ALA:O	2.16	0.46
1:E:147:LYS:HE2	1:E:147:LYS:HB2	1.66	0.46
1:E:253:GLU:O	1:E:256:GLY:N	2.49	0.46
1:G:33:TYR:HB2	1:G:253:GLU:CD	2.39	0.46
1:A:82:ILE:HG22	1:A:83:VAL:N	2.30	0.46
1:C:77:LYS:H	1:C:77:LYS:HG2	1.52	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:GLY:HA2	1:C:163:SER:HA	1.97	0.46
1:D:41:PHE:O	1:D:45:PHE:HD1	1.98	0.46
1:F:4:TYR:CD1	1:F:4:TYR:C	2.93	0.46
1:G:119:LEU:O	1:G:123:VAL:HG23	2.16	0.46
1:G:298:GLU:O	1:G:299:SER:C	2.57	0.46
1:H:336:GLY:HA2	1:H:362:LEU:CD2	2.46	0.46
1:B:24:ASP:HA	1:B:26:LYS:HZ2	1.80	0.46
1:B:287:HIS:CE1	1:B:288:PRO:HD2	2.50	0.46
1:C:380:ILE:HG22	1:C:381:ASP:N	2.30	0.46
1:D:202:ASP:CG	1:D:205:ILE:HG12	2.41	0.46
1:G:31:GLY:N	1:G:253:GLU:OE1	2.41	0.46
1:H:102:VAL:HG12	1:H:104:PHE:CE1	2.51	0.46
1:A:362:LEU:HD23	1:A:363:ASP:HA	1.97	0.46
1:B:19:ILE:O	1:B:20:GLN:C	2.57	0.46
1:B:150:GLY:HA2	1:B:151:GLY:HA2	1.55	0.46
1:B:252:LEU:O	1:B:253:GLU:C	2.59	0.46
1:C:36:GLN:HG2	1:C:260:ILE:CD1	2.45	0.46
1:D:22:VAL:O	1:D:25:SER:OG	2.34	0.46
1:E:287:HIS:CD2	1:E:384:ARG:NE	2.83	0.46
1:E:336:GLY:HA2	1:E:362:LEU:CD2	2.40	0.46
1:H:54:SER:OG	1:H:58:THR:HG21	2.16	0.46
1:H:380:ILE:O	1:H:383:LEU:HB3	2.16	0.46
1:A:81:ILE:HG13	1:A:82:ILE:N	2.29	0.46
1:A:238:GLU:OE1	1:A:238:GLU:HA	2.16	0.46
1:B:67:LEU:HD21	1:B:179:MET:HE1	1.97	0.46
1:B:120:LYS:HA	1:B:148:ILE:CG2	2.45	0.46
1:C:84:PRO:CB	1:C:114:ILE:HD12	2.46	0.46
1:C:149:ILE:O	1:C:149:ILE:HG23	2.16	0.46
1:G:93:TYR:HB2	1:G:94:PRO:HD3	1.97	0.46
1:G:253:GLU:OE1	1:G:253:GLU:HA	2.15	0.46
1:H:42:ALA:HB1	1:H:47:SER:O	2.16	0.46
1:H:137:GLY:HA2	1:H:163:SER:HA	1.97	0.46
1:H:161:CYS:HB2	1:H:188:LLP:C2	2.46	0.46
1:H:287:HIS:CE1	1:H:290:LEU:CD1	2.98	0.46
1:A:232:SER:OG	1:A:233:ASP:N	2.49	0.45
1:D:33:TYR:CG	1:D:257:ALA:HB2	2.51	0.45
1:F:361:TYR:O	1:F:362:LEU:C	2.59	0.45
1:G:70:THR:HG21	1:G:74:ARG:HE	1.82	0.45
1:G:209:LEU:HA	1:G:212:ILE:CG1	2.39	0.45
1:H:52:MET:O	1:H:251:PRO:HG3	2.15	0.45
1:H:124:THR:HG23	1:H:125:ASP:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:249:VAL:HG23	1:H:249:VAL:O	2.15	0.45
1:H:314:VAL:CG1	1:H:319:LEU:HD21	2.46	0.45
1:A:266:LEU:N	1:A:267:PRO:HD2	2.31	0.45
1:C:280:PHE:O	1:C:281:LEU:C	2.57	0.45
1:F:120:LYS:HB2	1:F:120:LYS:HE2	1.44	0.45
1:C:156:LEU:O	1:C:177:GLY:CA	2.64	0.45
1:D:69:PHE:CZ	1:D:245:PRO:HD2	2.50	0.45
1:D:346:LYS:HE2	1:D:346:LYS:HB2	1.54	0.45
1:E:203:GLU:O	1:E:206:TYR:HB3	2.16	0.45
1:E:345:LEU:O	1:E:346:LYS:C	2.57	0.45
1:F:26:LYS:HA	1:F:26:LYS:HZ3	1.81	0.45
1:F:48:LYS:HE3	1:F:201:ASP:O	2.17	0.45
1:H:37:TYR:HB2	1:H:260:ILE:HG12	1.98	0.45
1:H:168:PHE:O	1:H:169:ASN:C	2.59	0.45
1:H:379:GLU:O	1:H:382:TYR:HB3	2.16	0.45
1:A:203:GLU:O	1:A:206:TYR:HB3	2.16	0.45
1:B:27:MET:C	1:B:27:MET:SD	2.98	0.45
1:B:66:ALA:C	1:B:68:PHE:H	2.25	0.45
1:B:71:LYS:HE2	1:B:204:GLU:CD	2.41	0.45
1:C:72:LYS:HD2	1:C:72:LYS:HA	1.85	0.45
1:D:185:PHE:HB2	3:D:400:HOH:O	2.15	0.45
1:E:86:VAL:O	1:E:87:SER:HB2	2.16	0.45
1:G:235:GLN:C	1:G:237:GLU:N	2.73	0.45
1:A:136:LEU:C	1:A:302:PHE:CB	2.89	0.45
1:C:26:LYS:HA	1:C:28:PHE:CZ	2.51	0.45
1:C:101:ARG:HE	1:C:349:ASP:CG	2.24	0.45
1:E:266:LEU:N	1:E:267:PRO:CD	2.77	0.45
1:F:154:ILE:HD12	1:F:154:ILE:H	1.81	0.45
1:F:206:TYR:O	1:F:209:LEU:HB2	2.16	0.45
1:G:57:SER:HB2	1:H:248:ASN:HB3	1.98	0.45
1:B:221:LEU:O	1:B:231:LYS:NZ	2.47	0.45
1:C:245:PRO:HA	1:D:93:TYR:CD1	2.52	0.45
1:E:186:TYR:CD1	1:E:186:TYR:C	2.93	0.45
1:E:234:ASP:OD1	1:E:234:ASP:C	2.58	0.45
1:G:64:ILE:O	1:G:67:LEU:HB2	2.17	0.45
1:A:331:ARG:CB	1:A:332:PRO:HD2	2.46	0.45
1:B:387:LEU:HD23	1:B:387:LEU:HA	1.65	0.45
1:C:323:LEU:HD23	1:C:323:LEU:HA	1.62	0.45
1:C:384:ARG:HG3	1:C:384:ARG:O	2.15	0.45
1:D:76:LYS:O	1:D:79:ASP:HB2	2.17	0.45
1:F:368:PHE:CD1	1:F:368:PHE:C	2.94	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:36:GLN:HB3	1:G:260:ILE:HD11	1.98	0.45
1:G:137:GLY:HA2	1:G:163:SER:HA	1.99	0.45
1:H:331:ARG:O	1:H:368:PHE:N	2.43	0.45
1:F:102:VAL:O	1:F:350:TYR:HA	2.17	0.45
1:G:4:TYR:HB3	1:G:328:ILE:HA	1.99	0.45
1:G:88:TRP:HD1	1:G:90:THR:OG1	1.99	0.45
1:H:304:PHE:CE2	1:H:371:ASN:HB2	2.52	0.45
1:H:381:ASP:N	1:H:381:ASP:OD1	2.50	0.45
1:A:244:LEU:HA	1:A:245:PRO:HD3	1.67	0.45
1:D:273:ARG:HG2	1:D:371:ASN:ND2	2.32	0.45
1:F:182:PHE:HE1	1:F:199:VAL:HG22	1.82	0.45
1:G:379:GLU:CD	1:G:379:GLU:N	2.73	0.45
1:A:316:ARG:NH1	1:A:366:GLY:O	2.48	0.45
1:A:356:VAL:HG23	1:A:356:VAL:O	2.16	0.45
1:C:97:GLN:HB3	3:C:439:HOH:O	2.17	0.45
1:C:265:LYS:O	1:C:266:LEU:C	2.58	0.45
1:G:37:TYR:CE1	1:G:259:GLY:CA	3.00	0.45
1:H:139:PRO:HG3	1:H:166:ALA:HB1	1.99	0.45
1:A:289:TYR:HB2	1:A:312:SER:HB2	1.99	0.44
1:B:12:ASP:N	1:B:15:GLU:OE1	2.36	0.44
1:B:119:LEU:O	1:B:120:LYS:C	2.57	0.44
1:G:67:LEU:HD13	1:G:75:LEU:HD12	1.98	0.44
1:G:333:ILE:O	1:G:334:VAL:C	2.59	0.44
1:A:12:ASP:CG	1:A:265:LYS:HZ1	2.25	0.44
1:A:237:GLU:O	1:A:238:GLU:C	2.60	0.44
1:B:373:GLN:O	1:B:373:GLN:HG2	2.16	0.44
1:C:280:PHE:CZ	1:C:304:PHE:CB	2.98	0.44
1:C:320:VAL:O	1:C:321:GLU:C	2.56	0.44
1:D:137:GLY:HA2	1:D:163:SER:CB	2.47	0.44
1:E:106:ASP:CG	1:E:356:VAL:HA	2.42	0.44
1:F:289:TYR:CD1	1:F:290:LEU:CD2	3.00	0.44
1:A:161:CYS:HB2	1:A:188:LLP:C3	2.47	0.44
1:B:15:GLU:O	1:B:18:ALA:HB3	2.18	0.44
1:C:263:LEU:HD23	1:C:263:LEU:HA	1.58	0.44
1:D:81:ILE:HD11	1:D:131:LEU:HB2	1.98	0.44
1:E:35:LYS:HE2	1:E:35:LYS:HB2	1.74	0.44
1:E:67:LEU:CD2	1:E:74:ARG:HD3	2.48	0.44
1:E:190:ILE:CG2	1:E:266:LEU:HD13	2.47	0.44
1:F:106:ASP:OD1	1:F:358:ASN:HB2	2.18	0.44
1:F:385:GLU:O	1:F:388:LYS:HD2	2.18	0.44
1:G:94:PRO:HA	1:G:97:GLN:HE21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:10:THR:HG22	1:H:373:GLN:NE2	2.32	0.44
1:H:248:ASN:OD1	1:H:250:ARG:HB2	2.18	0.44
1:C:287:HIS:CG	1:C:288:PRO:HD2	2.52	0.44
1:D:277:ALA:O	1:D:280:PHE:HB3	2.17	0.44
1:D:368:PHE:CD1	1:D:368:PHE:C	2.96	0.44
1:E:130:ILE:HG22	1:E:132:THR:CG2	2.48	0.44
1:E:130:ILE:HG22	1:E:132:THR:HG23	1.98	0.44
1:G:234:ASP:O	1:G:237:GLU:N	2.51	0.44
1:G:250:ARG:HH21	1:H:194:GLU:CD	2.26	0.44
1:G:266:LEU:O	1:G:267:PRO:C	2.61	0.44
1:H:61:LEU:HD12	1:H:94:PRO:HB3	2.00	0.44
1:H:217:TRP:C	1:H:217:TRP:CD1	2.95	0.44
1:H:315:ILE:N	1:H:315:ILE:CD1	2.80	0.44
1:B:71:LYS:O	1:B:73:PRO:HD3	2.17	0.44
1:B:155:ILE:CG2	1:B:156:LEU:N	2.80	0.44
1:D:35:LYS:HB2	1:D:35:LYS:HZ1	1.83	0.44
1:D:83:VAL:HG12	1:D:131:LEU:HD23	1.99	0.44
1:H:375:GLU:O	1:H:375:GLU:HG2	2.17	0.44
1:A:271:SER:O	1:A:275:LYS:HB2	2.17	0.44
1:A:336:GLY:HA2	1:A:362:LEU:HD21	2.00	0.44
1:C:22:VAL:HG22	1:C:33:TYR:CE2	2.52	0.44
1:C:51:VAL:O	1:C:197[B]:CYS:HA	2.17	0.44
1:C:77:LYS:C	1:C:79:ASP:H	2.24	0.44
1:G:222:PRO:O	1:G:231:LYS:HD3	2.18	0.44
1:H:273:ARG:NH1	1:H:371:ASN:O	2.51	0.44
1:B:323:LEU:O	1:B:328:ILE:HB	2.18	0.44
1:E:136:LEU:HA	1:E:302:PHE:HB3	1.98	0.44
1:E:323:LEU:HD23	1:E:386:VAL:HG11	1.99	0.44
1:E:385:GLU:OE1	1:E:385:GLU:CA	2.64	0.44
1:G:141:ASN:OD1	1:G:141:ASN:O	2.36	0.44
1:G:213:ARG:HG3	1:G:249:VAL:HG23	1.99	0.44
1:H:118:SER:O	1:H:119:LEU:C	2.60	0.44
1:B:23:LEU:HD23	1:B:28:PHE:HE1	1.83	0.44
1:B:137:GLY:HA2	1:B:163:SER:HA	2.00	0.44
1:B:345:LEU:C	1:B:347:TYR:N	2.74	0.44
1:E:169:ASN:C	1:E:171:LYS:H	2.26	0.44
1:H:326:ALA:HB1	1:H:382:TYR:CZ	2.52	0.44
1:H:382:TYR:C	1:H:382:TYR:CD1	2.95	0.44
1:B:283:LYS:HA	1:B:283:LYS:HD2	1.75	0.44
1:B:340:LYS:NZ	3:B:409:HOH:O	2.50	0.44
1:C:58:THR:CG2	1:C:249:VAL:HG11	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:225:ASN:OD1	1:D:228:THR:OG1	2.31	0.44
1:D:263:LEU:HD23	1:D:263:LEU:HA	1.78	0.44
1:E:30:MET:CG	1:E:34:VAL:HG11	2.44	0.44
1:F:14:LEU:HD12	1:F:14:LEU:HA	1.73	0.44
1:F:287:HIS:CG	1:F:288:PRO:HD2	2.52	0.44
1:G:161:CYS:HB3	1:G:183:SER:HB3	2.00	0.44
1:G:334:VAL:HG12	1:G:335:THR:N	2.33	0.44
1:A:368:PHE:CD1	1:A:368:PHE:C	2.96	0.43
1:C:93:TYR:HB2	3:D:416:HOH:O	2.17	0.43
1:C:318:GLN:O	1:C:322:ASN:ND2	2.51	0.43
1:D:35:LYS:NZ	1:D:35:LYS:HB2	2.32	0.43
1:D:37:TYR:CE1	1:D:259:GLY:HA3	2.52	0.43
1:D:82:ILE:HD12	1:D:127:THR:HG23	2.00	0.43
1:D:310:LYS:HE2	1:D:310:LYS:HB2	1.65	0.43
1:E:5:PRO:HA	1:E:329:GLU:HB3	1.98	0.43
1:E:289:TYR:CD1	1:E:289:TYR:N	2.86	0.43
1:F:23:LEU:HD23	1:F:23:LEU:HA	1.76	0.43
1:F:76:LYS:HG2	1:F:79:ASP:OD2	2.18	0.43
1:G:119:LEU:HD11	1:G:130:ILE:CD1	2.48	0.43
1:G:225:ASN:HD21	1:G:231:LYS:HG3	1.83	0.43
1:G:244:LEU:HA	1:G:245:PRO:HD3	1.81	0.43
1:G:324:ASN:C	1:G:326:ALA:N	2.73	0.43
1:H:232:SER:OG	1:H:233:ASP:N	2.49	0.43
1:H:315:ILE:H	1:H:315:ILE:CD1	2.25	0.43
1:A:245:PRO:HA	1:B:93:TYR:CE1	2.54	0.43
1:C:58:THR:HG21	1:C:249:VAL:HG12	2.00	0.43
1:D:388:LYS:HA	1:D:388:LYS:HD2	1.51	0.43
1:E:169:ASN:O	1:E:171:LYS:N	2.51	0.43
1:E:193:MET:HB3	1:F:252:LEU:HD22	1.99	0.43
1:F:215:HIS:NE2	1:F:250:ARG:NH1	2.59	0.43
1:G:92:TYR:O	1:G:95:LEU:HG	2.18	0.43
1:G:331:ARG:HB2	1:G:331:ARG:HE	1.71	0.43
1:H:85:ALA:HB1	1:H:339:LEU:HD12	2.00	0.43
1:H:336:GLY:HA2	1:H:362:LEU:HD21	2.00	0.43
1:A:64:ILE:N	1:A:64:ILE:HD13	2.29	0.43
1:E:69:PHE:CZ	1:E:245:PRO:HG2	2.53	0.43
1:F:179:MET:HE3	1:F:179:MET:HB2	1.88	0.43
1:F:224:LYS:HE3	1:F:224:LYS:HB2	1.37	0.43
1:F:333:ILE:HB	1:F:362:LEU:HD21	2.00	0.43
1:G:234:ASP:O	1:G:235:GLN:C	2.62	0.43
1:G:333:ILE:CD1	1:G:367:LEU:N	2.81	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:77:LYS:H	1:H:77:LYS:HG2	1.64	0.43
1:H:265:LYS:O	1:H:266:LEU:C	2.62	0.43
1:A:283:LYS:O	1:A:384:ARG:HD3	2.17	0.43
1:E:155:ILE:H	1:E:155:ILE:HG13	1.50	0.43
1:F:21:SER:O	1:F:25:SER:HB3	2.18	0.43
1:F:145:ILE:HG12	1:F:145:ILE:H	1.24	0.43
1:F:289:TYR:HD1	1:F:290:LEU:CD2	2.31	0.43
1:G:114:ILE:O	1:G:114:ILE:HG23	2.17	0.43
1:G:209:LEU:O	1:G:213:ARG:N	2.48	0.43
1:G:384:ARG:HG3	1:G:384:ARG:HH11	1.82	0.43
1:H:372:HIS:C	1:H:374:ILE:H	2.26	0.43
1:A:160:ASN:ND2	1:A:182:PHE:CE2	2.78	0.43
1:A:202:ASP:HB3	1:A:205:ILE:HD12	2.01	0.43
1:B:13:ASP:O	1:B:17:LYS:HG2	2.18	0.43
1:E:92:TYR:O	1:E:95:LEU:HG	2.18	0.43
1:E:116:ILE:C	1:E:118:SER:N	2.76	0.43
1:F:50:ALA:HB2	1:F:199:VAL:HG12	2.00	0.43
1:F:150:GLY:O	1:F:152:ARG:N	2.52	0.43
1:G:65:ALA:O	1:G:66:ALA:C	2.60	0.43
1:G:177:GLY:C	1:G:179:MET:N	2.74	0.43
1:G:185:PHE:O	1:G:186:TYR:C	2.62	0.43
1:H:289:TYR:CD1	1:H:289:TYR:N	2.85	0.43
1:B:71:LYS:HB2	1:B:71:LYS:HE3	1.08	0.43
1:E:116:ILE:O	1:E:117:GLU:C	2.60	0.43
1:G:89:SER:HB2	1:G:93:TYR:CZ	2.54	0.43
1:H:20:GLN:OE1	1:H:23:LEU:HD12	2.18	0.43
1:H:182:PHE:CD1	1:H:182:PHE:N	2.86	0.43
1:B:145:ILE:HG22	1:B:149:ILE:CD1	2.49	0.43
1:C:152:ARG:CB	1:C:154:ILE:HD11	2.49	0.43
1:E:57:SER:HB2	1:F:248:ASN:HB3	2.00	0.43
1:F:142:PHE:HA	1:F:145:ILE:CG1	2.46	0.43
1:F:223:LYS:HD2	3:F:429:HOH:O	2.19	0.43
1:G:86:VAL:HG22	1:G:336:GLY:O	2.18	0.43
1:G:137:GLY:O	1:G:166:ALA:HB2	2.19	0.43
1:G:331:ARG:HD3	1:G:368:PHE:HD1	1.84	0.43
1:G:387:LEU:HD23	1:G:387:LEU:HA	1.75	0.43
1:H:287:HIS:CG	1:H:290:LEU:HB2	2.53	0.43
1:A:29:THR:O	1:A:30:MET:C	2.61	0.43
1:A:268:ARG:O	1:A:269:PHE:C	2.61	0.43
1:B:56:GLY:HA3	1:B:183:SER:HB2	2.01	0.43
1:B:70:THR:O	1:B:71:LYS:C	2.60	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:ASP:O	1:D:235:GLN:C	2.60	0.43
1:F:106:ASP:CG	1:F:356:VAL:HA	2.43	0.43
1:G:223:LYS:HD3	1:G:231:LYS:HB2	2.00	0.43
1:G:252:LEU:HD12	1:H:252:LEU:HD12	2.01	0.43
1:H:8:SER:OG	1:H:9:SER:N	2.52	0.43
1:H:238:GLU:O	1:H:240:PHE:N	2.52	0.43
1:H:254:MET:O	1:H:255:SER:C	2.61	0.43
1:H:263:LEU:HD23	1:H:263:LEU:HA	1.86	0.43
1:A:120:LYS:HG3	1:A:148:ILE:HD11	2.00	0.43
1:A:345:LEU:HD23	1:A:345:LEU:HA	1.80	0.43
1:B:266:LEU:HB3	1:B:267:PRO:CD	2.48	0.43
1:B:308:ILE:HB	1:B:365:ASN:HB3	2.01	0.43
1:C:109:ILE:HD12	1:C:307:ILE:CD1	2.49	0.43
1:C:155:ILE:HG22	1:C:156:LEU:N	2.34	0.43
1:D:14:LEU:HD12	1:D:265:LYS:NZ	2.34	0.43
1:E:209:LEU:O	1:E:210:LEU:C	2.61	0.43
1:F:310:LYS:O	1:F:311:ASP:CB	2.63	0.43
1:G:75:LEU:HA	1:G:79:ASP:OD2	2.18	0.43
1:G:253:GLU:O	1:G:254:MET:C	2.60	0.43
1:G:331:ARG:CB	1:G:332:PRO:HD2	2.49	0.43
1:G:333:ILE:CD1	1:G:366:GLY:C	2.92	0.43
1:H:42:ALA:O	1:H:43:LYS:C	2.61	0.43
1:H:270:ILE:C	1:H:272:VAL:N	2.77	0.43
1:A:250:ARG:NH2	1:B:185:PHE:CE1	2.87	0.43
1:A:292:VAL:HB	3:A:412:HOH:O	2.18	0.43
1:B:137:GLY:HA2	1:B:163:SER:CB	2.49	0.43
1:E:232:SER:OG	1:E:233:ASP:N	2.52	0.43
1:F:77:LYS:H	1:F:77:LYS:HG2	1.63	0.43
1:F:148:ILE:O	1:F:152:ARG:NH2	2.51	0.43
1:F:314:VAL:CG1	1:F:315:ILE:N	2.81	0.43
1:C:235:GLN:O	1:C:236:PHE:C	2.61	0.42
1:C:291:ASP:OD2	1:C:309:LYS:HG2	2.18	0.42
1:C:322:ASN:HA	1:C:325:SER:OG	2.19	0.42
1:E:52:MET:HG2	1:E:251:PRO:HG3	1.99	0.42
1:E:65:ALA:O	1:E:68:PHE:HB2	2.19	0.42
1:F:49:TYR:HE1	1:F:201:ASP:O	2.01	0.42
1:F:161:CYS:CB	1:F:188:LLP:C2	2.94	0.42
1:F:266:LEU:CB	1:F:267:PRO:CD	2.95	0.42
1:H:266:LEU:N	1:H:267:PRO:CD	2.82	0.42
1:H:266:LEU:CB	1:H:267:PRO:HD3	2.31	0.42
1:H:372:HIS:HB2	1:H:374:ILE:HG13	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:116:ILE:HG21	1:B:144:GLU:HG2	2.01	0.42
1:B:124:THR:CG2	1:B:125:ASP:N	2.62	0.42
1:B:299:SER:HB3	1:B:301:TRP:NE1	2.34	0.42
1:C:248:ASN:HB3	1:D:57:SER:HB2	2.00	0.42
1:D:34:VAL:O	1:D:38:GLU:HG3	2.19	0.42
1:E:185:PHE:CE1	1:F:250:ARG:NH2	2.87	0.42
1:F:130:ILE:O	1:F:156:LEU:HD12	2.19	0.42
1:G:105:VAL:CG1	1:G:118:SER:HB2	2.50	0.42
1:G:287:HIS:CE1	1:G:290:LEU:HD12	2.55	0.42
1:H:378:ASP:O	1:H:379:GLU:C	2.62	0.42
1:D:86:VAL:HG21	1:D:107:ILE:HD13	2.01	0.42
1:F:129:ALA:HA	1:F:154:ILE:HG23	2.01	0.42
1:A:264:LYS:O	1:A:267:PRO:HD2	2.20	0.42
1:B:62:LEU:O	1:B:63:MET:C	2.61	0.42
1:B:250:ARG:HA	1:B:251:PRO:HD3	1.85	0.42
1:D:120:LYS:CB	1:D:148:ILE:CD1	2.96	0.42
1:F:150:GLY:C	1:F:152:ARG:N	2.77	0.42
1:H:93:TYR:O	1:H:94:PRO:C	2.62	0.42
1:H:193:MET:HE2	1:H:258:ILE:CD1	2.49	0.42
1:A:371:ASN:C	1:A:372:HIS:CD2	2.97	0.42
1:A:375:GLU:O	1:A:375:GLU:HG2	2.18	0.42
1:B:210:LEU:HD23	1:B:210:LEU:HA	1.83	0.42
1:C:185:PHE:CG	1:C:186:TYR:N	2.87	0.42
1:C:331:ARG:HB2	1:C:332:PRO:CD	2.50	0.42
1:E:113:ASN:O	1:E:114:ILE:C	2.61	0.42
1:E:317:LYS:HB3	1:E:317:LYS:HE3	1.70	0.42
1:G:168:PHE:C	1:G:170:ASN:N	2.73	0.42
1:G:232:SER:HB3	1:G:238:GLU:OE1	2.19	0.42
1:G:337:ASN:O	1:G:340:LYS:HD3	2.19	0.42
1:H:111:THR:HG22	1:H:294:GLN:HB3	2.01	0.42
1:A:250:ARG:HA	1:A:251:PRO:HD3	1.93	0.42
1:A:266:LEU:N	1:A:267:PRO:CD	2.82	0.42
1:D:266:LEU:O	1:D:267:PRO:C	2.62	0.42
1:F:362:LEU:C	1:F:362:LEU:CD2	2.90	0.42
1:H:137:GLY:HA2	1:H:163:SER:CB	2.50	0.42
1:H:225:ASN:N	1:H:229:GLY:O	2.45	0.42
1:A:12:ASP:OD1	1:A:14:LEU:HG	2.20	0.42
1:A:136:LEU:CA	1:A:302:PHE:HB3	2.49	0.42
1:B:351:THR:OG1	1:B:352:VAL:N	2.52	0.42
1:C:284:PHE:CE1	1:C:384:ARG:HD2	2.55	0.42
1:D:287:HIS:HE1	1:D:289:TYR:CZ	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:339:LEU:HD13	1:E:339:LEU:HA	1.53	0.42
1:F:243:VAL:C	1:F:244:LEU:HD12	2.45	0.42
1:F:287:HIS:CE1	1:F:289:TYR:CE2	3.07	0.42
1:G:117:GLU:O	1:G:120:LYS:HB2	2.20	0.42
1:H:190:ILE:CG2	1:H:262:GLN:HB3	2.49	0.42
1:H:254:MET:C	1:H:256:GLY:N	2.74	0.42
1:A:323:LEU:HA	1:A:323:LEU:HD23	1.87	0.42
1:B:63:MET:HB2	1:B:63:MET:HE2	1.85	0.42
1:E:47:SER:OG	1:E:49:TYR:O	2.37	0.42
1:E:106:ASP:OD2	1:E:356:VAL:HA	2.19	0.42
1:E:184:SER:OG	1:E:192:THR:OG1	2.27	0.42
1:E:324:ASN:C	1:E:326:ALA:N	2.77	0.42
1:F:26:LYS:HZ3	1:F:26:LYS:CA	2.32	0.42
1:F:119:LEU:HD12	1:F:119:LEU:O	2.20	0.42
1:F:315:ILE:O	1:F:316:ARG:C	2.62	0.42
1:F:388:LYS:HE3	1:F:388:LYS:CA	2.47	0.42
1:G:128:LYS:HD2	1:G:128:LYS:HA	1.33	0.42
1:G:239:SER:HB3	1:G:240:PHE:CD2	2.55	0.42
1:H:80:GLU:HA	1:H:101:ARG:O	2.19	0.42
1:A:14:LEU:HG	1:A:14:LEU:H	1.74	0.42
1:A:279:TYR:CE2	1:A:381:ASP:OD1	2.72	0.42
1:B:7:ALA:HA	1:B:372:HIS:HE1	1.84	0.42
1:B:217:TRP:CD1	1:B:217:TRP:C	2.97	0.42
1:C:376:LEU:HA	1:C:379:GLU:OE1	2.20	0.42
1:E:268:ARG:CG	1:E:268:ARG:NH2	2.79	0.42
1:E:269:PHE:CD1	1:E:269:PHE:N	2.87	0.42
1:E:348:PHE:CD1	1:E:348:PHE:N	2.88	0.42
1:F:4:TYR:C	1:F:4:TYR:HD1	2.28	0.42
1:F:184:SER:O	1:F:191:ALA:HA	2.20	0.42
1:G:81:ILE:HD11	1:G:131:LEU:HB2	2.02	0.42
1:H:162:GLU:HG3	1:H:188:LLP:O3	2.20	0.42
1:H:303:GLY:CA	1:H:368:PHE:CE2	3.01	0.42
1:A:269:PHE:CE1	1:A:373:GLN:HG3	2.55	0.42
1:B:261:GLU:O	1:B:262:GLN:C	2.60	0.42
1:B:287:HIS:HA	1:B:288:PRO:HD3	1.77	0.42
1:C:310:LYS:HG3	1:C:361:TYR:CE2	2.55	0.42
1:E:207:HIS:CE1	1:E:226:LYS:H	2.37	0.42
1:F:111:THR:O	1:F:112:LEU:CB	2.68	0.42
1:F:323:LEU:HD23	1:F:323:LEU:HA	1.65	0.42
1:F:341:ASN:C	1:F:345:LEU:HD12	2.44	0.42
1:G:314:VAL:HG12	1:G:315:ILE:N	2.33	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:GLN:HA	1:A:23:LEU:HD12	2.02	0.41
1:B:49:TYR:O	1:B:199:VAL:HA	2.20	0.41
1:B:284:PHE:O	1:B:285:LYS:C	2.62	0.41
1:C:318:GLN:O	1:C:319:LEU:C	2.63	0.41
1:C:380:ILE:O	1:C:381:ASP:C	2.63	0.41
1:D:145:ILE:O	1:D:149:ILE:HG13	2.19	0.41
1:D:331:ARG:O	1:D:368:PHE:N	2.51	0.41
1:G:59:ALA:HB1	1:G:198:ILE:HG13	2.01	0.41
1:G:181:THR:C	1:G:182:PHE:CD1	2.98	0.41
1:G:287:HIS:ND1	1:G:288:PRO:HG2	2.33	0.41
1:G:341:ASN:O	1:G:344:VAL:HG12	2.19	0.41
1:G:378:ASP:O	1:G:381:ASP:HB2	2.20	0.41
1:G:384:ARG:HG3	1:G:384:ARG:NH1	2.35	0.41
1:H:172:CYS:O	1:H:173:ALA:C	2.63	0.41
1:H:266:LEU:CB	1:H:267:PRO:CD	2.91	0.41
1:A:333:ILE:HD12	1:A:366:GLY:HA3	2.02	0.41
1:B:12:ASP:O	1:B:16:TYR:HD1	2.03	0.41
1:B:52:MET:C	1:B:251:PRO:CG	2.93	0.41
1:B:306:PHE:HB2	1:B:367:LEU:HD12	2.02	0.41
1:C:171:LYS:HB3	1:C:176:PHE:CZ	2.54	0.41
1:C:265:LYS:HD3	1:C:269:PHE:CZ	2.55	0.41
1:E:88:TRP:CG	1:E:89:SER:N	2.88	0.41
1:F:6:LEU:O	1:F:372:HIS:CE1	2.73	0.41
1:F:58:THR:CG2	1:F:249:VAL:CG1	2.98	0.41
1:F:61:LEU:HD21	1:F:247:TYR:CZ	2.55	0.41
1:F:289:TYR:HA	1:F:309:LYS:CD	2.49	0.41
1:G:124:THR:HG22	1:G:126:SER:H	1.85	0.41
1:G:364:LYS:H	1:G:364:LYS:HG2	1.65	0.41
1:A:70:THR:O	1:A:73:PRO:HD3	2.20	0.41
1:A:81:ILE:HD11	1:A:131:LEU:HB2	2.02	0.41
1:A:279:TYR:HE2	1:A:381:ASP:OD1	2.02	0.41
1:B:36:GLN:O	1:B:39:THR:N	2.53	0.41
1:B:37:TYR:CE1	1:B:259:GLY:HA3	2.55	0.41
1:B:156:LEU:HD12	1:B:157:LEU:H	1.86	0.41
1:B:168:PHE:C	1:B:170:ASN:H	2.29	0.41
1:C:250:ARG:HA	1:C:251:PRO:HD3	1.84	0.41
1:E:202:ASP:OD2	1:E:205:ILE:HG12	2.19	0.41
1:E:259:GLY:O	1:E:260:ILE:C	2.64	0.41
1:E:321:GLU:O	1:E:322:ASN:C	2.63	0.41
1:F:78:GLY:O	1:F:79:ASP:C	2.61	0.41
1:F:138:ASN:OD1	1:F:139:PRO:HD2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:72:LYS:HA	1:G:73:PRO:HD3	1.81	0.41
1:H:286:ASP:O	1:H:287:HIS:C	2.61	0.41
1:B:7:ALA:HA	1:B:372:HIS:CE1	2.55	0.41
1:B:106:ASP:CG	1:B:358:ASN:HB2	2.45	0.41
1:B:107:ILE:HA	1:B:114:ILE:HA	2.02	0.41
1:B:318:GLN:HA	1:B:318:GLN:NE2	2.35	0.41
1:B:385:GLU:HA	1:B:388:LYS:HE2	2.01	0.41
1:C:324:ASN:O	1:C:325:SER:C	2.62	0.41
1:D:176:PHE:H	1:D:176:PHE:HD1	1.69	0.41
1:D:316:ARG:NH1	1:D:366:GLY:O	2.53	0.41
1:F:316:ARG:HE	1:F:316:ARG:HB3	1.64	0.41
1:A:70:THR:HG21	1:A:74:ARG:NE	2.35	0.41
1:B:36:GLN:O	1:B:37:TYR:C	2.64	0.41
1:B:223:LYS:O	1:B:230:VAL:HA	2.21	0.41
1:D:106:ASP:CG	1:D:356:VAL:HA	2.45	0.41
1:E:41:PHE:O	1:E:45:PHE:HD1	2.04	0.41
1:E:335:THR:HG21	1:F:242:PHE:CZ	2.56	0.41
1:F:143:ASP:O	1:F:147:LYS:HG3	2.20	0.41
1:G:61:LEU:HD21	1:G:247:TYR:CZ	2.56	0.41
1:G:185:PHE:HB2	3:G:420:HOH:O	2.20	0.41
1:C:29:THR:CG2	1:C:30:MET:N	2.81	0.41
1:C:122:ALA:HB2	1:C:353:HIS:CG	2.56	0.41
1:C:204:GLU:O	1:C:205:ILE:C	2.63	0.41
1:C:319:LEU:HD23	1:C:319:LEU:HA	1.73	0.41
1:D:334:VAL:HG12	1:D:335:THR:N	2.36	0.41
1:E:67:LEU:HD22	1:E:74:ARG:HD3	2.03	0.41
1:E:305:SER:N	3:E:408:HOH:O	2.53	0.41
1:G:149:ILE:N	1:G:149:ILE:CD1	2.81	0.41
1:G:250:ARG:HA	1:G:251:PRO:HD2	1.91	0.41
1:G:362:LEU:HD23	1:G:363:ASP:N	2.34	0.41
1:H:290:LEU:HD22	1:H:306:PHE:HB3	2.02	0.41
1:A:81:ILE:HD12	1:A:129:ALA:HB3	2.03	0.41
1:B:52:MET:C	1:B:251:PRO:HG2	2.46	0.41
1:B:63:MET:HE3	1:B:63:MET:HB3	1.80	0.41
1:C:268:ARG:O	1:C:272:VAL:HG23	2.20	0.41
1:E:250:ARG:NH2	2:F:405:AKG:O3	2.43	0.41
1:F:12:ASP:OD1	1:F:14:LEU:HB2	2.20	0.41
1:F:274:ARG:NH1	1:F:274:ARG:HG2	2.35	0.41
1:G:108:ASP:O	1:G:112:LEU:N	2.52	0.41
1:G:265:LYS:O	1:G:266:LEU:C	2.62	0.41
1:H:193:MET:HE2	1:H:258:ILE:HD11	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:277:ALA:O	1:H:280:PHE:HB3	2.21	0.41
1:A:12:ASP:CG	1:A:265:LYS:NZ	2.78	0.41
1:B:92:TYR:CE2	1:B:338:PHE:CG	3.09	0.41
1:C:105:VAL:HB	1:C:114:ILE:HD11	2.03	0.41
1:C:178:LEU:O	1:C:178:LEU:HG	2.21	0.41
1:D:22:VAL:HG22	1:D:33:TYR:CD2	2.55	0.41
1:D:137:GLY:HA2	1:D:163:SER:HA	2.03	0.41
1:E:77:LYS:HB3	1:E:77:LYS:HE2	1.15	0.41
1:E:82:ILE:HG23	1:E:83:VAL:N	2.35	0.41
1:E:331:ARG:HB2	1:E:332:PRO:HD2	2.02	0.41
1:H:337:ASN:HB3	1:H:340:LYS:HD3	2.02	0.41
1:A:88:TRP:CZ2	2:A:401:AKG:H41	2.56	0.41
1:A:304:PHE:O	1:A:368:PHE:HA	2.21	0.41
1:B:156:LEU:HD12	1:B:157:LEU:N	2.36	0.41
1:C:84:PRO:HA	1:C:114:ILE:CD1	2.51	0.41
1:C:252:LEU:HD23	1:C:252:LEU:HA	1.65	0.41
1:C:300:SER:O	1:C:301:TRP:C	2.63	0.41
1:C:310:LYS:HE2	1:C:310:LYS:HB3	1.45	0.41
1:D:156:LEU:CD1	1:D:157:LEU:N	2.78	0.41
1:E:240:PHE:CD2	1:F:332:PRO:HG2	2.56	0.41
1:F:140:ASN:HB2	1:F:142:PHE:CZ	2.56	0.41
1:F:193:MET:HB2	1:F:193:MET:HE3	1.93	0.41
1:F:314:VAL:HG12	1:F:315:ILE:N	2.35	0.41
1:G:29:THR:O	1:G:30:MET:C	2.64	0.41
1:G:49:TYR:OH	1:G:203:GLU:HB2	2.21	0.41
1:B:40:GLN:O	1:B:44:THR:OG1	2.30	0.41
1:B:106:ASP:OD2	1:B:358:ASN:HB2	2.21	0.41
1:C:192:THR:HA	1:C:258:ILE:HG21	2.02	0.41
1:C:244:LEU:HA	1:C:245:PRO:HD3	1.91	0.41
1:D:228:THR:H	1:D:228:THR:HG1	1.56	0.41
1:F:61:LEU:HA	1:F:94:PRO:HB3	2.02	0.41
1:F:354:ASN:CG	1:F:355:ASN:N	2.79	0.41
1:A:188:LLP:OP4	1:A:188:LLP:C4'	2.68	0.40
1:A:384:ARG:HD2	1:A:384:ARG:HA	1.76	0.40
1:C:150:GLY:HA3	1:C:151:GLY:HA3	1.39	0.40
1:E:217:TRP:C	1:E:217:TRP:HD1	2.29	0.40
1:E:316:ARG:HH22	1:E:364:LYS:HA	1.73	0.40
1:F:50:ALA:CB	1:F:199:VAL:HG12	2.51	0.40
1:F:64:ILE:HG23	1:F:64:ILE:HD12	1.83	0.40
1:F:376:LEU:HB2	1:F:380:ILE:CD1	2.51	0.40
1:H:29:THR:O	1:H:30:MET:C	2.63	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:279:TYR:HD2	1:H:380:ILE:HG21	1.85	0.40
1:B:49:TYR:OH	1:B:203:GLU:HG3	2.21	0.40
1:C:108:ASP:O	1:C:112:LEU:N	2.48	0.40
1:C:336:GLY:HA2	1:C:362:LEU:HD21	2.03	0.40
1:E:95:LEU:N	1:E:95:LEU:HD23	2.36	0.40
1:F:131:LEU:C	1:F:131:LEU:CD2	2.94	0.40
1:F:283:LYS:HD3	1:F:283:LYS:HA	1.30	0.40
1:G:192:THR:O	1:G:193:MET:CB	2.67	0.40
1:G:287:HIS:ND1	1:G:290:LEU:N	2.69	0.40
1:G:319:LEU:H	1:G:319:LEU:HG	1.76	0.40
1:A:95:LEU:H	1:A:95:LEU:HG	1.57	0.40
1:A:358:ASN:O	1:A:359:ALA:C	2.63	0.40
1:B:52:MET:O	1:B:213:ARG:NH1	2.42	0.40
1:B:346:LYS:HG2	1:B:346:LYS:H	1.52	0.40
1:B:376:LEU:HA	1:B:379:GLU:OE2	2.21	0.40
1:C:151:GLY:O	1:C:152:ARG:C	2.62	0.40
1:D:119:LEU:C	1:D:121:GLU:N	2.77	0.40
1:D:217:TRP:CD1	1:D:217:TRP:C	2.99	0.40
1:E:192:THR:O	1:E:193:MET:CB	2.69	0.40
1:E:269:PHE:H	1:E:269:PHE:HD1	1.70	0.40
1:F:69:PHE:CZ	1:F:245:PRO:HG2	2.56	0.40
1:G:209:LEU:O	1:G:210:LEU:C	2.65	0.40
1:H:304:PHE:CZ	1:H:371:ASN:HB2	2.55	0.40
1:A:109:ILE:HD12	1:A:109:ILE:HA	1.88	0.40
1:A:133:VAL:HG22	1:A:159:ASP:HB3	2.03	0.40
1:A:135:LEU:HD21	1:A:334:VAL:HG21	2.03	0.40
1:B:120:LYS:HA	1:B:148:ILE:HG23	2.02	0.40
1:B:221:LEU:O	1:B:231:LYS:HE2	2.22	0.40
1:B:244:LEU:HA	1:B:245:PRO:HD3	1.83	0.40
1:B:321:GLU:O	1:B:322:ASN:C	2.64	0.40
1:B:333:ILE:C	1:B:334:VAL:HG23	2.45	0.40
1:C:253:GLU:OE1	1:C:253:GLU:HA	2.21	0.40
1:D:34:VAL:HG23	1:D:253:GLU:HA	2.03	0.40
1:D:177:GLY:C	1:D:179:MET:N	2.78	0.40
1:D:185:PHE:CD1	1:D:194:GLU:OE1	2.74	0.40
1:E:139:PRO:O	1:E:296:THR:HB	2.21	0.40
1:E:277:ALA:C	1:E:281:LEU:HD12	2.46	0.40
1:E:335:THR:HG21	1:F:242:PHE:CE2	2.57	0.40
1:F:223:LYS:HB3	1:F:223:LYS:HE2	2.00	0.40
1:G:130:ILE:HD12	1:G:130:ILE:HG21	1.83	0.40
1:G:144:GLU:OE1	1:G:147:LYS:HD3	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:101:ARG:NH1	1:H:349:ASP:OD1	2.53	0.40
1:C:119:LEU:HD12	1:C:119:LEU:HA	1.76	0.40
1:C:235:GLN:O	1:C:237:GLU:N	2.55	0.40
1:C:306:PHE:HB2	1:C:367:LEU:HD13	2.03	0.40
1:D:167:THR:HG22	1:D:172:CYS:HA	2.03	0.40
1:F:287:HIS:HE1	1:F:289:TYR:CE2	2.37	0.40
1:H:225:ASN:O	1:H:229:GLY:HA2	2.21	0.40
1:H:304:PHE:HA	3:H:402:HOH:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	382/390 (98%)	352 (92%)	25 (6%)	5 (1%)	9	8
1	B	383/390 (98%)	342 (89%)	35 (9%)	6 (2%)	7	6
1	C	386/390 (99%)	336 (87%)	43 (11%)	7 (2%)	6	4
1	D	379/390 (97%)	354 (93%)	22 (6%)	3 (1%)	16	16
1	E	381/390 (98%)	337 (88%)	37 (10%)	7 (2%)	6	4
1	F	384/390 (98%)	338 (88%)	41 (11%)	5 (1%)	9	8
1	G	385/390 (99%)	339 (88%)	40 (10%)	6 (2%)	7	6
1	H	379/390 (97%)	327 (86%)	46 (12%)	6 (2%)	7	6
All	All	3059/3120 (98%)	2725 (89%)	289 (9%)	45 (2%)	8	6

All (45) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	312	SER
1	C	152	ARG

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Mol	Chain	Res	Type
1	G	354	ASN
1	A	311	ASP
1	B	150	GLY
1	C	301	TRP
1	C	311	ASP
1	D	186	TYR
1	E	186	TYR
1	E	193	MET
1	E	325	SER
1	G	186	TYR
1	G	193	MET
1	G	299	SER
1	H	193	MET
1	H	314	VAL
1	A	334	VAL
1	C	236	PHE
1	E	30	MET
1	E	334	VAL
1	F	151	GLY
1	F	193	MET
1	F	236	PHE
1	G	325	SER
1	G	334	VAL
1	H	239	SER
1	H	334	VAL
1	A	354	ASN
1	B	193	MET
1	B	235	GLN
1	B	285	LYS
1	B	334	VAL
1	C	334	VAL
1	C	354	ASN
1	D	334	VAL
1	F	334	VAL
1	A	30	MET
1	C	106	ASP
1	D	301	TRP
1	H	259	GLY
1	B	313	GLY
1	E	215	HIS
1	H	260	ILE
1	E	116	ILE

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Mol	Chain	Res	Type
1	F	4	TYR

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	340/344 (99%)	284 (84%)	56 (16%)	2	2
1	B	341/344 (99%)	274 (80%)	67 (20%)	1	1
1	C	344/344 (100%)	284 (83%)	60 (17%)	2	2
1	D	338/344 (98%)	287 (85%)	51 (15%)	3	2
1	E	339/344 (98%)	273 (80%)	66 (20%)	1	1
1	F	342/344 (99%)	275 (80%)	67 (20%)	1	1
1	G	343/344 (100%)	273 (80%)	70 (20%)	1	1
1	H	338/344 (98%)	265 (78%)	73 (22%)	1	1
All	All	2725/2752 (99%)	2215 (81%)	510 (19%)	1	1

All (510) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	ASP
1	A	14	LEU
1	A	17	LYS
1	A	21	SER
1	A	27	MET
1	A	28	PHE
1	A	47	SER
1	A	48	LYS
1	A	71	LYS
1	A	74	ARG
1	A	77	LYS
1	A	81	ILE
1	A	107	ILE
1	A	108	ASP

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Mol	Chain	Res	Type
1	A	109	ILE
1	A	118	SER
1	A	120	LYS
1	A	121	GLU
1	A	126	SER
1	A	132	THR
1	A	135	LEU
1	A	147	LYS
1	A	149	ILE
1	A	154	ILE
1	A	171	LYS
1	A	179	MET
1	A	205	ILE
1	A	221	LEU
1	A	226	LYS
1	A	232	SER
1	A	237	GLU
1	A	239	SER
1	A	241	LYS
1	A	244	LEU
1	A	249	VAL
1	A	252	LEU
1	A	260	ILE
1	A	268	ARG
1	A	270	ILE
1	A	283	LYS
1	A	314	VAL
1	A	317	LYS
1	A	319	LEU
1	A	331	ARG
1	A	339	LEU
1	A	340	LYS
1	A	342	THR
1	A	346	LYS
1	A	360	GLU
1	A	362	LEU
1	A	369	VAL
1	A	374	ILE
1	A	375	GLU
1	A	379	GLU
1	A	383	LEU
1	A	388	LYS

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Mol	Chain	Res	Type
1	B	17	LYS
1	B	20	GLN
1	B	21	SER
1	B	24	ASP
1	B	26	LYS
1	B	27	MET
1	B	29	THR
1	B	30	MET
1	B	35	LYS
1	B	43	LYS
1	B	48	LYS
1	B	64	ILE
1	B	71	LYS
1	B	81	ILE
1	B	82	ILE
1	B	101	ARG
1	B	107	ILE
1	B	108	ASP
1	B	117	GLU
1	B	120	LYS
1	B	121	GLU
1	B	128	LYS
1	B	130	ILE
1	B	131	LEU
1	B	135	LEU
1	B	144	GLU
1	B	155	ILE
1	B	158	GLU
1	B	164	MET
1	B	171	LYS
1	B	172	CYS
1	B	179	MET
1	B	184	SER
1	B	198	ILE
1	B	203	GLU
1	B	205	ILE
1	B	209	LEU
1	B	223	LYS
1	B	224	LYS
1	B	233	ASP
1	B	239	SER
1	B	241	LYS

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Mol	Chain	Res	Type
1	B	260	ILE
1	B	265	LYS
1	B	269	PHE
1	B	270	ILE
1	B	271	SER
1	B	285	LYS
1	B	290	LEU
1	B	292	VAL
1	B	300	SER
1	B	305	SER
1	B	307	ILE
1	B	309	LYS
1	B	310	LYS
1	B	314	VAL
1	B	318	GLN
1	B	325	SER
1	B	328	ILE
1	B	334	VAL
1	B	345	LEU
1	B	346	LYS
1	B	367	LEU
1	B	375	GLU
1	B	379	GLU
1	B	384	ARG
1	B	388	LYS
1	C	2	ILE
1	C	6	LEU
1	C	8	SER
1	C	14	LEU
1	C	17	LYS
1	C	20	GLN
1	C	24	ASP
1	C	27	MET
1	C	29	THR
1	C	35	LYS
1	C	58	THR
1	C	63	MET
1	C	72	LYS
1	C	76	LYS
1	C	77	LYS
1	C	103	LYS
1	C	109	ILE

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Mol	Chain	Res	Type
1	C	114	ILE
1	C	116	ILE
1	C	121	GLU
1	C	128	LYS
1	C	135	LEU
1	C	145	ILE
1	C	148	ILE
1	C	152	ARG
1	C	157	LEU
1	C	197[A]	CYS
1	C	197[B]	CYS
1	C	198	ILE
1	C	199	VAL
1	C	210	LEU
1	C	224	LYS
1	C	230	VAL
1	C	231	LYS
1	C	232	SER
1	C	241	LYS
1	C	258	ILE
1	C	264	LYS
1	C	265	LYS
1	C	271	SER
1	C	275	LYS
1	C	283	LYS
1	C	290	LEU
1	C	310	LYS
1	C	311	ASP
1	C	312	SER
1	C	314	VAL
1	C	316	ARG
1	C	322	ASN
1	C	325	SER
1	C	334	VAL
1	C	340	LYS
1	C	356	VAL
1	C	362	LEU
1	C	364	LYS
1	C	367	LEU
1	C	375	GLU
1	C	378	ASP
1	C	380	ILE

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Mol	Chain	Res	Type
1	C	388	LYS
1	D	10	THR
1	D	13	ASP
1	D	26	LYS
1	D	29	THR
1	D	35	LYS
1	D	48	LYS
1	D	62	LEU
1	D	72	LYS
1	D	82	ILE
1	D	108	ASP
1	D	120	LYS
1	D	128	LYS
1	D	135	LEU
1	D	136	LEU
1	D	145	ILE
1	D	147	LYS
1	D	171	LYS
1	D	178	LEU
1	D	184	SER
1	D	220	ASN
1	D	224	LYS
1	D	228	THR
1	D	232	SER
1	D	235	GLN
1	D	237	GLU
1	D	254	MET
1	D	268	ARG
1	D	271	SER
1	D	275	LYS
1	D	278	GLU
1	D	285	LYS
1	D	308	ILE
1	D	309	LYS
1	D	316	ARG
1	D	317	LYS
1	D	318	GLN
1	D	321	GLU
1	D	328	ILE
1	D	331	ARG
1	D	333	ILE
1	D	340	LYS

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Mol	Chain	Res	Type
1	D	346	LYS
1	D	355	ASN
1	D	367	LEU
1	D	368	PHE
1	D	369	VAL
1	D	373	GLN
1	D	374	ILE
1	D	383	LEU
1	D	384	ARG
1	D	388	LYS
1	E	6	LEU
1	E	10	THR
1	E	13	ASP
1	E	27	MET
1	E	34	VAL
1	E	36	GLN
1	E	40	GLN
1	E	43	LYS
1	E	47	SER
1	E	62	LEU
1	E	70	THR
1	E	72	LYS
1	E	76	LYS
1	E	77	LYS
1	E	97	GLN
1	E	103	LYS
1	E	107	ILE
1	E	108	ASP
1	E	118	SER
1	E	120	LYS
1	E	121	GLU
1	E	128	LYS
1	E	135	LEU
1	E	144	GLU
1	E	145	ILE
1	E	147	LYS
1	E	155	ILE
1	E	170	ASN
1	E	208	ILE
1	E	213	ARG
1	E	224	LYS
1	E	232	SER

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Mol	Chain	Res	Type
1	E	235	GLN
1	E	244	LEU
1	E	253	GLU
1	E	260	ILE
1	E	265	LYS
1	E	268	ARG
1	E	275	LYS
1	E	281	LEU
1	E	283	LYS
1	E	285	LYS
1	E	287	HIS
1	E	309	LYS
1	E	310	LYS
1	E	315	ILE
1	E	316	ARG
1	E	317	LYS
1	E	318	GLN
1	E	328	ILE
1	E	333	ILE
1	E	339	LEU
1	E	342	THR
1	E	344	VAL
1	E	345	LEU
1	E	346	LYS
1	E	350	TYR
1	E	351	THR
1	E	360	GLU
1	E	362	LEU
1	E	364	LYS
1	E	367	LEU
1	E	369	VAL
1	E	375	GLU
1	E	379	GLU
1	E	384	ARG
1	F	8	SER
1	F	14	LEU
1	F	19	ILE
1	F	21	SER
1	F	25	SER
1	F	26	LYS
1	F	43	LYS
1	F	48	LYS

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Mol	Chain	Res	Type
1	F	49	TYR
1	F	58	THR
1	F	61	LEU
1	F	62	LEU
1	F	71	LYS
1	F	72	LYS
1	F	77	LYS
1	F	107	ILE
1	F	116	ILE
1	F	119	LEU
1	F	120	LYS
1	F	125	ASP
1	F	126	SER
1	F	128	LYS
1	F	130	ILE
1	F	131	LEU
1	F	135	LEU
1	F	136	LEU
1	F	145	ILE
1	F	148	ILE
1	F	149	ILE
1	F	153	ASP
1	F	163	SER
1	F	171	LYS
1	F	178	LEU
1	F	179	MET
1	F	197[A]	CYS
1	F	197[B]	CYS
1	F	198	ILE
1	F	210	LEU
1	F	217	TRP
1	F	223	LYS
1	F	224	LYS
1	F	230	VAL
1	F	232	SER
1	F	239	SER
1	F	241	LYS
1	F	265	LYS
1	F	275	LYS
1	F	283	LYS
1	F	285	LYS
1	F	294	GLN

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Mol	Chain	Res	Type
1	F	299	SER
1	F	300	SER
1	F	307	ILE
1	F	309	LYS
1	F	312	SER
1	F	315	ILE
1	F	316	ARG
1	F	317	LYS
1	F	321	GLU
1	F	325	SER
1	F	340	LYS
1	F	352	VAL
1	F	367	LEU
1	F	368	PHE
1	F	383	LEU
1	F	384	ARG
1	F	388	LYS
1	G	3	ASN
1	G	5	PRO
1	G	6	LEU
1	G	9	SER
1	G	12	ASP
1	G	13	ASP
1	G	17	LYS
1	G	19	ILE
1	G	22	VAL
1	G	24	ASP
1	G	26	LYS
1	G	29	THR
1	G	32	GLU
1	G	40	GLN
1	G	43	LYS
1	G	48	LYS
1	G	49	TYR
1	G	52	MET
1	G	71	LYS
1	G	72	LYS
1	G	80	GLU
1	G	82	ILE
1	G	109	ILE
1	G	112	LEU
1	G	128	LYS

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Mol	Chain	Res	Type
1	G	130	ILE
1	G	131	LEU
1	G	141	ASN
1	G	145	ILE
1	G	148	ILE
1	G	149	ILE
1	G	152	ARG
1	G	170	ASN
1	G	179	MET
1	G	197[A]	CYS
1	G	197[B]	CYS
1	G	205	ILE
1	G	208	ILE
1	G	209	LEU
1	G	212	ILE
1	G	223	LYS
1	G	230	VAL
1	G	232	SER
1	G	235	GLN
1	G	237	GLU
1	G	260	ILE
1	G	263	LEU
1	G	264	LYS
1	G	265	LYS
1	G	267	PRO
1	G	268	ARG
1	G	271	SER
1	G	274	ARG
1	G	283	LYS
1	G	285	LYS
1	G	291	ASP
1	G	309	LYS
1	G	317	LYS
1	G	318	GLN
1	G	328	ILE
1	G	331	ARG
1	G	339	LEU
1	G	340	LYS
1	G	364	LYS
1	G	367	LEU
1	G	368	PHE
1	G	376	LEU

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Mol	Chain	Res	Type
1	G	380	ILE
1	G	385	GLU
1	G	388	LYS
1	H	17	LYS
1	H	20	GLN
1	H	21	SER
1	H	22	VAL
1	H	26	LYS
1	H	27	MET
1	H	29	THR
1	H	32	GLU
1	H	35	LYS
1	H	40	GLN
1	H	43	LYS
1	H	48	LYS
1	H	49	TYR
1	H	71	LYS
1	H	72	LYS
1	H	74	ARG
1	H	76	LYS
1	H	77	LYS
1	H	81	ILE
1	H	89	SER
1	H	97	GLN
1	H	100	LEU
1	H	120	LYS
1	H	124	THR
1	H	125	ASP
1	H	126	SER
1	H	135	LEU
1	H	136	LEU
1	H	144	GLU
1	H	154	ILE
1	H	169	ASN
1	H	170	ASN
1	H	172	CYS
1	H	197[A]	CYS
1	H	197[B]	CYS
1	H	223	LYS
1	H	224	LYS
1	H	230	VAL
1	H	232	SER

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Mol	Chain	Res	Type
1	H	235	GLN
1	H	239	SER
1	H	241	LYS
1	H	244	LEU
1	H	250	ARG
1	H	254	MET
1	H	265	LYS
1	H	272	VAL
1	H	273	ARG
1	H	275	LYS
1	H	278	GLU
1	H	282	ASP
1	H	285	LYS
1	H	286	ASP
1	H	307	ILE
1	H	310	LYS
1	H	315	ILE
1	H	316	ARG
1	H	318	GLN
1	H	319	LEU
1	H	324	ASN
1	H	328	ILE
1	H	329	GLU
1	H	330	CYS
1	H	331	ARG
1	H	339	LEU
1	H	340	LYS
1	H	342	THR
1	H	364	LYS
1	H	367	LEU
1	H	369	VAL
1	H	374	ILE
1	H	375	GLU
1	H	388	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (45) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	GLN
1	A	318	GLN
1	A	322	ASN
1	A	324	ASN

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Mol	Chain	Res	Type
1	A	337	ASN
1	A	353	HIS
1	B	36	GLN
1	B	318	GLN
1	B	322	ASN
1	B	324	ASN
1	B	372	HIS
1	C	294	GLN
1	C	322	ASN
1	D	20	GLN
1	D	235	GLN
1	D	322	ASN
1	D	353	HIS
1	D	355	ASN
1	D	371	ASN
1	E	97	GLN
1	E	287	HIS
1	E	322	ASN
1	E	353	HIS
1	E	372	HIS
1	F	170	ASN
1	F	287	HIS
1	F	294	GLN
1	F	337	ASN
1	F	354	ASN
1	G	36	GLN
1	G	40	GLN
1	G	97	GLN
1	G	140	ASN
1	G	170	ASN
1	G	322	ASN
1	G	324	ASN
1	G	365	ASN
1	G	372	HIS
1	H	20	GLN
1	H	36	GLN
1	H	97	GLN
1	H	170	ASN
1	H	324	ASN
1	H	353	HIS
1	H	372	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

8 non-standard protein/DNA/RNA residues 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
1	LLP	F	188	1	23,24,25	1.03	2 (8%)	25,32,34	1.15	1 (4%)
1	LLP	E	188	1	23,24,25	1.35	4 (17%)	25,32,34	1.16	1 (4%)
1	LLP	A	188	1	23,24,25	1.50	5 (21%)	25,32,34	1.30	2 (8%)
1	LLP	B	188	1	23,24,25	1.13	2 (8%)	25,32,34	1.16	2 (8%)
1	LLP	C	188	1	23,24,25	1.13	1 (4%)	25,32,34	0.99	2 (8%)
1	LLP	G	188	1	23,24,25	1.29	2 (8%)	25,32,34	1.22	2 (8%)
1	LLP	H	188	1	23,24,25	1.45	4 (17%)	25,32,34	1.21	2 (8%)
1	LLP	D	188	1	23,24,25	1.28	2 (8%)	25,32,34	1.04	3 (12%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	LLP	F	188	1	-	8/16/17/19	0/1/1/1
1	LLP	E	188	1	-	3/16/17/19	0/1/1/1
1	LLP	A	188	1	-	9/16/17/19	0/1/1/1
1	LLP	B	188	1	-	5/16/17/19	0/1/1/1
1	LLP	C	188	1	-	9/16/17/19	0/1/1/1
1	LLP	G	188	1	-	6/16/17/19	0/1/1/1
1	LLP	H	188	1	-	5/16/17/19	0/1/1/1
1	LLP	D	188	1	-	5/16/17/19	0/1/1/1

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	H	188	LLP	P-OP1	4.52	1.64	1.50
1	D	188	LLP	P-OP1	4.47	1.64	1.50
1	G	188	LLP	P-OP1	4.44	1.64	1.50
1	A	188	LLP	P-OP1	4.39	1.64	1.50
1	E	188	LLP	P-OP1	4.08	1.63	1.50
1	B	188	LLP	P-OP1	3.31	1.60	1.50
1	C	188	LLP	P-OP1	3.23	1.60	1.50
1	H	188	LLP	P-OP2	2.66	1.64	1.54
1	A	188	LLP	P-OP2	2.57	1.64	1.54
1	E	188	LLP	P-OP3	2.55	1.64	1.54
1	A	188	LLP	C3-C2	-2.52	1.38	1.41
1	B	188	LLP	P-OP2	2.38	1.63	1.54
1	H	188	LLP	P-OP3	2.37	1.63	1.54
1	D	188	LLP	P-OP2	2.36	1.63	1.54
1	E	188	LLP	C2-N1	-2.33	1.29	1.33
1	F	188	LLP	P-OP1	2.30	1.57	1.50
1	A	188	LLP	C2-N1	-2.28	1.29	1.33
1	H	188	LLP	C2-N1	-2.26	1.29	1.33
1	E	188	LLP	P-OP2	2.21	1.63	1.54
1	F	188	LLP	C3-C2	-2.17	1.38	1.41
1	G	188	LLP	C2-N1	-2.02	1.30	1.33
1	A	188	LLP	P-OP3	2.01	1.62	1.54

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	188	LLP	C4-C3-C2	-4.00	117.89	120.14
1	H	188	LLP	C4-C3-C2	-3.96	117.91	120.14
1	B	188	LLP	OP2-P-OP4	3.09	114.72	106.67
1	A	188	LLP	OP4-C5'-C5	-2.94	103.84	109.36
1	F	188	LLP	C5-C6-N1	-2.51	119.74	123.83
1	C	188	LLP	OP4-C5'-C5	-2.40	104.85	109.36
1	G	188	LLP	OP4-P-OP1	2.17	112.32	106.44
1	H	188	LLP	OP3-P-OP4	2.15	112.27	106.67
1	D	188	LLP	O3-C3-C2	2.14	122.01	117.58
1	C	188	LLP	OP2-P-OP4	2.12	112.20	106.67
1	D	188	LLP	C4-C3-C2	-2.06	118.98	120.14
1	A	188	LLP	CE-NZ-C4'	2.04	125.26	118.72
1	B	188	LLP	C2'-C2-C3	-2.03	118.42	120.80
1	E	188	LLP	C4-C3-C2	-2.02	119.00	120.14
1	D	188	LLP	CE-NZ-C4'	2.01	125.17	118.72

There are no chirality outliers.

All (50) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	188	LLP	C5'-OP4-P-OP3
1	A	188	LLP	N-CA-CB-CG
1	A	188	LLP	O-C-CA-CB
1	B	188	LLP	N-CA-CB-CG
1	B	188	LLP	O-C-CA-CB
1	C	188	LLP	C5'-OP4-P-OP1
1	C	188	LLP	C-CA-CB-CG
1	C	188	LLP	O-C-CA-CB
1	D	188	LLP	CG-CD-CE-NZ
1	F	188	LLP	C5'-OP4-P-OP2
1	F	188	LLP	C5'-OP4-P-OP3
1	F	188	LLP	CG-CD-CE-NZ
1	G	188	LLP	O-C-CA-CB
1	C	188	LLP	CG-CD-CE-NZ
1	G	188	LLP	CG-CD-CE-NZ
1	H	188	LLP	CG-CD-CE-NZ
1	F	188	LLP	C3-C4-C4'-NZ
1	A	188	LLP	CA-CB-CG-CD
1	H	188	LLP	CA-CB-CG-CD
1	D	188	LLP	CA-CB-CG-CD
1	E	188	LLP	CA-CB-CG-CD
1	F	188	LLP	CA-CB-CG-CD
1	G	188	LLP	CA-CB-CG-CD
1	F	188	LLP	C5'-OP4-P-OP1
1	B	188	LLP	CA-CB-CG-CD
1	H	188	LLP	CD-CE-NZ-C4'
1	A	188	LLP	CG-CD-CE-NZ
1	C	188	LLP	C5'-OP4-P-OP3
1	G	188	LLP	CD-CE-NZ-C4'
1	F	188	LLP	C5-C4-C4'-NZ
1	A	188	LLP	CD-CE-NZ-C4'
1	C	188	LLP	C4-C5-C5'-OP4
1	D	188	LLP	CD-CE-NZ-C4'
1	D	188	LLP	N-CA-CB-CG
1	C	188	LLP	C3-C4-C4'-NZ
1	D	188	LLP	C3-C4-C4'-NZ
1	E	188	LLP	C3-C4-C4'-NZ
1	G	188	LLP	C3-C4-C4'-NZ
1	A	188	LLP	C5'-OP4-P-OP1
1	B	188	LLP	CD-CE-NZ-C4'

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Mol	Chain	Res	Type	Atoms
1	A	188	LLP	C3-C4-C4'-NZ
1	B	188	LLP	C3-C4-C4'-NZ
1	H	188	LLP	C3-C4-C4'-NZ
1	C	188	LLP	CE-CD-CG-CB
1	F	188	LLP	CD-CE-NZ-C4'
1	A	188	LLP	C5'-OP4-P-OP2
1	C	188	LLP	C5'-OP4-P-OP2
1	E	188	LLP	CD-CE-NZ-C4'
1	G	188	LLP	N-CA-CB-CG
1	H	188	LLP	N-CA-CB-CG

There are no ring outliers.

8 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	F	188	LLP	7	0
1	E	188	LLP	2	0
1	A	188	LLP	4	0
1	B	188	LLP	6	0
1	C	188	LLP	4	0
1	G	188	LLP	4	0
1	H	188	LLP	3	0
1	D	188	LLP	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 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	AKG	C	403	-	9,9,9	1.73	2 (22%)	11,11,11	1.85	5 (45%)
2	AKG	A	401	-	9,9,9	1.97	2 (22%)	11,11,11	1.55	3 (27%)
2	AKG	H	406	-	9,9,9	1.96	2 (22%)	11,11,11	2.37	5 (45%)
2	AKG	B	402	-	9,9,9	2.06	2 (22%)	11,11,11	1.62	3 (27%)
2	AKG	D	404	-	9,9,9	1.49	1 (11%)	11,11,11	1.58	1 (9%)
2	AKG	F	405	-	9,9,9	2.40	3 (33%)	11,11,11	1.66	2 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AKG	C	403	-	-	4/9/9/9	-
2	AKG	A	401	-	-	4/9/9/9	-
2	AKG	H	406	-	-	0/9/9/9	-
2	AKG	B	402	-	-	3/9/9/9	-
2	AKG	D	404	-	-	4/9/9/9	-
2	AKG	F	405	-	-	2/9/9/9	-

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	405	AKG	C2-C1	-5.97	1.44	1.53
2	B	402	AKG	C2-C1	-4.50	1.46	1.53
2	H	406	AKG	O3-C5	4.32	1.36	1.22
2	A	401	AKG	O3-C5	4.27	1.36	1.22
2	C	403	AKG	O3-C5	3.62	1.33	1.22
2	D	404	AKG	C2-C1	-3.31	1.48	1.53
2	F	405	AKG	O2-C1	-3.25	1.21	1.30
2	A	401	AKG	C2-C1	-3.15	1.48	1.53
2	C	403	AKG	C2-C1	-2.50	1.49	1.53
2	F	405	AKG	O4-C5	-2.17	1.23	1.30
2	H	406	AKG	C2-C1	-2.01	1.50	1.53
2	B	402	AKG	O2-C1	-2.01	1.25	1.30

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	406	AKG	C4-C3-C2	-4.46	104.53	112.91
2	H	406	AKG	C3-C2-C1	3.96	122.58	115.86
2	F	405	AKG	C4-C3-C2	-3.75	105.86	112.91
2	B	402	AKG	C4-C3-C2	-3.19	106.92	112.91
2	D	404	AKG	C3-C4-C5	-2.81	106.20	113.67
2	C	403	AKG	O4-C5-C4	2.70	122.53	114.00
2	H	406	AKG	C3-C4-C5	-2.62	106.72	113.67
2	C	403	AKG	C3-C2-C1	2.52	120.14	115.86
2	A	401	AKG	C3-C2-C1	2.52	120.14	115.86
2	B	402	AKG	C3-C4-C5	-2.42	107.24	113.67
2	C	403	AKG	C4-C3-C2	-2.42	108.37	112.91
2	F	405	AKG	C3-C2-C1	2.38	119.89	115.86
2	H	406	AKG	O5-C2-C3	-2.32	116.19	121.17
2	C	403	AKG	O2-C1-C2	2.23	119.78	113.59
2	B	402	AKG	C3-C2-C1	2.20	119.59	115.86
2	H	406	AKG	O2-C1-C2	2.19	119.65	113.59
2	A	401	AKG	O2-C1-C2	2.12	119.46	113.59
2	C	403	AKG	O4-C5-O3	-2.09	117.97	123.33
2	A	401	AKG	O4-C5-C4	2.06	120.52	114.00

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	AKG	C1-C2-C3-C4
2	B	402	AKG	O2-C1-C2-C3
2	C	403	AKG	O2-C1-C2-C3
2	D	404	AKG	C1-C2-C3-C4
2	A	401	AKG	O5-C2-C3-C4
2	A	401	AKG	C3-C4-C5-O3
2	A	401	AKG	C3-C4-C5-O4
2	C	403	AKG	C3-C4-C5-O4
2	F	405	AKG	C3-C4-C5-O3
2	C	403	AKG	C3-C4-C5-O3
2	F	405	AKG	C3-C4-C5-O4
2	D	404	AKG	C3-C4-C5-O3
2	D	404	AKG	C3-C4-C5-O4
2	C	403	AKG	C1-C2-C3-C4
2	D	404	AKG	O5-C2-C3-C4
2	B	402	AKG	C3-C4-C5-O4
2	B	402	AKG	C3-C4-C5-O3

There are no ring outliers.

5 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	403	AKG	1	0
2	A	401	AKG	1	0
2	B	402	AKG	5	0
2	D	404	AKG	2	0
2	F	405	AKG	3	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	383/390 (98%)	-1.98	0 100 100	11, 37, 67, 96	1 (0%)
1	B	384/390 (98%)	-1.98	0 100 100	14, 36, 70, 88	1 (0%)
1	C	387/390 (99%)	-1.98	0 100 100	10, 38, 73, 89	1 (0%)
1	D	380/390 (97%)	-1.98	0 100 100	11, 37, 66, 94	1 (0%)
1	E	382/390 (97%)	-1.97	0 100 100	13, 42, 72, 94	1 (0%)
1	F	385/390 (98%)	-1.97	0 100 100	13, 40, 73, 92	1 (0%)
1	G	386/390 (98%)	-1.96	0 100 100	15, 45, 74, 98	1 (0%)
1	H	380/390 (97%)	-1.96	0 100 100	14, 45, 77, 100	1 (0%)
All	All	3067/3120 (98%)	-1.97	0 100 100	10, 40, 73, 100	8 (0%)

There are no RSRZ outliers to report.

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	LLP	A	188	24/25	1.00	0.01	7,34,55,78	0
1	LLP	B	188	24/25	1.00	0.01	11,28,86,99	0
1	LLP	C	188	24/25	1.00	0.01	10,26,55,83	0
1	LLP	D	188	24/25	1.00	0.01	14,36,61,69	0
1	LLP	E	188	24/25	1.00	0.01	5,40,99,99	0
1	LLP	F	188	24/25	1.00	0.02	32,59,99,99	0
1	LLP	G	188	24/25	1.00	0.01	13,26,57,66	0
1	LLP	H	188	24/25	1.00	0.01	13,39,98,99	0

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
2	AKG	A	401	10/10	1.00	0.01	34,66,99,99	0
2	AKG	B	402	10/10	1.00	0.01	16,32,70,79	0
2	AKG	C	403	10/10	1.00	0.01	16,32,99,99	0
2	AKG	D	404	10/10	1.00	0.01	23,42,99,99	0
2	AKG	F	405	10/10	1.00	0.01	43,62,99,99	0
2	AKG	H	406	10/10	1.00	0.01	15,37,99,99	0

6.5 Other polymers [i](#)

There are no such residues in this entry.