



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:17 AM UTC

PDB ID : 2JBP / pdb_00002jbp
Title : Protein kinase MK2 in complex with an inhibitor (crystal form-2, co-crystallization)
Authors : Hillig, R.C.; Eberspaecher, U.; Montecarlo, F.; Huber, M.; Nguyen, D.; Mengel, A.; Muller-Tiemann, B.; Egner, U.
Deposited on : 2006-12-09
Resolution : 3.31 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:

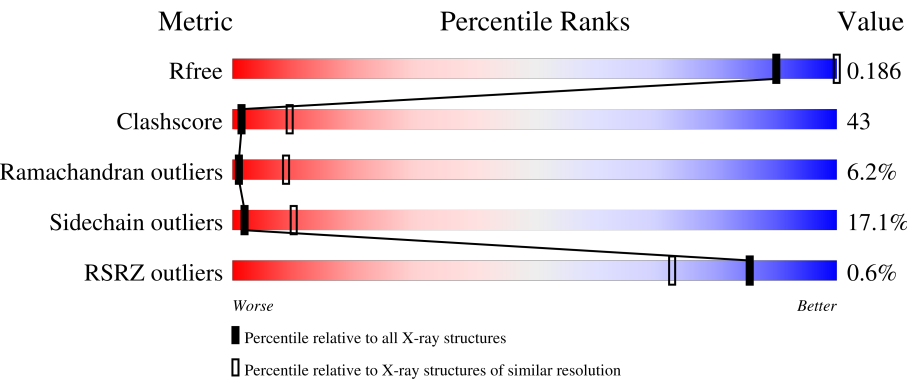
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance i

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

The reported resolution of this entry is 3.31 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	1153 (3.34-3.30)
Clashscore	190562	1193 (3.34-3.30)
Ramachandran outliers	187476	1172 (3.34-3.30)
Sidechain outliers	187428	1171 (3.34-3.30)
RSRZ outliers	180081	1153 (3.34-3.30)

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	326	42%34%10%•13%
1	B	326	34%40%13%•11%
1	C	326	% 31%43%12%•13%
1	D	326	% 33%39%15%•12%

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Mol	Chain	Length	Quality of chain
1	E	326	25%40%20%•13%
1	F	326	33%39%14%•12%
1	G	326	31%43%13%•12%
1	H	326	35%38%13%•13%
1	I	326	% 35%39%13%•11%
1	J	326	% 14%38%13%•31%
1	K	326	% 33%37%10%•19%
1	L	326	% 13%49%18%•18%

2 Entry composition

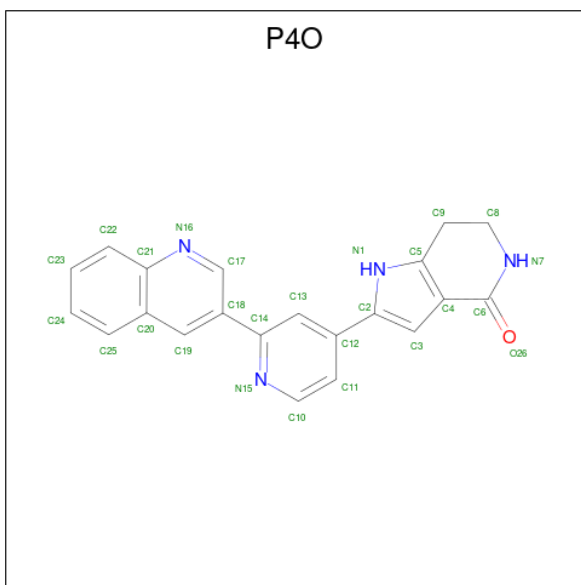
There are 3 unique types of molecules in this entry. The entry contains 27367 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 MAP KINASE-ACTIVATED PROTEIN KINASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	283	Total	C	N	O	S	0	0	0
			2298	1467	399	415	17			
1	B	290	Total	C	N	O	S	0	0	0
			2361	1510	407	427	17			
1	C	284	Total	C	N	O	S	0	0	0
			2316	1485	399	415	17			
1	D	286	Total	C	N	O	S	0	0	0
			2325	1486	402	420	17			
1	E	283	Total	C	N	O	S	0	0	1
			2291	1467	395	412	17			
1	F	288	Total	C	N	O	S	0	0	1
			2344	1499	405	423	17			
1	G	288	Total	C	N	O	S	0	0	1
			2343	1498	405	423	17			
1	H	283	Total	C	N	O	S	0	0	1
			2289	1464	396	412	17			
1	I	289	Total	C	N	O	S	0	0	0
			2354	1503	407	427	17			
1	J	225	Total	C	N	O	S	0	0	1
			1823	1167	315	326	15			
1	K	265	Total	C	N	O	S	0	0	1
			2142	1367	374	384	17			
1	L	268	Total	C	N	O	S	0	0	1
			2177	1390	379	391	17			

- Molecule 2 is 2-(2-QUINOLIN-3-YPYRIDIN-4-YL)-1,5,6,7-TETRAHYDRO-4H-PYRROLO[3,2-C]PYRIDIN-4-ONE (CCD ID: P4O) (formula: C₂₁H₁₆N₄O).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			26	21	4	1		
2	B	1	Total	C	N	O	0	0
			26	21	4	1		
2	C	1	Total	C	N	O	0	0
			26	21	4	1		
2	D	1	Total	C	N	O	0	0
			26	21	4	1		
2	E	1	Total	C	N	O	0	0
			26	21	4	1		
2	F	1	Total	C	N	O	0	0
			26	21	4	1		
2	G	1	Total	C	N	O	0	0
			26	21	4	1		
2	H	1	Total	C	N	O	0	0
			26	21	4	1		
2	I	1	Total	C	N	O	0	0
			26	21	4	1		
2	K	1	Total	C	N	O	0	0
			26	21	4	1		
2	L	1	Total	C	N	O	0	0
			26	21	4	1		

- Molecule 3 is water.

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

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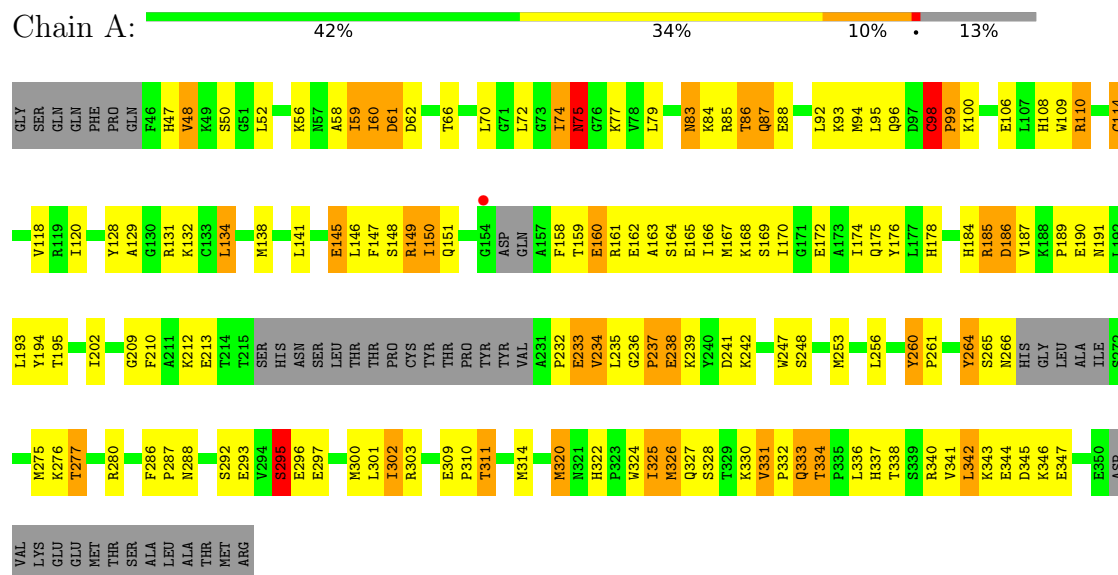
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total 2	O 2	0	0
3	C	2	Total 2	O 2	0	0
3	D	2	Total 2	O 2	0	0
3	E	1	Total 1	O 1	0	0
3	F	2	Total 2	O 2	0	0
3	G	3	Total 3	O 3	0	0
3	I	1	Total 1	O 1	0	0
3	L	1	Total 1	O 1	0	0

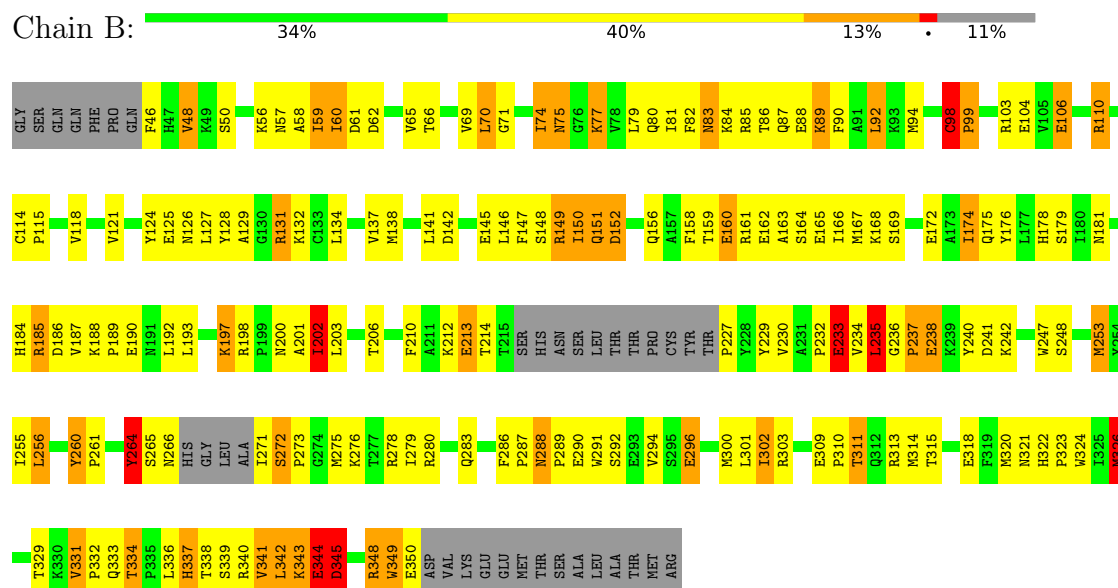
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

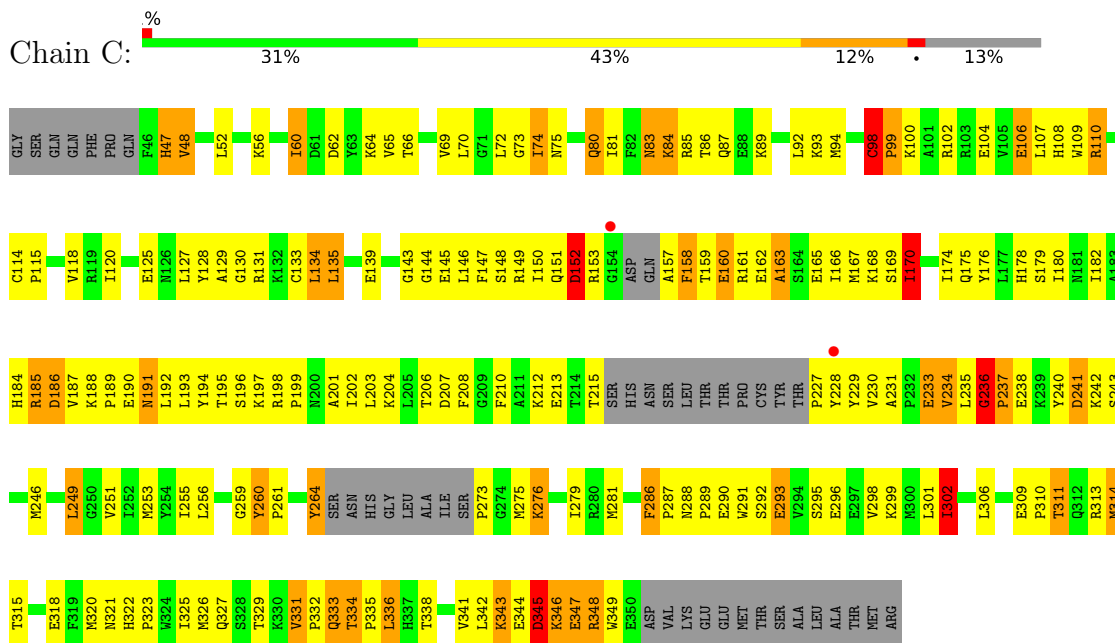
• Molecule 1: MAP KINASE-ACTIVATED PROTEIN KINASE 2



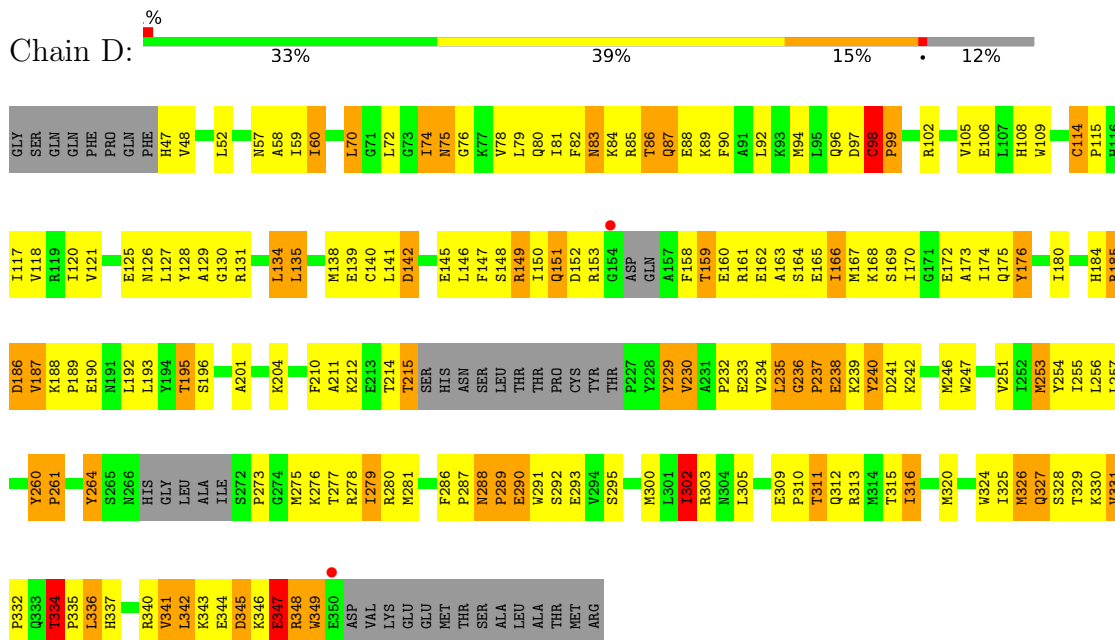
• Molecule 1: MAP KINASE-ACTIVATED PROTEIN KINASE 2



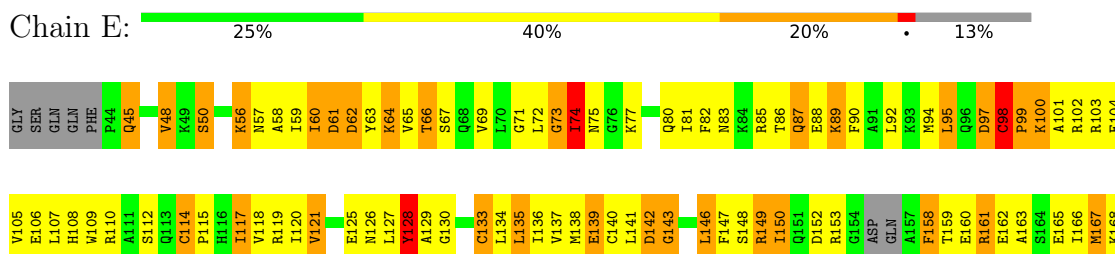
- Molecule 1: MAP KINASE-ACTIVATED PROTEIN KINASE 2

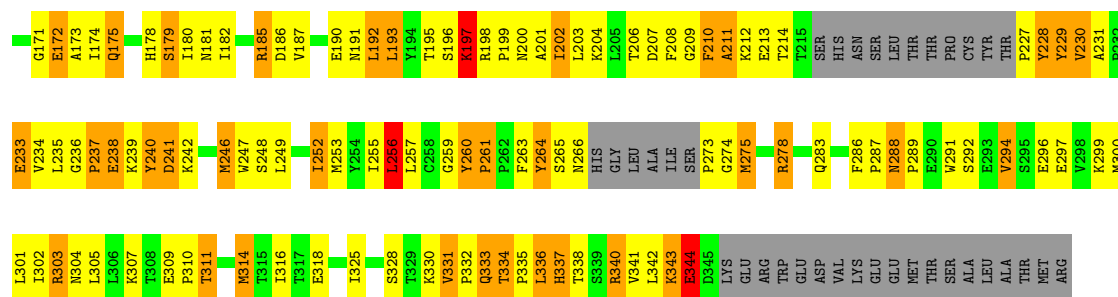


- Molecule 1: MAP KINASE-ACTIVATED PROTEIN KINASE 2



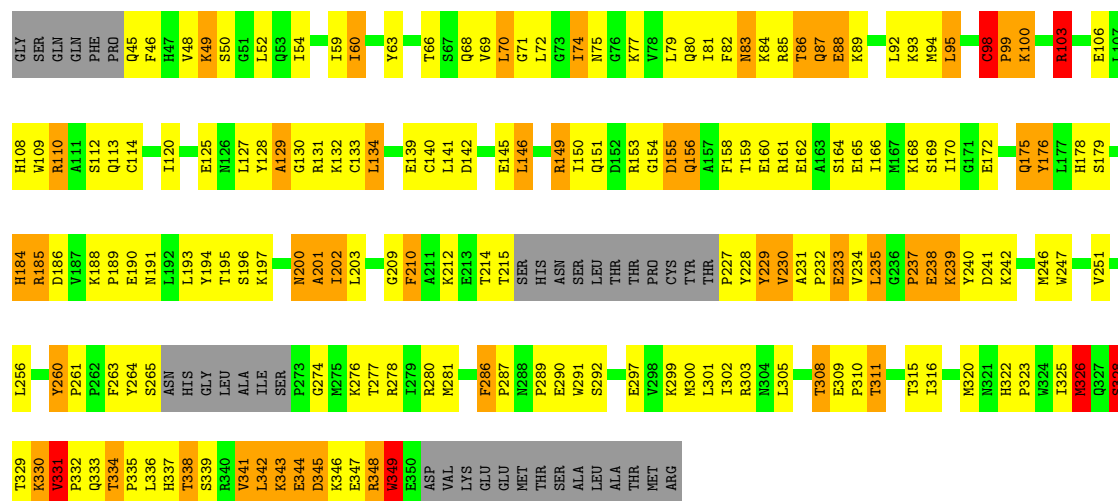
- Molecule 1: MAP KINASE-ACTIVATED PROTEIN KINASE 2





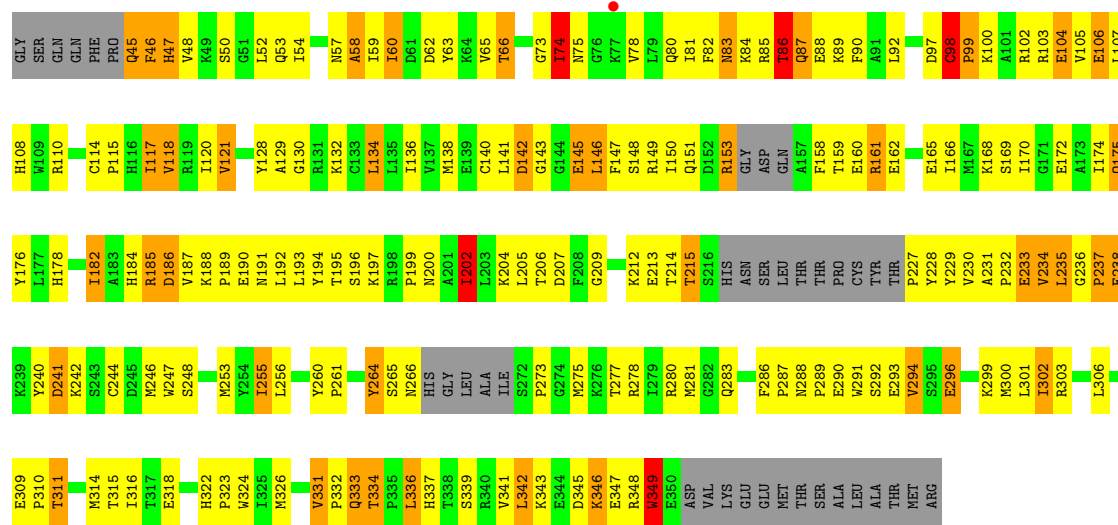
• Molecule 1: MAP KINASE-ACTIVATED PROTEIN KINASE 2

Chain F: 33% 39% 14% 12%

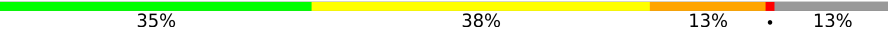


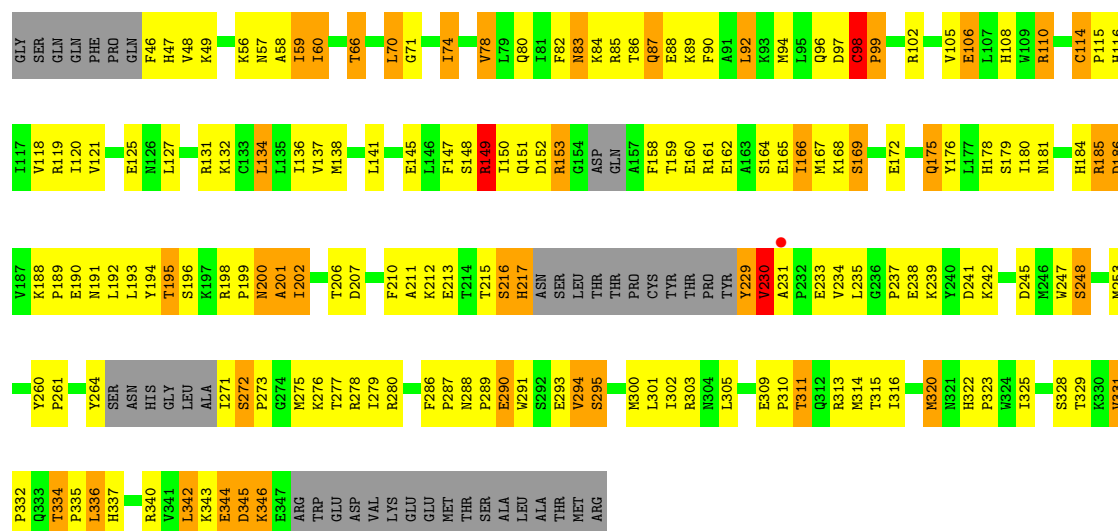
• Molecule 1: MAP KINASE-ACTIVATED PROTEIN KINASE 2

Chain G: 31% 43% 13% 12%

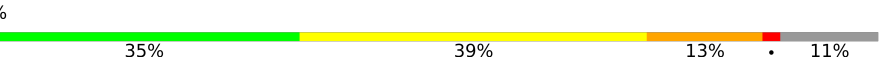


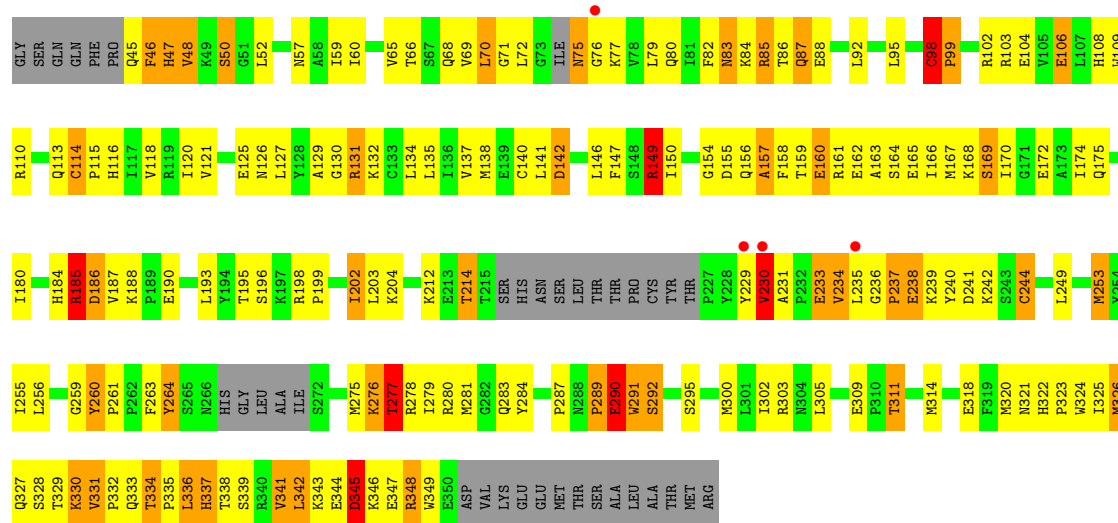
• Molecule 1: MAP KINASE-ACTIVATED PROTEIN KINASE 2

Chain H: 



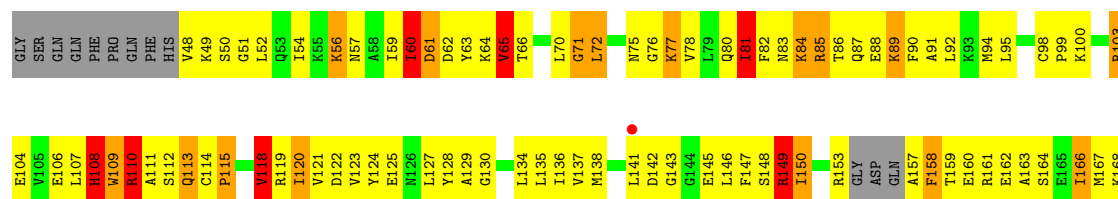
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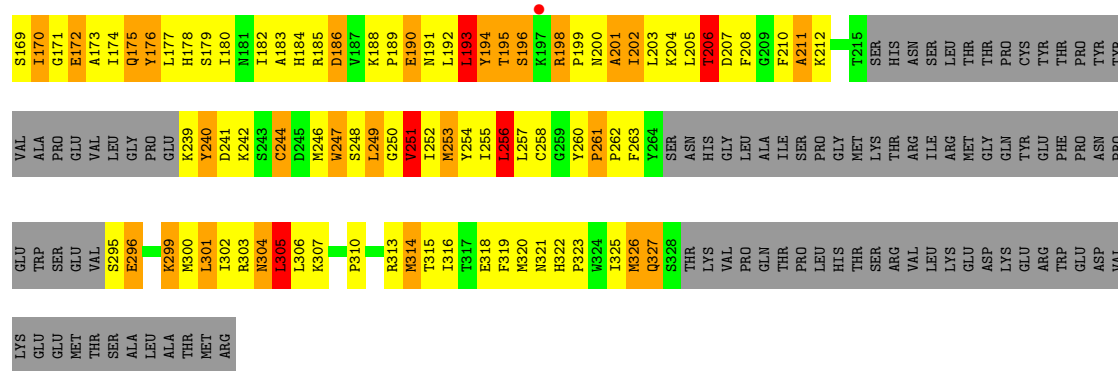
Chain I: 



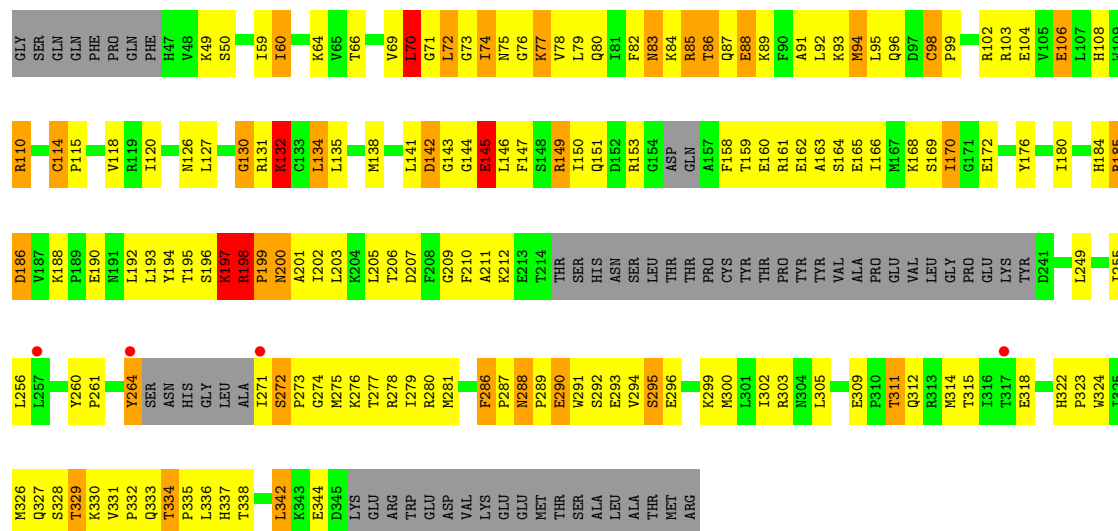
• Molecule 1: MAP KINASE-ACTIVATED PROTEIN KINASE 2

Chain J: 

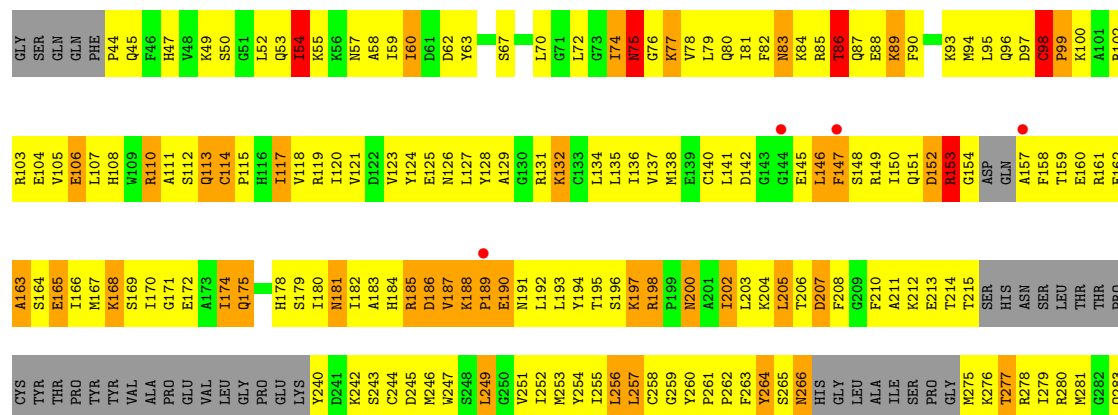
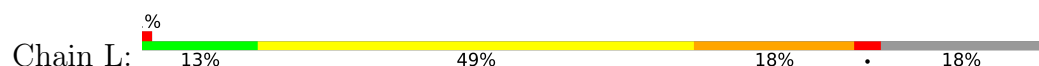




• Molecule 1: MAP KINASE-ACTIVATED PROTEIN KINASE 2



• Molecule 1: MAP KINASE-ACTIVATED PROTEIN KINASE 2



D345	LYS	Y284
GLU	E285	
ARG	F286	
TRP	P287	
GLU	N288	
ASP	P289	
VAL	E290	
GLU	W291	
GLU	E292	
GLU	S293	
GLU	V294	
MET	S295	
THR	E296	
SER	E297	
LEU	K298	
ALA	M300	
ALA	L301	
THR	L302	
MET	R303	
ARG	N304	
	L305	
	L306	
	K307	
	L308	
	E309	
	P310	
	T311	
	K312	
	R313	
	K314	
	T315	
	L316	
	T317	
	E318	
	F319	
	K320	
	N321	
	H322	
	K323	
	P324	
	K327	
	S328	
	T329	
	K330	
	V331	
	P332	
	K333	
	T334	
	P335	
	L336	
	H337	
	T338	
	S339	
	R340	
	V341	
	L342	
	K343	
	F344	

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	139.98Å 215.56Å 179.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.08 – 3.31 49.08 – 3.31	Depositor EDS
% Data completeness (in resolution range)	(Not available) (49.08-3.31) 96.5 (49.08-3.31)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 3.33Å)	Xtriage
Refinement program	CNX 2005	Depositor
R, R_{free}	0.215 , 0.279 0.195 , 0.186	Depositor DCC
R_{free} test set	3942 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	88.6	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 111.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	27367	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.95% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: P4O

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	1.21	6/2346 (0.3%)	1.31	21/3160 (0.7%)
1	B	1.04	5/2413 (0.2%)	1.21	18/3254 (0.6%)
1	C	1.10	7/2367 (0.3%)	1.31	22/3189 (0.7%)
1	D	1.14	8/2375 (0.3%)	1.34	29/3201 (0.9%)
1	E	0.82	2/2341 (0.1%)	1.23	24/3155 (0.8%)
1	F	1.24	8/2396 (0.3%)	1.43	25/3230 (0.8%)
1	G	1.00	7/2394 (0.3%)	1.27	18/3227 (0.6%)
1	H	0.86	3/2337 (0.1%)	1.17	12/3149 (0.4%)
1	I	0.95	2/2405 (0.1%)	1.23	22/3241 (0.7%)
1	J	0.70	1/1855 (0.1%)	1.09	14/2493 (0.6%)
1	K	0.71	2/2184 (0.1%)	1.03	10/2940 (0.3%)
1	L	0.72	2/2221 (0.1%)	1.14	15/2990 (0.5%)
All	All	0.98	53/27634 (0.2%)	1.24	230/37229 (0.6%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	2
1	F	0	2
1	G	0	2
1	I	0	1
All	All	0	8

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	320	MET	SD-CE	-16.73	1.37	1.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	138	MET	SD-CE	-12.92	1.47	1.79
1	B	253	MET	SD-CE	-10.51	1.53	1.79
1	B	320	MET	SD-CE	-10.09	1.54	1.79
1	A	320	MET	SD-CE	-9.43	1.55	1.79
1	C	320	MET	SD-CE	-8.98	1.57	1.79
1	D	187	VAL	CA-CB	-8.41	1.43	1.53
1	F	202	ILE	CA-CB	-7.94	1.43	1.55
1	H	320	MET	SD-CE	-7.72	1.60	1.79
1	D	105	VAL	CA-CB	-7.26	1.46	1.54
1	I	253	MET	SD-CE	-7.21	1.61	1.79
1	G	202	ILE	CA-CB	-7.15	1.46	1.54
1	C	246	MET	SD-CE	-7.04	1.61	1.79
1	A	314	MET	SD-CE	-6.93	1.62	1.79
1	B	138	MET	SD-CE	-6.88	1.62	1.79
1	I	202	ILE	CA-CB	-6.77	1.46	1.54
1	D	253	MET	SD-CE	-6.76	1.62	1.79
1	A	167	MET	SD-CE	-6.69	1.62	1.79
1	C	251	VAL	CA-CB	-6.61	1.46	1.54
1	A	253	MET	SD-CE	-6.60	1.63	1.79
1	F	170	ILE	CA-CB	-6.58	1.46	1.54
1	C	314	MET	SD-CE	-6.48	1.63	1.79
1	C	255	ILE	CA-CB	-6.46	1.47	1.54
1	B	341	VAL	CA-CB	-6.32	1.46	1.54
1	G	182	ILE	CA-CB	-6.32	1.46	1.54
1	G	255	ILE	CA-CB	-6.28	1.46	1.54
1	F	246	MET	SD-CE	-5.93	1.64	1.79
1	D	316	ILE	CA-CB	-5.92	1.46	1.54
1	D	320	MET	SD-CE	-5.88	1.64	1.79
1	F	230	VAL	CA-CB	5.86	1.60	1.53
1	D	302	ILE	CA-CB	-5.79	1.46	1.54
1	D	121	VAL	CA-CB	-5.77	1.46	1.54
1	E	344	GLU	C-N	-5.77	1.25	1.33
1	K	344	GLU	C-N	-5.73	1.25	1.33
1	C	167	MET	SD-CE	-5.69	1.65	1.79
1	J	327	GLN	C-N	-5.68	1.25	1.33
1	G	136	ILE	CA-CB	-5.63	1.47	1.54
1	L	344	GLU	C-N	-5.61	1.25	1.33
1	D	117	ILE	CA-CB	-5.55	1.47	1.54
1	L	54	ILE	CA-CB	-5.50	1.47	1.53
1	H	346	LYS	C-N	-5.47	1.25	1.33
1	G	54	ILE	CA-CB	-5.47	1.47	1.54
1	K	132	LYS	CA-C	5.46	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	251	VAL	CA-CB	-5.46	1.47	1.54
1	A	302	ILE	CA-CB	-5.42	1.48	1.54
1	H	138	MET	SD-CE	-5.35	1.66	1.79
1	E	230	VAL	CA-CB	5.33	1.61	1.54
1	G	58	ALA	CA-CB	-5.27	1.44	1.53
1	F	349	TRP	C-N	-5.21	1.26	1.33
1	F	54	ILE	CA-CB	-5.16	1.48	1.54
1	B	174	ILE	CA-CB	-5.14	1.47	1.54
1	G	349	TRP	C-N	-5.13	1.26	1.33
1	C	253	MET	SD-CE	-5.06	1.67	1.79

All (230) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	331	VAL	CA-C-N	14.19	135.12	119.93
1	C	331	VAL	C-N-CA	14.19	135.12	119.93
1	F	331	VAL	CA-C-N	12.95	136.03	119.84
1	F	331	VAL	C-N-CA	12.95	136.03	119.84
1	F	260	TYR	CA-C-N	12.22	128.46	119.66
1	F	260	TYR	C-N-CA	12.22	128.46	119.66
1	A	260	TYR	CA-C-N	11.06	127.62	119.66
1	A	260	TYR	C-N-CA	11.06	127.62	119.66
1	H	331	VAL	CA-C-N	10.88	131.57	119.93
1	H	331	VAL	C-N-CA	10.88	131.57	119.93
1	F	98	CYS	CA-C-N	-10.04	107.28	119.84
1	F	98	CYS	C-N-CA	-10.04	107.28	119.84
1	E	331	VAL	CA-C-N	9.82	129.58	119.76
1	E	331	VAL	C-N-CA	9.82	129.58	119.76
1	D	331	VAL	CA-C-N	9.81	129.91	119.90
1	D	331	VAL	C-N-CA	9.81	129.91	119.90
1	A	331	VAL	CA-C-N	9.47	130.07	119.93
1	A	331	VAL	C-N-CA	9.47	130.07	119.93
1	J	261	PRO	CA-C-N	-9.38	109.99	119.56
1	J	261	PRO	C-N-CA	-9.38	109.99	119.56
1	G	197	LYS	N-CA-C	-9.07	102.35	113.41
1	G	331	VAL	CA-C-N	8.99	129.03	119.76
1	G	331	VAL	C-N-CA	8.99	129.03	119.76
1	A	98	CYS	CA-C-N	-8.92	108.69	119.84
1	A	98	CYS	C-N-CA	-8.92	108.69	119.84
1	I	98	CYS	CA-C-N	-8.92	108.69	119.84
1	I	98	CYS	C-N-CA	-8.92	108.69	119.84
1	K	98	CYS	CA-C-N	-8.92	108.69	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	98	CYS	C-N-CA	-8.92	108.69	119.84
1	B	345	ASP	N-CA-C	-8.89	99.77	113.02
1	G	98	CYS	CA-C-N	-8.73	108.93	119.84
1	G	98	CYS	C-N-CA	-8.73	108.93	119.84
1	L	331	VAL	CA-C-N	8.37	130.31	119.84
1	L	331	VAL	C-N-CA	8.37	130.31	119.84
1	H	98	CYS	CA-C-N	-8.27	109.51	119.84
1	H	98	CYS	C-N-CA	-8.27	109.51	119.84
1	E	98	CYS	CA-C-N	-8.08	109.74	119.84
1	E	98	CYS	C-N-CA	-8.08	109.74	119.84
1	D	260	TYR	CA-C-N	7.93	128.55	120.38
1	D	260	TYR	C-N-CA	7.93	128.55	120.38
1	D	114	CYS	CA-C-N	7.77	127.83	119.28
1	D	114	CYS	C-N-CA	7.77	127.83	119.28
1	L	165	GLU	N-CA-C	-7.70	103.49	113.12
1	B	202	ILE	N-CA-C	7.67	119.65	108.53
1	A	295	SER	N-CA-C	7.58	120.96	110.35
1	H	114	CYS	CA-C-N	7.47	127.11	119.56
1	H	114	CYS	C-N-CA	7.47	127.11	119.56
1	D	334	THR	CA-C-N	7.43	128.02	119.99
1	D	334	THR	C-N-CA	7.43	128.02	119.99
1	F	286	PHE	CA-C-N	7.34	127.78	119.93
1	F	286	PHE	C-N-CA	7.34	127.78	119.93
1	G	104	GLU	N-CA-C	-7.25	102.18	111.02
1	G	202	ILE	N-CA-C	7.25	119.44	109.80
1	F	153	ARG	CA-C-N	-7.15	114.76	121.62
1	F	153	ARG	C-N-CA	-7.15	114.76	121.62
1	I	163	ALA	N-CA-C	-7.13	103.44	111.07
1	B	213	GLU	N-CA-C	-7.06	101.18	110.43
1	D	163	ALA	N-CA-C	-7.05	103.52	111.07
1	D	286	PHE	CA-C-N	7.00	126.99	119.78
1	D	286	PHE	C-N-CA	7.00	126.99	119.78
1	I	277	THR	N-CA-C	6.98	119.92	111.82
1	F	88	GLU	N-CA-C	6.90	120.01	110.35
1	A	286	PHE	CA-C-N	6.90	126.89	119.78
1	A	286	PHE	C-N-CA	6.90	126.89	119.78
1	J	61	ASP	N-CA-C	-6.86	105.85	114.56
1	B	241	ASP	N-CA-C	-6.76	105.16	113.41
1	G	145	GLU	N-CA-C	6.74	119.21	109.71
1	L	198	ARG	CA-C-N	6.73	126.99	119.32
1	L	198	ARG	C-N-CA	6.73	126.99	119.32
1	D	229	TYR	N-CA-C	-6.63	104.94	113.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	I	330	LYS	N-CA-C	-6.62	104.51	112.59
1	E	236	GLY	CA-C-N	6.61	128.10	119.84
1	E	236	GLY	C-N-CA	6.61	128.10	119.84
1	B	98	CYS	CA-C-N	-6.58	111.61	119.84
1	B	98	CYS	C-N-CA	-6.58	111.61	119.84
1	F	330	LYS	CA-C-N	-6.56	112.18	121.23
1	F	330	LYS	C-N-CA	-6.56	112.18	121.23
1	L	98	CYS	CA-C-N	-6.54	111.66	119.84
1	L	98	CYS	C-N-CA	-6.54	111.66	119.84
1	K	132	LYS	N-CA-C	6.52	119.32	108.96
1	C	260	TYR	CA-C-N	6.50	127.08	120.38
1	C	260	TYR	C-N-CA	6.50	127.08	120.38
1	D	121	VAL	CB-CA-C	-6.45	103.47	111.92
1	L	296	GLU	N-CA-C	-6.45	104.89	112.89
1	I	149	ARG	N-CA-C	-6.43	103.97	110.97
1	I	185	ARG	NE-CZ-NH1	-6.41	115.09	121.50
1	J	202	ILE	N-CA-C	6.41	118.37	108.44
1	E	114	CYS	CA-C-N	6.36	126.57	119.32
1	E	114	CYS	C-N-CA	6.36	126.57	119.32
1	L	322	HIS	CA-C-N	6.34	126.09	119.05
1	L	322	HIS	C-N-CA	6.34	126.09	119.05
1	B	331	VAL	CA-C-N	6.32	127.74	119.84
1	B	331	VAL	C-N-CA	6.32	127.74	119.84
1	E	74	ILE	N-CA-C	6.32	116.49	110.74
1	F	328	SER	N-CA-C	-6.31	105.55	113.18
1	G	110	ARG	CG-CD-NE	-6.26	98.22	112.00
1	G	121	VAL	CB-CA-C	-6.22	103.77	111.92
1	C	143	GLY	N-CA-C	6.19	121.27	114.40
1	F	103	ARG	NE-CZ-NH2	6.19	124.77	119.20
1	F	331	VAL	CA-C-O	6.19	124.54	119.47
1	C	163	ALA	N-CA-C	-6.18	104.47	111.14
1	C	234	VAL	N-CA-C	6.17	116.33	110.53
1	E	259	GLY	CA-C-N	-6.10	115.17	123.96
1	E	259	GLY	C-N-CA	-6.10	115.17	123.96
1	D	76	GLY	N-CA-C	6.09	127.62	113.18
1	D	98	CYS	CA-C-N	-6.05	112.27	119.84
1	D	98	CYS	C-N-CA	-6.05	112.27	119.84
1	E	330	LYS	N-CA-C	-6.05	105.71	114.12
1	H	286	PHE	CA-C-N	6.05	126.06	119.89
1	H	286	PHE	C-N-CA	6.05	126.06	119.89
1	B	288	ASN	CA-C-N	6.01	141.42	127.00
1	B	288	ASN	C-N-CA	6.01	141.42	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	146	LEU	N-CA-C	-5.95	104.71	111.14
1	G	47	HIS	N-CA-C	5.95	119.00	108.24
1	D	159	THR	N-CA-C	5.93	119.72	110.17
1	H	295	SER	N-CA-C	5.93	118.95	110.24
1	C	236	GLY	CA-C-N	5.90	127.22	119.84
1	C	236	GLY	C-N-CA	5.90	127.22	119.84
1	L	58	ALA	N-CA-C	-5.88	101.95	110.24
1	A	160	GLU	N-CA-C	-5.87	104.23	111.33
1	A	344	GLU	N-CA-C	-5.85	106.12	113.20
1	I	185	ARG	NE-CZ-NH2	5.84	124.46	119.20
1	F	49	LYS	N-CA-C	-5.84	101.55	110.14
1	J	122	ASP	CA-C-N	-5.83	114.84	122.94
1	J	122	ASP	C-N-CA	-5.83	114.84	122.94
1	C	286	PHE	CA-C-N	5.82	125.78	119.78
1	C	286	PHE	C-N-CA	5.82	125.78	119.78
1	C	98	CYS	CA-C-N	-5.81	112.57	119.84
1	C	98	CYS	C-N-CA	-5.81	112.57	119.84
1	B	288	ASN	C-N-CD	-5.81	107.82	120.60
1	E	263	PHE	N-CA-C	5.80	118.17	108.02
1	A	150	ILE	CB-CA-C	-5.80	104.43	112.02
1	G	347	GLU	N-CA-C	5.79	118.46	111.40
1	G	65	VAL	N-CA-C	5.78	116.13	107.51
1	I	331	VAL	CA-C-N	5.75	125.76	119.90
1	I	331	VAL	C-N-CA	5.75	125.76	119.90
1	L	286	PHE	CA-C-N	5.73	125.68	119.78
1	L	286	PHE	C-N-CA	5.73	125.68	119.78
1	B	160	GLU	N-CA-C	-5.70	104.28	111.11
1	F	292	SER	N-CA-C	5.69	117.48	111.28
1	J	305	LEU	N-CA-C	-5.68	104.48	111.75
1	D	236	GLY	CA-C-N	5.66	126.92	119.84
1	D	236	GLY	C-N-CA	5.66	126.92	119.84
1	E	50	SER	N-CA-C	5.66	117.37	110.41
1	C	160	GLU	N-CA-C	-5.64	104.34	111.11
1	H	294	VAL	N-CA-C	5.62	116.30	108.89
1	I	114	CYS	CA-C-N	5.57	125.41	119.28
1	I	114	CYS	C-N-CA	5.57	125.41	119.28
1	H	166	ILE	CB-CA-C	-5.57	104.84	111.97
1	K	331	VAL	CA-C-N	5.56	125.57	119.90
1	K	331	VAL	C-N-CA	5.56	125.57	119.90
1	G	273	PRO	N-CA-C	-5.55	107.20	114.03
1	E	260	TYR	CA-C-N	5.55	126.10	120.38
1	E	260	TYR	C-N-CA	5.55	126.10	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	296	GLU	N-CA-C	-5.53	105.15	111.07
1	I	46	PHE	N-CA-C	5.51	117.22	108.79
1	D	288	ASN	C-N-CD	-5.51	108.48	120.60
1	I	345	ASP	N-CA-C	-5.50	99.09	110.80
1	J	81	ILE	N-CA-C	5.50	116.28	108.42
1	J	299	LYS	N-CA-C	-5.50	106.70	113.41
1	E	65	VAL	N-CA-C	5.49	116.29	107.73
1	G	175	GLN	N-CA-C	-5.49	105.38	111.36
1	K	114	CYS	CA-C-N	5.48	125.15	119.56
1	K	114	CYS	C-N-CA	5.48	125.15	119.56
1	K	286	PHE	CA-C-N	5.47	125.42	119.78
1	K	286	PHE	C-N-CA	5.47	125.42	119.78
1	D	295	SER	N-CA-C	5.47	117.95	110.24
1	J	110	ARG	N-CA-C	-5.45	105.26	111.14
1	I	160	GLU	N-CA-C	-5.44	104.75	111.33
1	J	65	VAL	N-CA-C	5.44	114.57	106.85
1	D	166	ILE	CB-CA-C	-5.42	104.94	111.88
1	E	229	TYR	N-CA-C	-5.41	106.06	113.30
1	D	75	ASN	N-CA-C	-5.39	99.73	108.52
1	J	75	ASN	N-CA-C	5.39	117.12	107.80
1	G	296	GLU	N-CA-C	-5.38	105.45	112.23
1	D	254	TYR	N-CA-C	-5.38	105.32	111.07
1	E	197	LYS	N-CA-C	-5.38	108.49	114.62
1	F	184	HIS	N-CA-C	-5.37	104.98	112.45
1	E	172	GLU	N-CA-C	-5.37	105.54	111.71
1	I	50	SER	N-CA-C	5.36	117.61	110.53
1	L	187	VAL	CB-CA-C	-5.36	107.22	113.22
1	E	296	GLU	N-CA-C	-5.35	106.52	113.16
1	B	65	VAL	N-CA-C	5.35	115.48	107.51
1	C	69	VAL	N-CA-C	5.34	116.06	107.73
1	C	144	GLY	N-CA-C	5.32	120.69	112.81
1	B	260	TYR	CA-C-N	5.32	125.86	120.38
1	B	260	TYR	C-N-CA	5.32	125.86	120.38
1	B	163	ALA	N-CA-C	-5.32	105.38	111.07
1	A	114	CYS	CA-C-N	5.31	124.98	119.56
1	A	114	CYS	C-N-CA	5.31	124.98	119.56
1	A	75	ASN	N-CA-C	5.31	117.24	110.61
1	F	112	SER	N-CA-C	-5.30	106.32	112.89
1	I	65	VAL	N-CA-C	5.25	114.87	106.88
1	B	50	SER	N-CA-C	5.25	117.48	110.35
1	C	170	ILE	CB-CA-C	-5.23	105.08	112.14
1	K	197	LYS	N-CA-C	-5.22	106.97	113.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	173	ALA	N-CA-C	-5.20	105.30	110.97
1	G	78	VAL	CB-CA-C	-5.17	104.26	110.99
1	I	291	TRP	N-CA-C	5.17	119.74	113.38
1	J	206	THR	N-CA-C	5.16	115.10	108.34
1	J	120	ILE	N-CA-C	-5.16	101.05	108.53
1	C	234	VAL	CB-CA-C	-5.14	105.29	112.02
1	D	302	ILE	CB-CA-C	-5.14	104.55	112.05
1	H	132	LYS	N-CA-C	-5.14	101.59	109.76
1	E	45	GLN	N-CA-C	5.14	117.48	110.24
1	I	260	TYR	CA-C-N	5.13	125.67	120.38
1	I	260	TYR	C-N-CA	5.13	125.67	120.38
1	F	251	VAL	CB-CA-C	-5.13	105.14	112.22
1	A	302	ILE	CB-CA-C	-5.11	105.35	112.04
1	F	54	ILE	CB-CA-C	-5.09	103.75	111.33
1	C	233	GLU	CA-C-N	5.08	127.07	120.56
1	C	233	GLU	C-N-CA	5.08	127.07	120.56
1	A	163	ALA	N-CA-C	-5.08	105.63	111.07
1	D	261	PRO	CA-C-N	5.08	124.77	119.64
1	D	261	PRO	C-N-CA	5.08	124.77	119.64
1	E	192	LEU	N-CA-C	5.08	115.70	108.54
1	A	288	ASN	CA-C-N	5.07	139.16	127.00
1	A	288	ASN	C-N-CA	5.07	139.16	127.00
1	A	325	ILE	CB-CA-C	-5.06	105.83	111.80
1	I	341	VAL	CB-CA-C	-5.06	105.30	112.14
1	I	47	HIS	N-CA-C	5.06	118.28	107.70
1	G	110	ARG	NE-CZ-NH1	-5.06	116.44	121.50
1	B	302	ILE	CB-CA-C	-5.04	105.43	112.04
1	C	302	ILE	CB-CA-C	-5.04	105.34	112.14
1	C	47	HIS	N-CA-C	5.04	116.73	108.52
1	F	235	LEU	N-CA-C	-5.03	107.20	113.19
1	E	133	CYS	N-CA-C	5.03	116.61	108.26
1	L	168	LYS	N-CA-C	-5.03	107.11	113.20
1	F	129	ALA	N-CA-C	-5.01	105.05	110.91
1	D	279	ILE	CB-CA-C	-5.00	105.32	112.22

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	264	TYR	Sidechain
1	D	176	TYR	Sidechain
1	D	229	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	F	176	TYR	Sidechain
1	F	229	TYR	Sidechain
1	G	228	TYR	Sidechain
1	G	229	TYR	Sidechain
1	I	155	ASP	Peptide

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	2298	0	2326	142	0
1	B	2361	0	2385	199	0
1	C	2316	0	2346	187	0
1	D	2325	0	2352	185	0
1	E	2291	0	2325	252	0
1	F	2344	0	2370	181	0
1	G	2343	0	2369	195	0
1	H	2289	0	2325	170	0
1	I	2354	0	2370	189	0
1	J	1823	0	1868	280	0
1	K	2142	0	2186	168	0
1	L	2177	0	2212	345	0
2	A	26	0	16	2	0
2	B	26	0	16	1	0
2	C	26	0	16	4	0
2	D	26	0	16	5	0
2	E	26	0	16	4	0
2	F	26	0	16	5	0
2	G	26	0	16	5	0
2	H	26	0	16	4	0
2	I	26	0	16	3	0
2	K	26	0	16	3	0
2	L	26	0	16	4	0
3	A	4	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	0	0
3	D	2	0	0	0	0
3	E	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	F	2	0	0	0	0
3	G	3	0	0	0	0
3	I	1	0	0	0	0
3	L	1	0	0	0	0
All	All	27367	0	27610	2389	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 43.

All (2389) 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:G:45:GLN:HG3	1:G:46:PHE:H	1.03	1.17
1:L:275:MET:HA	1:L:278:ARG:NH1	1.60	1.16
1:L:275:MET:HG3	1:L:278:ARG:HH22	1.12	1.15
1:D:264:TYR:O	1:D:275:MET:HG3	1.43	1.14
1:F:151:GLN:HE22	1:F:346:LYS:HD3	1.01	1.13
1:C:150:ILE:HD12	1:C:158:PHE:HE1	1.07	1.13
1:G:233:GLU:HG2	1:H:310:PRO:HG3	1.24	1.13
1:J:149:ARG:HB3	1:J:149:ARG:HH11	0.96	1.12
1:B:264:TYR:O	1:B:275:MET:HG3	1.48	1.11
1:J:202:ILE:HD12	1:J:204:LYS:HE3	1.25	1.06
1:D:86:THR:HG22	1:D:88:GLU:H	1.09	1.06
1:E:343:LYS:HB2	1:E:344:GLU:OE2	1.56	1.06
1:K:86:THR:HG22	1:K:88:GLU:H	1.09	1.06
1:F:149:ARG:HH11	1:F:149:ARG:HG3	1.14	1.06
1:C:185:ARG:HH21	1:C:212:LYS:HD3	1.14	1.04
1:K:83:ASN:HD21	1:K:85:ARG:HG3	1.22	1.03
1:F:344:GLU:O	1:F:345:ASP:HB2	1.59	1.03
1:D:214:THR:O	1:D:215:THR:HG23	1.59	1.02
1:L:118:VAL:HG11	1:L:206:THR:HG22	1.40	1.02
1:G:310:PRO:HG3	1:I:233:GLU:HG2	1.39	1.02
1:F:86:THR:CG2	1:F:88:GLU:HB2	1.90	1.01
1:K:74:ILE:HG21	1:K:209:GLY:HA3	1.42	1.01
1:J:83:ASN:HD21	1:J:85:ARG:HB3	1.24	1.00
1:L:165:GLU:HG2	1:L:328:SER:HB3	1.42	1.00
1:C:150:ILE:HD12	1:C:158:PHE:CE1	1.97	1.00
1:G:74:ILE:HG21	1:G:209:GLY:HA3	1.43	1.00
1:A:149:ARG:HB3	1:A:149:ARG:HH11	1.26	1.00
1:D:230:VAL:HG11	1:D:235:LEU:HD21	1.40	1.00
1:A:149:ARG:HH11	1:A:149:ARG:CB	1.73	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:167:MET:HG3	1:J:253:MET:HG2	1.39	1.00
1:J:149:ARG:NH2	1:J:199:PRO:HA	1.76	0.99
1:J:195:THR:HG23	1:J:196:SER:H	1.22	0.99
1:L:275:MET:CA	1:L:278:ARG:HH12	1.75	0.99
1:J:193:LEU:HD23	1:J:193:LEU:H	1.28	0.99
1:E:246:MET:HE1	1:E:316:ILE:HD12	1.42	0.98
1:E:288:ASN:HB3	1:E:289:PRO:HA	1.44	0.98
1:J:251:VAL:HG12	1:J:252:ILE:HG13	1.41	0.98
1:L:300:MET:HE1	1:L:303:ARG:HH21	1.27	0.97
1:E:227:PRO:HB3	1:E:229:TYR:CE2	2.00	0.97
1:J:149:ARG:HB3	1:J:149:ARG:NH1	1.79	0.97
1:E:180:ILE:HG13	1:E:182:ILE:HD12	1.47	0.97
1:L:281:MET:HB2	1:L:283:GLN:HG3	1.44	0.97
1:D:151:GLN:HE22	1:D:346:LYS:HD2	1.28	0.97
1:E:264:TYR:O	1:E:275:MET:HG3	1.64	0.96
1:J:195:THR:HG21	1:J:202:ILE:H	1.29	0.96
1:D:70:LEU:HD21	1:D:80:GLN:HB2	1.47	0.95
1:E:233:GLU:HG2	1:F:310:PRO:HG3	1.46	0.95
1:K:118:VAL:HG11	1:K:206:THR:HG22	1.46	0.95
1:K:288:ASN:HB3	1:K:289:PRO:HA	1.49	0.95
1:J:149:ARG:HH11	1:J:149:ARG:CB	1.80	0.94
1:L:263:PHE:CE2	1:L:279:ILE:HA	2.03	0.94
1:K:86:THR:HG22	1:K:88:GLU:N	1.83	0.94
1:A:310:PRO:HG3	1:C:233:GLU:CG	1.96	0.94
1:G:45:GLN:HG3	1:G:46:PHE:N	1.83	0.93
1:J:83:ASN:ND2	1:J:85:ARG:HB3	1.82	0.93
1:I:289:PRO:O	1:I:291:TRP:N	2.01	0.93
1:F:86:THR:HG21	1:F:88:GLU:HB2	1.50	0.93
1:A:310:PRO:HG3	1:C:233:GLU:HG2	1.50	0.93
1:L:83:ASN:C	1:L:83:ASN:HD22	1.77	0.92
1:C:348:ARG:HH21	1:C:348:ARG:HG2	1.35	0.92
1:B:227:PRO:HG2	1:B:230:VAL:HB	1.52	0.92
1:B:80:GLN:NE2	1:B:89:LYS:HD2	1.83	0.91
1:L:275:MET:HG3	1:L:278:ARG:NH2	1.84	0.91
1:L:332:PRO:HB2	1:L:334:THR:HG22	1.49	0.91
1:J:301:LEU:HD13	1:J:322:HIS:CD2	2.06	0.91
1:I:83:ASN:OD1	1:I:86:THR:HG22	1.71	0.91
1:F:149:ARG:HG3	1:F:149:ARG:NH1	1.83	0.90
1:F:151:GLN:NE2	1:F:346:LYS:HD3	1.86	0.90
1:J:107:LEU:HD22	1:J:182:ILE:CG2	2.01	0.90
1:J:198:ARG:HG2	1:J:198:ARG:HH11	1.35	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:83:ASN:HD22	1:F:84:LYS:N	1.68	0.90
1:G:143:GLY:HA3	1:G:196:SER:O	1.72	0.90
1:B:343:LYS:O	1:B:344:GLU:HB3	1.72	0.90
1:L:246:MET:SD	1:L:316:ILE:HB	2.12	0.90
1:F:185:ARG:HH21	1:F:212:LYS:HD3	1.37	0.89
1:H:149:ARG:HB3	1:H:149:ARG:HH11	1.36	0.89
1:L:275:MET:HA	1:L:278:ARG:HH12	0.79	0.89
1:C:331:VAL:HG13	1:C:332:PRO:HD2	1.54	0.89
1:G:74:ILE:HG23	1:G:75:ASN:H	1.35	0.89
1:E:299:LYS:O	1:E:303:ARG:HG3	1.72	0.89
1:L:181:ASN:HB3	1:L:214:THR:OG1	1.71	0.89
1:J:195:THR:HB	1:J:202:ILE:HG13	1.52	0.88
1:B:86:THR:HG23	1:B:88:GLU:HB2	1.55	0.88
1:F:344:GLU:O	1:F:344:GLU:HG2	1.72	0.88
1:J:143:GLY:O	1:J:149:ARG:HD2	1.74	0.88
1:D:238:GLU:OE1	1:D:242:LYS:HE3	1.74	0.88
1:E:235:LEU:HD13	1:F:276:LYS:HG3	1.56	0.88
1:E:66:THR:HG23	1:E:80:GLN:O	1.73	0.87
1:L:86:THR:O	1:L:88:GLU:N	2.08	0.87
1:H:74:ILE:HG21	1:H:210:PHE:CE2	2.10	0.87
1:E:227:PRO:HB3	1:E:229:TYR:CZ	2.10	0.87
1:E:73:GLY:HA3	2:E:1345:P4O:H8C2	1.57	0.87
1:F:83:ASN:HD22	1:F:83:ASN:C	1.80	0.86
1:K:74:ILE:CG2	1:K:209:GLY:HA3	2.05	0.86
1:K:196:SER:HB2	1:K:198:ARG:HB2	1.56	0.86
1:B:147:PHE:HD1	1:B:349:TRP:CZ2	1.93	0.86
1:L:343:LYS:H	1:L:343:LYS:HE2	1.40	0.86
1:E:167:MET:HG3	1:E:253:MET:HE2	1.57	0.85
1:K:83:ASN:HD21	1:K:85:ARG:CG	1.89	0.85
1:C:338:THR:O	1:C:342:LEU:HD13	1.76	0.85
1:A:233:GLU:HG2	1:B:310:PRO:HG3	1.57	0.85
1:J:110:ARG:HG2	1:J:110:ARG:HH11	1.38	0.85
1:J:114:CYS:HB2	1:J:176:TYR:CD2	2.12	0.85
1:E:60:ILE:HG12	1:E:61:ASP:H	1.40	0.85
1:B:276:LYS:O	1:B:280:ARG:HG3	1.77	0.85
1:E:60:ILE:HG12	1:E:61:ASP:N	1.92	0.85
1:G:185:ARG:HH21	1:G:212:LYS:HD2	1.41	0.85
1:H:152:ASP:O	1:H:153:ARG:HG3	1.76	0.85
1:E:121:VAL:HG23	1:E:137:VAL:O	1.77	0.84
1:E:185:ARG:CB	1:E:185:ARG:HH11	1.89	0.84
1:J:114:CYS:HB2	1:J:176:TYR:HD2	1.42	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:160:GLU:OE1	1:K:294:VAL:HG13	1.78	0.84
1:E:198:ARG:HH21	1:E:200:ASN:HD21	1.26	0.84
1:D:337:HIS:CD2	1:D:340:ARG:HH12	1.96	0.84
1:J:169:SER:C	1:J:171:GLY:H	1.85	0.84
1:K:151:GLN:HB2	1:K:342:LEU:HD23	1.59	0.84
1:L:166:ILE:HG21	1:L:256:LEU:HD11	1.59	0.84
1:E:60:ILE:O	1:E:62:ASP:N	2.11	0.83
1:L:255:ILE:HG12	1:L:261:PRO:HA	1.59	0.83
1:E:146:LEU:HD11	1:E:166:ILE:HD13	1.59	0.83
1:E:101:ALA:O	1:E:105:VAL:HG23	1.78	0.83
1:D:86:THR:HG21	1:D:88:GLU:HB2	1.61	0.83
1:E:83:ASN:HB3	1:E:86:THR:HG22	1.59	0.83
1:C:185:ARG:NH2	1:C:212:LYS:HD3	1.93	0.83
1:G:192:LEU:C	1:G:193:LEU:HD23	2.04	0.83
1:I:149:ARG:HB3	1:I:149:ARG:HH11	1.43	0.83
1:I:57:ASN:HA	1:K:50:SER:OG	1.79	0.82
1:E:85:ARG:HD2	1:E:85:ARG:O	1.79	0.82
1:E:185:ARG:HH11	1:E:185:ARG:HB3	1.43	0.82
1:E:195:THR:HG21	1:E:202:ILE:HG12	1.59	0.82
1:H:149:ARG:HH11	1:H:149:ARG:CB	1.91	0.82
1:L:300:MET:CE	1:L:303:ARG:HH21	1.93	0.82
1:L:275:MET:CG	1:L:278:ARG:HH22	1.92	0.82
1:H:74:ILE:HG21	1:H:210:PHE:HE2	1.44	0.82
1:D:230:VAL:CG1	1:D:235:LEU:HD21	2.09	0.82
1:D:332:PRO:HB2	1:D:334:THR:HG22	1.59	0.82
1:L:331:VAL:HG13	1:L:332:PRO:HD2	1.61	0.81
1:I:195:THR:HG23	1:I:202:ILE:O	1.80	0.81
1:B:331:VAL:HG13	1:B:332:PRO:HD2	1.59	0.81
1:F:86:THR:CG2	1:F:88:GLU:H	1.92	0.81
1:J:143:GLY:HA3	1:J:196:SER:O	1.80	0.81
1:B:233:GLU:HG2	1:C:310:PRO:HG3	1.61	0.81
1:G:151:GLN:O	1:G:343:LYS:HE2	1.81	0.81
1:J:158:PHE:HZ	1:J:163:ALA:HB2	1.46	0.81
1:J:174:ILE:HB	1:J:316:ILE:HD13	1.62	0.81
1:E:195:THR:HG23	1:E:202:ILE:O	1.81	0.80
1:G:118:VAL:HG11	1:G:206:THR:HG22	1.62	0.80
1:L:185:ARG:CB	1:L:185:ARG:HH11	1.94	0.80
1:G:233:GLU:CG	1:H:310:PRO:HG3	2.10	0.80
1:I:83:ASN:CG	1:I:86:THR:HG22	2.07	0.80
1:A:327:GLN:HE21	1:A:330:LYS:HG3	1.47	0.79
1:J:158:PHE:CZ	1:J:163:ALA:HB2	2.17	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:59:ILE:HG13	1:L:124:TYR:CD1	2.16	0.79
1:G:148:SER:O	1:G:150:ILE:N	2.16	0.79
1:K:80:GLN:NE2	1:K:89:LYS:HG2	1.97	0.79
1:C:83:ASN:HD22	1:C:84:LYS:N	1.80	0.79
1:D:86:THR:O	1:D:87:GLN:HB2	1.82	0.79
1:J:304:ASN:O	1:J:307:LYS:HG2	1.83	0.79
1:K:271:ILE:CG2	1:K:278:ARG:HH12	1.95	0.79
1:K:86:THR:HG21	1:K:88:GLU:OE1	1.82	0.79
1:K:118:VAL:CG1	1:K:206:THR:HG22	2.11	0.79
1:H:331:VAL:HG13	1:H:332:PRO:HD2	1.65	0.79
1:E:260:TYR:HB2	1:E:261:PRO:HD2	1.65	0.79
1:L:300:MET:HE1	1:L:303:ARG:NH2	1.96	0.79
1:B:83:ASN:HD22	1:B:83:ASN:C	1.90	0.78
1:H:260:TYR:OH	1:H:287:PRO:HG2	1.84	0.78
1:J:107:LEU:HD22	1:J:182:ILE:HG23	1.64	0.78
1:K:83:ASN:ND2	1:K:85:ARG:HG3	1.98	0.78
1:F:149:ARG:HH11	1:F:149:ARG:CG	1.95	0.78
1:H:98:CYS:HB2	1:H:99:PRO:HD3	1.64	0.78
1:E:246:MET:CE	1:E:316:ILE:HD12	2.13	0.78
1:J:149:ARG:HH21	1:J:199:PRO:HA	1.45	0.78
1:L:74:ILE:HG23	1:L:75:ASN:ND2	1.98	0.78
1:D:83:ASN:C	1:D:83:ASN:HD22	1.90	0.78
1:L:67:SER:HA	1:L:79:LEU:HD22	1.63	0.78
1:C:273:PRO:HB3	1:K:131:ARG:HH12	1.46	0.78
1:D:332:PRO:HB2	1:D:334:THR:CG2	2.12	0.78
1:G:86:THR:O	1:G:88:GLU:N	2.17	0.78
1:L:121:VAL:HB	1:L:137:VAL:HG12	1.66	0.78
1:C:227:PRO:HG2	1:C:229:TYR:CZ	2.19	0.78
1:E:198:ARG:HH21	1:E:200:ASN:ND2	1.81	0.77
1:K:275:MET:HE3	1:K:279:ILE:HD11	1.66	0.77
1:F:347:GLU:C	1:F:349:TRP:H	1.90	0.77
1:L:74:ILE:HG23	1:L:75:ASN:H	1.49	0.77
1:G:83:ASN:C	1:G:83:ASN:HD22	1.92	0.77
1:H:98:CYS:HB2	1:H:99:PRO:CD	2.14	0.77
1:E:121:VAL:HG23	1:E:137:VAL:HG12	1.67	0.77
1:C:152:ASP:O	1:C:153:ARG:HG3	1.85	0.77
1:G:337:HIS:O	1:G:341:VAL:HG23	1.83	0.77
1:C:65:VAL:O	1:L:44:PRO:HA	1.84	0.76
1:G:99:PRO:HD2	1:G:100:LYS:H	1.50	0.76
1:K:84:LYS:O	1:K:84:LYS:HD2	1.85	0.76
1:C:64:LYS:HE3	1:L:44:PRO:CG	2.16	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:77:LYS:H	1:L:77:LYS:HD3	1.49	0.76
1:A:70:LEU:HD13	2:A:1351:P4O:C17	2.15	0.76
1:G:147:PHE:CE1	1:G:255:ILE:HG21	2.21	0.76
1:E:60:ILE:C	1:E:62:ASP:H	1.93	0.76
1:L:152:ASP:O	1:L:153:ARG:HG3	1.86	0.76
1:H:158:PHE:HD1	1:H:336:LEU:HD23	1.49	0.76
1:E:260:TYR:HB2	1:E:261:PRO:CD	2.15	0.76
1:J:146:LEU:O	1:J:150:ILE:HG12	1.85	0.76
1:D:151:GLN:NE2	1:D:346:LYS:HD2	1.99	0.76
1:J:107:LEU:HD22	1:J:182:ILE:HG21	1.68	0.76
1:K:290:GLU:OE2	1:K:337:HIS:HB2	1.86	0.76
1:B:275:MET:HE3	1:B:279:ILE:CD1	2.15	0.76
1:E:233:GLU:CG	1:F:310:PRO:HG3	2.15	0.76
1:K:83:ASN:C	1:K:83:ASN:HD22	1.93	0.76
1:E:195:THR:CG2	1:E:202:ILE:HG12	2.16	0.75
1:D:96:GLN:OE1	1:D:131:ARG:HD3	1.87	0.75
1:J:189:PRO:HA	1:J:192:LEU:HD12	1.68	0.75
1:A:233:GLU:CG	1:B:310:PRO:HG3	2.17	0.75
1:J:108:HIS:O	1:J:111:ALA:N	2.18	0.75
1:L:184:HIS:ND1	1:L:205:LEU:HD21	2.01	0.75
1:E:181:ASN:HB3	1:E:214:THR:OG1	1.87	0.75
1:E:198:ARG:NH2	1:E:200:ASN:HD21	1.84	0.75
1:F:276:LYS:O	1:F:280:ARG:HG3	1.87	0.75
1:A:264:TYR:O	1:A:275:MET:HG3	1.85	0.75
1:D:276:LYS:O	1:D:280:ARG:HG3	1.86	0.75
1:B:83:ASN:HD22	1:B:84:LYS:N	1.82	0.74
1:E:202:ILE:HD11	1:E:204:LYS:CE	2.17	0.74
1:F:239:LYS:HB2	1:F:241:ASP:OD2	1.86	0.74
1:L:82:PHE:CD1	1:L:89:LYS:HB3	2.22	0.74
1:C:260:TYR:HE1	1:C:290:GLU:HG2	1.52	0.74
1:D:70:LEU:HD12	2:D:1351:P4O:C17	2.17	0.74
1:I:332:PRO:HB2	1:I:334:THR:HG22	1.69	0.74
1:C:64:LYS:HE3	1:L:44:PRO:HG3	1.70	0.74
1:D:86:THR:HG22	1:D:88:GLU:N	1.94	0.74
1:F:86:THR:HG22	1:F:88:GLU:H	1.51	0.74
1:L:327:GLN:HB3	1:L:330:LYS:HB2	1.68	0.74
1:C:264:TYR:O	1:C:275:MET:HG3	1.87	0.74
1:B:300:MET:CE	1:B:303:ARG:HH21	2.00	0.74
1:E:344:GLU:H	1:E:344:GLU:CD	1.96	0.74
1:J:189:PRO:HD2	1:J:190:GLU:OE1	1.88	0.74
1:J:195:THR:HG23	1:J:196:SER:N	2.01	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:254:TYR:HB3	1:J:262:PRO:HG3	1.70	0.73
1:I:130:GLY:HA3	1:K:180:ILE:HB	1.71	0.73
1:L:83:ASN:HD21	1:L:85:ARG:HG3	1.53	0.73
1:J:193:LEU:HD23	1:J:193:LEU:N	1.96	0.73
1:D:239:LYS:HB3	1:D:241:ASP:OD2	1.88	0.73
1:I:52:LEU:HD13	1:I:109:TRP:CE3	2.22	0.73
1:D:332:PRO:CB	1:D:334:THR:HG22	2.19	0.73
1:E:125:GLU:C	1:E:126:ASN:HD22	1.96	0.73
1:F:80:GLN:NE2	1:F:89:LYS:HD3	2.03	0.73
1:G:145:GLU:HG3	1:G:145:GLU:O	1.88	0.73
1:C:331:VAL:CG1	1:C:332:PRO:HD2	2.18	0.73
1:D:234:VAL:C	1:D:236:GLY:H	1.96	0.73
1:E:332:PRO:HB2	1:E:334:THR:HG22	1.70	0.73
1:C:83:ASN:HD22	1:C:83:ASN:C	1.97	0.73
1:D:74:ILE:O	1:D:74:ILE:HD12	1.89	0.73
1:E:141:LEU:HD13	1:E:193:LEU:HB2	1.70	0.73
1:J:118:VAL:HG12	1:J:205:LEU:O	1.89	0.73
1:J:195:THR:CG2	1:J:202:ILE:H	2.02	0.73
1:J:175:GLN:O	1:J:177:LEU:N	2.22	0.73
1:K:332:PRO:HB2	1:K:334:THR:HG22	1.71	0.73
1:L:78:VAL:HG12	1:L:79:LEU:N	2.04	0.73
1:L:82:PHE:HD1	1:L:89:LYS:HB3	1.54	0.73
1:B:260:TYR:HB2	1:B:261:PRO:HD2	1.71	0.72
1:C:227:PRO:HB2	1:C:229:TYR:CE2	2.24	0.72
1:J:256:LEU:HD13	1:J:256:LEU:O	1.89	0.72
1:H:83:ASN:ND2	1:H:85:ARG:H	1.87	0.72
1:K:309:GLU:OE2	1:K:311:THR:HG23	1.89	0.72
1:A:60:ILE:HD13	1:F:48:VAL:HG23	1.72	0.72
1:K:147:PHE:CZ	1:K:255:ILE:HG21	2.24	0.72
1:D:141:LEU:HD13	1:D:193:LEU:HB2	1.72	0.72
1:L:185:ARG:HH11	1:L:185:ARG:HB3	1.54	0.72
1:L:205:LEU:HD12	1:L:206:THR:N	2.05	0.72
1:J:168:LYS:O	1:J:168:LYS:HG2	1.88	0.72
1:L:63:TYR:CD1	1:L:81:ILE:HD12	2.25	0.72
1:L:142:ASP:HA	2:L:1345:P4O:N16	2.04	0.72
1:G:45:GLN:CG	1:G:46:PHE:H	1.93	0.72
1:G:86:THR:O	1:G:86:THR:CG2	2.37	0.72
1:L:337:HIS:O	1:L:341:VAL:HG23	1.90	0.72
1:D:78:VAL:C	1:D:79:LEU:HD23	2.14	0.71
1:E:73:GLY:HA3	2:E:1345:P4O:C8	2.20	0.71
1:J:188:LYS:O	1:J:192:LEU:HG	1.90	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:166:ILE:HG21	1:L:256:LEU:CD1	2.20	0.71
1:J:167:MET:HA	1:J:167:MET:HE3	1.70	0.71
1:L:98:CYS:HB2	1:L:99:PRO:CD	2.20	0.71
1:G:214:THR:O	1:G:215:THR:HB	1.90	0.71
1:I:345:ASP:O	1:I:347:GLU:N	2.23	0.71
1:E:233:GLU:HG2	1:F:310:PRO:CG	2.20	0.71
1:H:83:ASN:HD22	1:H:84:LYS:N	1.88	0.71
1:I:156:GLN:O	1:I:158:PHE:N	2.23	0.71
1:I:241:ASP:O	1:I:244:CYS:HB2	1.89	0.71
1:B:275:MET:HE3	1:B:279:ILE:HD11	1.71	0.71
1:C:345:ASP:O	1:C:347:GLU:N	2.23	0.71
1:I:260:TYR:OH	1:I:287:PRO:HG2	1.90	0.71
1:F:154:GLY:O	1:F:156:GLN:OE1	2.07	0.71
1:L:80:GLN:NE2	1:L:89:LYS:HB2	2.05	0.71
1:B:343:LYS:O	1:B:344:GLU:CB	2.37	0.71
1:C:86:THR:O	1:C:87:GLN:HB2	1.91	0.71
1:C:322:HIS:ND1	1:C:323:PRO:HD2	2.06	0.71
1:K:141:LEU:HD13	1:K:193:LEU:HB2	1.73	0.71
1:C:83:ASN:ND2	1:C:85:ARG:H	1.89	0.71
1:F:98:CYS:HB2	1:F:99:PRO:HD3	1.73	0.71
1:J:254:TYR:CB	1:J:262:PRO:HG3	2.21	0.71
1:D:149:ARG:HB3	1:D:149:ARG:HH11	1.56	0.70
1:G:80:GLN:NE2	1:G:89:LYS:HG2	2.05	0.70
1:J:299:LYS:O	1:J:303:ARG:HG3	1.91	0.70
1:H:200:ASN:HD22	1:H:200:ASN:N	1.87	0.70
1:C:309:GLU:OE2	1:C:311:THR:HG23	1.92	0.70
1:F:344:GLU:O	1:F:345:ASP:CB	2.38	0.70
1:L:284:TYR:OH	1:L:303:ARG:HA	1.91	0.70
1:J:314:MET:HG3	1:J:318:GLU:OE1	1.91	0.70
1:L:77:LYS:HD3	1:L:77:LYS:N	2.05	0.70
1:J:195:THR:CB	1:J:202:ILE:HG13	2.20	0.70
1:L:184:HIS:CE1	1:L:205:LEU:HD11	2.26	0.70
1:L:247:TRP:HB2	1:L:313:ARG:NH1	2.06	0.70
1:E:314:MET:HG3	1:E:318:GLU:HB2	1.72	0.70
1:H:309:GLU:OE2	1:H:311:THR:HG23	1.92	0.70
1:C:52:LEU:HD13	1:C:109:TRP:CD2	2.27	0.70
1:E:80:GLN:HE22	1:E:89:LYS:HG2	1.56	0.70
1:G:296:GLU:OE2	1:G:303:ARG:NH2	2.24	0.70
1:J:110:ARG:HG2	1:J:110:ARG:NH1	2.03	0.70
1:K:260:TYR:OH	1:K:287:PRO:HG2	1.90	0.70
1:L:255:ILE:CG1	1:L:261:PRO:HA	2.21	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:ASN:OD1	1:B:292:SER:HB3	1.91	0.70
1:E:121:VAL:CG2	1:E:137:VAL:HG12	2.22	0.70
1:L:263:PHE:HE2	1:L:279:ILE:HA	1.56	0.70
1:I:347:GLU:HG3	1:I:348:ARG:N	2.06	0.70
1:L:77:LYS:H	1:L:77:LYS:CD	2.05	0.70
1:C:348:ARG:HG2	1:C:348:ARG:NH2	2.05	0.70
1:E:193:LEU:HD23	1:E:193:LEU:N	2.06	0.70
1:L:83:ASN:C	1:L:83:ASN:ND2	2.50	0.70
1:C:127:LEU:HD23	1:C:131:ARG:O	1.92	0.69
1:L:285:GLU:O	1:L:287:PRO:HD3	1.92	0.69
1:A:74:ILE:CG2	1:A:210:PHE:HE2	2.05	0.69
1:J:246:MET:HA	1:J:246:MET:HE3	1.74	0.69
1:D:151:GLN:HE22	1:D:346:LYS:CD	2.03	0.69
1:L:324:TRP:HE1	1:L:331:VAL:HG11	1.57	0.69
1:B:179:SER:HB3	1:C:281:MET:HE2	1.73	0.69
1:D:313:ARG:NH1	1:F:233:GLU:OE1	2.25	0.69
1:D:337:HIS:O	1:D:341:VAL:HG23	1.93	0.69
1:G:141:LEU:HD13	1:G:193:LEU:HB2	1.73	0.69
1:J:148:SER:C	1:J:150:ILE:H	1.98	0.69
1:L:78:VAL:CG1	1:L:79:LEU:N	2.54	0.69
1:H:276:LYS:O	1:H:280:ARG:HG3	1.92	0.69
1:A:74:ILE:HG21	1:A:210:PHE:CE2	2.28	0.69
1:H:74:ILE:CG2	1:H:210:PHE:HE2	2.05	0.69
1:J:195:THR:HG22	1:J:202:ILE:O	1.93	0.69
1:K:281:MET:HE2	1:L:179:SER:HB3	1.74	0.69
1:D:83:ASN:HD22	1:D:84:LYS:N	1.90	0.69
1:G:301:LEU:HD13	1:G:322:HIS:CD2	2.28	0.69
1:J:166:ILE:HG21	1:J:256:LEU:HG	1.75	0.69
1:G:118:VAL:CG1	1:G:206:THR:HG22	2.23	0.69
1:K:185:ARG:HB3	1:K:185:ARG:HH11	1.58	0.69
1:D:309:GLU:OE2	1:D:311:THR:HG23	1.93	0.68
1:K:276:LYS:O	1:K:280:ARG:HG3	1.92	0.68
1:E:288:ASN:CB	1:E:289:PRO:HA	2.18	0.68
1:H:83:ASN:HD22	1:H:83:ASN:C	2.01	0.68
1:E:278:ARG:HG3	1:E:283:GLN:HB2	1.75	0.68
1:F:337:HIS:O	1:F:339:SER:N	2.26	0.68
1:L:70:LEU:HD22	2:L:1345:P4O:C21	2.24	0.68
1:B:201:ALA:C	1:B:202:ILE:HD13	2.18	0.68
1:D:52:LEU:HD13	1:D:109:TRP:CE3	2.29	0.68
1:D:81:ILE:HD13	1:D:92:LEU:HB2	1.75	0.68
1:I:327:GLN:HE21	1:I:330:LYS:HD3	1.57	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:83:ASN:ND2	1:L:85:ARG:H	1.92	0.68
1:C:153:ARG:HH21	1:C:157:ALA:C	2.02	0.68
1:I:69:VAL:C	1:I:70:LEU:HD23	2.18	0.68
1:J:118:VAL:O	1:J:118:VAL:HG22	1.94	0.68
1:L:316:ILE:HG13	1:L:316:ILE:O	1.92	0.68
1:C:48:VAL:HG22	1:D:60:ILE:HD13	1.74	0.68
1:F:331:VAL:CG1	1:F:332:PRO:HD2	2.24	0.68
1:L:86:THR:C	1:L:88:GLU:H	1.99	0.68
1:A:276:LYS:O	1:A:280:ARG:HG3	1.93	0.68
1:I:154:GLY:C	1:I:156:GLN:H	2.00	0.68
1:J:167:MET:SD	1:J:252:ILE:O	2.52	0.68
1:L:315:THR:OG1	1:L:317:THR:HG22	1.93	0.68
1:E:99:PRO:HA	1:E:102:ARG:HB2	1.76	0.67
1:E:159:THR:OG1	1:E:162:GLU:HG3	1.93	0.67
1:B:181:ASN:HB3	1:B:214:THR:HG22	1.76	0.67
1:F:260:TYR:HB2	1:F:261:PRO:HD2	1.76	0.67
1:H:47:HIS:HB3	1:H:49:LYS:NZ	2.09	0.67
1:J:111:ALA:O	1:J:113:GLN:N	2.28	0.67
1:K:83:ASN:HD22	1:K:84:LYS:N	1.93	0.67
1:K:96:GLN:CD	1:K:131:ARG:HH21	2.01	0.67
1:A:310:PRO:HG3	1:C:233:GLU:HG3	1.75	0.67
1:C:153:ARG:NH2	1:C:157:ALA:O	2.28	0.67
1:B:260:TYR:OH	1:B:287:PRO:HG2	1.94	0.67
1:J:86:THR:O	1:J:86:THR:HG22	1.93	0.67
1:K:114:CYS:HB2	1:K:176:TYR:CD2	2.29	0.67
1:F:142:ASP:OD2	1:F:196:SER:HA	1.95	0.67
1:A:337:HIS:CD2	1:A:340:ARG:HH11	2.12	0.67
1:H:271:ILE:CD1	1:H:278:ARG:HH12	2.07	0.67
1:A:83:ASN:C	1:A:83:ASN:HD22	2.00	0.67
1:A:85:ARG:O	1:A:85:ARG:HG2	1.94	0.67
1:B:343:LYS:O	1:B:343:LYS:HG2	1.93	0.67
1:B:233:GLU:CG	1:C:310:PRO:HG3	2.24	0.67
1:E:83:ASN:CB	1:E:86:THR:HG22	2.25	0.67
1:L:291:TRP:HA	1:L:294:VAL:HG23	1.76	0.67
1:B:83:ASN:ND2	1:B:85:ARG:H	1.93	0.67
1:G:80:GLN:OE1	1:G:89:LYS:HE2	1.95	0.67
1:J:103:ARG:CB	1:J:103:ARG:HH11	2.07	0.67
1:J:168:LYS:HB2	1:J:325:ILE:HG23	1.76	0.67
1:K:275:MET:HE3	1:K:279:ILE:CD1	2.25	0.67
1:E:148:SER:O	1:E:150:ILE:N	2.28	0.66
1:L:344:GLU:N	1:L:344:GLU:CD	2.53	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:86:THR:CG2	1:J:88:GLU:HB2	2.26	0.66
1:L:94:MET:C	1:L:95:LEU:HD23	2.20	0.66
1:L:309:GLU:OE2	1:L:310:PRO:HD2	1.96	0.66
1:C:147:PHE:CD1	1:C:189:PRO:HB3	2.30	0.66
1:B:235:LEU:N	1:B:235:LEU:HD23	2.09	0.66
1:F:322:HIS:ND1	1:F:323:PRO:HD2	2.10	0.66
1:I:327:GLN:HE21	1:I:330:LYS:CD	2.09	0.66
1:I:149:ARG:HH11	1:I:149:ARG:CB	2.08	0.66
1:I:300:MET:CE	1:I:303:ARG:HH21	2.09	0.66
1:A:145:GLU:HA	1:A:193:LEU:CD2	2.24	0.66
1:L:302:ILE:HG22	1:L:306:LEU:HD12	1.75	0.66
1:L:184:HIS:HE1	1:L:205:LEU:HD11	1.60	0.66
1:A:310:PRO:CG	1:C:233:GLU:HG2	2.26	0.66
1:E:202:ILE:HD11	1:E:204:LYS:HE3	1.76	0.66
1:J:188:LYS:HB2	1:J:189:PRO:CD	2.25	0.66
1:J:186:ASP:OD2	1:J:188:LYS:HE3	1.96	0.66
1:K:141:LEU:CD1	1:K:193:LEU:HB2	2.25	0.66
1:E:48:VAL:HG13	1:H:60:ILE:HD13	1.77	0.66
1:L:59:ILE:HG13	1:L:124:TYR:CE1	2.30	0.66
1:J:319:PHE:O	1:J:321:ASN:N	2.29	0.65
1:L:118:VAL:HG11	1:L:206:THR:CG2	2.22	0.65
1:L:331:VAL:CG1	1:L:332:PRO:HD2	2.24	0.65
1:G:66:THR:HG21	1:G:82:PHE:HE2	1.60	0.65
1:L:263:PHE:CD2	1:L:279:ILE:HG12	2.31	0.65
1:L:333:GLN:O	1:L:335:PRO:HD3	1.95	0.65
1:A:74:ILE:HB	1:A:210:PHE:HE2	1.62	0.65
1:B:291:TRP:CE3	1:B:294:VAL:HG21	2.30	0.65
1:F:70:LEU:HD21	1:F:80:GLN:HB2	1.76	0.65
1:K:288:ASN:HD22	1:K:288:ASN:N	1.92	0.65
1:L:119:ARG:NH1	1:L:119:ARG:HB2	2.10	0.65
1:L:192:LEU:HB3	1:L:203:LEU:HD11	1.76	0.65
1:D:86:THR:CG2	1:D:88:GLU:H	1.96	0.65
1:D:98:CYS:HB2	1:D:99:PRO:HD3	1.77	0.65
1:D:237:PRO:O	1:D:238:GLU:HB3	1.97	0.65
1:L:247:TRP:HB2	1:L:313:ARG:HH11	1.61	0.65
1:A:145:GLU:HA	1:A:193:LEU:HD23	1.78	0.65
1:D:167:MET:HG3	1:D:253:MET:HG3	1.77	0.65
1:E:117:ILE:HD12	1:E:208:PHE:HZ	1.61	0.65
1:J:185:ARG:O	1:J:186:ASP:HB2	1.96	0.65
1:B:337:HIS:O	1:B:341:VAL:HG23	1.96	0.65
1:E:60:ILE:C	1:E:62:ASP:N	2.50	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:162:GLU:O	1:C:166:ILE:HG13	1.96	0.65
1:K:83:ASN:HB3	1:K:86:THR:HB	1.76	0.65
1:L:108:HIS:O	1:L:108:HIS:HD2	1.79	0.65
1:A:260:TYR:OH	1:A:287:PRO:HG2	1.96	0.65
1:B:235:LEU:HD23	1:B:235:LEU:H	1.61	0.65
1:H:328:SER:O	1:H:331:VAL:HB	1.97	0.65
1:B:260:TYR:HB2	1:B:261:PRO:CD	2.27	0.64
1:E:202:ILE:HD11	1:E:204:LYS:HE2	1.79	0.64
1:G:238:GLU:OE1	1:G:242:LYS:HE3	1.97	0.64
1:H:229:TYR:O	1:H:230:VAL:HG13	1.97	0.64
1:B:185:ARG:HB3	1:B:185:ARG:HH11	1.62	0.64
1:L:301:LEU:HD12	1:L:314:MET:HE1	1.78	0.64
1:J:167:MET:HG3	1:J:253:MET:CG	2.24	0.64
1:K:271:ILE:HG22	1:K:278:ARG:HH12	1.60	0.64
1:L:52:LEU:HD12	1:L:53:GLN:H	1.62	0.64
1:L:158:PHE:CZ	1:L:163:ALA:HB2	2.33	0.64
1:C:52:LEU:HD13	1:C:109:TRP:CE3	2.33	0.64
1:F:114:CYS:HB2	1:F:176:TYR:CD2	2.32	0.64
1:I:86:THR:C	1:I:88:GLU:H	2.04	0.64
1:J:310:PRO:O	1:J:313:ARG:HB3	1.97	0.64
1:A:309:GLU:OE2	1:A:311:THR:HG23	1.97	0.64
1:A:331:VAL:HG13	1:A:332:PRO:HD2	1.79	0.64
1:B:114:CYS:HB2	1:B:176:TYR:CD2	2.31	0.64
1:E:291:TRP:O	1:E:294:VAL:HB	1.97	0.64
1:J:296:GLU:HA	1:J:299:LYS:HD2	1.80	0.64
1:L:111:ALA:HB1	1:L:117:ILE:HD12	1.79	0.64
1:L:281:MET:CB	1:L:283:GLN:HG3	2.26	0.64
1:E:80:GLN:NE2	1:E:89:LYS:HG2	2.12	0.64
1:L:105:VAL:HG22	1:L:136:ILE:HD11	1.79	0.64
1:I:156:GLN:HB3	1:I:339:SER:HB3	1.78	0.64
1:L:192:LEU:O	1:L:193:LEU:HD23	1.98	0.64
1:D:70:LEU:CD2	1:D:70:LEU:H	2.11	0.64
1:E:74:ILE:HG21	1:E:209:GLY:HA3	1.80	0.64
1:H:98:CYS:O	1:H:102:ARG:HG2	1.98	0.64
1:I:83:ASN:CB	1:I:86:THR:HG22	2.28	0.64
1:K:71:GLY:O	1:K:72:LEU:HD22	1.98	0.64
1:L:161:ARG:HB2	1:L:332:PRO:O	1.98	0.64
1:L:281:MET:HG3	1:L:283:GLN:HE21	1.63	0.64
1:G:143:GLY:CA	1:G:196:SER:O	2.44	0.64
1:L:184:HIS:CD2	1:L:184:HIS:C	2.75	0.64
1:A:74:ILE:HB	1:A:210:PHE:CE2	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:83:ASN:HD21	1:D:85:ARG:HG3	1.63	0.64
1:E:237:PRO:O	1:E:238:GLU:HB2	1.96	0.64
1:H:200:ASN:HD22	1:H:200:ASN:H	1.46	0.64
1:J:124:TYR:HB2	1:J:135:LEU:HB2	1.80	0.64
1:B:69:VAL:HG23	1:B:77:LYS:HG3	1.80	0.63
1:B:184:HIS:HD2	1:B:186:ASP:H	1.46	0.63
1:E:291:TRP:HE3	1:E:294:VAL:HG11	1.62	0.63
1:G:291:TRP:HA	1:G:294:VAL:CG2	2.27	0.63
1:I:328:SER:O	1:I:331:VAL:HB	1.98	0.63
1:J:319:PHE:C	1:J:321:ASN:H	2.05	0.63
1:A:337:HIS:O	1:A:341:VAL:HG23	1.98	0.63
1:E:95:LEU:HD13	1:E:101:ALA:HB1	1.80	0.63
1:K:72:LEU:HD11	1:K:77:LYS:HE3	1.81	0.63
1:K:73:GLY:HA2	2:K:1345:P4O:H8C1	1.80	0.63
1:L:205:LEU:HD12	1:L:206:THR:H	1.63	0.63
1:A:332:PRO:HB2	1:A:334:THR:CG2	2.28	0.63
1:B:77:LYS:H	1:B:77:LYS:HD3	1.63	0.63
1:B:214:THR:HG23	1:B:214:THR:O	1.97	0.63
1:I:130:GLY:O	1:K:110:ARG:NH1	2.31	0.63
1:I:142:ASP:OD2	1:I:196:SER:HA	1.99	0.63
1:L:108:HIS:O	1:L:108:HIS:CD2	2.52	0.63
1:A:149:ARG:HB3	1:A:149:ARG:NH1	2.07	0.63
1:B:178:HIS:CG	1:B:242:LYS:HD3	2.32	0.63
1:D:337:HIS:CD2	1:D:340:ARG:NH1	2.65	0.63
1:G:195:THR:HG23	1:G:202:ILE:O	1.98	0.63
1:H:344:GLU:O	1:H:344:GLU:HG2	1.99	0.63
1:J:148:SER:O	1:J:150:ILE:N	2.31	0.63
1:A:74:ILE:HG21	1:A:210:PHE:CD2	2.33	0.63
1:I:158:PHE:O	1:I:336:LEU:HD22	1.99	0.63
1:J:166:ILE:HG21	1:J:256:LEU:CG	2.29	0.63
1:J:198:ARG:HH11	1:J:198:ARG:CG	2.10	0.63
1:J:252:ILE:O	1:J:252:ILE:HG22	1.97	0.63
1:L:52:LEU:HD12	1:L:53:GLN:N	2.13	0.63
1:L:191:ASN:O	1:L:205:LEU:HD12	1.99	0.63
1:L:301:LEU:HD13	1:L:322:HIS:CD2	2.33	0.63
1:C:238:GLU:OE1	1:C:242:LYS:HE3	1.99	0.63
1:L:49:LYS:HE3	1:L:113:GLN:OE1	1.98	0.63
1:L:168:LYS:O	1:L:172:GLU:HG3	1.98	0.63
1:E:300:MET:HE2	1:E:300:MET:HA	1.81	0.63
1:G:83:ASN:ND2	1:G:85:ARG:H	1.97	0.63
1:G:260:TYR:HB2	1:G:261:PRO:HD2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:TYR:O	1:A:129:ALA:HB3	1.99	0.63
1:D:149:ARG:HH11	1:D:149:ARG:CB	2.12	0.63
1:I:214:THR:HB	1:I:238:GLU:HG3	1.80	0.63
1:B:147:PHE:HD1	1:B:349:TRP:HZ2	1.47	0.62
1:F:70:LEU:HD11	1:F:80:GLN:HA	1.80	0.62
1:G:300:MET:CE	1:G:303:ARG:HE	2.12	0.62
1:H:114:CYS:HB2	1:H:176:TYR:CD2	2.34	0.62
1:J:302:ILE:CG2	1:J:306:LEU:HD12	2.28	0.62
1:C:150:ILE:CD1	1:C:158:PHE:HE1	1.98	0.62
1:K:192:LEU:C	1:K:193:LEU:HD23	2.24	0.62
1:C:83:ASN:C	1:C:83:ASN:ND2	2.55	0.62
1:E:246:MET:HE2	1:E:316:ILE:HA	1.82	0.62
1:G:80:GLN:CD	1:G:89:LYS:HE2	2.23	0.62
1:G:98:CYS:HB2	1:G:99:PRO:HD3	1.82	0.62
1:L:260:TYR:HB2	1:L:261:PRO:HD2	1.80	0.62
1:A:149:ARG:HH11	1:A:149:ARG:CG	2.12	0.62
1:A:260:TYR:HB2	1:A:261:PRO:HD2	1.81	0.62
1:G:86:THR:O	1:G:86:THR:HG23	2.00	0.62
1:G:264:TYR:O	1:G:275:MET:HG3	1.99	0.62
1:I:167:MET:HG3	1:I:253:MET:HE2	1.81	0.62
1:J:56:LYS:HZ1	1:J:125:GLU:CD	2.07	0.62
1:J:175:GLN:C	1:J:177:LEU:H	2.06	0.62
1:J:261:PRO:HG2	1:J:263:PHE:O	1.99	0.62
1:L:186:ASP:OD1	1:L:188:LYS:HE3	1.98	0.62
1:E:69:VAL:HG12	1:E:71:GLY:H	1.64	0.62
1:J:103:ARG:HH11	1:J:103:ARG:HB2	1.62	0.62
1:L:146:LEU:C	1:L:148:SER:H	2.07	0.62
1:B:338:THR:O	1:B:342:LEU:HB2	1.99	0.62
1:D:165:GLU:HG2	1:D:328:SER:OG	1.98	0.62
1:F:86:THR:CG2	1:F:88:GLU:CB	2.73	0.62
1:J:255:ILE:HD11	1:J:261:PRO:HA	1.81	0.62
1:A:237:PRO:O	1:A:238:GLU:HB3	1.98	0.62
1:B:332:PRO:HB2	1:B:334:THR:CG2	2.29	0.62
1:D:195:THR:HG22	1:D:196:SER:N	2.14	0.62
1:F:83:ASN:C	1:F:83:ASN:ND2	2.51	0.62
1:J:149:ARG:HH22	1:J:199:PRO:HA	1.59	0.62
1:L:154:GLY:HA3	1:L:157:ALA:HB2	1.82	0.62
1:L:260:TYR:OH	1:L:287:PRO:HG2	1.99	0.62
1:L:312:GLN:O	1:L:313:ARG:O	2.18	0.62
1:B:300:MET:HE2	1:B:303:ARG:HH21	1.65	0.62
1:G:74:ILE:HG23	1:G:75:ASN:N	2.12	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:193:LEU:HD23	1:G:193:LEU:N	2.14	0.62
1:G:214:THR:O	1:G:215:THR:CB	2.48	0.62
1:J:121:VAL:HB	1:J:137:VAL:HG12	1.81	0.62
1:K:158:PHE:HD2	1:K:159:THR:N	1.97	0.62
1:K:332:PRO:HB2	1:K:334:THR:CG2	2.29	0.62
1:L:80:GLN:HE21	1:L:89:LYS:HB2	1.64	0.62
1:L:83:ASN:HD22	1:L:85:ARG:H	1.46	0.62
1:L:108:HIS:CD2	1:L:120:ILE:HD11	2.35	0.62
1:L:174:ILE:HD11	1:L:187:VAL:HG21	1.81	0.62
1:L:285:GLU:C	1:L:287:PRO:HD3	2.25	0.62
1:B:237:PRO:O	1:B:238:GLU:HB3	1.98	0.62
1:E:99:PRO:O	1:E:102:ARG:N	2.33	0.62
1:L:44:PRO:O	1:L:45:GLN:HG2	1.99	0.62
1:D:86:THR:CG2	1:D:88:GLU:HB2	2.30	0.61
1:I:332:PRO:HB2	1:I:334:THR:CG2	2.30	0.61
1:J:255:ILE:HG12	1:J:260:TYR:O	1.99	0.61
1:A:74:ILE:CG2	1:A:210:PHE:CE2	2.83	0.61
1:I:83:ASN:HB3	1:I:86:THR:HG22	1.80	0.61
1:J:108:HIS:HA	1:J:208:PHE:CD2	2.34	0.61
1:K:83:ASN:ND2	1:K:85:ARG:CG	2.58	0.61
1:C:160:GLU:O	1:C:163:ALA:HB3	2.00	0.61
1:I:149:ARG:O	1:I:150:ILE:C	2.43	0.61
1:L:184:HIS:CD2	1:L:184:HIS:O	2.53	0.61
1:L:258:CYS:SG	1:L:259:GLY:N	2.73	0.61
1:F:330:LYS:O	1:F:332:PRO:HD3	2.01	0.61
1:I:289:PRO:C	1:I:291:TRP:H	2.03	0.61
1:A:99:PRO:HD2	1:A:100:LYS:H	1.64	0.61
1:B:238:GLU:OE1	1:B:242:LYS:HE3	1.99	0.61
1:C:260:TYR:CE1	1:C:290:GLU:HG2	2.34	0.61
1:A:86:THR:HG22	1:A:88:GLU:H	1.65	0.61
1:D:108:HIS:CG	1:D:120:ILE:HD11	2.35	0.61
1:D:185:ARG:CB	1:D:185:ARG:HH11	2.13	0.61
1:G:74:ILE:HD13	1:G:75:ASN:HB2	1.82	0.61
1:E:130:GLY:HA3	1:J:180:ILE:HG21	1.83	0.61
1:E:337:HIS:O	1:E:341:VAL:HG23	2.00	0.61
1:G:145:GLU:O	1:G:147:PHE:N	2.34	0.61
1:D:74:ILE:HG13	1:D:75:ASN:N	2.16	0.61
1:J:255:ILE:HG12	1:J:260:TYR:C	2.25	0.61
1:J:296:GLU:CD	1:J:296:GLU:H	2.09	0.61
1:K:69:VAL:O	1:K:69:VAL:HG12	1.98	0.61
1:D:115:PRO:O	1:D:204:LYS:HE2	2.01	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:278:ARG:CG	1:E:283:GLN:HB2	2.30	0.61
1:I:180:ILE:HG13	1:I:180:ILE:O	1.99	0.61
1:J:260:TYR:HB2	1:J:261:PRO:HD2	1.81	0.61
1:B:344:GLU:O	1:B:344:GLU:HG2	2.00	0.61
1:C:259:GLY:HA2	1:C:342:LEU:HD11	1.82	0.61
1:E:58:ALA:N	1:J:50:SER:HB3	2.16	0.61
1:F:347:GLU:O	1:F:349:TRP:N	2.33	0.61
1:G:332:PRO:HB2	1:G:334:THR:HG22	1.82	0.61
1:H:102:ARG:HD2	1:H:134:LEU:HD21	1.82	0.61
1:J:108:HIS:HA	1:J:208:PHE:CE2	2.36	0.61
1:K:158:PHE:HD2	1:K:159:THR:H	1.49	0.61
1:C:333:GLN:HE21	1:C:333:GLN:HA	1.66	0.60
1:D:186:ASP:OD2	1:D:188:LYS:NZ	2.34	0.60
1:D:251:VAL:O	1:D:255:ILE:HG13	2.00	0.60
1:D:289:PRO:O	1:D:291:TRP:N	2.34	0.60
1:J:255:ILE:CG1	1:J:261:PRO:HA	2.31	0.60
1:L:146:LEU:O	1:L:148:SER:N	2.33	0.60
1:L:151:GLN:O	1:L:151:GLN:HG3	2.01	0.60
1:E:82:PHE:HA	1:E:88:GLU:O	2.01	0.60
1:F:129:ALA:O	1:F:131:ARG:N	2.34	0.60
1:H:234:VAL:O	1:H:234:VAL:CG1	2.49	0.60
1:H:288:ASN:HB3	1:H:289:PRO:HA	1.83	0.60
1:B:309:GLU:OE2	1:B:311:THR:HG23	2.01	0.60
1:C:345:ASP:C	1:C:347:GLU:H	2.08	0.60
1:E:133:CYS:HB3	1:E:135:LEU:HD21	1.83	0.60
1:G:291:TRP:HA	1:G:294:VAL:HG21	1.84	0.60
1:K:288:ASN:HB3	1:K:289:PRO:CA	2.28	0.60
1:C:118:VAL:HG11	1:C:206:THR:HG22	1.83	0.60
1:B:110:ARG:HG2	1:B:110:ARG:HH11	1.66	0.60
1:E:300:MET:HE2	1:E:300:MET:CA	2.31	0.60
1:I:57:ASN:HA	1:K:50:SER:HG	1.64	0.60
1:A:74:ILE:CB	1:A:210:PHE:HE2	2.15	0.60
1:G:128:TYR:O	1:G:129:ALA:HB3	2.01	0.60
1:G:292:SER:HB2	1:G:293:GLU:OE2	2.02	0.60
1:H:47:HIS:HB3	1:H:49:LYS:HZ3	1.66	0.60
1:C:322:HIS:CE1	1:C:323:PRO:HD2	2.37	0.60
1:E:343:LYS:N	1:E:343:LYS:HD3	2.16	0.60
1:I:147:PHE:HE1	1:I:256:LEU:HD23	1.66	0.60
1:J:143:GLY:HA3	1:J:196:SER:C	2.26	0.60
1:L:171:GLY:O	1:L:175:GLN:HB3	2.02	0.60
1:L:332:PRO:CB	1:L:334:THR:HG22	2.27	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:GLU:OE1	1:B:313:ARG:NH2	2.35	0.60
1:A:237:PRO:O	1:A:238:GLU:CB	2.49	0.60
1:K:196:SER:CB	1:K:198:ARG:HB2	2.30	0.60
1:L:337:HIS:ND1	1:L:337:HIS:N	2.50	0.60
1:L:344:GLU:CD	1:L:344:GLU:H	2.10	0.60
1:D:341:VAL:O	1:D:345:ASP:HB2	2.01	0.60
1:F:86:THR:HG23	1:F:88:GLU:H	1.67	0.60
1:I:263:PHE:CZ	1:I:284:TYR:HD1	2.19	0.60
1:L:112:SER:OG	1:L:119:ARG:HA	2.01	0.60
1:D:86:THR:O	1:D:87:GLN:CB	2.49	0.60
1:I:82:PHE:HA	1:I:88:GLU:O	2.02	0.60
1:I:198:ARG:HB3	1:I:199:PRO:HD2	1.83	0.60
1:L:162:GLU:C	1:L:164:SER:H	2.10	0.60
1:A:52:LEU:HD13	1:A:109:TRP:CE3	2.37	0.59
1:A:185:ARG:HH21	1:A:212:LYS:CD	2.15	0.59
1:B:83:ASN:C	1:B:83:ASN:ND2	2.55	0.59
1:F:155:ASP:O	1:F:156:GLN:HB2	2.01	0.59
1:F:260:TYR:OH	1:F:287:PRO:HG2	2.02	0.59
1:H:116:HIS:CE1	1:H:169:SER:HB3	2.37	0.59
1:L:314:MET:SD	1:L:319:PHE:HB2	2.42	0.59
1:B:233:GLU:OE1	1:C:313:ARG:NH1	2.34	0.59
1:D:278:ARG:HH11	1:D:278:ARG:HG3	1.67	0.59
1:F:86:THR:HG22	1:F:88:GLU:N	2.17	0.59
1:L:119:ARG:CB	1:L:119:ARG:HH11	2.15	0.59
1:L:301:LEU:CD1	1:L:314:MET:HE1	2.32	0.59
1:C:70:LEU:HD22	2:C:1351:P4O:N16	2.17	0.59
1:E:64:LYS:N	1:E:82:PHE:O	2.31	0.59
1:I:185:ARG:HH21	1:I:212:LYS:HD3	1.67	0.59
1:K:82:PHE:HD1	1:K:88:GLU:O	1.85	0.59
1:L:127:LEU:HD23	1:L:132:LYS:HA	1.84	0.59
1:C:93:LYS:HE3	2:C:1351:P4O:O26	2.03	0.59
1:D:47:HIS:O	1:D:47:HIS:ND1	2.35	0.59
1:D:289:PRO:HG2	1:D:290:GLU:H	1.68	0.59
1:F:82:PHE:CE1	1:F:89:LYS:HG2	2.37	0.59
1:G:247:TRP:O	1:G:248:SER:C	2.45	0.59
1:I:159:THR:C	1:I:336:LEU:HD21	2.27	0.59
1:J:171:GLY:C	1:J:173:ALA:H	2.07	0.59
1:J:70:LEU:O	1:J:70:LEU:HD23	2.02	0.59
1:L:180:ILE:O	1:L:182:ILE:HG13	2.03	0.59
1:E:121:VAL:HG23	1:E:137:VAL:C	2.27	0.59
1:F:69:VAL:HG12	1:F:71:GLY:H	1.68	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:300:MET:CE	1:F:303:ARG:HH21	2.14	0.59
1:H:168:LYS:O	1:H:172:GLU:HG3	2.03	0.59
1:J:158:PHE:HA	1:J:162:GLU:OE2	2.03	0.59
1:E:60:ILE:CG1	1:E:61:ASP:N	2.65	0.59
1:E:190:GLU:OE1	1:E:190:GLU:N	2.31	0.59
1:H:191:ASN:ND2	2:H:1347:P4O:H8C2	2.17	0.59
1:J:128:TYR:O	1:J:129:ALA:HB3	2.02	0.59
1:K:260:TYR:HB2	1:K:261:PRO:HD2	1.84	0.59
1:L:75:ASN:ND2	1:L:75:ASN:H	2.00	0.59
1:L:99:PRO:HD2	1:L:100:LYS:H	1.67	0.59
1:B:275:MET:HE3	1:B:279:ILE:HD12	1.84	0.59
1:C:146:LEU:HD12	1:C:146:LEU:O	2.02	0.59
1:G:148:SER:C	1:G:150:ILE:H	2.10	0.59
1:H:162:GLU:O	1:H:166:ILE:HG13	2.02	0.59
1:H:344:GLU:O	1:H:344:GLU:CG	2.51	0.59
1:K:314:MET:HG3	1:K:318:GLU:HB2	1.85	0.59
1:L:324:TRP:NE1	1:L:331:VAL:HG11	2.17	0.59
1:B:321:ASN:O	1:B:326:MET:HG3	2.03	0.59
1:D:79:LEU:HD23	1:D:79:LEU:N	2.15	0.59
1:I:264:TYR:O	1:I:275:MET:HG3	2.03	0.59
1:I:345:ASP:O	1:I:348:ARG:N	2.35	0.59
1:J:149:ARG:C	1:J:150:ILE:HD13	2.28	0.59
1:E:143:GLY:CA	1:E:196:SER:O	2.51	0.59
1:E:237:PRO:O	1:E:238:GLU:CB	2.50	0.59
1:F:227:PRO:HB3	1:F:229:TYR:CZ	2.38	0.59
1:F:301:LEU:HD13	1:F:322:HIS:CD2	2.38	0.59
1:G:88:GLU:CG	1:G:89:LYS:H	2.16	0.59
1:J:64:LYS:HB2	1:J:84:LYS:HG3	1.85	0.59
1:A:235:LEU:HB2	1:B:280:ARG:NH1	2.18	0.58
1:G:147:PHE:HD1	1:G:349:TRP:CZ2	2.20	0.58
1:I:276:LYS:O	1:I:280:ARG:HG3	2.02	0.58
1:I:322:HIS:ND1	1:I:323:PRO:HD2	2.18	0.58
1:J:86:THR:O	1:J:86:THR:CG2	2.50	0.58
1:J:86:THR:HG22	1:J:88:GLU:HB2	1.85	0.58
1:A:114:CYS:HB2	1:A:176:TYR:CD2	2.38	0.58
1:D:239:LYS:HG3	1:D:240:TYR:H	1.68	0.58
1:G:288:ASN:HB3	1:G:289:PRO:HA	1.85	0.58
1:H:159:THR:OG1	1:H:162:GLU:HG3	2.03	0.58
1:I:154:GLY:C	1:I:156:GLN:N	2.60	0.58
1:I:275:MET:O	1:I:279:ILE:HG13	2.03	0.58
1:J:248:SER:O	1:J:250:GLY:N	2.36	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:ILE:HG13	1:B:75:ASN:CG	2.28	0.58
1:F:168:LYS:O	1:F:172:GLU:HG3	2.03	0.58
1:H:88:GLU:HG2	1:H:90:PHE:CE1	2.38	0.58
1:J:169:SER:C	1:J:171:GLY:N	2.52	0.58
1:B:86:THR:C	1:B:88:GLU:H	2.11	0.58
1:D:150:ILE:CD1	1:D:158:PHE:HE2	2.16	0.58
1:D:214:THR:O	1:D:215:THR:CG2	2.43	0.58
1:A:98:CYS:HB2	1:A:99:PRO:HD3	1.85	0.58
1:C:150:ILE:HG23	1:C:158:PHE:CD1	2.39	0.58
1:E:344:GLU:CD	1:E:344:GLU:N	2.61	0.58
1:F:110:ARG:HH11	1:F:110:ARG:HG2	1.68	0.58
1:I:260:TYR:HB2	1:I:261:PRO:HD2	1.85	0.58
1:I:278:ARG:HB3	1:I:283:GLN:HB2	1.85	0.58
1:J:160:GLU:C	1:J:162:GLU:H	2.11	0.58
1:J:160:GLU:O	1:J:162:GLU:N	2.37	0.58
1:E:235:LEU:HD13	1:F:276:LYS:CG	2.32	0.58
1:E:274:GLY:O	1:E:278:ARG:HB2	2.03	0.58
1:G:310:PRO:HG3	1:I:233:GLU:CG	2.26	0.58
1:H:233:GLU:O	1:H:233:GLU:HG2	2.02	0.58
1:J:148:SER:C	1:J:150:ILE:N	2.60	0.58
1:G:86:THR:C	1:G:88:GLU:H	2.12	0.58
1:I:86:THR:O	1:I:88:GLU:N	2.35	0.58
1:J:158:PHE:HZ	1:J:163:ALA:CB	2.17	0.58
1:A:141:LEU:HD13	1:A:193:LEU:HB2	1.86	0.58
1:E:134:LEU:C	1:E:135:LEU:HD23	2.29	0.58
1:K:108:HIS:CG	1:K:120:ILE:HD11	2.39	0.58
1:L:310:PRO:N	1:L:313:ARG:HH21	2.01	0.58
1:J:59:ILE:C	1:J:61:ASP:H	2.12	0.58
1:L:178:HIS:CE1	1:L:242:LYS:HB3	2.39	0.58
1:L:188:LYS:HB3	1:L:189:PRO:CD	2.34	0.58
1:E:287:PRO:O	1:E:291:TRP:HD1	1.87	0.58
1:H:97:ASP:OD1	1:H:102:ARG:NH2	2.26	0.58
1:H:110:ARG:HG2	1:H:110:ARG:HH11	1.69	0.58
1:I:72:LEU:HG	1:I:77:LYS:HB3	1.85	0.58
1:I:195:THR:CG2	1:I:202:ILE:HB	2.33	0.58
1:I:327:GLN:NE2	1:I:330:LYS:HD3	2.19	0.58
1:F:74:ILE:HD12	1:F:74:ILE:O	2.04	0.57
1:H:200:ASN:C	1:H:201:ALA:O	2.46	0.57
1:I:82:PHE:HB3	1:I:87:GLN:O	2.03	0.57
1:J:83:ASN:HD22	1:J:83:ASN:C	2.10	0.57
1:L:119:ARG:HB2	1:L:119:ARG:HH11	1.68	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:239:LYS:C	1:D:241:ASP:H	2.10	0.57
1:G:159:THR:OG1	1:G:162:GLU:HG3	2.05	0.57
1:I:83:ASN:C	1:I:83:ASN:HD22	2.10	0.57
1:I:234:VAL:HG12	1:I:235:LEU:HD23	1.86	0.57
1:J:63:TYR:HE1	1:J:90:PHE:CD1	2.22	0.57
1:J:205:LEU:HD12	1:J:206:THR:H	1.69	0.57
1:K:84:LYS:C	1:K:85:ARG:HG2	2.29	0.57
1:C:234:VAL:O	1:C:236:GLY:N	2.34	0.57
1:E:63:TYR:CB	1:E:81:ILE:HD12	2.35	0.57
1:E:185:ARG:HH11	1:E:185:ARG:CG	2.14	0.57
1:G:264:TYR:C	1:G:278:ARG:HH21	2.11	0.57
1:H:271:ILE:HD11	1:H:278:ARG:HH12	1.69	0.57
1:J:65:VAL:HA	1:J:81:ILE:HG22	1.87	0.57
1:J:316:ILE:O	1:J:316:ILE:HG13	2.02	0.57
1:A:178:HIS:CG	1:A:242:LYS:HD3	2.38	0.57
1:H:289:PRO:O	1:H:290:GLU:C	2.48	0.57
1:J:189:PRO:C	1:J:191:ASN:H	2.12	0.57
1:L:174:ILE:O	1:L:178:HIS:HD2	1.88	0.57
1:D:147:PHE:HE2	1:D:256:LEU:HD23	1.69	0.57
1:D:313:ARG:NH2	1:F:233:GLU:OE1	2.36	0.57
1:F:349:TRP:HA	1:F:349:TRP:CE3	2.39	0.57
1:J:149:ARG:NH2	1:J:199:PRO:CA	2.60	0.57
1:A:148:SER:O	1:A:149:ARG:C	2.45	0.57
1:E:57:ASN:ND2	1:E:58:ALA:O	2.38	0.57
1:G:74:ILE:CG2	1:G:209:GLY:HA3	2.27	0.57
1:H:141:LEU:CD1	1:H:193:LEU:HB2	2.35	0.57
1:I:300:MET:HE1	1:I:303:ARG:HE	1.70	0.57
1:L:332:PRO:HB2	1:L:334:THR:CG2	2.29	0.57
1:D:164:SER:HA	1:D:324:TRP:CH2	2.39	0.57
1:D:278:ARG:HG3	1:D:278:ARG:NH1	2.18	0.57
1:H:260:TYR:HB2	1:H:261:PRO:HD2	1.86	0.57
1:J:254:TYR:CD1	1:J:262:PRO:HD3	2.40	0.57
1:K:197:LYS:CE	1:K:197:LYS:H	2.17	0.57
1:B:126:ASN:HB3	1:I:48:VAL:CG2	2.34	0.57
1:B:129:ALA:C	1:B:131:ARG:H	2.13	0.57
1:A:332:PRO:CB	1:A:334:THR:HG22	2.35	0.57
1:G:240:TYR:O	1:G:241:ASP:C	2.47	0.57
1:J:195:THR:HG21	1:J:202:ILE:N	2.09	0.57
1:F:128:TYR:O	1:F:129:ALA:HB3	2.05	0.57
1:J:183:ALA:O	1:J:211:ALA:HA	2.04	0.57
1:L:83:ASN:O	1:L:85:ARG:N	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:189:PRO:HD2	1:L:190:GLU:OE1	2.05	0.57
1:L:291:TRP:HA	1:L:294:VAL:CG2	2.34	0.57
1:C:227:PRO:HG2	1:C:229:TYR:CE1	2.40	0.56
1:C:322:HIS:ND1	1:C:323:PRO:CD	2.68	0.56
1:E:246:MET:CE	1:E:316:ILE:HA	2.35	0.56
1:I:168:LYS:O	1:I:172:GLU:HG3	2.05	0.56
1:L:108:HIS:CE1	1:L:138:MET:HE1	2.40	0.56
1:B:69:VAL:CG2	1:B:77:LYS:HG3	2.34	0.56
1:D:260:TYR:HB2	1:D:261:PRO:HD2	1.86	0.56
1:E:168:LYS:HD2	1:E:325:ILE:O	2.05	0.56
1:G:231:ALA:O	1:G:234:VAL:HB	2.05	0.56
1:L:212:LYS:HG2	1:L:213:GLU:O	2.04	0.56
1:A:238:GLU:OE1	1:A:242:LYS:HE3	2.04	0.56
1:B:150:ILE:C	1:B:152:ASP:H	2.12	0.56
1:C:108:HIS:CG	1:C:120:ILE:HD11	2.40	0.56
1:C:118:VAL:CG1	1:C:206:THR:HG22	2.35	0.56
1:C:275:MET:HE3	1:C:279:ILE:HD11	1.87	0.56
1:D:185:ARG:HH11	1:D:185:ARG:HB3	1.70	0.56
1:D:280:ARG:HG2	1:F:235:LEU:HD12	1.87	0.56
1:F:200:ASN:HD22	1:F:201:ALA:N	2.03	0.56
1:G:212:LYS:HG2	1:G:213:GLU:O	2.05	0.56
1:H:184:HIS:HD2	1:H:186:ASP:H	1.52	0.56
1:J:178:HIS:HD2	1:J:182:ILE:O	1.88	0.56
1:L:86:THR:O	1:L:86:THR:CG2	2.53	0.56
1:L:304:ASN:HD22	1:L:307:LYS:HE2	1.70	0.56
1:A:162:GLU:O	1:A:166:ILE:HG13	2.06	0.56
1:D:146:LEU:HD11	1:D:166:ILE:HD13	1.87	0.56
1:D:192:LEU:C	1:D:193:LEU:HD23	2.31	0.56
1:H:195:THR:HG22	1:H:201:ALA:HB1	1.86	0.56
1:J:158:PHE:HA	1:J:162:GLU:CD	2.30	0.56
1:L:95:LEU:HD23	1:L:95:LEU:N	2.21	0.56
1:L:277:THR:C	1:L:279:ILE:N	2.62	0.56
1:D:159:THR:O	1:D:160:GLU:C	2.47	0.56
1:H:234:VAL:O	1:H:234:VAL:HG12	2.05	0.56
1:C:107:LEU:HD22	1:C:182:ILE:HD13	1.87	0.56
1:F:52:LEU:HD13	1:F:109:TRP:CD2	2.40	0.56
1:I:141:LEU:HD21	1:I:204:LYS:HD2	1.88	0.56
1:B:300:MET:HE1	1:B:303:ARG:HH21	1.70	0.56
1:G:45:GLN:O	1:G:46:PHE:HB2	2.05	0.56
1:I:314:MET:HG3	1:I:318:GLU:HB2	1.88	0.56
1:I:337:HIS:O	1:I:341:VAL:HG23	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:252:ILE:O	1:J:252:ILE:CG2	2.54	0.56
1:L:128:TYR:O	1:L:129:ALA:HB3	2.03	0.56
1:D:234:VAL:C	1:D:236:GLY:N	2.63	0.56
1:F:158:PHE:CZ	1:F:256:LEU:HD22	2.41	0.56
1:F:274:GLY:O	1:F:278:ARG:HG3	2.06	0.56
1:H:147:PHE:CD1	1:H:189:PRO:HB3	2.41	0.56
1:I:83:ASN:C	1:I:83:ASN:ND2	2.62	0.56
1:J:195:THR:CG2	1:J:196:SER:H	2.05	0.56
1:J:251:VAL:HG12	1:J:252:ILE:N	2.21	0.56
1:E:240:TYR:O	1:E:241:ASP:C	2.48	0.56
1:E:291:TRP:CE3	1:E:294:VAL:HG11	2.41	0.56
1:I:70:LEU:HD13	2:I:1351:P4O:C17	2.36	0.56
1:L:189:PRO:HA	1:L:192:LEU:HD12	1.88	0.56
1:C:195:THR:OG1	1:C:201:ALA:HB1	2.06	0.56
1:E:110:ARG:HG2	1:E:110:ARG:HH11	1.70	0.56
1:E:125:GLU:O	1:E:126:ASN:ND2	2.26	0.56
1:E:174:ILE:HG21	1:E:316:ILE:HD13	1.87	0.56
1:G:83:ASN:HD22	1:G:84:LYS:N	2.04	0.56
1:G:107:LEU:HD22	1:G:182:ILE:HD13	1.87	0.56
1:H:141:LEU:HD13	1:H:193:LEU:HB2	1.87	0.56
1:H:198:ARG:HB3	1:H:199:PRO:HD2	1.87	0.56
1:K:197:LYS:H	1:K:197:LYS:HE2	1.70	0.56
1:F:184:HIS:O	1:F:185:ARG:HB2	2.06	0.55
1:G:174:ILE:HD11	1:G:187:VAL:HG21	1.87	0.55
1:I:68:GLN:HG2	1:I:70:LEU:CD2	2.36	0.55
1:E:143:GLY:HA3	1:E:196:SER:O	2.06	0.55
1:I:77:LYS:HD2	1:I:79:LEU:HD21	1.87	0.55
1:I:230:VAL:HG21	1:I:235:LEU:HD21	1.87	0.55
1:J:198:ARG:HD3	1:J:201:ALA:HB2	1.87	0.55
1:K:72:LEU:HD13	1:K:77:LYS:HA	1.88	0.55
1:E:273:PRO:HB3	1:L:131:ARG:NH2	2.21	0.55
1:G:184:HIS:HD2	1:G:186:ASP:H	1.54	0.55
1:G:310:PRO:CG	1:I:233:GLU:HG2	2.24	0.55
1:L:254:TYR:CD1	1:L:262:PRO:HD3	2.42	0.55
1:B:178:HIS:CD2	1:B:242:LYS:HD3	2.41	0.55
1:E:264:TYR:O	1:E:275:MET:CG	2.49	0.55
1:H:74:ILE:HG21	1:H:210:PHE:CD2	2.41	0.55
1:I:259:GLY:HA2	1:I:342:LEU:HD13	1.89	0.55
1:J:166:ILE:HG21	1:J:256:LEU:HD11	1.88	0.55
1:F:239:LYS:HE2	1:F:239:LYS:N	2.22	0.55
1:I:121:VAL:HB	1:I:137:VAL:HG12	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:166:ILE:HG21	1:J:256:LEU:CD1	2.36	0.55
1:L:275:MET:O	1:L:279:ILE:HG13	2.06	0.55
1:C:227:PRO:CG	1:C:229:TYR:CZ	2.90	0.55
1:D:96:GLN:CD	1:D:131:ARG:HD3	2.32	0.55
1:G:280:ARG:HH12	1:I:236:GLY:HA3	1.70	0.55
1:I:290:GLU:CD	1:I:290:GLU:H	2.14	0.55
1:I:344:GLU:O	1:I:345:ASP:OD1	2.25	0.55
1:J:56:LYS:NZ	1:J:125:GLU:CD	2.65	0.55
1:J:71:GLY:O	1:J:72:LEU:C	2.49	0.55
1:L:174:ILE:HG22	1:L:178:HIS:CD2	2.41	0.55
1:D:150:ILE:C	1:D:152:ASP:H	2.14	0.55
1:E:73:GLY:CA	2:E:1345:P4O:H8C2	2.34	0.55
1:E:119:ARG:HG2	1:E:120:ILE:N	2.22	0.55
1:J:88:GLU:HG3	1:J:89:LYS:N	2.21	0.55
1:D:260:TYR:OH	1:D:287:PRO:HG2	2.06	0.55
1:E:210:PHE:CD2	1:E:210:PHE:N	2.75	0.55
1:H:83:ASN:ND2	1:H:83:ASN:C	2.64	0.55
1:C:158:PHE:HD2	1:C:158:PHE:C	2.15	0.55
1:D:74:ILE:HD12	1:D:74:ILE:C	2.32	0.55
1:D:184:HIS:O	1:D:184:HIS:CD2	2.60	0.55
1:F:60:ILE:HD13	1:G:48:VAL:CG1	2.36	0.55
1:F:140:CYS:SG	2:F:1350:P4O:H17	2.47	0.55
1:H:235:LEU:HD12	1:I:280:ARG:HG2	1.88	0.55
1:L:53:GLN:NE2	1:L:53:GLN:HA	2.22	0.55
1:L:343:LYS:HE2	1:L:343:LYS:N	2.15	0.55
1:A:295:SER:OG	1:A:297:GLU:HB3	2.06	0.55
1:B:233:GLU:HG2	1:C:310:PRO:CG	2.36	0.55
1:B:348:ARG:O	1:B:350:GLU:N	2.31	0.55
1:G:63:TYR:C	1:G:84:LYS:HG3	2.31	0.55
1:G:161:ARG:O	1:G:165:GLU:HG3	2.07	0.55
1:J:188:LYS:HB2	1:J:189:PRO:HD2	1.87	0.55
1:A:233:GLU:HG2	1:B:310:PRO:CG	2.34	0.54
1:B:190:GLU:H	1:B:190:GLU:CD	2.16	0.54
1:B:265:SER:O	1:B:271:ILE:O	2.24	0.54
1:D:141:LEU:CD1	1:D:193:LEU:HB2	2.36	0.54
1:G:147:PHE:HE1	1:G:255:ILE:HG21	1.69	0.54
1:G:151:GLN:HB2	1:G:342:LEU:HB3	1.88	0.54
1:L:160:GLU:O	1:L:160:GLU:HG2	2.08	0.54
1:L:278:ARG:O	1:L:283:GLN:HB2	2.06	0.54
1:L:335:PRO:C	1:L:336:LEU:HD13	2.32	0.54
1:D:159:THR:C	1:D:336:LEU:HD21	2.32	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:300:MET:HA	1:E:300:MET:CE	2.36	0.54
1:H:71:GLY:O	1:H:78:VAL:HG23	2.07	0.54
1:I:83:ASN:HD22	1:I:84:LYS:N	2.05	0.54
1:L:258:CYS:HB3	1:L:291:TRP:CZ2	2.43	0.54
1:B:278:ARG:HB3	1:B:283:GLN:HB2	1.88	0.54
1:E:229:TYR:CD2	1:E:229:TYR:N	2.71	0.54
1:F:200:ASN:O	1:F:201:ALA:O	2.25	0.54
1:G:74:ILE:HG21	1:G:209:GLY:CA	2.28	0.54
1:H:145:GLU:O	1:H:148:SER:HB2	2.07	0.54
1:L:167:MET:HE2	1:L:253:MET:HB2	1.88	0.54
1:B:141:LEU:HD13	1:B:193:LEU:HB2	1.89	0.54
1:C:145:GLU:HA	1:C:193:LEU:HD23	1.88	0.54
1:C:343:LYS:C	1:C:345:ASP:H	2.15	0.54
1:D:83:ASN:ND2	1:D:85:ARG:H	2.06	0.54
1:E:255:ILE:O	1:E:257:LEU:N	2.41	0.54
1:E:265:SER:O	1:E:266:ASN:HB2	2.08	0.54
1:F:74:ILE:HG21	1:F:209:GLY:HA3	1.87	0.54
1:G:289:PRO:HD2	1:G:290:GLU:OE2	2.07	0.54
1:I:321:ASN:HA	1:I:326:MET:HG3	1.90	0.54
1:J:170:ILE:O	1:J:170:ILE:HG22	2.07	0.54
1:L:277:THR:O	1:L:280:ARG:N	2.41	0.54
1:B:227:PRO:HG2	1:B:230:VAL:CB	2.34	0.54
1:D:142:ASP:HA	2:D:1351:P4O:N16	2.23	0.54
1:E:159:THR:HB	1:E:333:GLN:HA	1.90	0.54
1:E:301:LEU:CD1	1:E:314:MET:HE1	2.37	0.54
1:F:210:PHE:CD2	1:F:210:PHE:N	2.76	0.54
1:G:331:VAL:HG13	1:G:332:PRO:HD2	1.88	0.54
1:H:151:GLN:O	1:H:343:LYS:HE3	2.07	0.54
1:A:83:ASN:C	1:A:83:ASN:ND2	2.65	0.54
1:A:168:LYS:O	1:A:172:GLU:HG3	2.08	0.54
1:C:315:THR:OG1	1:C:318:GLU:HG3	2.08	0.54
1:E:159:THR:HG23	1:E:162:GLU:OE2	2.08	0.54
1:G:281:MET:HB2	1:G:283:GLN:HG3	1.88	0.54
1:B:69:VAL:HG13	1:B:69:VAL:O	2.08	0.54
1:D:327:GLN:HG3	1:D:330:LYS:HG2	1.89	0.54
1:E:83:ASN:OD1	1:E:86:THR:N	2.41	0.54
1:G:185:ARG:NH2	1:G:212:LYS:HD2	2.18	0.54
1:L:246:MET:HG3	1:L:314:MET:O	2.08	0.54
1:L:277:THR:HG22	1:L:280:ARG:HD3	1.90	0.54
1:B:168:LYS:O	1:B:172:GLU:HG3	2.08	0.54
1:C:301:LEU:HD13	1:C:322:HIS:CD2	2.43	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:70:LEU:CD2	1:D:80:GLN:HB2	2.31	0.54
1:D:337:HIS:HD2	1:D:340:ARG:NH1	2.05	0.54
1:E:98:CYS:HB2	1:E:99:PRO:CD	2.38	0.54
1:K:296:GLU:OE2	1:K:299:LYS:HD2	2.07	0.54
1:L:208:PHE:C	1:L:210:PHE:H	2.15	0.54
1:E:74:ILE:HD12	1:E:74:ILE:O	2.07	0.54
1:F:99:PRO:HD2	1:F:100:LYS:H	1.73	0.54
1:F:323:PRO:HA	1:F:326:MET:HB2	1.90	0.54
1:L:85:ARG:O	1:L:85:ARG:HD2	2.08	0.54
1:A:48:VAL:HG13	1:G:60:ILE:HD13	1.90	0.53
1:E:146:LEU:HD13	1:E:203:LEU:HD22	1.89	0.53
1:E:148:SER:C	1:E:150:ILE:H	2.16	0.53
1:F:86:THR:O	1:F:87:GLN:CB	2.56	0.53
1:G:309:GLU:OE2	1:G:310:PRO:HD2	2.08	0.53
1:I:156:GLN:O	1:I:157:ALA:C	2.51	0.53
1:B:185:ARG:HH11	1:B:185:ARG:CB	2.20	0.53
1:D:150:ILE:C	1:D:152:ASP:N	2.66	0.53
1:G:99:PRO:CD	1:G:100:LYS:H	2.21	0.53
1:J:72:LEU:C	1:J:72:LEU:HD23	2.33	0.53
1:L:255:ILE:HG12	1:L:261:PRO:CA	2.36	0.53
1:F:108:HIS:CG	1:F:120:ILE:HD11	2.43	0.53
1:F:237:PRO:O	1:F:238:GLU:HB3	2.07	0.53
1:G:300:MET:HE1	1:G:303:ARG:HE	1.73	0.53
1:H:87:GLN:HA	1:H:87:GLN:NE2	2.24	0.53
1:J:255:ILE:C	1:J:257:LEU:H	2.17	0.53
1:K:332:PRO:CB	1:K:334:THR:HG22	2.37	0.53
1:B:147:PHE:CD1	1:B:349:TRP:CZ2	2.86	0.53
1:B:272:SER:H	1:B:273:PRO:CD	2.21	0.53
1:D:150:ILE:O	1:D:152:ASP:N	2.41	0.53
1:E:341:VAL:O	1:E:344:GLU:OE1	2.26	0.53
1:F:289:PRO:HD2	1:F:290:GLU:OE2	2.08	0.53
1:F:322:HIS:ND1	1:F:323:PRO:CD	2.72	0.53
1:I:309:GLU:OE2	1:I:311:THR:HG23	2.08	0.53
1:K:141:LEU:H	2:K:1345:P4O:C10	2.21	0.53
1:L:180:ILE:O	1:L:181:ASN:C	2.51	0.53
1:L:192:LEU:C	1:L:193:LEU:HD23	2.32	0.53
1:C:158:PHE:C	1:C:158:PHE:CD2	2.85	0.53
1:F:195:THR:HG23	1:F:202:ILE:O	2.09	0.53
1:H:147:PHE:HB3	1:H:342:LEU:HD11	1.89	0.53
1:I:69:VAL:HG11	1:I:72:LEU:HD11	1.89	0.53
1:K:287:PRO:C	1:K:288:ASN:HD22	2.16	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:86:THR:HG22	1:L:88:GLU:HB2	1.89	0.53
1:B:129:ALA:O	1:B:131:ARG:N	2.41	0.53
1:F:110:ARG:HG2	1:F:110:ARG:NH1	2.24	0.53
1:F:239:LYS:C	1:F:241:ASP:H	2.16	0.53
1:F:260:TYR:HB2	1:F:261:PRO:CD	2.39	0.53
1:G:148:SER:C	1:G:150:ILE:N	2.65	0.53
1:H:200:ASN:O	1:H:201:ALA:O	2.26	0.53
1:J:195:THR:HG21	1:J:201:ALA:HB3	1.91	0.53
1:K:195:THR:HG22	1:K:202:ILE:H	1.74	0.53
1:L:150:ILE:HG23	1:L:151:GLN:N	2.22	0.53
1:L:277:THR:C	1:L:279:ILE:H	2.16	0.53
1:C:228:TYR:C	1:C:228:TYR:CD1	2.86	0.53
1:F:86:THR:HG21	1:F:88:GLU:CB	2.29	0.53
1:J:108:HIS:O	1:J:110:ARG:N	2.41	0.53
1:A:74:ILE:CB	1:A:210:PHE:CE2	2.92	0.53
1:C:114:CYS:HB2	1:C:176:TYR:CD2	2.44	0.53
1:C:190:GLU:H	1:C:190:GLU:CD	2.17	0.53
1:E:59:ILE:N	1:E:126:ASN:OD1	2.42	0.53
1:F:289:PRO:O	1:F:290:GLU:C	2.52	0.53
1:I:174:ILE:HD11	1:I:187:VAL:HG21	1.91	0.53
1:I:300:MET:CE	1:I:303:ARG:HE	2.21	0.53
1:J:103:ARG:HA	1:J:106:GLU:HB2	1.89	0.53
1:J:119:ARG:CZ	1:J:119:ARG:HB2	2.39	0.53
1:B:59:ILE:HG13	1:B:124:TYR:CE1	2.44	0.53
1:C:302:ILE:HG22	1:C:306:LEU:HD12	1.91	0.53
1:D:83:ASN:C	1:D:83:ASN:ND2	2.60	0.53
1:F:98:CYS:HB2	1:F:99:PRO:CD	2.38	0.53
1:I:168:LYS:HB2	1:I:325:ILE:HG23	1.89	0.53
1:J:62:ASP:O	1:J:84:LYS:N	2.42	0.53
1:B:86:THR:CG2	1:B:88:GLU:HB2	2.35	0.53
1:B:164:SER:HA	1:B:324:TRP:CH2	2.44	0.53
1:C:345:ASP:C	1:C:347:GLU:N	2.64	0.53
1:F:191:ASN:ND2	2:F:1350:P4O:H8C2	2.24	0.53
1:J:248:SER:C	1:J:250:GLY:N	2.66	0.53
1:E:233:GLU:CD	1:F:310:PRO:HG3	2.33	0.52
1:G:83:ASN:C	1:G:83:ASN:ND2	2.63	0.52
1:G:114:CYS:HB2	1:G:176:TYR:CD2	2.43	0.52
1:I:337:HIS:ND1	1:I:337:HIS:N	2.56	0.52
1:L:78:VAL:CG1	1:L:79:LEU:H	2.21	0.52
1:C:158:PHE:O	1:C:336:LEU:HD22	2.09	0.52
1:F:190:GLU:CD	1:F:190:GLU:H	2.16	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:250:GLY:O	1:J:251:VAL:C	2.52	0.52
1:J:304:ASN:C	1:J:306:LEU:N	2.63	0.52
1:L:90:PHE:HA	1:L:140:CYS:HB2	1.91	0.52
1:L:340:ARG:H	1:L:340:ARG:HD3	1.74	0.52
1:C:147:PHE:HD1	1:C:189:PRO:HB3	1.74	0.52
1:E:97:ASP:HB2	1:E:134:LEU:HD22	1.92	0.52
1:I:164:SER:HA	1:I:324:TRP:CH2	2.44	0.52
1:I:300:MET:HE2	1:I:303:ARG:HH21	1.73	0.52
1:J:239:LYS:O	1:J:241:ASP:N	2.43	0.52
1:K:118:VAL:HG12	1:K:205:LEU:O	2.09	0.52
1:L:108:HIS:CG	1:L:120:ILE:HD11	2.45	0.52
1:L:159:THR:C	1:L:336:LEU:CD2	2.83	0.52
1:A:195:THR:HG23	1:A:202:ILE:O	2.09	0.52
1:D:125:GLU:C	1:D:126:ASN:HD22	2.17	0.52
1:F:239:LYS:HE2	1:F:239:LYS:CA	2.39	0.52
1:I:98:CYS:HB2	1:I:99:PRO:CD	2.39	0.52
1:I:237:PRO:O	1:I:238:GLU:HB3	2.10	0.52
1:A:332:PRO:HB2	1:A:334:THR:HG22	1.92	0.52
1:C:150:ILE:HG23	1:C:158:PHE:HD1	1.73	0.52
1:E:185:ARG:CG	1:E:185:ARG:NH1	2.72	0.52
1:K:158:PHE:CD2	1:K:159:THR:N	2.77	0.52
1:B:125:GLU:C	1:B:126:ASN:HD22	2.17	0.52
1:C:333:GLN:HE21	1:C:333:GLN:CA	2.22	0.52
1:J:171:GLY:C	1:J:173:ALA:N	2.67	0.52
1:K:86:THR:O	1:K:87:GLN:HB2	2.09	0.52
1:L:310:PRO:HA	1:L:313:ARG:NH2	2.25	0.52
1:A:129:ALA:C	1:A:131:ARG:H	2.17	0.52
1:B:272:SER:N	1:B:273:PRO:CD	2.73	0.52
1:C:47:HIS:CG	1:C:47:HIS:O	2.62	0.52
1:D:239:LYS:HG3	1:D:240:TYR:N	2.25	0.52
1:E:110:ARG:HG2	1:E:110:ARG:NH1	2.24	0.52
1:G:309:GLU:OE2	1:G:311:THR:HG23	2.09	0.52
1:L:145:GLU:O	1:L:147:PHE:N	2.42	0.52
1:L:255:ILE:HA	1:L:260:TYR:O	2.09	0.52
1:L:310:PRO:CA	1:L:313:ARG:HH21	2.22	0.52
1:C:147:PHE:CE1	1:C:189:PRO:HB3	2.44	0.52
1:F:345:ASP:OD1	1:F:348:ARG:HB2	2.08	0.52
1:H:185:ARG:HH21	1:H:212:LYS:CD	2.23	0.52
1:I:75:ASN:HD22	1:I:75:ASN:N	2.07	0.52
1:I:338:THR:HG22	1:I:342:LEU:HD22	1.91	0.52
1:J:48:VAL:O	1:J:48:VAL:HG13	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:175:GLN:C	1:J:177:LEU:N	2.68	0.52
1:A:151:GLN:O	1:A:343:LYS:HE3	2.10	0.52
1:A:185:ARG:HH21	1:A:212:LYS:HD3	1.74	0.52
1:B:341:VAL:O	1:B:345:ASP:HB2	2.10	0.52
1:E:198:ARG:O	1:E:201:ALA:N	2.43	0.52
1:E:210:PHE:N	1:E:210:PHE:HD2	2.07	0.52
1:F:300:MET:HE1	1:F:303:ARG:HH21	1.74	0.52
1:G:345:ASP:O	1:G:346:LYS:C	2.52	0.52
1:I:202:ILE:HG22	1:I:203:LEU:N	2.25	0.52
1:J:83:ASN:HD21	1:J:85:ARG:HE	1.58	0.52
1:J:149:ARG:O	1:J:150:ILE:HD13	2.10	0.52
1:K:164:SER:HA	1:K:324:TRP:CH2	2.45	0.52
1:L:208:PHE:O	1:L:210:PHE:N	2.43	0.52
1:A:277:THR:HG21	1:C:179:SER:O	2.10	0.52
1:B:147:PHE:HD1	1:B:349:TRP:CH2	2.27	0.52
1:B:159:THR:OG1	1:B:162:GLU:HG3	2.09	0.52
1:E:108:HIS:O	1:E:109:TRP:C	2.52	0.52
1:E:338:THR:O	1:E:342:LEU:HB2	2.10	0.52
1:F:151:GLN:HG3	1:F:342:LEU:HB3	1.90	0.52
1:G:168:LYS:O	1:G:172:GLU:HG3	2.10	0.52
1:J:321:ASN:HA	1:J:326:MET:HG2	1.92	0.52
1:K:49:LYS:HD2	1:K:50:SER:H	1.74	0.52
1:A:83:ASN:HD22	1:A:84:LYS:N	2.07	0.51
1:A:151:GLN:O	1:A:151:GLN:HG2	2.09	0.51
1:B:110:ARG:HG2	1:B:110:ARG:NH1	2.26	0.51
1:B:332:PRO:CB	1:B:334:THR:HG22	2.39	0.51
1:C:74:ILE:HG13	1:C:75:ASN:ND2	2.25	0.51
1:E:127:LEU:O	1:E:128:TYR:HB2	2.10	0.51
1:I:156:GLN:HB3	1:I:339:SER:CB	2.41	0.51
1:J:78:VAL:HG11	1:J:91:ALA:HB1	1.92	0.51
1:J:255:ILE:CD1	1:J:261:PRO:HA	2.41	0.51
1:D:114:CYS:HB2	1:D:176:TYR:CD2	2.45	0.51
1:E:210:PHE:O	1:E:211:ALA:C	2.52	0.51
1:E:230:VAL:HG22	1:E:231:ALA:N	2.25	0.51
1:F:162:GLU:O	1:F:166:ILE:HG13	2.11	0.51
1:F:309:GLU:OE2	1:F:311:THR:HG23	2.10	0.51
1:G:227:PRO:O	1:H:275:MET:HE1	2.10	0.51
1:H:151:GLN:HG3	1:H:342:LEU:HB3	1.91	0.51
1:I:83:ASN:OD1	1:I:86:THR:CG2	2.52	0.51
1:J:167:MET:HE3	1:J:167:MET:CA	2.33	0.51
1:K:83:ASN:CB	1:K:86:THR:HB	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:188:LYS:O	1:L:192:LEU:HD12	2.09	0.51
1:C:260:TYR:OH	1:C:287:PRO:HG2	2.11	0.51
1:D:52:LEU:HD13	1:D:109:TRP:CD2	2.46	0.51
1:E:302:ILE:HG22	1:E:302:ILE:O	2.09	0.51
1:H:70:LEU:HD22	1:H:80:GLN:HB2	1.92	0.51
1:I:83:ASN:HB3	1:I:86:THR:CG2	2.40	0.51
1:K:69:VAL:O	1:K:71:GLY:N	2.44	0.51
1:B:74:ILE:HD12	1:B:74:ILE:O	2.10	0.51
1:F:349:TRP:HA	1:F:349:TRP:HE3	1.73	0.51
1:J:195:THR:HG21	1:J:201:ALA:CB	2.40	0.51
1:K:146:LEU:HD13	1:K:203:LEU:HD11	1.93	0.51
1:L:180:ILE:O	1:L:180:ILE:HG13	2.11	0.51
1:L:189:PRO:C	1:L:191:ASN:H	2.17	0.51
1:B:80:GLN:CD	1:B:89:LYS:HD2	2.34	0.51
1:D:98:CYS:HB2	1:D:99:PRO:CD	2.39	0.51
1:D:128:TYR:O	1:D:129:ALA:HB3	2.10	0.51
1:F:86:THR:HG23	1:F:88:GLU:HB2	1.86	0.51
1:H:105:VAL:HG22	1:H:136:ILE:HD11	1.92	0.51
1:K:78:VAL:C	1:K:79:LEU:HD23	2.36	0.51
1:L:184:HIS:O	1:L:184:HIS:HD2	1.94	0.51
1:B:60:ILE:O	1:B:61:ASP:C	2.53	0.51
1:C:145:GLU:HA	1:C:193:LEU:CD2	2.40	0.51
1:C:227:PRO:CG	1:C:229:TYR:OH	2.58	0.51
1:D:92:LEU:HD11	1:D:135:LEU:HB3	1.92	0.51
1:E:158:PHE:HE1	1:E:256:LEU:HD22	1.75	0.51
1:G:97:ASP:O	1:G:98:CYS:HB3	2.10	0.51
1:G:147:PHE:CE1	1:G:255:ILE:CG2	2.93	0.51
1:G:247:TRP:NE1	1:I:230:VAL:O	2.44	0.51
1:H:172:GLU:HG2	1:H:320:MET:HE1	1.93	0.51
1:I:195:THR:CG2	1:I:202:ILE:H	2.23	0.51
1:K:83:ASN:CG	1:K:86:THR:HB	2.35	0.51
1:L:153:ARG:CB	1:L:153:ARG:CZ	2.88	0.51
1:C:168:LYS:HB2	1:C:325:ILE:HG23	1.93	0.51
1:D:70:LEU:HD22	1:D:70:LEU:N	2.26	0.51
1:K:288:ASN:N	1:K:288:ASN:ND2	2.57	0.51
1:A:146:LEU:HD11	1:A:166:ILE:HD13	1.93	0.51
1:B:48:VAL:HG13	1:K:60:ILE:HD13	1.92	0.51
1:C:152:ASP:N	1:C:152:ASP:OD1	2.44	0.51
1:D:281:MET:HE2	1:F:179:SER:HB3	1.93	0.51
1:E:127:LEU:HB2	1:J:49:LYS:HB2	1.91	0.51
1:E:160:GLU:O	1:E:163:ALA:N	2.44	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:86:THR:O	1:F:87:GLN:HB2	2.10	0.51
1:G:241:ASP:O	1:G:244:CYS:HB3	2.11	0.51
1:I:345:ASP:HB3	1:I:348:ARG:HG3	1.92	0.51
1:I:347:GLU:HG3	1:I:348:ARG:H	1.74	0.51
1:J:103:ARG:HG3	1:J:104:GLU:N	2.24	0.51
1:J:176:TYR:CD2	1:J:176:TYR:O	2.64	0.51
1:J:179:SER:HA	1:L:281:MET:SD	2.51	0.51
1:J:300:MET:O	1:J:302:ILE:N	2.44	0.51
1:K:74:ILE:HG22	1:K:207:ASP:OD1	2.11	0.51
1:C:170:ILE:CD1	1:C:192:LEU:HD13	2.41	0.51
1:D:158:PHE:O	1:D:336:LEU:HD22	2.10	0.51
1:E:118:VAL:CG1	1:E:206:THR:HG22	2.41	0.51
1:J:302:ILE:HG22	1:J:306:LEU:HD12	1.91	0.51
1:L:160:GLU:HB3	1:L:334:THR:HG23	1.93	0.51
1:B:314:MET:HG3	1:B:318:GLU:HB2	1.93	0.51
1:C:341:VAL:O	1:C:341:VAL:HG12	2.10	0.51
1:E:115:PRO:O	1:E:204:LYS:HE2	2.10	0.51
1:G:185:ARG:HB3	1:G:185:ARG:HH11	1.74	0.51
1:K:294:VAL:O	1:K:295:SER:C	2.54	0.51
1:L:240:TYR:CD1	1:L:240:TYR:C	2.89	0.51
1:A:87:GLN:NE2	1:A:87:GLN:HA	2.26	0.50
1:C:237:PRO:O	1:C:238:GLU:HB3	2.11	0.50
1:F:149:ARG:O	1:F:150:ILE:C	2.52	0.50
1:H:184:HIS:HD2	1:H:186:ASP:N	2.09	0.50
1:J:193:LEU:N	1:J:193:LEU:CD2	2.68	0.50
1:K:93:LYS:NZ	1:K:104:GLU:OE1	2.36	0.50
1:K:102:ARG:O	1:K:106:GLU:HB2	2.11	0.50
1:K:168:LYS:O	1:K:172:GLU:HG3	2.12	0.50
1:C:202:ILE:HD13	1:C:202:ILE:N	2.25	0.50
1:E:89:LYS:O	1:E:90:PHE:CD2	2.64	0.50
1:G:88:GLU:HG3	1:G:89:LYS:H	1.77	0.50
1:G:147:PHE:CZ	1:G:255:ILE:CG2	2.95	0.50
1:H:110:ARG:HG2	1:H:110:ARG:NH1	2.26	0.50
1:K:196:SER:CB	1:K:198:ARG:HD3	2.41	0.50
1:A:149:ARG:NH1	1:A:149:ARG:CG	2.72	0.50
1:E:167:MET:HE2	1:E:253:MET:HB2	1.94	0.50
1:G:195:THR:CG2	1:G:202:ILE:HB	2.41	0.50
1:L:94:MET:HE3	1:L:135:LEU:HD21	1.94	0.50
1:A:118:VAL:O	1:A:118:VAL:HG13	2.12	0.50
1:A:343:LYS:C	1:A:345:ASP:H	2.20	0.50
1:C:129:ALA:O	1:C:131:ARG:HG3	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:196:SER:OG	1:C:201:ALA:HB2	2.11	0.50
1:E:99:PRO:O	1:E:101:ALA:N	2.44	0.50
1:F:331:VAL:HG13	1:F:332:PRO:HD2	1.91	0.50
1:G:159:THR:O	1:G:160:GLU:C	2.54	0.50
1:G:166:ILE:HG21	1:G:256:LEU:HD11	1.94	0.50
1:H:272:SER:H	1:H:273:PRO:CD	2.25	0.50
1:J:301:LEU:HD22	1:J:322:HIS:CE1	2.47	0.50
1:K:329:THR:CG2	1:K:330:LYS:HE2	2.41	0.50
1:L:255:ILE:HG12	1:L:260:TYR:O	2.12	0.50
1:E:180:ILE:CG1	1:E:182:ILE:HD12	2.31	0.50
1:F:80:GLN:HE22	1:F:89:LYS:HD3	1.73	0.50
1:F:290:GLU:OE2	1:F:290:GLU:N	2.41	0.50
1:K:110:ARG:HG2	1:K:110:ARG:HH11	1.76	0.50
1:L:118:VAL:O	1:L:118:VAL:HG13	2.11	0.50
1:L:189:PRO:O	1:L:191:ASN:N	2.45	0.50
1:A:56:LYS:O	1:F:50:SER:HB2	2.11	0.50
1:C:288:ASN:N	1:C:288:ASN:OD1	2.45	0.50
1:H:149:ARG:HH11	1:H:149:ARG:CG	2.25	0.50
1:I:190:GLU:CD	1:I:190:GLU:H	2.19	0.50
1:J:62:ASP:HB2	1:J:63:TYR:CD2	2.47	0.50
1:L:90:PHE:CD2	1:L:121:VAL:HG21	2.47	0.50
1:L:158:PHE:CE1	1:L:163:ALA:HB2	2.47	0.50
1:G:286:PHE:O	1:G:291:TRP:HB2	2.11	0.50
1:H:200:ASN:N	1:H:200:ASN:ND2	2.57	0.50
1:H:247:TRP:O	1:H:248:SER:C	2.55	0.50
1:I:71:GLY:O	1:I:72:LEU:HD12	2.12	0.50
1:I:338:THR:O	1:I:342:LEU:HB2	2.11	0.50
1:L:153:ARG:HB3	1:L:153:ARG:NH1	2.26	0.50
1:L:169:SER:C	1:L:171:GLY:N	2.67	0.50
1:L:175:GLN:O	1:L:175:GLN:HG3	2.09	0.50
1:L:202:ILE:HG22	1:L:204:LYS:HG3	1.94	0.50
1:L:251:VAL:HG13	1:L:262:PRO:HD2	1.94	0.50
1:C:151:GLN:HE22	1:C:346:LYS:HG3	1.76	0.50
1:C:198:ARG:HB3	1:C:199:PRO:HD2	1.94	0.50
1:G:48:VAL:O	1:G:48:VAL:HG13	2.12	0.50
1:J:107:LEU:O	1:J:108:HIS:C	2.55	0.50
1:J:240:TYR:CD2	1:J:240:TYR:N	2.79	0.50
1:K:338:THR:O	1:K:342:LEU:HB2	2.12	0.50
1:B:323:PRO:HA	1:B:326:MET:HB2	1.93	0.49
1:C:74:ILE:HD12	1:C:74:ILE:O	2.12	0.49
1:C:134:LEU:C	1:C:135:LEU:HD23	2.37	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:189:PRO:C	1:L:191:ASN:N	2.69	0.49
1:B:233:GLU:OE1	1:C:313:ARG:NH2	2.45	0.49
1:D:192:LEU:O	1:D:193:LEU:HD23	2.12	0.49
1:D:340:ARG:O	1:D:344:GLU:HB2	2.12	0.49
1:E:48:VAL:HG13	1:E:48:VAL:O	2.11	0.49
1:F:227:PRO:HB2	1:F:230:VAL:HB	1.94	0.49
1:I:195:THR:HG21	1:I:202:ILE:HB	1.94	0.49
1:I:345:ASP:C	1:I:347:GLU:N	2.69	0.49
1:J:303:ARG:O	1:J:306:LEU:O	2.30	0.49
1:K:146:LEU:HD12	1:K:194:TYR:CE2	2.46	0.49
1:A:165:GLU:HG2	1:A:328:SER:HB3	1.93	0.49
1:C:174:ILE:HD11	1:C:187:VAL:HG21	1.94	0.49
1:F:139:GLU:O	2:F:1350:P4O:H10	2.12	0.49
1:C:333:GLN:HA	1:C:333:GLN:NE2	2.27	0.49
1:E:118:VAL:HA	1:E:139:GLU:OE1	2.12	0.49
1:E:239:LYS:HE3	1:E:240:TYR:HE1	1.77	0.49
1:F:49:LYS:HG3	1:F:113:GLN:CD	2.37	0.49
1:G:88:GLU:CG	1:G:89:LYS:N	2.75	0.49
1:H:161:ARG:O	1:H:164:SER:HB3	2.10	0.49
1:B:74:ILE:CG2	1:B:210:PHE:HE2	2.25	0.49
1:B:247:TRP:O	1:B:248:SER:C	2.55	0.49
1:D:168:LYS:O	1:D:172:GLU:HG3	2.13	0.49
1:F:277:THR:HA	1:F:280:ARG:HG3	1.94	0.49
1:F:332:PRO:HB2	1:F:334:THR:CG2	2.43	0.49
1:H:105:VAL:CG2	1:H:136:ILE:HD11	2.43	0.49
1:J:300:MET:C	1:J:302:ILE:N	2.70	0.49
1:K:80:GLN:NE2	1:K:89:LYS:CG	2.71	0.49
1:L:98:CYS:O	1:L:102:ARG:HG2	2.13	0.49
1:L:338:THR:O	1:L:339:SER:C	2.56	0.49
1:A:239:LYS:C	1:A:241:ASP:H	2.21	0.49
1:B:147:PHE:CD1	1:B:349:TRP:CH2	3.01	0.49
1:E:60:ILE:O	1:E:61:ASP:C	2.56	0.49
1:F:347:GLU:C	1:F:349:TRP:N	2.62	0.49
1:I:83:ASN:O	1:I:87:GLN:N	2.45	0.49
1:J:251:VAL:CG1	1:J:252:ILE:HG13	2.29	0.49
1:K:70:LEU:HG	2:K:1345:P4O:C17	2.43	0.49
1:L:158:PHE:HE1	1:L:256:LEU:O	1.96	0.49
1:L:169:SER:C	1:L:171:GLY:H	2.19	0.49
1:L:258:CYS:O	1:L:338:THR:HA	2.12	0.49
1:C:80:GLN:NE2	1:C:89:LYS:HB2	2.28	0.49
1:F:286:PHE:CE1	1:F:299:LYS:HB3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:194:TYR:O	1:J:195:THR:C	2.55	0.49
1:L:125:GLU:O	1:L:126:ASN:ND2	2.45	0.49
1:A:52:LEU:HD13	1:A:109:TRP:CD2	2.47	0.49
1:A:74:ILE:C	1:A:74:ILE:HD12	2.38	0.49
1:A:83:ASN:ND2	1:A:85:ARG:H	2.11	0.49
1:C:159:THR:O	1:C:160:GLU:C	2.56	0.49
1:D:237:PRO:O	1:D:238:GLU:CB	2.60	0.49
1:F:247:TRP:CZ2	1:F:263:PHE:HE1	2.31	0.49
1:G:166:ILE:CG2	1:G:256:LEU:HD11	2.43	0.49
1:J:247:TRP:O	1:J:248:SER:C	2.56	0.49
1:J:254:TYR:HD1	1:J:262:PRO:HD3	1.75	0.49
1:J:302:ILE:HG23	1:J:306:LEU:HD12	1.94	0.49
1:A:190:GLU:CD	1:A:190:GLU:H	2.21	0.49
1:B:74:ILE:HB	1:B:210:PHE:HE2	1.77	0.49
1:B:151:GLN:HG3	1:B:151:GLN:O	2.13	0.49
1:F:60:ILE:HD13	1:G:48:VAL:HG12	1.95	0.49
1:F:331:VAL:HG12	1:F:332:PRO:HD2	1.95	0.49
1:H:207:ASP:HB2	2:H:1347:P4O:N7	2.28	0.49
1:J:119:ARG:HB2	1:J:119:ARG:NH1	2.28	0.49
1:K:329:THR:HG23	1:K:330:LYS:HE2	1.93	0.49
1:B:198:ARG:O	1:B:201:ALA:HB2	2.13	0.49
1:B:332:PRO:HB2	1:B:334:THR:HG22	1.93	0.49
1:C:227:PRO:HG2	1:C:229:TYR:OH	2.12	0.49
1:G:199:PRO:HD2	1:G:200:ASN:OD1	2.12	0.49
1:H:172:GLU:HG2	1:H:320:MET:CE	2.43	0.49
1:A:233:GLU:CD	1:B:313:ARG:HH22	2.21	0.48
1:B:59:ILE:HG13	1:B:124:TYR:CD1	2.47	0.48
1:C:148:SER:O	1:C:149:ARG:C	2.54	0.48
1:D:118:VAL:O	1:D:118:VAL:HG13	2.13	0.48
1:E:80:GLN:HE21	1:E:81:ILE:N	2.10	0.48
1:E:133:CYS:HB3	1:E:135:LEU:CD2	2.43	0.48
1:E:148:SER:C	1:E:150:ILE:N	2.70	0.48
1:F:191:ASN:HD21	2:F:1350:P4O:H8C2	1.78	0.48
1:G:66:THR:HG21	1:G:82:PHE:CE2	2.45	0.48
1:J:261:PRO:HB2	1:J:263:PHE:O	2.12	0.48
1:K:314:MET:CG	1:K:318:GLU:HB2	2.43	0.48
1:L:253:MET:HE1	1:L:301:LEU:CD2	2.43	0.48
1:L:277:THR:HA	1:L:280:ARG:CD	2.42	0.48
1:L:291:TRP:CE3	1:L:294:VAL:HG21	2.48	0.48
1:L:319:PHE:O	1:L:319:PHE:CG	2.66	0.48
1:A:58:ALA:H	1:F:50:SER:HB3	1.77	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:PHE:HE2	1:A:256:LEU:HD23	1.78	0.48
1:F:196:SER:OG	1:F:201:ALA:HB2	2.13	0.48
1:I:108:HIS:CG	1:I:120:ILE:HD11	2.48	0.48
1:J:76:GLY:O	1:J:77:LYS:HB2	2.13	0.48
1:J:81:ILE:HG13	1:J:90:PHE:O	2.12	0.48
1:K:149:ARG:NH2	1:K:197:LYS:O	2.46	0.48
1:K:194:TYR:HB3	1:K:201:ALA:HB1	1.96	0.48
1:L:161:ARG:O	1:L:165:GLU:HG3	2.12	0.48
1:L:316:ILE:O	1:L:316:ILE:CG1	2.59	0.48
1:A:108:HIS:CG	1:A:120:ILE:HD11	2.48	0.48
1:B:271:ILE:CG1	1:B:273:PRO:HD2	2.43	0.48
1:C:240:TYR:O	1:C:243:SER:N	2.46	0.48
1:C:309:GLU:OE2	1:C:311:THR:CG2	2.59	0.48
1:D:330:LYS:HD3	1:D:330:LYS:N	2.27	0.48
1:E:142:ASP:HA	2:E:1345:P4O:N16	2.27	0.48
1:F:184:HIS:HD2	1:F:186:ASP:H	1.60	0.48
1:G:103:ARG:O	1:G:104:GLU:C	2.55	0.48
1:G:191:ASN:ND2	2:G:1350:P4O:H8C2	2.29	0.48
1:J:60:ILE:HG22	1:J:65:VAL:HG21	1.96	0.48
1:J:300:MET:C	1:J:302:ILE:H	2.21	0.48
1:A:185:ARG:HH21	1:A:212:LYS:HD2	1.78	0.48
1:A:233:GLU:CD	1:B:310:PRO:HG3	2.39	0.48
1:B:340:ARG:O	1:B:343:LYS:O	2.31	0.48
1:C:240:TYR:O	1:C:241:ASP:C	2.56	0.48
1:D:159:THR:OG1	1:D:162:GLU:HG3	2.14	0.48
1:E:83:ASN:OD1	1:E:85:ARG:HB3	2.13	0.48
1:E:147:PHE:CE1	1:E:255:ILE:HG21	2.47	0.48
1:F:178:HIS:CG	1:F:242:LYS:HD3	2.48	0.48
1:G:115:PRO:O	1:G:204:LYS:HE2	2.14	0.48
1:H:178:HIS:CG	1:H:242:LYS:HD3	2.48	0.48
1:I:86:THR:C	1:I:88:GLU:N	2.71	0.48
1:K:274:GLY:O	1:K:278:ARG:HG3	2.12	0.48
1:B:188:LYS:HB2	1:B:189:PRO:CD	2.42	0.48
1:D:129:ALA:C	1:D:131:ARG:H	2.22	0.48
1:F:155:ASP:O	1:F:156:GLN:O	2.32	0.48
1:I:150:ILE:CD1	1:I:158:PHE:CE2	2.97	0.48
1:C:146:LEU:HD12	1:C:146:LEU:C	2.37	0.48
1:E:193:LEU:O	1:E:203:LEU:HD12	2.14	0.48
1:F:79:LEU:N	1:F:79:LEU:HD23	2.28	0.48
1:G:291:TRP:CE3	1:G:294:VAL:HG21	2.49	0.48
1:H:121:VAL:HB	1:H:137:VAL:HG12	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:70:LEU:HD22	1:K:79:LEU:C	2.39	0.48
1:K:196:SER:HB3	1:K:198:ARG:HD3	1.96	0.48
1:L:86:THR:O	1:L:86:THR:HG22	2.13	0.48
1:L:152:ASP:C	1:L:153:ARG:HG3	2.39	0.48
1:L:185:ARG:HH11	1:L:185:ARG:CG	2.25	0.48
1:L:337:HIS:O	1:L:338:THR:C	2.56	0.48
1:B:57:ASN:O	1:B:58:ALA:C	2.57	0.48
1:E:341:VAL:C	1:E:343:LYS:H	2.22	0.48
1:F:52:LEU:HD13	1:F:109:TRP:CE3	2.49	0.48
1:G:141:LEU:CD1	1:G:193:LEU:HB2	2.41	0.48
1:I:45:GLN:O	1:I:46:PHE:CD2	2.67	0.48
1:L:262:PRO:C	1:L:263:PHE:CD1	2.92	0.48
1:D:70:LEU:CD2	1:D:70:LEU:N	2.75	0.48
1:F:202:ILE:HG22	1:F:203:LEU:N	2.28	0.48
1:G:192:LEU:O	1:G:193:LEU:HD23	2.13	0.48
1:G:289:PRO:O	1:G:292:SER:OG	2.30	0.48
1:H:78:VAL:HA	1:H:92:LEU:O	2.14	0.48
1:J:123:VAL:HG22	1:J:136:ILE:HA	1.94	0.48
1:L:183:ALA:O	1:L:211:ALA:HA	2.13	0.48
1:L:278:ARG:CZ	1:L:278:ARG:HB2	2.40	0.48
1:B:74:ILE:HG21	1:B:210:PHE:CE2	2.49	0.48
1:C:161:ARG:O	1:C:165:GLU:HG3	2.13	0.48
1:C:332:PRO:HB2	1:C:334:THR:CG2	2.44	0.48
1:D:145:GLU:HA	1:D:193:LEU:CD2	2.44	0.48
1:E:66:THR:OG1	1:E:67:SER:N	2.44	0.48
1:E:304:ASN:HA	1:E:307:LYS:HE2	1.94	0.48
1:F:68:GLN:O	1:F:79:LEU:HA	2.14	0.48
1:G:146:LEU:HA	1:G:194:TYR:HE2	1.79	0.48
1:I:98:CYS:HB2	1:I:99:PRO:HD3	1.96	0.48
1:I:146:LEU:HD11	1:I:166:ILE:HD13	1.95	0.48
1:K:83:ASN:ND2	1:K:83:ASN:C	2.65	0.48
1:L:188:LYS:O	1:L:192:LEU:CD1	2.61	0.48
1:L:243:SER:C	1:L:245:ASP:H	2.21	0.48
1:L:309:GLU:HG3	1:L:311:THR:HG23	1.96	0.48
1:C:130:GLY:HA3	1:L:180:ILE:CG2	2.44	0.48
1:D:129:ALA:O	1:D:131:ARG:N	2.47	0.48
1:E:117:ILE:HD12	1:E:208:PHE:CZ	2.47	0.48
1:E:138:MET:O	1:E:139:GLU:O	2.32	0.48
1:E:252:ILE:O	1:E:256:LEU:HB2	2.14	0.48
1:F:151:GLN:O	1:F:151:GLN:HG2	2.14	0.48
1:G:290:GLU:H	1:G:290:GLU:CD	2.22	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:103:ARG:O	1:I:104:GLU:C	2.55	0.48
1:J:174:ILE:HB	1:J:316:ILE:CD1	2.39	0.48
1:J:304:ASN:O	1:J:307:LYS:N	2.47	0.48
1:K:300:MET:CE	1:K:303:ARG:HE	2.27	0.48
1:L:86:THR:HG22	1:L:88:GLU:CB	2.44	0.48
1:A:58:ALA:N	1:F:50:SER:HB3	2.29	0.47
1:D:275:MET:HE3	1:D:279:ILE:CD1	2.44	0.47
1:E:174:ILE:CG2	1:E:316:ILE:HD13	2.43	0.47
1:F:129:ALA:C	1:F:131:ARG:H	2.21	0.47
1:F:175:GLN:HA	1:F:316:ILE:HG12	1.96	0.47
1:F:256:LEU:HA	1:F:256:LEU:HD23	1.66	0.47
1:I:277:THR:O	1:I:281:MET:HG2	2.14	0.47
1:K:199:PRO:HG2	1:K:200:ASN:H	1.79	0.47
1:L:47:HIS:O	1:L:47:HIS:CG	2.66	0.47
1:A:212:LYS:HG2	1:A:213:GLU:O	2.14	0.47
1:B:150:ILE:O	1:B:152:ASP:N	2.39	0.47
1:E:341:VAL:O	1:E:341:VAL:HG12	2.14	0.47
1:F:276:LYS:O	1:F:280:ARG:CG	2.61	0.47
1:G:73:GLY:O	1:G:74:ILE:C	2.57	0.47
1:J:72:LEU:HG	1:J:77:LYS:HG2	1.94	0.47
1:J:160:GLU:C	1:J:162:GLU:N	2.72	0.47
1:J:254:TYR:HB3	1:J:262:PRO:CG	2.42	0.47
1:L:158:PHE:CE2	1:L:162:GLU:HB2	2.49	0.47
1:D:233:GLU:CB	1:E:310:PRO:HG3	2.44	0.47
1:F:93:LYS:HE3	2:F:1350:P4O:O26	2.13	0.47
1:G:190:GLU:H	1:G:190:GLU:CD	2.21	0.47
1:H:212:LYS:HG2	1:H:213:GLU:O	2.14	0.47
1:I:59:ILE:HG21	1:I:135:LEU:CD1	2.44	0.47
1:K:86:THR:O	1:K:87:GLN:CB	2.61	0.47
1:L:284:TYR:OH	1:L:303:ARG:HG3	2.14	0.47
1:L:343:LYS:HB2	1:L:344:GLU:OE2	2.13	0.47
1:A:265:SER:O	1:A:266:ASN:HB2	2.15	0.47
1:B:82:PHE:CD1	1:B:89:LYS:HG2	2.48	0.47
1:E:253:MET:HG2	1:E:302:ILE:HD11	1.96	0.47
1:J:108:HIS:O	1:J:109:TRP:C	2.58	0.47
1:L:249:LEU:HD21	1:L:319:PHE:CE2	2.49	0.47
1:L:317:THR:O	1:L:321:ASN:ND2	2.47	0.47
1:L:333:GLN:O	1:L:335:PRO:CD	2.61	0.47
1:B:106:GLU:OE2	1:K:132:LYS:NZ	2.47	0.47
1:B:271:ILE:HG12	1:B:273:PRO:HD2	1.96	0.47
1:C:56:LYS:O	1:L:50:SER:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:ILE:CD1	1:C:75:ASN:ND2	2.77	0.47
1:C:128:TYR:O	1:C:129:ALA:HB3	2.14	0.47
1:C:197:LYS:C	1:C:198:ARG:O	2.56	0.47
1:D:70:LEU:HD12	2:D:1351:P4O:N16	2.29	0.47
1:E:309:GLU:HG3	1:E:311:THR:HG23	1.96	0.47
1:H:300:MET:CE	1:H:303:ARG:HE	2.28	0.47
1:I:190:GLU:OE1	1:I:190:GLU:N	2.43	0.47
1:J:100:LYS:O	1:J:103:ARG:HG2	2.14	0.47
1:J:255:ILE:HD11	1:J:261:PRO:CA	2.44	0.47
1:L:86:THR:CG2	1:L:88:GLU:HB2	2.44	0.47
1:L:180:ILE:O	1:L:182:ILE:N	2.48	0.47
1:B:145:GLU:HA	1:B:193:LEU:CD2	2.45	0.47
1:B:202:ILE:CG2	1:B:203:LEU:N	2.77	0.47
1:C:185:ARG:HB3	1:C:185:ARG:HH11	1.79	0.47
1:G:90:PHE:CE2	1:G:121:VAL:HG21	2.49	0.47
1:G:118:VAL:HG12	1:G:205:LEU:O	2.15	0.47
1:I:185:ARG:HE	1:I:185:ARG:HB3	1.57	0.47
1:I:255:ILE:HG12	1:I:261:PRO:HA	1.96	0.47
1:J:261:PRO:CG	1:J:263:PHE:O	2.60	0.47
1:B:74:ILE:CB	1:B:210:PHE:HE2	2.27	0.47
1:C:230:VAL:HG22	1:C:231:ALA:H	1.79	0.47
1:E:340:ARG:HA	1:E:343:LYS:HE2	1.96	0.47
1:F:202:ILE:CG2	1:F:203:LEU:N	2.78	0.47
1:G:52:LEU:HD12	1:G:53:GLN:N	2.29	0.47
1:G:63:TYR:CB	1:G:81:ILE:HD12	2.45	0.47
1:G:140:CYS:SG	2:G:1350:P4O:H17	2.55	0.47
1:G:146:LEU:HA	1:G:194:TYR:CE2	2.50	0.47
1:H:149:ARG:HG3	1:H:194:TYR:CD2	2.50	0.47
1:H:309:GLU:CD	1:H:310:PRO:HD2	2.40	0.47
1:I:83:ASN:ND2	1:I:85:ARG:H	2.13	0.47
1:I:141:LEU:CD1	1:I:193:LEU:HB2	2.45	0.47
1:A:96:GLN:OE1	1:A:131:ARG:HD2	2.13	0.47
1:B:83:ASN:OD1	1:B:86:THR:HG22	2.14	0.47
1:D:184:HIS:CD2	1:D:184:HIS:C	2.92	0.47
1:D:233:GLU:HB3	1:E:310:PRO:HG3	1.97	0.47
1:E:230:VAL:O	1:F:247:TRP:NE1	2.48	0.47
1:F:83:ASN:ND2	1:F:85:ARG:H	2.13	0.47
1:G:178:HIS:CG	1:G:242:LYS:HD3	2.49	0.47
1:H:191:ASN:HD21	2:H:1347:P4O:H8C2	1.79	0.47
1:I:147:PHE:HD2	1:I:349:TRP:HZ2	1.61	0.47
1:K:127:LEU:HD23	1:K:127:LEU:HA	1.60	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:288:ASN:HB3	1:L:289:PRO:HA	1.97	0.47
1:B:77:LYS:HE3	1:B:79:LEU:HD21	1.96	0.47
1:B:127:LEU:HD13	1:I:113:GLN:HE21	1.79	0.47
1:D:134:LEU:C	1:D:135:LEU:HD23	2.40	0.47
1:G:108:HIS:CG	1:G:120:ILE:HD11	2.50	0.47
1:G:316:ILE:O	1:G:316:ILE:HG13	2.15	0.47
1:H:167:MET:HG3	1:H:253:MET:HG3	1.97	0.47
1:I:75:ASN:HD22	1:I:76:GLY:N	2.13	0.47
1:J:98:CYS:O	1:J:99:PRO:C	2.57	0.47
1:J:146:LEU:C	1:J:148:SER:H	2.23	0.47
1:K:162:GLU:O	1:K:166:ILE:HG13	2.15	0.47
1:L:70:LEU:HB3	2:L:1345:P4O:C19	2.45	0.47
1:L:150:ILE:CG2	1:L:151:GLN:N	2.78	0.47
1:L:197:LYS:O	1:L:198:ARG:C	2.58	0.47
1:B:118:VAL:HG13	1:B:118:VAL:O	2.13	0.47
1:B:159:THR:O	1:B:160:GLU:C	2.57	0.47
1:H:96:GLN:NE2	1:H:131:ARG:HH21	2.13	0.47
1:H:192:LEU:C	1:H:193:LEU:HD23	2.40	0.47
1:H:289:PRO:CD	1:H:290:GLU:H	2.27	0.47
1:B:301:LEU:HD13	1:B:322:HIS:CD2	2.49	0.46
1:E:72:LEU:HD13	1:E:77:LYS:HG2	1.98	0.46
1:E:191:ASN:ND2	1:E:207:ASP:HB2	2.30	0.46
1:G:238:GLU:CD	1:G:242:LYS:HE3	2.40	0.46
1:H:185:ARG:HB3	1:H:185:ARG:HH11	1.79	0.46
1:H:329:THR:C	1:H:331:VAL:H	2.22	0.46
1:L:107:LEU:HD23	1:L:110:ARG:HH21	1.80	0.46
1:D:138:MET:C	1:D:139:GLU:O	2.58	0.46
1:D:196:SER:O	1:D:201:ALA:HB2	2.15	0.46
1:E:98:CYS:HB2	1:E:99:PRO:HD3	1.96	0.46
1:E:230:VAL:CG2	1:E:231:ALA:N	2.78	0.46
1:E:309:GLU:OE2	1:E:310:PRO:HD2	2.15	0.46
1:F:230:VAL:O	1:F:230:VAL:HG13	2.14	0.46
1:G:331:VAL:CG1	1:G:332:PRO:HD2	2.45	0.46
1:H:97:ASP:OD1	1:H:102:ARG:HD3	2.16	0.46
1:H:301:LEU:CD1	1:H:314:MET:HE1	2.45	0.46
1:J:256:LEU:O	1:J:256:LEU:CD1	2.61	0.46
1:L:55:LYS:HD2	1:L:124:TYR:CE2	2.50	0.46
1:L:315:THR:HG1	1:L:317:THR:HG22	1.81	0.46
1:A:159:THR:OG1	1:A:162:GLU:HG3	2.15	0.46
1:D:147:PHE:HE2	1:D:256:LEU:CD2	2.28	0.46
1:E:99:PRO:O	1:E:100:LYS:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:241:ASP:O	1:G:244:CYS:CB	2.63	0.46
1:G:343:LYS:O	1:G:346:LYS:HB2	2.15	0.46
1:H:196:SER:H	1:H:201:ALA:HB1	1.80	0.46
1:J:258:CYS:SG	1:J:260:TYR:CE1	3.09	0.46
1:K:142:ASP:C	1:K:144:GLY:H	2.22	0.46
1:D:70:LEU:H	1:D:70:LEU:HD22	1.77	0.46
1:D:82:PHE:HD1	1:D:87:GLN:O	1.98	0.46
1:D:289:PRO:CG	1:D:290:GLU:H	2.28	0.46
1:E:234:VAL:O	1:E:234:VAL:HG12	2.15	0.46
1:E:331:VAL:HA	1:E:332:PRO:HD3	1.67	0.46
1:G:188:LYS:HB2	1:G:189:PRO:CD	2.45	0.46
1:G:189:PRO:HD2	1:G:190:GLU:OE1	2.15	0.46
1:H:102:ARG:O	1:H:106:GLU:HB2	2.16	0.46
1:H:293:GLU:HA	1:H:293:GLU:OE2	2.15	0.46
1:I:129:ALA:C	1:I:131:ARG:H	2.23	0.46
1:I:331:VAL:HA	1:I:332:PRO:HD3	1.81	0.46
1:J:82:PHE:HA	1:J:88:GLU:O	2.15	0.46
1:K:72:LEU:CD1	1:K:77:LYS:HA	2.45	0.46
1:A:74:ILE:HG12	1:A:209:GLY:HA3	1.96	0.46
1:A:332:PRO:HB3	1:A:334:THR:HG22	1.97	0.46
1:E:64:LYS:C	1:E:64:LYS:HD3	2.40	0.46
1:F:74:ILE:HD12	1:F:74:ILE:C	2.41	0.46
1:G:265:SER:O	1:G:266:ASN:HB2	2.15	0.46
1:H:70:LEU:HG	2:H:1347:P4O:C17	2.46	0.46
1:I:140:CYS:HG	2:I:1351:P4O:H17	1.81	0.46
1:I:188:LYS:HD2	1:I:190:GLU:OE2	2.16	0.46
1:J:295:SER:O	1:J:299:LYS:HE3	2.14	0.46
1:K:188:LYS:HD2	1:K:190:GLU:OE2	2.15	0.46
1:K:330:LYS:HD3	1:K:330:LYS:N	2.31	0.46
1:B:145:GLU:HA	1:B:193:LEU:HD23	1.96	0.46
1:B:151:GLN:HE21	1:B:343:LYS:HB3	1.80	0.46
1:B:237:PRO:O	1:B:238:GLU:CB	2.64	0.46
1:C:72:LEU:HD12	1:C:73:GLY:H	1.80	0.46
1:C:321:ASN:O	1:C:326:MET:HG3	2.16	0.46
1:D:70:LEU:HD21	1:D:80:GLN:CB	2.33	0.46
1:E:286:PHE:CD1	1:E:299:LYS:HD3	2.51	0.46
1:F:200:ASN:HD22	1:F:200:ASN:H	1.63	0.46
1:G:232:PRO:HB3	1:H:279:ILE:HG22	1.97	0.46
1:J:153:ARG:NH2	1:J:162:GLU:OE1	2.49	0.46
1:J:190:GLU:O	1:J:191:ASN:ND2	2.49	0.46
1:K:300:MET:CE	1:K:303:ARG:HH21	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:47:HIS:O	1:L:47:HIS:ND1	2.47	0.46
1:L:184:HIS:CE1	1:L:205:LEU:HD21	2.50	0.46
1:B:188:LYS:HD2	1:B:190:GLU:OE2	2.16	0.46
1:D:246:MET:HE2	1:D:315:THR:C	2.40	0.46
1:E:191:ASN:ND2	1:E:207:ASP:CB	2.78	0.46
1:E:212:LYS:HG2	1:E:213:GLU:O	2.16	0.46
1:E:257:LEU:HD13	1:E:291:TRP:HZ3	1.81	0.46
1:G:278:ARG:HH11	1:G:278:ARG:HG3	1.81	0.46
1:H:119:ARG:HG2	1:H:120:ILE:N	2.30	0.46
1:H:148:SER:O	1:H:150:ILE:N	2.49	0.46
1:I:127:LEU:HA	1:I:127:LEU:HD23	1.68	0.46
1:J:296:GLU:O	1:J:300:MET:N	2.39	0.46
1:J:301:LEU:HD22	1:J:322:HIS:CG	2.51	0.46
1:J:321:ASN:OD1	1:J:326:MET:HE2	2.15	0.46
1:K:256:LEU:HA	1:K:256:LEU:HD23	1.79	0.46
1:K:287:PRO:O	1:K:291:TRP:HD1	1.97	0.46
1:B:167:MET:HG3	1:B:253:MET:HG3	1.97	0.46
1:B:233:GLU:HG2	1:C:310:PRO:HD3	1.98	0.46
1:D:90:PHE:HA	1:D:140:CYS:HB2	1.96	0.46
1:D:275:MET:HE3	1:D:279:ILE:HD11	1.97	0.46
1:G:207:ASP:HB2	2:G:1350:P4O:N7	2.31	0.46
1:G:300:MET:CE	1:G:303:ARG:HH21	2.28	0.46
1:G:302:ILE:HG22	1:G:306:LEU:HD12	1.98	0.46
1:H:186:ASP:OD1	1:H:188:LYS:HE3	2.15	0.46
1:L:172:GLU:HG2	1:L:320:MET:HE1	1.98	0.46
1:L:178:HIS:ND1	1:L:242:LYS:CD	2.79	0.46
1:L:324:TRP:CD1	1:L:331:VAL:HG21	2.50	0.46
1:B:83:ASN:CG	1:B:86:THR:HG22	2.41	0.46
1:D:340:ARG:HG2	1:D:344:GLU:OE1	2.16	0.46
1:E:264:TYR:CB	1:E:278:ARG:HH22	2.28	0.46
1:F:145:GLU:HA	1:F:193:LEU:HD23	1.98	0.46
1:I:162:GLU:O	1:I:166:ILE:HG13	2.16	0.46
1:K:286:PHE:HE1	1:K:303:ARG:NH1	2.13	0.46
1:B:89:LYS:C	1:B:90:PHE:CD1	2.94	0.46
1:B:161:ARG:O	1:B:165:GLU:HG3	2.15	0.46
1:C:256:LEU:HA	1:C:256:LEU:HD23	1.66	0.46
1:E:130:GLY:HA3	1:J:180:ILE:CG2	2.45	0.46
1:F:134:LEU:HD12	1:F:134:LEU:HA	1.60	0.46
1:H:108:HIS:CG	1:H:120:ILE:HD11	2.51	0.46
1:H:331:VAL:HG13	1:H:332:PRO:CD	2.41	0.46
1:I:140:CYS:SG	2:I:1351:P4O:H17	2.56	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:195:THR:HG23	1:I:202:ILE:N	2.31	0.46
1:J:304:ASN:O	1:J:305:LEU:C	2.58	0.46
1:K:49:LYS:CD	1:K:50:SER:H	2.28	0.46
1:L:149:ARG:O	1:L:153:ARG:HD3	2.16	0.46
1:A:94:MET:SD	1:F:46:PHE:HZ	2.40	0.45
1:B:181:ASN:CB	1:B:214:THR:HG22	2.45	0.45
1:B:349:TRP:CG	1:B:349:TRP:O	2.69	0.45
1:C:139:GLU:O	2:C:1351:P4O:H10	2.15	0.45
1:D:150:ILE:CD1	1:D:158:PHE:CE2	2.98	0.45
1:G:134:LEU:HA	1:G:134:LEU:HD12	1.58	0.45
1:G:147:PHE:CZ	1:G:255:ILE:HG22	2.51	0.45
1:J:210:PHE:O	1:J:211:ALA:C	2.59	0.45
1:L:252:ILE:O	1:L:252:ILE:CG2	2.64	0.45
1:L:304:ASN:HD22	1:L:307:LYS:CE	2.29	0.45
1:A:131:ARG:HH11	1:D:273:PRO:HB3	1.81	0.45
1:A:185:ARG:HB3	1:A:185:ARG:HH11	1.80	0.45
1:B:202:ILE:HD13	1:B:202:ILE:N	2.27	0.45
1:F:337:HIS:C	1:F:341:VAL:HG23	2.41	0.45
1:H:59:ILE:O	1:H:59:ILE:HG12	2.15	0.45
1:I:70:LEU:HD21	1:I:80:GLN:HB2	1.98	0.45
1:I:141:LEU:HD13	1:I:193:LEU:HB2	1.98	0.45
1:K:194:TYR:HA	1:K:202:ILE:O	2.17	0.45
1:L:53:GLN:HA	1:L:53:GLN:HE21	1.80	0.45
1:L:63:TYR:CG	1:L:81:ILE:HD12	2.51	0.45
1:L:120:ILE:HD13	1:L:138:MET:CE	2.47	0.45
1:B:286:PHE:HE1	1:B:303:ARG:NH1	2.13	0.45
1:D:246:MET:CE	1:D:316:ILE:HA	2.46	0.45
1:E:48:VAL:CG1	1:H:60:ILE:HD13	2.43	0.45
1:H:332:PRO:CB	1:H:334:THR:HG22	2.45	0.45
1:J:189:PRO:O	1:J:191:ASN:N	2.47	0.45
1:J:248:SER:C	1:J:250:GLY:H	2.24	0.45
1:K:159:THR:OG1	1:K:162:GLU:HG3	2.16	0.45
1:L:141:LEU:HB2	1:L:193:LEU:HD12	1.98	0.45
1:L:170:ILE:O	1:L:170:ILE:HG22	2.16	0.45
1:B:174:ILE:HD11	1:B:187:VAL:HG21	1.97	0.45
1:C:287:PRO:O	1:C:291:TRP:HD1	1.99	0.45
1:D:264:TYR:HE2	1:D:348:ARG:HH12	1.63	0.45
1:E:171:GLY:O	1:E:175:GLN:HB3	2.16	0.45
1:E:210:PHE:O	1:E:211:ALA:O	2.34	0.45
1:E:247:TRP:O	1:E:248:SER:C	2.56	0.45
1:G:86:THR:HG22	1:G:88:GLU:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:331:VAL:HA	1:H:332:PRO:HD3	1.72	0.45
1:K:271:ILE:HG12	1:K:274:GLY:H	1.82	0.45
1:L:146:LEU:C	1:L:148:SER:N	2.74	0.45
1:L:162:GLU:C	1:L:164:SER:N	2.75	0.45
1:B:158:PHE:HE1	1:B:256:LEU:HD22	1.82	0.45
1:B:181:ASN:HD22	1:B:214:THR:CG2	2.29	0.45
1:B:229:TYR:CD2	1:B:229:TYR:N	2.82	0.45
1:C:127:LEU:HD23	1:C:127:LEU:HA	1.79	0.45
1:I:150:ILE:HD12	1:I:158:PHE:CE2	2.52	0.45
1:J:166:ILE:CG2	1:J:256:LEU:HD11	2.46	0.45
1:K:311:THR:HG21	1:L:311:THR:OG1	2.17	0.45
1:L:255:ILE:CD1	1:L:261:PRO:HA	2.46	0.45
1:A:134:LEU:HD12	1:A:134:LEU:HA	1.72	0.45
1:C:227:PRO:HD2	1:C:230:VAL:HB	1.98	0.45
1:D:159:THR:C	1:D:336:LEU:CD2	2.90	0.45
1:E:128:TYR:HD1	1:E:129:ALA:N	2.14	0.45
1:E:128:TYR:C	1:E:130:GLY:N	2.74	0.45
1:E:343:LYS:O	1:E:344:GLU:C	2.60	0.45
1:F:100:LYS:O	1:F:103:ARG:HB3	2.16	0.45
1:G:184:HIS:HD2	1:G:186:ASP:N	2.14	0.45
1:J:60:ILE:O	1:J:60:ILE:CG1	2.62	0.45
1:B:98:CYS:HB2	1:B:99:PRO:CD	2.46	0.45
1:B:158:PHE:CE1	1:B:256:LEU:HD22	2.52	0.45
1:C:260:TYR:HB2	1:C:261:PRO:HD2	1.99	0.45
1:C:334:THR:HA	1:C:335:PRO:HD3	1.67	0.45
1:D:161:ARG:O	1:D:165:GLU:HG3	2.16	0.45
1:E:192:LEU:C	1:E:193:LEU:HD23	2.42	0.45
1:F:125:GLU:HA	1:F:133:CYS:O	2.17	0.45
1:G:142:ASP:HA	2:G:1350:P4O:N16	2.32	0.45
1:G:161:ARG:NH1	1:G:333:GLN:OE1	2.50	0.45
1:G:314:MET:CG	1:G:318:GLU:HB2	2.47	0.45
1:H:87:GLN:NE2	1:H:87:GLN:CA	2.78	0.45
1:H:88:GLU:HG3	1:H:89:LYS:N	2.32	0.45
1:H:271:ILE:CD1	1:H:278:ARG:NH1	2.79	0.45
1:I:116:HIS:CE1	1:I:169:SER:HB3	2.52	0.45
1:I:164:SER:HA	1:I:324:TRP:CZ3	2.51	0.45
1:K:134:LEU:C	1:K:135:LEU:HD23	2.41	0.45
1:L:94:MET:O	1:L:95:LEU:HD23	2.16	0.45
1:A:110:ARG:NH1	1:G:130:GLY:O	2.47	0.45
1:A:128:TYR:O	1:A:129:ALA:CB	2.65	0.45
1:C:343:LYS:O	1:C:345:ASP:N	2.46	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:160:GLU:HB2	1:E:334:THR:HG23	1.97	0.45
1:E:198:ARG:O	1:E:199:PRO:C	2.59	0.45
1:G:158:PHE:O	1:G:336:LEU:HD22	2.17	0.45
1:G:234:VAL:C	1:G:236:GLY:N	2.75	0.45
1:I:278:ARG:HA	1:I:283:GLN:HG3	1.99	0.45
1:J:301:LEU:HD22	1:J:322:HIS:ND1	2.32	0.45
1:J:302:ILE:O	1:J:306:LEU:HB2	2.17	0.45
1:K:72:LEU:HD13	1:K:72:LEU:HA	1.52	0.45
1:K:110:ARG:NH1	1:K:110:ARG:HG2	2.31	0.45
1:A:159:THR:O	1:A:160:GLU:C	2.58	0.45
1:C:74:ILE:HD11	1:C:75:ASN:HD21	1.82	0.45
1:D:300:MET:HE2	1:D:303:ARG:HH21	1.82	0.45
1:E:301:LEU:HD12	1:E:314:MET:HE1	1.98	0.45
1:F:70:LEU:HD11	1:F:80:GLN:CA	2.44	0.45
1:F:332:PRO:C	1:F:334:THR:H	2.25	0.45
1:F:334:THR:HA	1:F:335:PRO:HD3	1.75	0.45
1:F:343:LYS:O	1:F:346:LYS:HB2	2.17	0.45
1:G:286:PHE:CE1	1:G:299:LYS:HB3	2.51	0.45
1:H:151:GLN:NE2	1:H:346:LYS:HD2	2.32	0.45
1:J:71:GLY:O	1:J:72:LEU:O	2.34	0.45
1:L:202:ILE:N	1:L:202:ILE:CD1	2.80	0.45
1:B:56:LYS:NZ	1:I:52:LEU:O	2.50	0.45
1:D:247:TRP:CE2	1:F:231:ALA:HA	2.52	0.45
1:D:278:ARG:HH11	1:D:278:ARG:CG	2.30	0.45
1:E:99:PRO:C	1:E:101:ALA:N	2.73	0.45
1:F:74:ILE:CG2	1:F:209:GLY:HA3	2.46	0.45
1:I:75:ASN:N	1:I:75:ASN:ND2	2.64	0.45
1:J:59:ILE:C	1:J:61:ASP:N	2.75	0.45
1:J:167:MET:C	1:J:169:SER:H	2.25	0.45
1:L:208:PHE:C	1:L:210:PHE:N	2.75	0.45
1:L:251:VAL:O	1:L:255:ILE:HG13	2.16	0.45
1:A:74:ILE:HD12	1:A:74:ILE:O	2.17	0.44
1:A:333:GLN:HE21	1:A:333:GLN:HB3	1.43	0.44
1:B:86:THR:O	1:B:88:GLU:N	2.50	0.44
1:D:86:THR:HG21	1:D:88:GLU:CB	2.39	0.44
1:D:174:ILE:HD11	1:D:187:VAL:HG21	1.99	0.44
1:E:158:PHE:O	1:E:335:PRO:HA	2.16	0.44
1:F:160:GLU:HA	1:F:336:LEU:HD11	1.99	0.44
1:H:344:GLU:O	1:H:345:ASP:HB2	2.17	0.44
1:J:157:ALA:O	1:J:158:PHE:HB3	2.17	0.44
1:J:304:ASN:N	1:J:304:ASN:OD1	2.49	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:266:ASN:HD22	1:L:266:ASN:HA	1.53	0.44
1:L:319:PHE:CD1	1:L:319:PHE:C	2.94	0.44
1:B:86:THR:HG23	1:B:88:GLU:CB	2.36	0.44
1:B:147:PHE:CE1	1:B:255:ILE:HG21	2.52	0.44
1:C:94:MET:HE2	1:C:94:MET:HB3	1.71	0.44
1:E:108:HIS:CD2	1:E:120:ILE:HD11	2.53	0.44
1:G:234:VAL:C	1:G:236:GLY:H	2.24	0.44
1:G:253:MET:HE2	1:G:324:TRP:HZ3	1.82	0.44
1:I:86:THR:HG23	1:I:88:GLU:H	1.82	0.44
1:I:110:ARG:HG2	1:I:110:ARG:HH11	1.82	0.44
1:I:300:MET:HE1	1:I:303:ARG:HH21	1.82	0.44
1:J:83:ASN:ND2	1:J:83:ASN:C	2.75	0.44
1:J:198:ARG:CG	1:J:198:ARG:NH1	2.74	0.44
1:K:170:ILE:HG22	1:K:249:LEU:HD11	1.99	0.44
1:B:94:MET:HE2	1:B:94:MET:HB3	1.68	0.44
1:B:118:VAL:HG11	1:B:206:THR:HG22	2.00	0.44
1:B:296:GLU:O	1:B:300:MET:HB2	2.17	0.44
1:B:331:VAL:HA	1:B:332:PRO:HD3	1.81	0.44
1:C:104:GLU:HG3	1:C:208:PHE:C	2.42	0.44
1:C:343:LYS:H	1:C:343:LYS:HG2	1.63	0.44
1:D:232:PRO:HD3	1:E:247:TRP:CZ2	2.52	0.44
1:D:313:ARG:CZ	1:F:233:GLU:OE1	2.65	0.44
1:F:86:THR:CG2	1:F:88:GLU:N	2.71	0.44
1:G:230:VAL:HG21	1:G:235:LEU:HD23	1.97	0.44
1:H:300:MET:HE1	1:H:303:ARG:HE	1.82	0.44
1:K:75:ASN:CB	1:K:95:LEU:HD22	2.47	0.44
1:L:74:ILE:HG13	1:L:75:ASN:N	2.31	0.44
1:L:111:ALA:O	1:L:113:GLN:N	2.50	0.44
1:L:190:GLU:C	1:L:191:ASN:HD22	2.25	0.44
1:L:277:THR:O	1:L:279:ILE:N	2.50	0.44
1:A:70:LEU:HD23	1:A:70:LEU:HA	1.80	0.44
1:B:103:ARG:O	1:B:104:GLU:C	2.61	0.44
1:D:97:ASP:OD1	1:D:102:ARG:NH2	2.45	0.44
1:E:83:ASN:O	1:E:87:GLN:N	2.51	0.44
1:E:108:HIS:CG	1:E:120:ILE:HD11	2.52	0.44
1:E:128:TYR:C	1:E:130:GLY:H	2.25	0.44
1:E:178:HIS:CG	1:E:242:LYS:HD3	2.53	0.44
1:E:336:LEU:HD13	1:E:336:LEU:HA	1.56	0.44
1:F:231:ALA:HB1	1:F:232:PRO:HD2	2.00	0.44
1:G:63:TYR:CA	1:G:84:LYS:HG3	2.48	0.44
1:G:84:LYS:HB3	1:G:84:LYS:HE2	1.55	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:332:PRO:HB2	1:G:334:THR:CG2	2.45	0.44
1:H:66:THR:HG21	1:H:82:PHE:HE2	1.81	0.44
1:H:114:CYS:HA	1:H:115:PRO:HD3	1.75	0.44
1:H:217:HIS:CD2	1:H:217:HIS:N	2.85	0.44
1:H:309:GLU:OE2	1:H:310:PRO:HD2	2.17	0.44
1:J:113:GLN:H	1:J:113:GLN:HG2	1.58	0.44
1:J:244:CYS:O	1:J:247:TRP:HB3	2.17	0.44
1:J:296:GLU:CD	1:J:296:GLU:N	2.74	0.44
1:K:272:SER:H	1:K:273:PRO:CD	2.30	0.44
1:L:74:ILE:O	1:L:75:ASN:O	2.34	0.44
1:L:113:GLN:O	1:L:114:CYS:C	2.61	0.44
1:L:115:PRO:O	1:L:204:LYS:HG2	2.17	0.44
1:A:70:LEU:HD13	2:A:1351:P4O:C18	2.46	0.44
1:B:158:PHE:HZ	1:B:166:ILE:HD12	1.82	0.44
1:B:192:LEU:C	1:B:193:LEU:HD23	2.42	0.44
1:B:212:LYS:HG2	1:B:213:GLU:O	2.17	0.44
1:E:227:PRO:HB2	1:E:230:VAL:HB	1.98	0.44
1:G:80:GLN:NE2	1:G:89:LYS:HE2	2.33	0.44
1:G:237:PRO:O	1:G:238:GLU:CB	2.66	0.44
1:H:85:ARG:O	1:H:85:ARG:HG2	2.18	0.44
1:H:184:HIS:HE1	1:H:206:THR:O	2.00	0.44
1:I:69:VAL:HG11	1:I:72:LEU:CD1	2.48	0.44
1:I:86:THR:HG23	1:I:88:GLU:CB	2.47	0.44
1:J:178:HIS:CD2	1:J:182:ILE:O	2.69	0.44
1:K:309:GLU:HB3	1:K:312:GLN:HB2	1.99	0.44
1:L:136:ILE:CG2	1:L:138:MET:HE3	2.48	0.44
1:L:166:ILE:O	1:L:169:SER:HB2	2.18	0.44
1:A:174:ILE:HD11	1:A:187:VAL:HG21	1.99	0.44
1:D:343:LYS:C	1:D:345:ASP:H	2.26	0.44
1:E:107:LEU:HD23	1:E:107:LEU:HA	1.52	0.44
1:E:180:ILE:HG13	1:E:180:ILE:O	2.16	0.44
1:E:234:VAL:O	1:E:234:VAL:CG1	2.65	0.44
1:F:86:THR:HG22	1:F:87:GLN:N	2.32	0.44
1:I:166:ILE:O	1:I:167:MET:C	2.61	0.44
1:I:195:THR:HG23	1:I:202:ILE:C	2.42	0.44
1:I:195:THR:HG21	1:I:202:ILE:CB	2.47	0.44
1:J:72:LEU:HA	1:J:77:LYS:HA	1.99	0.44
1:J:195:THR:CG2	1:J:201:ALA:HB3	2.47	0.44
1:J:313:ARG:O	1:J:314:MET:O	2.35	0.44
1:K:158:PHE:HE2	1:K:163:ALA:N	2.16	0.44
1:L:44:PRO:O	1:L:45:GLN:CG	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:89:LYS:O	1:L:140:CYS:HB2	2.18	0.44
1:A:233:GLU:OE1	1:B:313:ARG:NH1	2.47	0.44
1:B:81:ILE:HD13	1:B:92:LEU:HB2	1.99	0.44
1:G:104:GLU:O	1:G:105:VAL:C	2.61	0.44
1:H:110:ARG:NH1	1:J:130:GLY:O	2.51	0.44
1:H:175:GLN:HA	1:H:316:ILE:HG12	2.00	0.44
1:K:143:GLY:CA	1:K:196:SER:C	2.91	0.44
1:L:72:LEU:HD12	1:L:77:LYS:HB3	1.99	0.44
1:L:99:PRO:HA	1:L:102:ARG:HB2	2.00	0.44
1:L:165:GLU:HG2	1:L:328:SER:CB	2.31	0.44
1:A:256:LEU:HD23	1:A:256:LEU:HA	1.76	0.44
1:B:256:LEU:HA	1:B:256:LEU:HD23	1.35	0.44
1:C:74:ILE:CG2	1:C:207:ASP:OD2	2.66	0.44
1:C:178:HIS:CE1	1:C:242:LYS:HB3	2.53	0.44
1:C:331:VAL:HA	1:C:332:PRO:HD3	1.61	0.44
1:D:230:VAL:HG11	1:D:235:LEU:CD2	2.30	0.44
1:E:175:GLN:O	1:E:175:GLN:HG3	2.18	0.44
1:E:264:TYR:HB3	1:E:278:ARG:HH22	1.82	0.44
1:E:302:ILE:O	1:E:302:ILE:CG2	2.65	0.44
1:H:56:LYS:HD3	1:H:125:GLU:HB3	1.98	0.44
1:H:87:GLN:CA	1:H:87:GLN:HE21	2.30	0.44
1:H:147:PHE:O	1:H:151:GLN:HB2	2.17	0.44
1:J:147:PHE:CZ	1:J:255:ILE:HG21	2.53	0.44
1:J:315:THR:OG1	1:J:318:GLU:HG3	2.17	0.44
1:C:191:ASN:HD22	1:C:191:ASN:HA	1.50	0.44
1:C:293:GLU:OE2	1:C:293:GLU:N	2.47	0.44
1:D:334:THR:HA	1:D:335:PRO:HD3	1.74	0.44
1:F:300:MET:HE1	1:F:303:ARG:NH2	2.33	0.44
1:F:337:HIS:O	1:F:338:THR:C	2.60	0.44
1:G:60:ILE:C	1:G:62:ASP:N	2.75	0.44
1:G:322:HIS:ND1	1:G:323:PRO:HD2	2.32	0.44
1:H:345:ASP:O	1:H:346:LYS:C	2.61	0.44
1:I:79:LEU:N	1:I:79:LEU:HD23	2.33	0.44
1:I:156:GLN:HE21	1:I:156:GLN:HB2	1.55	0.44
1:I:322:HIS:CE1	1:I:323:PRO:HD2	2.52	0.44
1:J:167:MET:HA	1:J:167:MET:CE	2.41	0.44
1:K:86:THR:HG21	1:K:88:GLU:HB2	2.00	0.44
1:L:145:GLU:O	1:L:145:GLU:HG3	2.17	0.44
1:L:290:GLU:HA	1:L:337:HIS:CE1	2.53	0.44
1:A:325:ILE:HD12	1:A:325:ILE:HG23	1.74	0.43
1:B:233:GLU:H	1:B:233:GLU:HG3	1.08	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:ILE:C	1:C:62:ASP:N	2.74	0.43
1:D:114:CYS:SG	1:D:115:PRO:HD2	2.58	0.43
1:D:309:GLU:HB3	1:D:312:GLN:HB2	2.00	0.43
1:E:179:SER:OG	1:E:180:ILE:HG23	2.18	0.43
1:H:46:PHE:HE2	1:J:65:VAL:HG11	1.83	0.43
1:I:85:ARG:O	1:I:85:ARG:HG3	2.17	0.43
1:I:154:GLY:O	1:I:156:GLN:N	2.50	0.43
1:J:99:PRO:O	1:J:100:LYS:C	2.60	0.43
1:K:134:LEU:HD12	1:K:134:LEU:HA	1.59	0.43
1:K:271:ILE:CG2	1:K:278:ARG:NH1	2.74	0.43
1:L:96:GLN:HG2	1:L:97:ASP:N	2.33	0.43
1:L:298:VAL:O	1:L:298:VAL:HG12	2.18	0.43
1:A:161:ARG:O	1:A:165:GLU:HG3	2.18	0.43
1:C:110:ARG:HG2	1:C:110:ARG:HH11	1.84	0.43
1:D:134:LEU:HD12	1:D:134:LEU:HA	1.84	0.43
1:D:180:ILE:HG13	1:D:180:ILE:O	2.18	0.43
1:D:239:LYS:C	1:D:241:ASP:N	2.77	0.43
1:E:74:ILE:HD12	1:E:74:ILE:C	2.44	0.43
1:F:127:LEU:HD23	1:F:127:LEU:HA	1.82	0.43
1:F:210:PHE:N	1:F:210:PHE:HD2	2.15	0.43
1:H:47:HIS:HB3	1:H:49:LYS:HZ1	1.82	0.43
1:I:159:THR:O	1:I:160:GLU:C	2.62	0.43
1:I:184:HIS:HD2	1:I:186:ASP:H	1.65	0.43
1:J:163:ALA:CB	1:J:257:LEU:HG	2.48	0.43
1:J:176:TYR:HA	1:J:179:SER:OG	2.18	0.43
1:L:184:HIS:C	1:L:184:HIS:HD2	2.26	0.43
1:A:184:HIS:HD2	1:A:186:ASP:H	1.66	0.43
1:A:234:VAL:C	1:A:236:GLY:H	2.25	0.43
1:E:66:THR:HG21	1:E:82:PHE:HE2	1.83	0.43
1:E:110:ARG:HD3	1:H:127:LEU:HD21	1.99	0.43
1:H:88:GLU:HG2	1:H:90:PHE:CZ	2.52	0.43
1:H:305:LEU:O	1:H:313:ARG:HD3	2.18	0.43
1:L:257:LEU:HD23	1:L:336:LEU:HG	1.98	0.43
1:A:164:SER:HA	1:A:324:TRP:CH2	2.54	0.43
1:D:52:LEU:HA	1:D:52:LEU:HD12	1.65	0.43
1:D:280:ARG:HG2	1:F:235:LEU:CD1	2.47	0.43
1:E:197:LYS:O	1:E:198:ARG:C	2.62	0.43
1:E:202:ILE:HG13	1:E:203:LEU:N	2.32	0.43
1:E:257:LEU:HD13	1:E:291:TRP:CZ3	2.54	0.43
1:E:287:PRO:O	1:E:291:TRP:CD1	2.70	0.43
1:G:86:THR:CG2	1:G:88:GLU:HB2	2.47	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:130:GLY:CA	1:K:180:ILE:HB	2.46	0.43
1:K:77:LYS:HB3	1:K:77:LYS:HE2	1.37	0.43
1:K:103:ARG:O	1:K:104:GLU:C	2.62	0.43
1:L:170:ILE:CD1	1:L:192:LEU:HD22	2.48	0.43
1:L:214:THR:O	1:L:215:THR:HG23	2.18	0.43
1:L:341:VAL:O	1:L:341:VAL:HG12	2.17	0.43
1:A:60:ILE:C	1:A:62:ASP:N	2.75	0.43
1:E:230:VAL:CG2	1:E:231:ALA:H	2.31	0.43
1:G:63:TYR:CG	1:G:81:ILE:HD12	2.54	0.43
1:H:46:PHE:CE2	1:J:65:VAL:HG11	2.54	0.43
1:H:332:PRO:HB2	1:H:334:THR:HG22	1.99	0.43
1:I:98:CYS:CB	1:I:99:PRO:CD	2.95	0.43
1:J:143:GLY:CA	1:J:196:SER:O	2.59	0.43
1:J:254:TYR:CD1	1:J:262:PRO:CD	3.02	0.43
1:L:249:LEU:HD21	1:L:319:PHE:CZ	2.54	0.43
1:D:57:ASN:O	1:D:58:ALA:C	2.61	0.43
1:D:70:LEU:HD12	2:D:1351:P4O:C18	2.48	0.43
1:D:346:LYS:O	1:D:347:GLU:O	2.37	0.43
1:E:134:LEU:O	1:E:135:LEU:HD23	2.18	0.43
1:H:127:LEU:HD23	1:H:127:LEU:HA	1.75	0.43
1:H:242:LYS:O	1:H:245:ASP:N	2.52	0.43
1:K:83:ASN:ND2	1:K:85:ARG:HG2	2.33	0.43
1:K:161:ARG:O	1:K:165:GLU:HG3	2.17	0.43
1:L:304:ASN:HD22	1:L:304:ASN:HA	1.66	0.43
1:A:74:ILE:HG13	1:A:75:ASN:N	2.33	0.43
1:A:86:THR:O	1:A:87:GLN:HB2	2.18	0.43
1:A:129:ALA:O	1:A:131:ARG:N	2.52	0.43
1:B:86:THR:C	1:B:88:GLU:N	2.76	0.43
1:B:127:LEU:O	1:I:48:VAL:HG23	2.19	0.43
1:B:201:ALA:O	1:B:202:ILE:HD13	2.18	0.43
1:C:323:PRO:HA	1:C:326:MET:HB2	2.01	0.43
1:D:327:GLN:C	1:D:329:THR:H	2.26	0.43
1:E:56:LYS:O	1:J:51:GLY:N	2.50	0.43
1:G:83:ASN:HD22	1:G:85:ARG:H	1.65	0.43
1:G:146:LEU:HD11	1:G:166:ILE:HD13	2.00	0.43
1:H:271:ILE:HD11	1:H:278:ARG:NH1	2.33	0.43
1:H:322:HIS:HA	1:H:323:PRO:HD3	1.80	0.43
1:I:161:ARG:O	1:I:165:GLU:HG3	2.18	0.43
1:J:127:LEU:HD23	1:J:127:LEU:HA	1.68	0.43
1:J:300:MET:HE2	1:J:300:MET:HB2	1.84	0.43
1:K:150:ILE:O	1:K:150:ILE:HG12	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:170:ILE:HG12	1:L:192:LEU:CD2	2.49	0.43
1:L:314:MET:HG3	1:L:318:GLU:HB2	2.00	0.43
1:A:301:LEU:HD13	1:A:322:HIS:CD2	2.54	0.43
1:E:58:ALA:HA	1:E:126:ASN:OD1	2.19	0.43
1:E:305:LEU:HA	1:E:305:LEU:HD23	1.82	0.43
1:F:322:HIS:CE1	1:F:323:PRO:HD2	2.54	0.43
1:G:45:GLN:CG	1:G:46:PHE:N	2.63	0.43
1:G:102:ARG:O	1:G:106:GLU:HB2	2.19	0.43
1:H:210:PHE:O	1:H:211:ALA:C	2.59	0.43
1:H:337:HIS:CD2	1:H:340:ARG:NH1	2.86	0.43
1:I:195:THR:HG21	1:I:202:ILE:CG1	2.49	0.43
1:I:321:ASN:C	1:I:326:MET:HG3	2.44	0.43
1:J:59:ILE:O	1:J:61:ASP:N	2.43	0.43
1:J:89:LYS:O	1:J:90:PHE:CD2	2.71	0.43
1:J:247:TRP:HA	1:J:247:TRP:CE3	2.54	0.43
1:K:70:LEU:HD23	1:K:91:ALA:CB	2.49	0.43
1:K:160:GLU:CD	1:K:294:VAL:HG13	2.41	0.43
1:L:75:ASN:HB2	1:L:76:GLY:H	1.69	0.43
1:B:114:CYS:HA	1:B:115:PRO:HD3	1.91	0.43
1:C:99:PRO:HD2	1:C:100:LYS:H	1.83	0.43
1:C:129:ALA:C	1:C:131:ARG:H	2.26	0.43
1:C:134:LEU:HD12	1:C:134:LEU:HA	1.85	0.43
1:D:74:ILE:HB	1:D:210:PHE:CE2	2.54	0.43
1:D:331:VAL:HA	1:D:332:PRO:HD3	1.79	0.43
1:E:159:THR:O	1:E:160:GLU:C	2.61	0.43
1:E:168:LYS:O	1:E:172:GLU:HG3	2.19	0.43
1:H:134:LEU:HA	1:H:134:LEU:HD12	1.62	0.43
1:H:329:THR:C	1:H:331:VAL:N	2.76	0.43
1:I:114:CYS:HA	1:I:115:PRO:HD3	1.87	0.43
1:J:157:ALA:O	1:J:158:PHE:CB	2.66	0.43
1:A:60:ILE:O	1:A:61:ASP:C	2.62	0.43
1:C:74:ILE:CB	1:C:210:PHE:HE2	2.32	0.43
1:C:98:CYS:HB2	1:C:99:PRO:HD3	2.00	0.43
1:F:214:THR:O	1:F:215:THR:C	2.62	0.43
1:F:287:PRO:O	1:F:291:TRP:HB2	2.19	0.43
1:H:118:VAL:O	1:H:118:VAL:HG13	2.18	0.43
1:H:185:ARG:HH21	1:H:212:LYS:HD2	1.84	0.43
1:H:289:PRO:O	1:H:291:TRP:N	2.51	0.43
1:J:166:ILE:HD13	1:J:203:LEU:HD21	2.01	0.43
1:J:247:TRP:HA	1:J:247:TRP:HE3	1.84	0.43
1:K:114:CYS:HA	1:K:115:PRO:HD3	1.84	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:142:ASP:C	1:K:144:GLY:N	2.77	0.43
1:L:97:ASP:HB2	1:L:132:LYS:O	2.19	0.43
1:A:60:ILE:HD13	1:F:48:VAL:CG2	2.47	0.42
1:A:247:TRP:O	1:A:248:SER:C	2.60	0.42
1:B:82:PHE:HA	1:B:88:GLU:O	2.19	0.42
1:B:121:VAL:HB	1:B:137:VAL:HG12	2.00	0.42
1:C:74:ILE:HG22	1:C:207:ASP:OD2	2.19	0.42
1:C:275:MET:HE3	1:C:279:ILE:CD1	2.47	0.42
1:D:74:ILE:HG21	1:D:210:PHE:CE2	2.55	0.42
1:D:145:GLU:O	1:D:148:SER:HB2	2.19	0.42
1:E:153:ARG:NH2	1:E:162:GLU:OE1	2.50	0.42
1:E:180:ILE:HG13	1:E:182:ILE:CD1	2.32	0.42
1:F:305:LEU:HD23	1:F:305:LEU:HA	1.74	0.42
1:H:151:GLN:CD	1:H:346:LYS:HD2	2.44	0.42
1:I:150:ILE:HD13	1:I:150:ILE:HA	1.85	0.42
1:J:83:ASN:HB3	1:J:88:GLU:H	1.84	0.42
1:J:108:HIS:CA	1:J:208:PHE:CD2	3.02	0.42
1:K:300:MET:HE2	1:K:303:ARG:HH21	1.83	0.42
1:L:55:LYS:HB2	1:L:124:TYR:CD2	2.54	0.42
1:L:200:ASN:OD1	1:L:200:ASN:N	2.46	0.42
1:L:265:SER:OG	1:L:266:ASN:N	2.50	0.42
1:B:192:LEU:O	1:B:193:LEU:HD23	2.19	0.42
1:C:195:THR:HG23	1:C:202:ILE:O	2.19	0.42
1:G:99:PRO:CD	1:G:100:LYS:N	2.82	0.42
1:H:332:PRO:HB2	1:H:334:THR:CG2	2.48	0.42
1:I:147:PHE:HE1	1:I:256:LEU:CD2	2.31	0.42
1:I:147:PHE:CE1	1:I:256:LEU:HD23	2.51	0.42
1:J:78:VAL:CG1	1:J:91:ALA:HB1	2.48	0.42
1:J:176:TYR:O	1:J:176:TYR:CG	2.72	0.42
1:L:78:VAL:HG13	1:L:79:LEU:H	1.83	0.42
1:L:105:VAL:O	1:L:106:GLU:C	2.58	0.42
1:L:285:GLU:O	1:L:287:PRO:CD	2.63	0.42
1:A:79:LEU:N	1:A:79:LEU:HD23	2.34	0.42
1:A:98:CYS:HB2	1:A:99:PRO:CD	2.50	0.42
1:B:289:PRO:HG2	1:B:290:GLU:N	2.35	0.42
1:C:150:ILE:CG2	1:C:158:PHE:CD1	3.02	0.42
1:C:178:HIS:CG	1:C:242:LYS:HD3	2.54	0.42
1:D:288:ASN:OD1	1:D:292:SER:HB3	2.19	0.42
1:E:85:ARG:HD2	1:E:85:ARG:C	2.44	0.42
1:E:300:MET:O	1:E:303:ARG:HB2	2.19	0.42
1:E:314:MET:HE2	1:E:314:MET:HB2	1.78	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:300:MET:HE1	1:G:303:ARG:NE	2.34	0.42
1:G:300:MET:HE2	1:G:303:ARG:HH21	1.84	0.42
1:H:159:THR:O	1:H:160:GLU:C	2.63	0.42
1:I:69:VAL:O	1:I:70:LEU:HD23	2.19	0.42
1:I:184:HIS:HD2	1:I:186:ASP:N	2.17	0.42
1:I:241:ASP:O	1:I:244:CYS:CB	2.65	0.42
1:I:331:VAL:HG13	1:I:332:PRO:HD2	2.00	0.42
1:J:83:ASN:O	1:J:85:ARG:N	2.49	0.42
1:J:107:LEU:CD2	1:J:182:ILE:HG23	2.42	0.42
1:J:198:ARG:HG2	1:J:198:ARG:NH1	2.15	0.42
1:J:198:ARG:HH22	1:J:200:ASN:HD22	1.67	0.42
1:K:69:VAL:C	1:K:71:GLY:N	2.77	0.42
1:L:310:PRO:HA	1:L:313:ARG:HH21	1.80	0.42
1:B:337:HIS:ND1	1:B:337:HIS:N	2.66	0.42
1:C:259:GLY:HA2	1:C:342:LEU:CD1	2.48	0.42
1:C:286:PHE:CE1	1:C:299:LYS:HB3	2.55	0.42
1:E:103:ARG:O	1:E:104:GLU:C	2.62	0.42
1:G:195:THR:HG21	1:G:202:ILE:HB	2.01	0.42
1:H:195:THR:HB	1:H:202:ILE:H	1.84	0.42
1:H:331:VAL:CG1	1:H:332:PRO:N	2.82	0.42
1:I:71:GLY:C	1:I:72:LEU:HD12	2.44	0.42
1:J:86:THR:C	1:J:88:GLU:N	2.77	0.42
1:J:184:HIS:O	1:J:185:ARG:HB2	2.19	0.42
1:K:293:GLU:HG3	1:K:294:VAL:HG23	2.01	0.42
1:L:318:GLU:C	1:L:320:MET:N	2.77	0.42
1:L:331:VAL:O	1:L:332:PRO:O	2.37	0.42
1:A:129:ALA:C	1:A:131:ARG:N	2.76	0.42
1:A:150:ILE:CD1	1:A:158:PHE:CE2	3.03	0.42
1:A:184:HIS:HD2	1:A:186:ASP:N	2.18	0.42
1:C:296:GLU:OE1	1:C:296:GLU:HA	2.20	0.42
1:F:72:LEU:HD12	1:F:72:LEU:HA	1.60	0.42
1:F:184:HIS:HD2	1:F:186:ASP:N	2.17	0.42
1:F:309:GLU:O	1:F:310:PRO:C	2.62	0.42
1:J:178:HIS:HB3	1:J:242:LYS:HD3	2.01	0.42
1:J:314:MET:HG2	1:J:315:THR:N	2.34	0.42
1:K:59:ILE:O	1:K:59:ILE:HG12	2.19	0.42
1:K:94:MET:HE3	1:K:94:MET:HB3	1.79	0.42
1:L:54:ILE:CG2	1:L:125:GLU:HB2	2.49	0.42
1:L:57:ASN:OD1	1:L:57:ASN:N	2.50	0.42
1:L:180:ILE:O	1:L:180:ILE:CG1	2.67	0.42
1:L:191:ASN:N	1:L:191:ASN:HD22	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:THR:C	1:A:88:GLU:H	2.26	0.42
1:A:145:GLU:HA	1:A:193:LEU:HD22	2.02	0.42
1:B:48:VAL:CG1	1:K:60:ILE:HD13	2.50	0.42
1:B:74:ILE:HD12	1:B:74:ILE:C	2.44	0.42
1:B:98:CYS:CB	1:B:99:PRO:CD	2.98	0.42
1:B:184:HIS:HD2	1:B:186:ASP:N	2.15	0.42
1:B:202:ILE:HG22	1:B:203:LEU:N	2.32	0.42
1:C:74:ILE:HD11	1:C:75:ASN:ND2	2.35	0.42
1:C:174:ILE:HG13	1:C:249:LEU:HD13	2.01	0.42
1:D:190:GLU:CD	1:D:190:GLU:H	2.28	0.42
1:E:173:ALA:O	1:E:174:ILE:C	2.59	0.42
1:F:161:ARG:O	1:F:165:GLU:HG3	2.20	0.42
1:F:308:THR:O	1:F:310:PRO:HD3	2.20	0.42
1:G:331:VAL:HA	1:G:332:PRO:HD3	1.78	0.42
1:H:325:ILE:HD12	1:H:325:ILE:HG23	1.76	0.42
1:J:59:ILE:HG21	1:J:135:LEU:CD1	2.50	0.42
1:J:80:GLN:O	1:J:81:ILE:HG23	2.19	0.42
1:L:59:ILE:CG2	1:L:60:ILE:N	2.79	0.42
1:A:338:THR:O	1:A:342:LEU:HB2	2.19	0.42
1:C:102:ARG:O	1:C:106:GLU:HB2	2.19	0.42
1:D:184:HIS:HD2	1:D:186:ASP:N	2.17	0.42
1:D:188:LYS:HB2	1:D:189:PRO:CD	2.49	0.42
1:D:310:PRO:HG3	1:F:233:GLU:CD	2.45	0.42
1:D:326:MET:O	1:D:328:SER:N	2.44	0.42
1:E:88:GLU:HG2	1:E:89:LYS:N	2.35	0.42
1:F:63:TYR:HB3	1:F:81:ILE:HD12	2.01	0.42
1:G:184:HIS:O	1:G:185:ARG:HB2	2.19	0.42
1:H:114:CYS:SG	1:H:115:PRO:HD2	2.60	0.42
1:J:89:LYS:HD3	1:J:89:LYS:HA	1.73	0.42
1:J:166:ILE:CG2	1:J:256:LEU:HG	2.46	0.42
1:J:185:ARG:HE	1:J:212:LYS:HB2	1.83	0.42
1:L:275:MET:C	1:L:277:THR:H	2.27	0.42
1:L:304:ASN:HA	1:L:307:LYS:HE2	2.02	0.42
1:L:313:ARG:HE	1:L:313:ARG:HB2	1.75	0.42
1:L:323:PRO:O	1:L:324:TRP:C	2.62	0.42
1:A:300:MET:CE	1:A:303:ARG:HH21	2.33	0.42
1:D:329:THR:C	1:D:331:VAL:H	2.27	0.42
1:D:347:GLU:O	1:D:349:TRP:N	2.52	0.42
1:E:227:PRO:C	1:E:228:TYR:CD2	2.98	0.42
1:F:75:ASN:HB2	1:F:95:LEU:HD22	2.01	0.42
1:H:185:ARG:HH21	1:H:212:LYS:HD3	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:286:PHE:O	1:K:291:TRP:HB2	2.20	0.42
1:B:48:VAL:HG23	1:K:126:ASN:HB3	2.02	0.42
1:B:118:VAL:CG1	1:B:206:THR:HG22	2.50	0.42
1:B:185:ARG:HH21	1:B:212:LYS:HD2	1.85	0.42
1:B:315:THR:OG1	1:B:318:GLU:HG3	2.20	0.42
1:C:83:ASN:ND2	1:C:84:LYS:N	2.59	0.42
1:C:295:SER:OG	1:C:298:VAL:HG23	2.20	0.42
1:D:232:PRO:C	1:D:234:VAL:H	2.28	0.42
1:F:228:TYR:CD1	1:F:228:TYR:C	2.97	0.42
1:G:114:CYS:HA	1:G:115:PRO:HD3	1.85	0.42
1:G:215:THR:O	1:G:215:THR:CG2	2.67	0.42
1:H:301:LEU:O	1:H:302:ILE:C	2.63	0.42
1:I:276:LYS:O	1:I:279:ILE:HB	2.19	0.42
1:J:56:LYS:HZ3	1:J:56:LYS:HG3	1.55	0.42
1:J:296:GLU:O	1:J:299:LYS:N	2.45	0.42
1:K:49:LYS:CG	1:K:50:SER:N	2.82	0.42
1:K:281:MET:O	1:L:317:THR:HG21	2.19	0.42
1:C:74:ILE:HB	1:C:210:PHE:HE2	1.85	0.42
1:C:288:ASN:HB3	1:C:289:PRO:HA	2.02	0.42
1:E:165:GLU:HG3	1:E:328:SER:HB3	2.00	0.42
1:G:57:ASN:O	1:G:58:ALA:C	2.63	0.42
1:H:216:SER:HB2	1:H:217:HIS:HD2	1.84	0.42
1:H:260:TYR:HB2	1:H:261:PRO:CD	2.50	0.42
1:H:337:HIS:CD2	1:H:340:ARG:HH12	2.38	0.42
1:I:320:MET:O	1:I:326:MET:HG2	2.20	0.42
1:J:158:PHE:HZ	1:J:163:ALA:CA	2.33	0.42
1:J:200:ASN:OD1	1:J:200:ASN:O	2.38	0.42
1:J:248:SER:O	1:J:249:LEU:C	2.61	0.42
1:K:145:GLU:HA	1:K:193:LEU:HD22	2.02	0.42
1:L:114:CYS:HA	1:L:115:PRO:HD3	1.69	0.42
1:L:253:MET:HE1	1:L:301:LEU:HD21	2.02	0.42
1:L:293:GLU:HA	1:L:293:GLU:OE2	2.18	0.42
1:A:86:THR:CG2	1:A:88:GLU:HB3	2.50	0.41
1:B:69:VAL:O	1:B:69:VAL:CG1	2.68	0.41
1:B:150:ILE:HD13	1:B:150:ILE:HG23	1.71	0.41
1:B:229:TYR:CZ	1:C:188:LYS:HD3	2.55	0.41
1:B:331:VAL:CG1	1:B:332:PRO:HD2	2.40	0.41
1:D:162:GLU:O	1:D:166:ILE:HG13	2.20	0.41
1:E:80:GLN:NE2	1:E:89:LYS:CG	2.83	0.41
1:F:154:GLY:O	1:F:155:ASP:C	2.64	0.41
1:I:203:LEU:HD12	1:I:203:LEU:HA	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:289:PRO:O	1:I:292:SER:N	2.45	0.41
1:I:334:THR:HA	1:I:335:PRO:HD3	1.73	0.41
1:K:210:PHE:O	1:K:211:ALA:C	2.63	0.41
1:L:107:LEU:HD23	1:L:110:ARG:NH2	2.35	0.41
1:L:111:ALA:C	1:L:113:GLN:N	2.76	0.41
1:L:314:MET:SD	1:L:319:PHE:CA	3.08	0.41
1:C:203:LEU:HA	1:C:203:LEU:HD12	1.76	0.41
1:C:227:PRO:HB2	1:C:229:TYR:CZ	2.53	0.41
1:D:305:LEU:O	1:D:313:ARG:HD3	2.19	0.41
1:F:194:TYR:CZ	1:F:203:LEU:HD13	2.55	0.41
1:F:325:ILE:HA	1:F:325:ILE:HD13	1.80	0.41
1:J:301:LEU:CD1	1:J:322:HIS:CD2	2.93	0.41
1:K:184:HIS:HD2	1:K:186:ASP:H	1.66	0.41
1:K:264:TYR:O	1:K:275:MET:HG3	2.20	0.41
1:K:322:HIS:HA	1:K:323:PRO:HD3	1.94	0.41
1:A:86:THR:HG22	1:A:88:GLU:HB3	2.02	0.41
1:A:158:PHE:CZ	1:A:256:LEU:HD22	2.56	0.41
1:B:60:ILE:C	1:B:62:ASP:N	2.79	0.41
1:B:86:THR:HG23	1:B:88:GLU:H	1.85	0.41
1:B:289:PRO:HG2	1:B:290:GLU:CD	2.45	0.41
1:B:290:GLU:CD	1:B:290:GLU:H	2.28	0.41
1:B:343:LYS:O	1:B:343:LYS:CG	2.67	0.41
1:C:184:HIS:HD2	1:C:186:ASP:N	2.18	0.41
1:D:98:CYS:CB	1:D:99:PRO:CD	2.98	0.41
1:E:95:LEU:HD12	1:E:134:LEU:HB2	2.01	0.41
1:E:127:LEU:O	1:J:48:VAL:HA	2.20	0.41
1:G:232:PRO:HD3	1:H:247:TRP:CZ2	2.55	0.41
1:H:102:ARG:HD2	1:H:134:LEU:CD2	2.48	0.41
1:I:68:GLN:HG2	1:I:70:LEU:HD21	2.01	0.41
1:K:75:ASN:HB2	1:K:95:LEU:HD22	2.02	0.41
1:K:311:THR:CG2	1:L:311:THR:OG1	2.69	0.41
1:L:207:ASP:HB2	2:L:1345:P4O:N7	2.34	0.41
1:L:333:GLN:HE21	1:L:333:GLN:HB3	1.56	0.41
1:B:89:LYS:O	1:B:90:PHE:CD1	2.73	0.41
1:C:234:VAL:C	1:C:236:GLY:N	2.78	0.41
1:F:300:MET:HE2	1:F:303:ARG:HH21	1.82	0.41
1:G:151:GLN:HB2	1:G:342:LEU:HD23	2.02	0.41
1:H:161:ARG:O	1:H:165:GLU:HG3	2.19	0.41
1:I:305:LEU:HD23	1:I:305:LEU:HA	1.79	0.41
1:K:147:PHE:HZ	1:K:255:ILE:HG21	1.79	0.41
1:L:62:ASP:O	1:L:63:TYR:CD2	2.73	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:98:CYS:CB	1:L:99:PRO:CD	2.92	0.41
1:A:93:LYS:HD3	1:A:95:LEU:HD21	2.01	0.41
1:A:149:ARG:HG3	1:A:194:TYR:CD2	2.56	0.41
1:B:58:ALA:HB3	1:B:61:ASP:OD2	2.20	0.41
1:B:70:LEU:HD22	2:B:1351:P4O:C17	2.51	0.41
1:C:115:PRO:O	1:C:204:LYS:HE2	2.21	0.41
1:C:331:VAL:CG1	1:C:332:PRO:CD	2.93	0.41
1:E:210:PHE:C	1:E:211:ALA:O	2.63	0.41
1:G:159:THR:C	1:G:336:LEU:HD21	2.45	0.41
1:G:264:TYR:C	1:G:278:ARG:NH2	2.78	0.41
1:G:265:SER:HA	1:G:275:MET:HB2	2.01	0.41
1:I:98:CYS:O	1:I:102:ARG:HG2	2.21	0.41
1:J:172:GLU:H	1:J:172:GLU:HG3	1.58	0.41
1:K:141:LEU:HD12	1:K:193:LEU:HB2	2.02	0.41
1:L:158:PHE:HD1	1:L:338:THR:CB	2.33	0.41
1:L:257:LEU:O	1:L:336:LEU:HG	2.19	0.41
1:B:71:GLY:O	1:B:77:LYS:HB2	2.20	0.41
1:C:135:LEU:HD23	1:C:135:LEU:N	2.36	0.41
1:D:153:ARG:NH2	1:D:162:GLU:OE1	2.54	0.41
1:E:118:VAL:HG11	1:E:206:THR:HG22	2.00	0.41
1:E:158:PHE:O	1:E:336:LEU:N	2.52	0.41
1:I:345:ASP:C	1:I:347:GLU:H	2.27	0.41
1:J:254:TYR:HB3	1:J:262:PRO:HD3	2.02	0.41
1:K:149:ARG:HG3	1:K:194:TYR:CD2	2.56	0.41
1:K:334:THR:HA	1:K:335:PRO:HD3	1.82	0.41
1:L:103:ARG:O	1:L:104:GLU:C	2.62	0.41
1:L:138:MET:HE2	1:L:138:MET:HB3	1.60	0.41
1:A:86:THR:CG2	1:A:88:GLU:CB	2.98	0.41
1:A:295:SER:HG	1:A:297:GLU:HB3	1.84	0.41
1:B:260:TYR:CB	1:B:261:PRO:CD	2.93	0.41
1:D:161:ARG:HA	1:D:331:VAL:CG1	2.51	0.41
1:E:237:PRO:HB2	1:E:238:GLU:H	1.68	0.41
1:E:342:LEU:HD12	1:E:342:LEU:HA	1.92	0.41
1:F:155:ASP:O	1:F:156:GLN:CB	2.64	0.41
1:G:246:MET:HE2	1:G:315:THR:C	2.46	0.41
1:H:180:ILE:O	1:H:181:ASN:HB2	2.19	0.41
1:H:184:HIS:O	1:H:185:ARG:HB2	2.20	0.41
1:I:102:ARG:O	1:I:106:GLU:HB2	2.20	0.41
1:I:195:THR:CG2	1:I:202:ILE:CB	2.98	0.41
1:I:289:PRO:O	1:I:290:GLU:C	2.59	0.41
1:A:331:VAL:CG1	1:A:332:PRO:HD2	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:150:ILE:C	1:B:152:ASP:N	2.78	0.41
1:C:70:LEU:HD22	2:C:1351:P4O:C21	2.51	0.41
1:C:322:HIS:ND1	1:C:323:PRO:N	2.69	0.41
1:D:257:LEU:HD23	1:D:257:LEU:HA	1.90	0.41
1:E:64:LYS:HB3	1:E:82:PHE:HB2	2.03	0.41
1:E:286:PHE:CE1	1:E:299:LYS:HB3	2.55	0.41
1:F:191:ASN:HD22	1:F:191:ASN:HA	1.67	0.41
1:F:286:PHE:HA	1:F:287:PRO:HD2	1.82	0.41
1:G:158:PHE:HE1	1:G:256:LEU:O	2.04	0.41
1:H:176:TYR:O	1:H:179:SER:OG	2.35	0.41
1:I:242:LYS:C	1:I:244:CYS:N	2.77	0.41
1:J:52:LEU:HG	1:J:54:ILE:CD1	2.51	0.41
1:L:206:THR:HB	1:L:207:ASP:H	1.54	0.41
1:L:318:GLU:O	1:L:320:MET:N	2.53	0.41
1:L:334:THR:O	1:L:334:THR:OG1	2.33	0.41
1:B:128:TYR:O	1:B:129:ALA:HB3	2.21	0.41
1:B:149:ARG:HG3	1:B:149:ARG:NH1	2.36	0.41
1:B:300:MET:CE	1:B:303:ARG:HE	2.34	0.41
1:B:326:MET:C	1:B:326:MET:HE2	2.45	0.41
1:C:110:ARG:NH2	1:C:213:GLU:OE1	2.53	0.41
1:C:149:ARG:HD3	1:C:194:TYR:CD2	2.55	0.41
1:C:343:LYS:C	1:C:345:ASP:N	2.77	0.41
1:D:256:LEU:HD23	1:D:256:LEU:HA	1.77	0.41
1:D:302:ILE:O	1:D:302:ILE:HG22	2.21	0.41
1:E:56:LYS:C	1:E:57:ASN:O	2.64	0.41
1:E:160:GLU:HB3	1:E:331:VAL:CG1	2.51	0.41
1:E:168:LYS:HB2	1:E:325:ILE:HG23	2.01	0.41
1:F:164:SER:OG	1:F:328:SER:HB2	2.20	0.41
1:G:60:ILE:C	1:G:62:ASP:H	2.29	0.41
1:I:338:THR:CG2	1:I:342:LEU:HD22	2.51	0.41
1:I:347:GLU:C	1:I:349:TRP:N	2.78	0.41
1:J:95:LEU:HD23	1:J:95:LEU:HA	1.82	0.41
1:J:147:PHE:CZ	1:J:255:ILE:CG2	3.04	0.41
1:J:255:ILE:HG13	1:J:261:PRO:HA	2.03	0.41
1:K:86:THR:HG22	1:K:87:GLN:N	2.36	0.41
1:K:184:HIS:HD2	1:K:186:ASP:N	2.19	0.41
1:L:63:TYR:CD1	1:L:81:ILE:CD1	2.99	0.41
1:L:127:LEU:CD2	1:L:132:LYS:HA	2.48	0.41
1:L:244:CYS:O	1:L:244:CYS:SG	2.79	0.41
1:L:275:MET:C	1:L:277:THR:N	2.79	0.41
1:L:286:PHE:HD2	1:L:291:TRP:CE3	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:337:HIS:CD2	1:A:340:ARG:NH1	2.84	0.41
1:B:179:SER:CB	1:C:281:MET:HE2	2.47	0.41
1:C:180:ILE:O	1:C:180:ILE:HG13	2.21	0.41
1:D:150:ILE:HG12	1:D:158:PHE:CE2	2.56	0.41
1:G:128:TYR:O	1:G:129:ALA:CB	2.67	0.41
1:G:247:TRP:CD1	1:I:231:ALA:HB2	2.55	0.41
1:H:71:GLY:C	1:H:78:VAL:HG23	2.46	0.41
1:H:158:PHE:O	1:H:335:PRO:HA	2.20	0.41
1:J:114:CYS:O	1:J:115:PRO:C	2.63	0.41
1:J:141:LEU:HD22	1:J:195:THR:HA	2.03	0.41
1:K:158:PHE:CD1	1:K:338:THR:HB	2.56	0.41
1:K:161:ARG:NH1	1:K:333:GLN:OE1	2.54	0.41
1:L:60:ILE:C	1:L:62:ASP:H	2.28	0.41
1:L:136:ILE:HG21	1:L:138:MET:HE3	2.03	0.41
1:L:194:TYR:O	1:L:195:THR:C	2.64	0.41
1:L:295:SER:HB2	1:L:298:VAL:HG23	2.01	0.41
1:C:80:GLN:HG3	1:C:81:ILE:N	2.34	0.40
1:C:114:CYS:HA	1:C:115:PRO:HD3	1.88	0.40
1:D:289:PRO:O	1:D:290:GLU:C	2.64	0.40
1:E:195:THR:OG1	1:E:196:SER:N	2.54	0.40
1:F:159:THR:O	1:F:160:GLU:C	2.62	0.40
1:F:200:ASN:O	1:F:201:ALA:C	2.63	0.40
1:G:184:HIS:CD2	1:G:184:HIS:C	2.99	0.40
1:G:278:ARG:HG3	1:G:278:ARG:NH1	2.35	0.40
1:G:332:PRO:CB	1:G:334:THR:HG22	2.51	0.40
1:H:57:ASN:O	1:H:58:ALA:C	2.63	0.40
1:J:52:LEU:HG	1:J:54:ILE:HD13	2.03	0.40
1:J:200:ASN:O	1:J:200:ASN:CG	2.64	0.40
1:L:70:LEU:HB2	1:L:78:VAL:CG1	2.51	0.40
1:L:256:LEU:O	1:L:256:LEU:CD2	2.70	0.40
1:L:264:TYR:O	1:L:278:ARG:NH2	2.54	0.40
1:L:275:MET:O	1:L:277:THR:N	2.54	0.40
1:A:232:PRO:HB3	1:B:280:ARG:HA	2.03	0.40
1:B:197:LYS:O	1:B:198:ARG:C	2.65	0.40
1:C:60:ILE:C	1:C:62:ASP:H	2.29	0.40
1:C:125:GLU:HA	1:C:133:CYS:O	2.21	0.40
1:C:275:MET:O	1:C:276:LYS:C	2.64	0.40
1:C:286:PHE:CD1	1:C:299:LYS:HD3	2.56	0.40
1:E:198:ARG:HH21	1:E:200:ASN:CG	2.28	0.40
1:F:188:LYS:HB2	1:F:189:PRO:HD2	2.02	0.40
1:F:325:ILE:HD12	1:F:325:ILE:HG23	1.69	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:74:ILE:CG1	1:G:75:ASN:N	2.80	0.40
1:G:191:ASN:HD21	2:G:1350:P4O:H8C2	1.86	0.40
1:G:260:TYR:OH	1:G:287:PRO:HG2	2.20	0.40
1:H:149:ARG:CG	1:H:149:ARG:NH1	2.81	0.40
1:I:118:VAL:HG13	1:I:118:VAL:O	2.20	0.40
1:J:142:ASP:OD2	1:J:196:SER:HA	2.21	0.40
1:J:159:THR:N	1:J:162:GLU:HG3	2.36	0.40
1:J:322:HIS:HA	1:J:323:PRO:HD3	1.90	0.40
1:L:243:SER:C	1:L:245:ASP:N	2.79	0.40
1:A:59:ILE:O	1:A:59:ILE:HG12	2.21	0.40
1:A:343:LYS:C	1:A:345:ASP:N	2.79	0.40
1:B:110:ARG:CG	1:K:130:GLY:O	2.69	0.40
1:B:232:PRO:C	1:B:234:VAL:H	2.30	0.40
1:B:235:LEU:H	1:B:235:LEU:CD2	2.28	0.40
1:C:130:GLY:HA3	1:L:180:ILE:HG22	2.03	0.40
1:C:151:GLN:HG2	1:C:342:LEU:HB3	2.03	0.40
1:C:314:MET:HG3	1:C:318:GLU:HB2	2.03	0.40
1:D:127:LEU:HA	1:D:127:LEU:HD23	1.74	0.40
1:D:289:PRO:HG2	1:D:290:GLU:CD	2.46	0.40
1:E:63:TYR:HB3	1:E:81:ILE:HD12	2.03	0.40
1:E:152:ASP:C	1:E:153:ARG:HG3	2.46	0.40
1:E:246:MET:HG3	1:E:314:MET:O	2.21	0.40
1:G:114:CYS:SG	1:G:117:ILE:HG13	2.61	0.40
1:G:153:ARG:CG	1:G:153:ARG:HH11	2.35	0.40
1:I:45:GLN:O	1:I:45:GLN:HG2	2.20	0.40
1:I:125:GLU:C	1:I:126:ASN:HD22	2.30	0.40
1:J:153:ARG:HD2	1:J:157:ALA:HB3	2.02	0.40
1:J:158:PHE:CZ	1:J:163:ALA:N	2.90	0.40
1:L:147:PHE:CZ	1:L:255:ILE:CG2	3.04	0.40
1:L:149:ARG:HH11	1:L:197:LYS:HA	1.86	0.40
1:A:151:GLN:O	1:A:151:GLN:CG	2.69	0.40
1:A:320:MET:O	1:A:326:MET:HG2	2.21	0.40
1:B:321:ASN:HA	1:B:326:MET:HG2	2.02	0.40
1:D:185:ARG:HH21	1:D:212:LYS:HD3	1.86	0.40
1:D:325:ILE:HD12	1:D:325:ILE:HG23	1.73	0.40
1:E:200:ASN:CG	1:E:200:ASN:O	2.64	0.40
1:G:153:ARG:HB2	1:G:339:SER:OG	2.21	0.40
1:H:85:ARG:O	1:H:86:THR:HG23	2.21	0.40
1:I:342:LEU:HD12	1:I:342:LEU:HA	1.71	0.40
1:J:153:ARG:HH22	1:J:158:PHE:HD2	1.70	0.40
1:K:190:GLU:H	1:K:190:GLU:CD	2.30	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:305:LEU:HD23	1:K:314:MET:HB3	2.04	0.40
1:L:159:THR:C	1:L:336:LEU:HD22	2.47	0.40
1:L:247:TRP:CZ3	1:L:306:LEU:HA	2.57	0.40
1:A:99:PRO:CD	1:A:100:LYS:H	2.32	0.40
1:A:147:PHE:CD1	1:A:189:PRO:HB3	2.57	0.40
1:A:191:ASN:HD22	1:A:191:ASN:HA	1.62	0.40
1:D:83:ASN:ND2	1:D:85:ARG:HG3	2.34	0.40
1:D:141:LEU:O	2:D:1351:P4O:C17	2.69	0.40
1:D:210:PHE:O	1:D:211:ALA:C	2.64	0.40
1:D:342:LEU:HD12	1:D:342:LEU:HA	1.96	0.40
1:E:195:THR:HG23	1:E:202:ILE:HG12	2.01	0.40
1:E:239:LYS:HG3	1:E:240:TYR:CD1	2.57	0.40
1:E:333:GLN:HE21	1:E:333:GLN:HB3	1.62	0.40
1:H:190:GLU:H	1:H:190:GLU:CD	2.28	0.40
1:H:230:VAL:HB	1:H:231:ALA:H	1.59	0.40
1:H:290:GLU:H	1:H:290:GLU:HG2	1.73	0.40
1:I:277:THR:O	1:I:281:MET:HB2	2.22	0.40
1:J:108:HIS:C	1:J:110:ARG:N	2.80	0.40
1:J:128:TYR:O	1:J:129:ALA:CB	2.68	0.40
1:J:258:CYS:HB2	1:J:260:TYR:CE1	2.57	0.40
1:K:74:ILE:HG12	1:K:210:PHE:CE2	2.56	0.40
1:K:145:GLU:OE1	1:K:147:PHE:HB2	2.22	0.40
1:L:147:PHE:CZ	1:L:255:ILE:HG21	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	275/326 (84%)	244 (89%)	23 (8%)	8 (3%)	3	22
1	B	284/326 (87%)	238 (84%)	32 (11%)	14 (5%)	1	12

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	276/326 (85%)	245 (89%)	19 (7%)	12 (4%)	2	15
1	D	278/326 (85%)	236 (85%)	26 (9%)	16 (6%)	1	9
1	E	275/326 (84%)	210 (76%)	47 (17%)	18 (6%)	1	8
1	F	282/326 (86%)	248 (88%)	21 (7%)	13 (5%)	2	13
1	G	280/326 (86%)	238 (85%)	26 (9%)	16 (6%)	1	9
1	H	275/326 (84%)	239 (87%)	23 (8%)	13 (5%)	2	13
1	I	281/326 (86%)	245 (87%)	22 (8%)	14 (5%)	1	12
1	J	217/326 (67%)	142 (65%)	40 (18%)	35 (16%)	0	1
1	K	257/326 (79%)	221 (86%)	22 (9%)	14 (5%)	1	10
1	L	260/326 (80%)	187 (72%)	44 (17%)	29 (11%)	0	2
All	All	3240/3912 (83%)	2693 (83%)	345 (11%)	202 (6%)	1	9

All (202) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	98	CYS
1	A	237	PRO
1	B	98	CYS
1	B	156	GLN
1	B	235	LEU
1	B	349	TRP
1	C	235	LEU
1	C	237	PRO
1	C	241	ASP
1	D	98	CYS
1	D	237	PRO
1	D	290	GLU
1	D	327	GLN
1	D	347	GLU
1	E	61	ASP
1	E	98	CYS
1	E	139	GLU
1	E	149	ARG
1	E	211	ALA
1	E	237	PRO
1	E	238	GLU
1	E	241	ASP
1	E	256	LEU

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Mol	Chain	Res	Type
1	F	98	CYS
1	F	99	PRO
1	F	201	ALA
1	F	338	THR
1	F	345	ASP
1	F	348	ARG
1	G	46	PHE
1	G	74	ILE
1	G	87	GLN
1	G	98	CYS
1	G	146	LEU
1	G	149	ARG
1	G	215	THR
1	G	238	GLU
1	G	241	ASP
1	G	349	TRP
1	H	98	CYS
1	H	99	PRO
1	H	149	ARG
1	H	201	ALA
1	H	230	VAL
1	I	87	GLN
1	I	98	CYS
1	I	157	ALA
1	I	229	TYR
1	J	60	ILE
1	J	72	LEU
1	J	85	ARG
1	J	112	SER
1	J	145	GLU
1	J	175	GLN
1	J	176	TYR
1	J	186	ASP
1	J	190	GLU
1	J	193	LEU
1	J	195	THR
1	J	201	ALA
1	J	211	ALA
1	J	240	TYR
1	J	314	MET
1	J	320	MET
1	K	70	LEU

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Mol	Chain	Res	Type
1	K	85	ARG
1	K	88	GLU
1	K	98	CYS
1	K	145	GLU
1	K	295	SER
1	L	75	ASN
1	L	86	THR
1	L	87	GLN
1	L	146	LEU
1	L	147	PHE
1	L	181	ASN
1	L	207	ASP
1	L	313	ARG
1	L	332	PRO
1	A	99	PRO
1	A	238	GLU
1	A	346	LYS
1	B	236	GLY
1	B	344	GLU
1	C	152	ASP
1	C	345	ASP
1	C	346	LYS
1	D	86	THR
1	D	130	GLY
1	D	186	ASP
1	D	238	GLU
1	E	99	PRO
1	E	344	GLU
1	F	130	GLY
1	F	240	TYR
1	G	99	PRO
1	G	235	LEU
1	G	237	PRO
1	H	345	ASP
1	I	290	GLU
1	I	346	LYS
1	J	109	TRP
1	J	149	ARG
1	J	161	ARG
1	J	170	ILE
1	J	207	ASP
1	J	251	VAL

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Mol	Chain	Res	Type
1	J	256	LEU
1	J	301	LEU
1	K	130	GLY
1	L	84	LYS
1	L	113	GLN
1	L	152	ASP
1	L	311	THR
1	L	319	PHE
1	A	186	ASP
1	B	151	GLN
1	C	186	ASP
1	C	344	GLU
1	D	87	GLN
1	D	99	PRO
1	D	151	GLN
1	D	326	MET
1	D	349	TRP
1	E	73	GLY
1	E	128	TYR
1	E	143	GLY
1	E	186	ASP
1	F	156	GLN
1	G	186	ASP
1	H	290	GLU
1	I	99	PRO
1	I	237	PRO
1	I	239	LYS
1	J	71	GLY
1	J	108	HIS
1	J	158	PHE
1	J	164	SER
1	K	99	PRO
1	K	186	ASP
1	L	98	CYS
1	L	190	GLU
1	L	316	ILE
1	A	347	GLU
1	B	87	GLN
1	B	233	GLU
1	D	235	LEU
1	D	289	PRO
1	F	238	GLU

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Mol	Chain	Res	Type
1	F	326	MET
1	G	86	THR
1	H	216	SER
1	H	237	PRO
1	H	272	SER
1	I	186	ASP
1	J	77	LYS
1	J	84	LYS
1	J	247	TRP
1	L	153	ARG
1	L	163	ALA
1	L	186	ASP
1	L	189	PRO
1	A	61	ASP
1	B	238	GLU
1	B	326	MET
1	C	98	CYS
1	C	236	GLY
1	C	349	TRP
1	E	87	GLN
1	E	97	ASP
1	E	161	ARG
1	F	237	PRO
1	G	346	LYS
1	H	186	ASP
1	H	215	THR
1	I	238	GLU
1	I	345	ASP
1	J	87	GLN
1	K	292	SER
1	L	99	PRO
1	L	188	LYS
1	L	286	PHE
1	L	301	LEU
1	L	334	THR
1	B	99	PRO
1	F	343	LYS
1	H	153	ARG
1	J	172	GLU
1	K	76	GLY
1	K	199	PRO
1	L	276	LYS

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Mol	Chain	Res	Type
1	L	298	VAL
1	C	99	PRO
1	K	198	ARG
1	K	272	SER
1	L	310	PRO
1	J	118	VAL
1	B	237	PRO
1	B	272	SER
1	I	230	VAL
1	J	115	PRO
1	I	289	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	255/294 (87%)	217 (85%)	38 (15%)	3	14
1	B	262/294 (89%)	212 (81%)	50 (19%)	1	7
1	C	256/294 (87%)	220 (86%)	36 (14%)	3	15
1	D	258/294 (88%)	224 (87%)	34 (13%)	4	17
1	E	255/294 (87%)	192 (75%)	63 (25%)	1	3
1	F	260/294 (88%)	210 (81%)	50 (19%)	1	7
1	G	261/294 (89%)	223 (85%)	38 (15%)	3	14
1	H	255/294 (87%)	217 (85%)	38 (15%)	3	14
1	I	261/294 (89%)	215 (82%)	46 (18%)	2	9
1	J	202/294 (69%)	167 (83%)	35 (17%)	2	9
1	K	239/294 (81%)	198 (83%)	41 (17%)	2	10
1	L	243/294 (83%)	197 (81%)	46 (19%)	1	7
All	All	3007/3528 (85%)	2492 (83%)	515 (17%)	2	10

All (515) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	48	VAL
1	A	50	SER
1	A	59	ILE
1	A	60	ILE
1	A	66	THR
1	A	72	LEU
1	A	74	ILE
1	A	75	ASN
1	A	77	LYS
1	A	83	ASN
1	A	86	THR
1	A	87	GLN
1	A	92	LEU
1	A	106	GLU
1	A	110	ARG
1	A	132	LYS
1	A	134	LEU
1	A	145	GLU
1	A	149	ARG
1	A	169	SER
1	A	170	ILE
1	A	175	GLN
1	A	185	ARG
1	A	233	GLU
1	A	234	VAL
1	A	264	TYR
1	A	277	THR
1	A	292	SER
1	A	293	GLU
1	A	295	SER
1	A	302	ILE
1	A	311	THR
1	A	326	MET
1	A	333	GLN
1	A	334	THR
1	A	336	LEU
1	A	342	LEU
1	B	46	PHE
1	B	48	VAL
1	B	59	ILE
1	B	60	ILE
1	B	66	THR

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Mol	Chain	Res	Type
1	B	70	LEU
1	B	74	ILE
1	B	75	ASN
1	B	77	LYS
1	B	83	ASN
1	B	89	LYS
1	B	92	LEU
1	B	106	GLU
1	B	110	ARG
1	B	131	ARG
1	B	132	LYS
1	B	134	LEU
1	B	142	ASP
1	B	146	LEU
1	B	148	SER
1	B	149	ARG
1	B	150	ILE
1	B	152	ASP
1	B	169	SER
1	B	175	GLN
1	B	185	ARG
1	B	197	LYS
1	B	200	ASN
1	B	202	ILE
1	B	233	GLU
1	B	235	LEU
1	B	240	TYR
1	B	256	LEU
1	B	264	TYR
1	B	266	ASN
1	B	296	GLU
1	B	302	ILE
1	B	311	THR
1	B	326	MET
1	B	329	THR
1	B	333	GLN
1	B	334	THR
1	B	336	LEU
1	B	337	HIS
1	B	339	SER
1	B	342	LEU
1	B	343	LYS

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Mol	Chain	Res	Type
1	B	344	GLU
1	B	345	ASP
1	B	348	ARG
1	C	48	VAL
1	C	60	ILE
1	C	66	THR
1	C	74	ILE
1	C	80	GLN
1	C	83	ASN
1	C	84	LYS
1	C	92	LEU
1	C	106	GLU
1	C	110	ARG
1	C	134	LEU
1	C	135	LEU
1	C	152	ASP
1	C	158	PHE
1	C	169	SER
1	C	170	ILE
1	C	175	GLN
1	C	185	ARG
1	C	191	ASN
1	C	215	THR
1	C	249	LEU
1	C	264	TYR
1	C	276	LYS
1	C	292	SER
1	C	293	GLU
1	C	302	ILE
1	C	311	THR
1	C	327	GLN
1	C	329	THR
1	C	333	GLN
1	C	334	THR
1	C	336	LEU
1	C	343	LYS
1	C	345	ASP
1	C	347	GLU
1	C	348	ARG
1	D	48	VAL
1	D	59	ILE
1	D	60	ILE

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Mol	Chain	Res	Type
1	D	70	LEU
1	D	72	LEU
1	D	74	ILE
1	D	83	ASN
1	D	89	LYS
1	D	94	MET
1	D	106	GLU
1	D	134	LEU
1	D	135	LEU
1	D	142	ASP
1	D	149	ARG
1	D	169	SER
1	D	170	ILE
1	D	175	GLN
1	D	185	ARG
1	D	195	THR
1	D	215	THR
1	D	230	VAL
1	D	240	TYR
1	D	264	TYR
1	D	277	THR
1	D	293	GLU
1	D	302	ILE
1	D	311	THR
1	D	334	THR
1	D	336	LEU
1	D	341	VAL
1	D	342	LEU
1	D	345	ASP
1	D	347	GLU
1	D	348	ARG
1	E	45	GLN
1	E	48	VAL
1	E	50	SER
1	E	56	LYS
1	E	60	ILE
1	E	62	ASP
1	E	64	LYS
1	E	66	THR
1	E	74	ILE
1	E	75	ASN
1	E	89	LYS

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Mol	Chain	Res	Type
1	E	92	LEU
1	E	94	MET
1	E	95	LEU
1	E	100	LYS
1	E	106	GLU
1	E	112	SER
1	E	114	CYS
1	E	117	ILE
1	E	121	VAL
1	E	128	TYR
1	E	135	LEU
1	E	136	ILE
1	E	140	CYS
1	E	142	ASP
1	E	146	LEU
1	E	149	ARG
1	E	150	ILE
1	E	158	PHE
1	E	161	ARG
1	E	167	MET
1	E	175	GLN
1	E	179	SER
1	E	185	ARG
1	E	187	VAL
1	E	193	LEU
1	E	197	LYS
1	E	202	ILE
1	E	210	PHE
1	E	228	TYR
1	E	233	GLU
1	E	240	TYR
1	E	246	MET
1	E	249	LEU
1	E	252	ILE
1	E	256	LEU
1	E	261	PRO
1	E	264	TYR
1	E	275	MET
1	E	278	ARG
1	E	288	ASN
1	E	292	SER
1	E	294	VAL

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Mol	Chain	Res	Type
1	E	297	GLU
1	E	303	ARG
1	E	311	THR
1	E	314	MET
1	E	333	GLN
1	E	334	THR
1	E	336	LEU
1	E	337	HIS
1	E	340	ARG
1	E	343	LYS
1	F	45	GLN
1	F	59	ILE
1	F	60	ILE
1	F	66	THR
1	F	70	LEU
1	F	74	ILE
1	F	77	LYS
1	F	83	ASN
1	F	86	THR
1	F	87	GLN
1	F	92	LEU
1	F	94	MET
1	F	95	LEU
1	F	100	LYS
1	F	103	ARG
1	F	106	GLU
1	F	110	ARG
1	F	132	LYS
1	F	134	LEU
1	F	141	LEU
1	F	146	LEU
1	F	149	ARG
1	F	155	ASP
1	F	169	SER
1	F	175	GLN
1	F	185	ARG
1	F	197	LYS
1	F	200	ASN
1	F	210	PHE
1	F	233	GLU
1	F	234	VAL
1	F	239	LYS

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Mol	Chain	Res	Type
1	F	264	TYR
1	F	265	SER
1	F	281	MET
1	F	297	GLU
1	F	302	ILE
1	F	308	THR
1	F	311	THR
1	F	315	THR
1	F	326	MET
1	F	328	SER
1	F	329	THR
1	F	331	VAL
1	F	333	GLN
1	F	334	THR
1	F	341	VAL
1	F	342	LEU
1	F	344	GLU
1	F	349	TRP
1	G	45	GLN
1	G	47	HIS
1	G	50	SER
1	G	59	ILE
1	G	60	ILE
1	G	66	THR
1	G	74	ILE
1	G	83	ASN
1	G	86	THR
1	G	87	GLN
1	G	92	LEU
1	G	106	GLU
1	G	117	ILE
1	G	118	VAL
1	G	132	LYS
1	G	134	LEU
1	G	138	MET
1	G	142	ASP
1	G	153	ARG
1	G	161	ARG
1	G	169	SER
1	G	170	ILE
1	G	175	GLN
1	G	185	ARG

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Mol	Chain	Res	Type
1	G	202	ILE
1	G	233	GLU
1	G	234	VAL
1	G	264	TYR
1	G	277	THR
1	G	294	VAL
1	G	302	ILE
1	G	311	THR
1	G	326	MET
1	G	333	GLN
1	G	334	THR
1	G	336	LEU
1	G	342	LEU
1	G	348	ARG
1	H	48	VAL
1	H	59	ILE
1	H	60	ILE
1	H	66	THR
1	H	70	LEU
1	H	74	ILE
1	H	78	VAL
1	H	83	ASN
1	H	87	GLN
1	H	92	LEU
1	H	94	MET
1	H	106	GLU
1	H	110	ARG
1	H	134	LEU
1	H	149	ARG
1	H	169	SER
1	H	175	GLN
1	H	185	ARG
1	H	195	THR
1	H	200	ASN
1	H	202	ILE
1	H	217	HIS
1	H	229	TYR
1	H	230	VAL
1	H	238	GLU
1	H	239	LYS
1	H	241	ASP
1	H	248	SER

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Mol	Chain	Res	Type
1	H	264	TYR
1	H	277	THR
1	H	294	VAL
1	H	295	SER
1	H	311	THR
1	H	315	THR
1	H	334	THR
1	H	336	LEU
1	H	342	LEU
1	H	344	GLU
1	I	47	HIS
1	I	48	VAL
1	I	50	SER
1	I	60	ILE
1	I	66	THR
1	I	70	LEU
1	I	75	ASN
1	I	83	ASN
1	I	85	ARG
1	I	92	LEU
1	I	95	LEU
1	I	106	GLU
1	I	131	ARG
1	I	132	LYS
1	I	134	LEU
1	I	138	MET
1	I	142	ASP
1	I	149	ARG
1	I	169	SER
1	I	170	ILE
1	I	175	GLN
1	I	185	ARG
1	I	214	THR
1	I	230	VAL
1	I	233	GLU
1	I	234	VAL
1	I	240	TYR
1	I	244	CYS
1	I	249	LEU
1	I	264	TYR
1	I	276	LYS
1	I	277	THR

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Mol	Chain	Res	Type
1	I	290	GLU
1	I	292	SER
1	I	295	SER
1	I	302	ILE
1	I	311	THR
1	I	326	MET
1	I	329	THR
1	I	333	GLN
1	I	334	THR
1	I	336	LEU
1	I	337	HIS
1	I	342	LEU
1	I	343	LYS
1	I	348	ARG
1	J	56	LYS
1	J	57	ASN
1	J	60	ILE
1	J	65	VAL
1	J	66	THR
1	J	81	ILE
1	J	89	LYS
1	J	92	LEU
1	J	94	MET
1	J	103	ARG
1	J	108	HIS
1	J	110	ARG
1	J	113	GLN
1	J	118	VAL
1	J	120	ILE
1	J	134	LEU
1	J	138	MET
1	J	149	ARG
1	J	150	ILE
1	J	166	ILE
1	J	193	LEU
1	J	194	TYR
1	J	196	SER
1	J	198	ARG
1	J	206	THR
1	J	244	CYS
1	J	249	LEU
1	J	251	VAL

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Mol	Chain	Res	Type
1	J	253	MET
1	J	256	LEU
1	J	296	GLU
1	J	304	ASN
1	J	305	LEU
1	J	326	MET
1	J	327	GLN
1	K	60	ILE
1	K	64	LYS
1	K	66	THR
1	K	70	LEU
1	K	72	LEU
1	K	74	ILE
1	K	77	LYS
1	K	83	ASN
1	K	86	THR
1	K	92	LEU
1	K	94	MET
1	K	106	GLU
1	K	110	ARG
1	K	132	LYS
1	K	134	LEU
1	K	138	MET
1	K	142	ASP
1	K	145	GLU
1	K	149	ARG
1	K	153	ARG
1	K	169	SER
1	K	170	ILE
1	K	185	ARG
1	K	197	LYS
1	K	198	ARG
1	K	200	ASN
1	K	212	LYS
1	K	264	TYR
1	K	277	THR
1	K	288	ASN
1	K	290	GLU
1	K	302	ILE
1	K	311	THR
1	K	315	THR
1	K	326	MET

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Mol	Chain	Res	Type
1	K	327	GLN
1	K	328	SER
1	K	329	THR
1	K	334	THR
1	K	336	LEU
1	K	342	LEU
1	L	54	ILE
1	L	60	ILE
1	L	74	ILE
1	L	75	ASN
1	L	77	LYS
1	L	83	ASN
1	L	86	THR
1	L	89	LYS
1	L	93	LYS
1	L	98	CYS
1	L	106	GLU
1	L	110	ARG
1	L	114	CYS
1	L	117	ILE
1	L	123	VAL
1	L	132	LYS
1	L	134	LEU
1	L	153	ARG
1	L	174	ILE
1	L	175	GLN
1	L	185	ARG
1	L	196	SER
1	L	197	LYS
1	L	200	ASN
1	L	202	ILE
1	L	205	LEU
1	L	249	LEU
1	L	256	LEU
1	L	257	LEU
1	L	264	TYR
1	L	266	ASN
1	L	277	THR
1	L	285	GLU
1	L	290	GLU
1	L	293	GLU
1	L	294	VAL

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Mol	Chain	Res	Type
1	L	296	GLU
1	L	304	ASN
1	L	311	THR
1	L	313	ARG
1	L	315	THR
1	L	333	GLN
1	L	334	THR
1	L	336	LEU
1	L	337	HIS
1	L	342	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (120) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	83	ASN
1	A	87	GLN
1	A	116	HIS
1	A	184	HIS
1	A	191	ASN
1	A	304	ASN
1	A	312	GLN
1	A	327	GLN
1	A	333	GLN
1	A	337	HIS
1	B	68	GLN
1	B	83	ASN
1	B	96	GLN
1	B	116	HIS
1	B	151	GLN
1	B	178	HIS
1	B	181	ASN
1	B	184	HIS
1	B	191	ASN
1	B	266	ASN
1	B	304	ASN
1	B	333	GLN
1	C	75	ASN
1	C	80	GLN
1	C	83	ASN
1	C	96	GLN
1	C	151	GLN

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Mol	Chain	Res	Type
1	C	184	HIS
1	C	191	ASN
1	C	327	GLN
1	C	333	GLN
1	C	337	HIS
1	D	68	GLN
1	D	83	ASN
1	D	87	GLN
1	D	96	GLN
1	D	126	ASN
1	D	151	GLN
1	D	184	HIS
1	D	191	ASN
1	D	304	ASN
1	D	337	HIS
1	E	45	GLN
1	E	57	ASN
1	E	96	GLN
1	E	184	HIS
1	E	200	ASN
1	E	266	ASN
1	E	283	GLN
1	E	288	ASN
1	E	333	GLN
1	F	68	GLN
1	F	80	GLN
1	F	83	ASN
1	F	151	GLN
1	F	184	HIS
1	F	191	ASN
1	F	200	ASN
1	F	304	ASN
1	G	45	GLN
1	G	68	GLN
1	G	83	ASN
1	G	96	GLN
1	G	116	HIS
1	G	184	HIS
1	G	191	ASN
1	G	288	ASN
1	G	304	ASN
1	H	68	GLN

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Mol	Chain	Res	Type
1	H	83	ASN
1	H	87	GLN
1	H	96	GLN
1	H	184	HIS
1	H	200	ASN
1	H	217	HIS
1	H	304	ASN
1	H	337	HIS
1	I	68	GLN
1	I	75	ASN
1	I	83	ASN
1	I	96	GLN
1	I	113	GLN
1	I	116	HIS
1	I	151	GLN
1	I	156	GLN
1	I	184	HIS
1	I	191	ASN
1	I	304	ASN
1	I	321	ASN
1	I	327	GLN
1	I	333	GLN
1	J	75	ASN
1	J	96	GLN
1	J	151	GLN
1	J	178	HIS
1	J	200	ASN
1	K	68	GLN
1	K	80	GLN
1	K	83	ASN
1	K	96	GLN
1	K	181	ASN
1	K	184	HIS
1	K	288	ASN
1	K	304	ASN
1	K	337	HIS
1	L	45	GLN
1	L	53	GLN
1	L	75	ASN
1	L	83	ASN
1	L	108	HIS
1	L	126	ASN

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Mol	Chain	Res	Type
1	L	181	ASN
1	L	184	HIS
1	L	191	ASN
1	L	266	ASN
1	L	283	GLN
1	L	304	ASN
1	L	321	ASN
1	L	333	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

11 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	P4O	I	1351	-	29,30,30	2.32	7 (24%)	39,43,43	1.81	9 (23%)
2	P4O	A	1351	-	29,30,30	2.27	7 (24%)	39,43,43	1.85	12 (30%)
2	P4O	C	1351	-	29,30,30	2.31	7 (24%)	39,43,43	1.76	10 (25%)
2	P4O	G	1350	-	29,30,30	2.33	7 (24%)	39,43,43	1.82	9 (23%)
2	P4O	D	1351	-	29,30,30	2.33	7 (24%)	39,43,43	1.91	12 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	P4O	H	1347	-	29,30,30	2.33	7 (24%)	39,43,43	1.81	10 (25%)
2	P4O	L	1345	-	29,30,30	2.34	7 (24%)	39,43,43	1.89	11 (28%)
2	P4O	K	1345	-	29,30,30	2.33	7 (24%)	39,43,43	1.90	9 (23%)
2	P4O	E	1345	-	29,30,30	2.32	7 (24%)	39,43,43	1.89	12 (30%)
2	P4O	B	1351	-	29,30,30	2.33	7 (24%)	39,43,43	1.85	9 (23%)
2	P4O	F	1350	-	29,30,30	2.33	7 (24%)	39,43,43	1.94	9 (23%)

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	P4O	I	1351	-	-	4/8/18/18	0/5/5/5
2	P4O	A	1351	-	-	0/8/18/18	0/5/5/5
2	P4O	C	1351	-	-	0/8/18/18	0/5/5/5
2	P4O	G	1350	-	-	0/8/18/18	0/5/5/5
2	P4O	D	1351	-	-	0/8/18/18	0/5/5/5
2	P4O	H	1347	-	-	0/8/18/18	0/5/5/5
2	P4O	L	1345	-	-	0/8/18/18	0/5/5/5
2	P4O	K	1345	-	-	0/8/18/18	0/5/5/5
2	P4O	E	1345	-	-	0/8/18/18	0/5/5/5
2	P4O	B	1351	-	-	0/8/18/18	0/5/5/5
2	P4O	F	1350	-	-	0/8/18/18	0/5/5/5

All (77) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	1350	P4O	C6-N7	6.42	1.41	1.34
2	L	1345	P4O	C6-N7	6.40	1.41	1.34
2	D	1351	P4O	C6-N7	6.29	1.40	1.34
2	E	1345	P4O	C6-N7	6.29	1.40	1.34
2	B	1351	P4O	C6-N7	6.27	1.40	1.34
2	H	1347	P4O	C6-N7	6.27	1.40	1.34
2	K	1345	P4O	C6-N7	6.17	1.40	1.34
2	I	1351	P4O	C6-N7	6.13	1.40	1.34
2	C	1351	P4O	C6-N7	6.09	1.40	1.34
2	F	1350	P4O	C18-C14	-6.09	1.39	1.49
2	F	1350	P4O	C6-N7	6.05	1.40	1.34
2	C	1351	P4O	C18-C14	-6.04	1.39	1.49
2	K	1345	P4O	C18-C14	-6.04	1.39	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1351	P4O	C18-C14	-6.03	1.39	1.49
2	I	1351	P4O	C18-C14	-6.03	1.39	1.49
2	H	1347	P4O	C18-C14	-6.02	1.39	1.49
2	L	1345	P4O	C18-C14	-6.02	1.39	1.49
2	B	1351	P4O	C18-C14	-6.00	1.39	1.49
2	G	1350	P4O	C18-C14	-5.98	1.39	1.49
2	E	1345	P4O	C18-C14	-5.91	1.39	1.49
2	A	1351	P4O	C6-N7	5.90	1.40	1.34
2	A	1351	P4O	C18-C14	-5.83	1.40	1.49
2	F	1350	P4O	C12-C2	-4.97	1.39	1.47
2	B	1351	P4O	C12-C2	-4.86	1.39	1.47
2	D	1351	P4O	C12-C2	-4.85	1.39	1.47
2	K	1345	P4O	C12-C2	-4.81	1.39	1.47
2	C	1351	P4O	C12-C2	-4.81	1.39	1.47
2	E	1345	P4O	C12-C2	-4.79	1.39	1.47
2	H	1347	P4O	C12-C2	-4.79	1.39	1.47
2	I	1351	P4O	C12-C2	-4.77	1.39	1.47
2	A	1351	P4O	C12-C2	-4.72	1.39	1.47
2	L	1345	P4O	C12-C2	-4.71	1.39	1.47
2	G	1350	P4O	C12-C2	-4.71	1.39	1.47
2	L	1345	P4O	C3-C4	-4.00	1.33	1.42
2	B	1351	P4O	C3-C4	-3.99	1.33	1.42
2	F	1350	P4O	C3-C4	-3.99	1.33	1.42
2	K	1345	P4O	C3-C4	-3.99	1.33	1.42
2	E	1345	P4O	C3-C4	-3.96	1.33	1.42
2	D	1351	P4O	C3-C4	-3.96	1.33	1.42
2	H	1347	P4O	C3-C4	-3.93	1.33	1.42
2	I	1351	P4O	C3-C4	-3.92	1.33	1.42
2	G	1350	P4O	C3-C4	-3.92	1.33	1.42
2	C	1351	P4O	C3-C4	-3.91	1.33	1.42
2	A	1351	P4O	C3-C4	-3.90	1.33	1.42
2	A	1351	P4O	C4-C6	-2.85	1.39	1.45
2	L	1345	P4O	C4-C6	-2.84	1.39	1.45
2	B	1351	P4O	C4-C6	-2.83	1.39	1.45
2	K	1345	P4O	C4-C6	-2.82	1.39	1.45
2	D	1351	P4O	C4-C6	-2.82	1.39	1.45
2	I	1351	P4O	C4-C6	-2.81	1.39	1.45
2	E	1345	P4O	C4-C6	-2.81	1.39	1.45
2	F	1350	P4O	C4-C6	-2.79	1.39	1.45
2	C	1351	P4O	C4-C6	-2.78	1.39	1.45
2	H	1347	P4O	C4-C6	-2.75	1.39	1.45
2	G	1350	P4O	C4-C6	-2.75	1.39	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1350	P4O	C3-C2	-2.67	1.33	1.38
2	I	1351	P4O	C3-C2	-2.60	1.33	1.38
2	L	1345	P4O	C3-C2	-2.60	1.33	1.38
2	D	1351	P4O	C3-C2	-2.58	1.33	1.38
2	G	1350	P4O	C3-C2	-2.58	1.33	1.38
2	B	1351	P4O	C3-C2	-2.57	1.33	1.38
2	C	1351	P4O	C3-C2	-2.57	1.33	1.38
2	A	1351	P4O	C3-C2	-2.57	1.33	1.38
2	H	1347	P4O	C3-C2	-2.56	1.33	1.38
2	E	1345	P4O	C3-C2	-2.55	1.33	1.38
2	K	1345	P4O	C3-C2	-2.53	1.33	1.38
2	G	1350	P4O	C9-C5	2.25	1.53	1.49
2	I	1351	P4O	C9-C5	2.24	1.53	1.49
2	K	1345	P4O	C9-C5	2.24	1.53	1.49
2	E	1345	P4O	C9-C5	2.22	1.53	1.49
2	H	1347	P4O	C9-C5	2.22	1.53	1.49
2	B	1351	P4O	C9-C5	2.20	1.53	1.49
2	C	1351	P4O	C9-C5	2.20	1.53	1.49
2	F	1350	P4O	C9-C5	2.19	1.53	1.49
2	L	1345	P4O	C9-C5	2.19	1.53	1.49
2	D	1351	P4O	C9-C5	2.19	1.53	1.49
2	A	1351	P4O	C9-C5	2.13	1.53	1.49

All (112) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	1345	P4O	C18-C17-N16	-5.34	120.77	125.48
2	D	1351	P4O	C18-C17-N16	-5.21	120.89	125.48
2	B	1351	P4O	C18-C17-N16	-5.10	120.98	125.48
2	F	1350	P4O	C18-C17-N16	-5.07	121.01	125.48
2	I	1351	P4O	C18-C17-N16	-4.95	121.12	125.48
2	G	1350	P4O	C18-C17-N16	-4.95	121.12	125.48
2	C	1351	P4O	C18-C17-N16	-4.88	121.17	125.48
2	H	1347	P4O	C18-C17-N16	-4.88	121.17	125.48
2	L	1345	P4O	C18-C17-N16	-4.81	121.24	125.48
2	E	1345	P4O	C18-C17-N16	-4.76	121.28	125.48
2	B	1351	P4O	C17-N16-C21	4.58	122.26	116.96
2	K	1345	P4O	C17-N16-C21	4.57	122.25	116.96
2	D	1351	P4O	C17-N16-C21	4.56	122.24	116.96
2	E	1345	P4O	C17-N16-C21	4.46	122.12	116.96
2	H	1347	P4O	C17-N16-C21	4.45	122.11	116.96
2	A	1351	P4O	C18-C17-N16	-4.45	121.56	125.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1351	P4O	C17-N16-C21	4.39	122.04	116.96
2	I	1351	P4O	C17-N16-C21	4.38	122.03	116.96
2	F	1350	P4O	C17-N16-C21	4.38	122.03	116.96
2	G	1350	P4O	C17-N16-C21	4.31	121.95	116.96
2	L	1345	P4O	C17-N16-C21	4.30	121.94	116.96
2	C	1351	P4O	C17-N16-C21	4.28	121.92	116.96
2	E	1345	P4O	C10-N15-C14	4.21	123.13	117.24
2	F	1350	P4O	C12-C2-C3	-3.94	124.98	131.03
2	L	1345	P4O	C10-N15-C14	3.91	122.72	117.24
2	B	1351	P4O	C10-N15-C14	3.83	122.60	117.24
2	G	1350	P4O	C10-N15-C14	3.82	122.59	117.24
2	F	1350	P4O	C10-N15-C14	3.78	122.53	117.24
2	H	1347	P4O	C10-N15-C14	3.77	122.51	117.24
2	I	1351	P4O	C10-N15-C14	3.76	122.50	117.24
2	K	1345	P4O	C10-N15-C14	3.75	122.49	117.24
2	A	1351	P4O	C10-N15-C14	3.74	122.48	117.24
2	C	1351	P4O	C10-N15-C14	3.74	122.48	117.24
2	D	1351	P4O	C12-C2-C3	-3.74	125.29	131.03
2	D	1351	P4O	C10-N15-C14	3.73	122.46	117.24
2	L	1345	P4O	C12-C2-C3	-3.56	125.56	131.03
2	E	1345	P4O	C12-C2-C3	-3.36	125.88	131.03
2	K	1345	P4O	C12-C2-C3	-3.35	125.89	131.03
2	B	1351	P4O	C12-C2-C3	-3.33	125.92	131.03
2	H	1347	P4O	C12-C2-C3	-3.24	126.05	131.03
2	E	1345	P4O	C11-C10-N15	-3.24	120.00	123.97
2	A	1351	P4O	C4-C6-N7	3.16	120.26	113.59
2	L	1345	P4O	C11-C10-N15	-3.16	120.10	123.97
2	G	1350	P4O	C11-C10-N15	-3.12	120.15	123.97
2	I	1351	P4O	C12-C2-C3	-3.07	126.32	131.03
2	K	1345	P4O	C11-C10-N15	-3.04	120.25	123.97
2	K	1345	P4O	C4-C6-N7	3.01	119.93	113.59
2	E	1345	P4O	C4-C6-N7	2.99	119.89	113.59
2	A	1351	P4O	C12-C2-C3	-2.98	126.45	131.03
2	F	1350	P4O	C9-C5-C4	-2.97	123.34	125.13
2	G	1350	P4O	C4-C6-N7	2.94	119.78	113.59
2	I	1351	P4O	C4-C6-N7	2.93	119.77	113.59
2	G	1350	P4O	C12-C2-C3	-2.90	126.58	131.03
2	F	1350	P4O	C4-C6-N7	2.89	119.68	113.59
2	I	1351	P4O	C11-C10-N15	-2.88	120.45	123.97
2	A	1351	P4O	C11-C10-N15	-2.86	120.47	123.97
2	D	1351	P4O	C9-C5-C4	-2.85	123.41	125.13
2	B	1351	P4O	C4-C6-N7	2.84	119.58	113.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	1345	P4O	C4-C6-N7	2.84	119.58	113.59
2	C	1351	P4O	C4-C6-N7	2.83	119.57	113.59
2	D	1351	P4O	C4-C6-N7	2.80	119.50	113.59
2	C	1351	P4O	C12-C2-C3	-2.79	126.74	131.03
2	H	1347	P4O	C11-C10-N15	-2.76	120.60	123.97
2	H	1347	P4O	C4-C6-N7	2.75	119.39	113.59
2	A	1351	P4O	O26-C6-N7	-2.72	118.53	123.24
2	D	1351	P4O	C11-C10-N15	-2.72	120.64	123.97
2	F	1350	P4O	C11-C10-N15	-2.65	120.72	123.97
2	K	1345	P4O	O26-C6-C4	-2.64	120.16	125.98
2	L	1345	P4O	O26-C6-C4	-2.56	120.34	125.98
2	E	1345	P4O	O26-C6-C4	-2.56	120.35	125.98
2	B	1351	P4O	C11-C10-N15	-2.55	120.85	123.97
2	B	1351	P4O	O26-C6-C4	-2.52	120.42	125.98
2	G	1350	P4O	O26-C6-C4	-2.51	120.44	125.98
2	F	1350	P4O	O26-C6-C4	-2.51	120.44	125.98
2	I	1351	P4O	O26-C6-C4	-2.49	120.50	125.98
2	G	1350	P4O	C4-C5-N1	-2.45	107.13	109.75
2	C	1351	P4O	C11-C10-N15	-2.45	120.97	123.97
2	A	1351	P4O	C13-C14-N15	-2.44	119.05	122.13
2	L	1345	P4O	C12-C2-N1	2.44	125.85	122.76
2	I	1351	P4O	C4-C5-N1	-2.41	107.18	109.75
2	K	1345	P4O	C4-C5-N1	-2.40	107.18	109.75
2	C	1351	P4O	C13-C14-N15	-2.39	119.11	122.13
2	A	1351	P4O	C9-C5-C4	-2.37	123.70	125.13
2	L	1345	P4O	C4-C5-N1	-2.37	107.22	109.75
2	E	1345	P4O	C13-C14-N15	-2.36	119.15	122.13
2	F	1350	P4O	C12-C2-N1	2.36	125.75	122.76
2	D	1351	P4O	O26-C6-C4	-2.34	120.83	125.98
2	D	1351	P4O	C12-C2-N1	2.34	125.72	122.76
2	C	1351	P4O	O26-C6-N7	-2.33	119.22	123.24
2	E	1345	P4O	C4-C5-N1	-2.31	107.28	109.75
2	H	1347	P4O	O26-C6-N7	-2.31	119.24	123.24
2	A	1351	P4O	C4-C5-N1	-2.30	107.29	109.75
2	E	1345	P4O	C9-C5-C4	-2.28	123.75	125.13
2	B	1351	P4O	C13-C14-N15	-2.27	119.27	122.13
2	A	1351	P4O	C12-C2-N1	2.21	125.56	122.76
2	B	1351	P4O	C4-C5-N1	-2.20	107.40	109.75
2	C	1351	P4O	C4-C5-N1	-2.19	107.41	109.75
2	A	1351	P4O	O26-C6-C4	-2.19	121.16	125.98
2	C	1351	P4O	O26-C6-C4	-2.16	121.21	125.98
2	E	1345	P4O	C12-C2-N1	2.16	125.50	122.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	L	1345	P4O	C9-C5-C4	-2.15	123.83	125.13
2	H	1347	P4O	O26-C6-C4	-2.14	121.27	125.98
2	D	1351	P4O	C13-C14-N15	-2.09	119.49	122.13
2	H	1347	P4O	C4-C5-N1	-2.09	107.52	109.75
2	D	1351	P4O	O26-C6-N7	-2.08	119.64	123.24
2	K	1345	P4O	C12-C2-N1	2.08	125.39	122.76
2	H	1347	P4O	C13-C14-N15	-2.05	119.54	122.13
2	G	1350	P4O	O26-C6-N7	-2.05	119.70	123.24
2	L	1345	P4O	C13-C14-N15	-2.05	119.55	122.13
2	E	1345	P4O	O26-C6-N7	-2.04	119.71	123.24
2	I	1351	P4O	O26-C6-N7	-2.03	119.73	123.24
2	D	1351	P4O	C4-C5-N1	-2.02	107.59	109.75

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	I	1351	P4O	C13-C14-C18-C17
2	I	1351	P4O	N15-C14-C18-C17
2	I	1351	P4O	C13-C14-C18-C19
2	I	1351	P4O	N15-C14-C18-C19

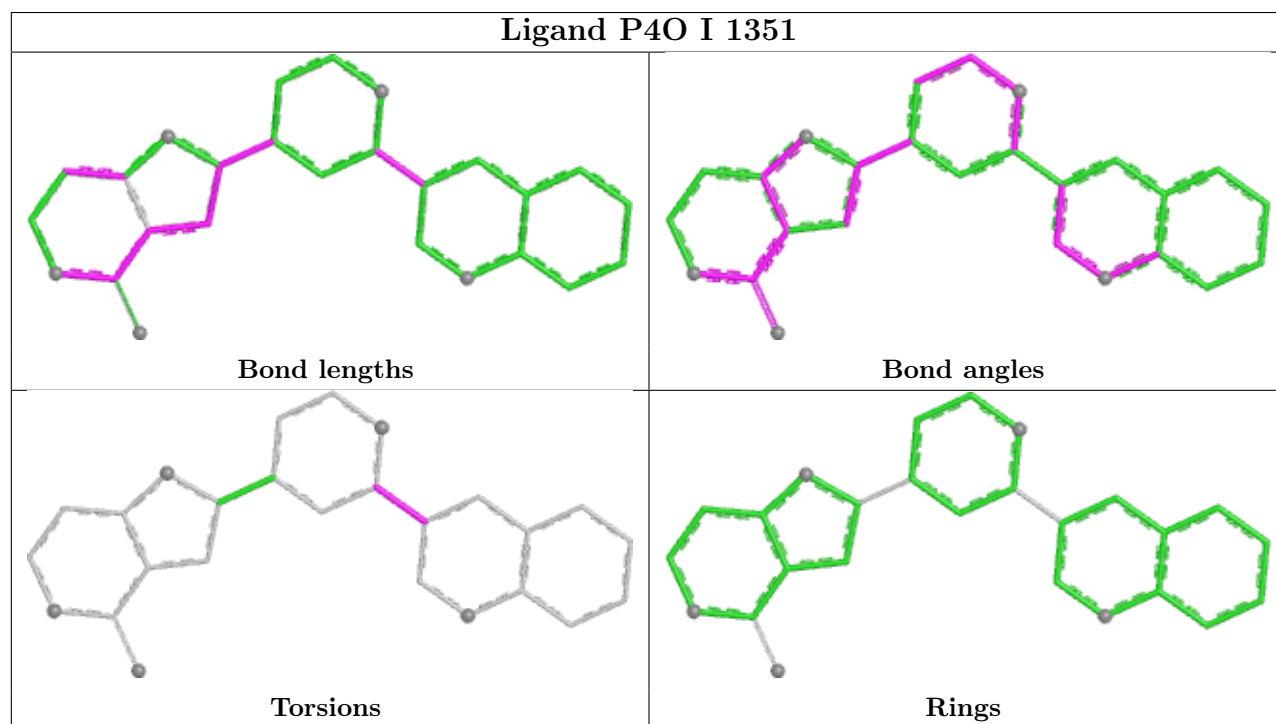
There are no ring outliers.

11 monomers are involved in 40 short contacts:

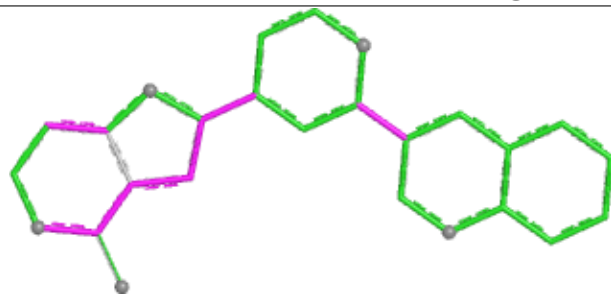
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	I	1351	P4O	3	0
2	A	1351	P4O	2	0
2	C	1351	P4O	4	0
2	G	1350	P4O	5	0
2	D	1351	P4O	5	0
2	H	1347	P4O	4	0
2	L	1345	P4O	4	0
2	K	1345	P4O	3	0
2	E	1345	P4O	4	0
2	B	1351	P4O	1	0
2	F	1350	P4O	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

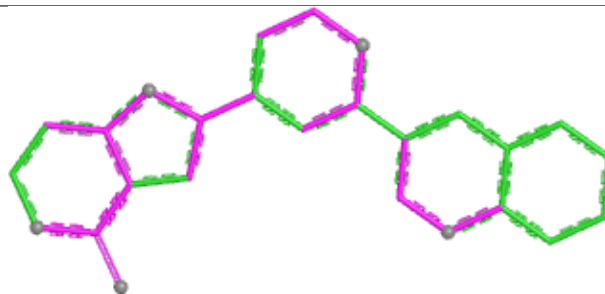
also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



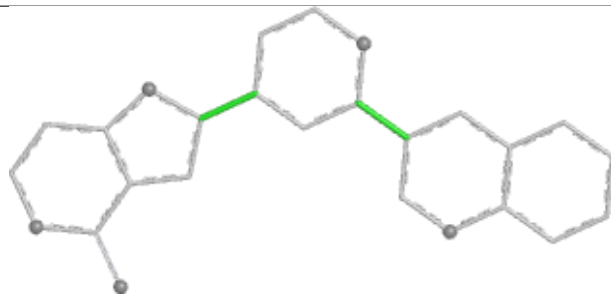
Ligand P4O A 1351



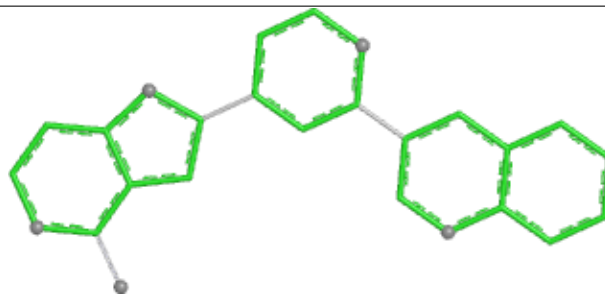
Bond lengths



Bond angles

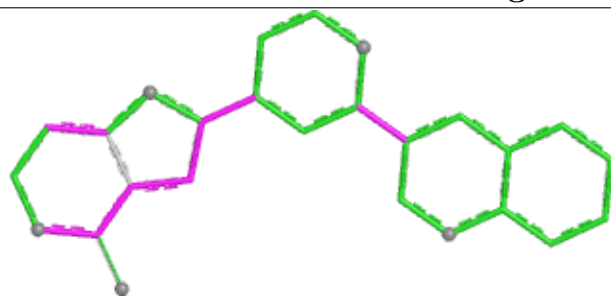


Torsions

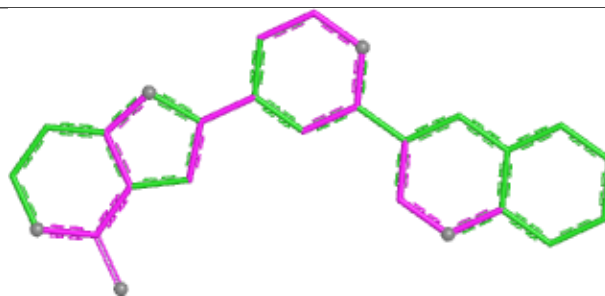


Rings

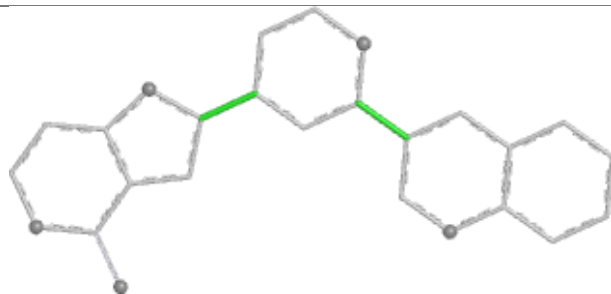
Ligand P4O C 1351



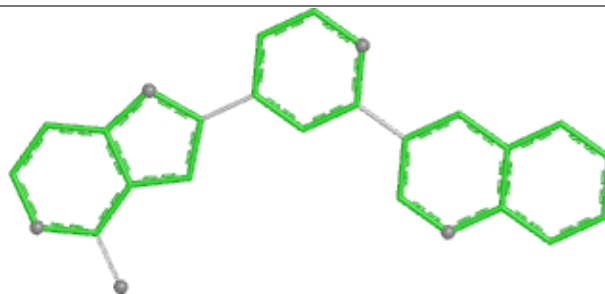
Bond lengths



Bond angles

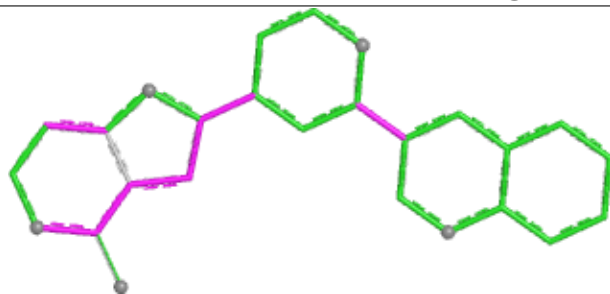


Torsions

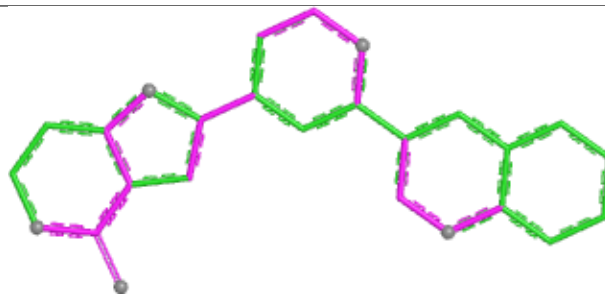


Rings

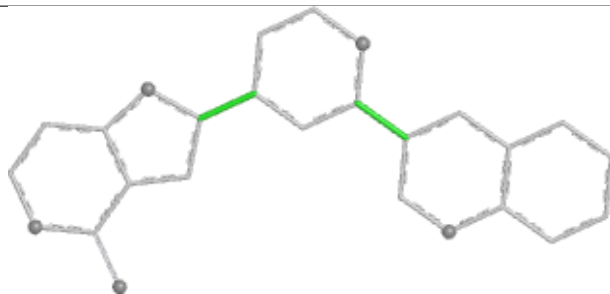
Ligand P4O G 1350



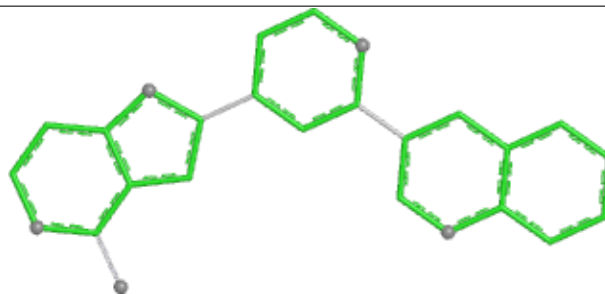
Bond lengths



Bond angles

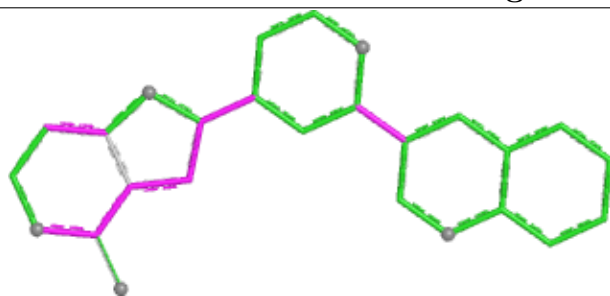


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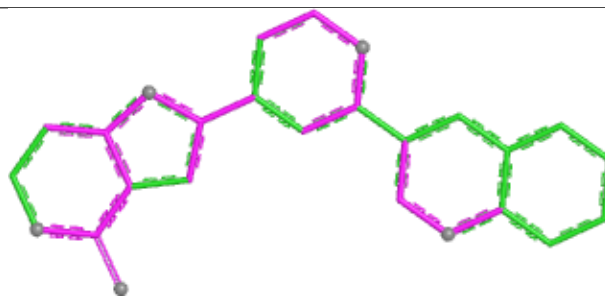


Rings

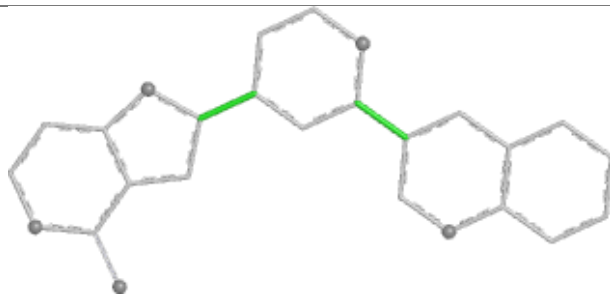
Ligand P4O D 1351



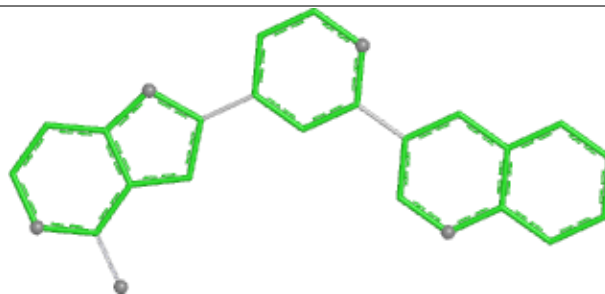
Bond lengths



Bond angles

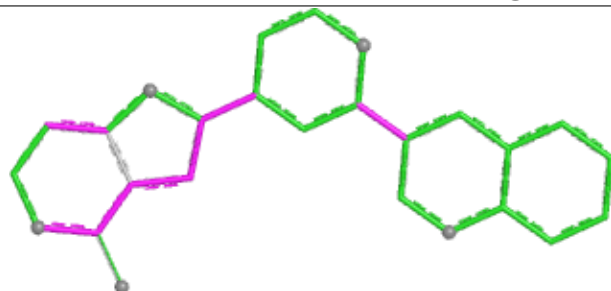


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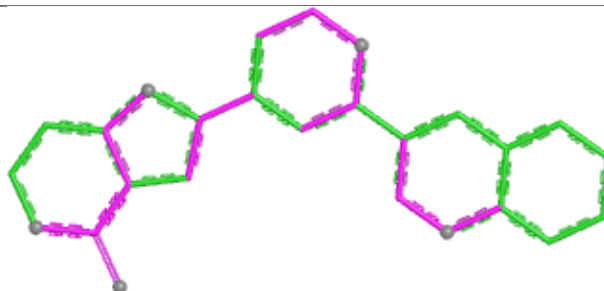


Rings

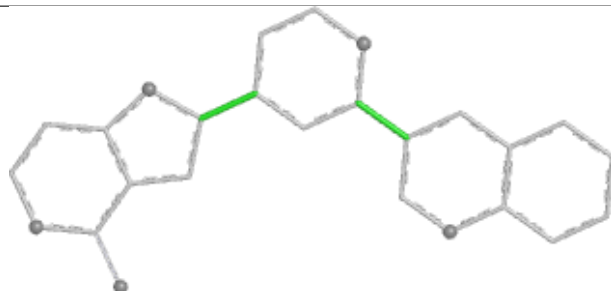
Ligand P4O H 1347



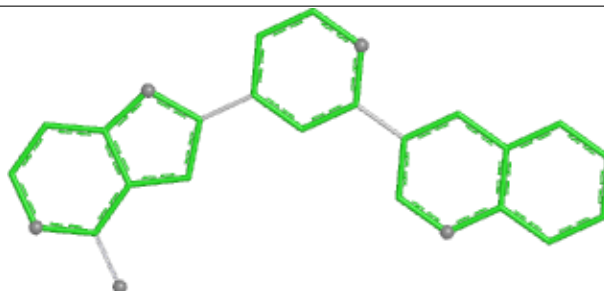
Bond lengths



Bond angles

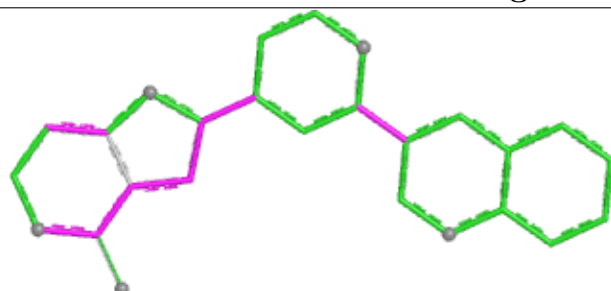


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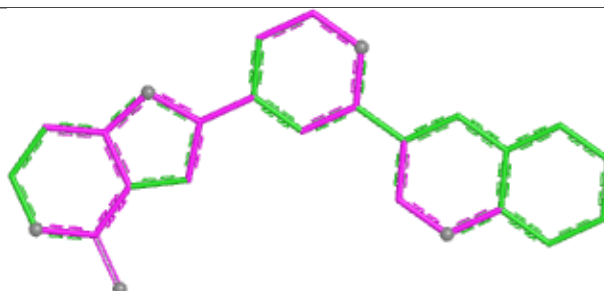


Rings

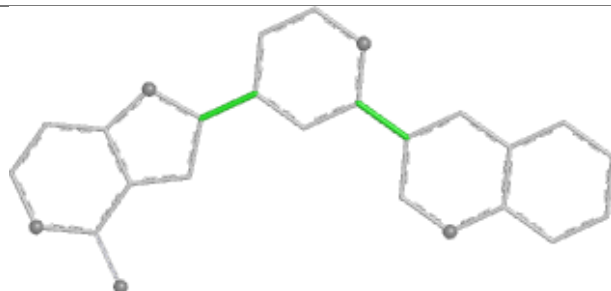
Ligand P4O L 1345



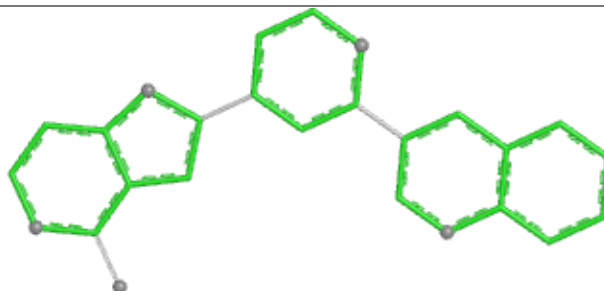
Bond lengths



Bond angles

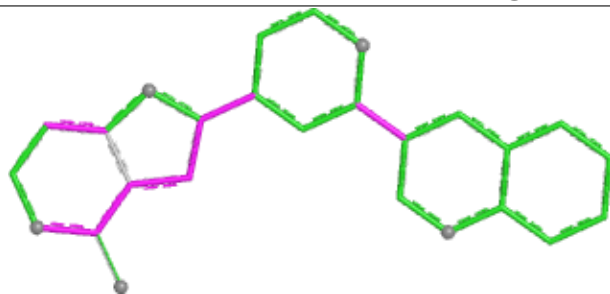


Torsions

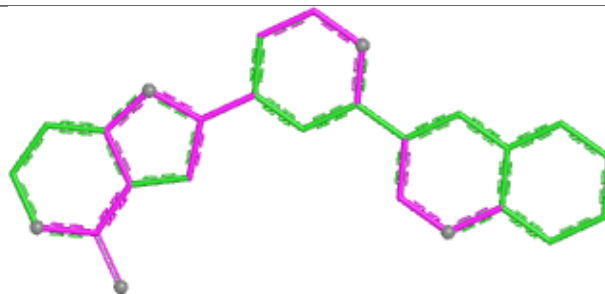


Rings

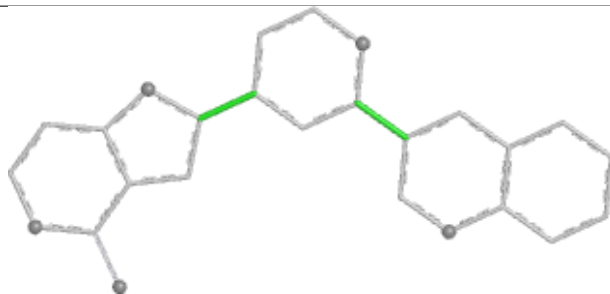
Ligand P4O K 1345



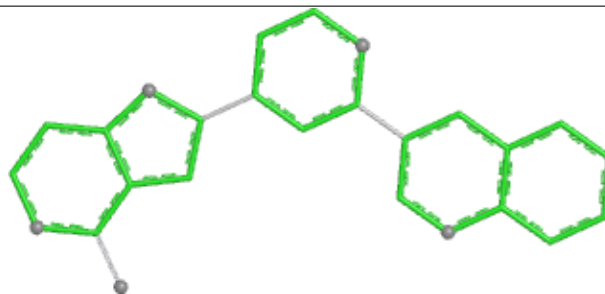
Bond lengths



Bond angles

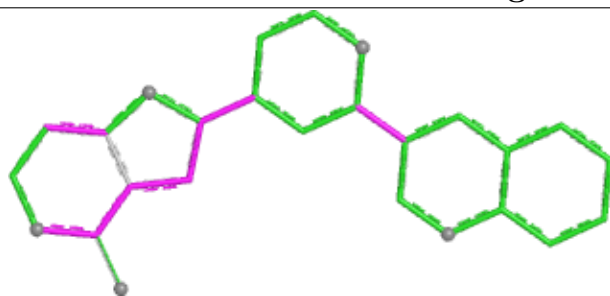


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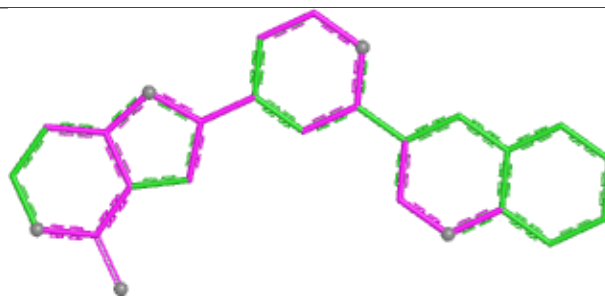


Rings

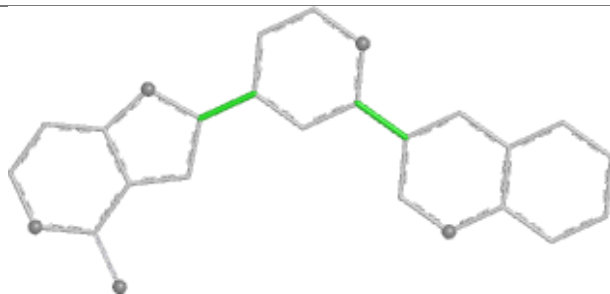
Ligand P4O E 1345



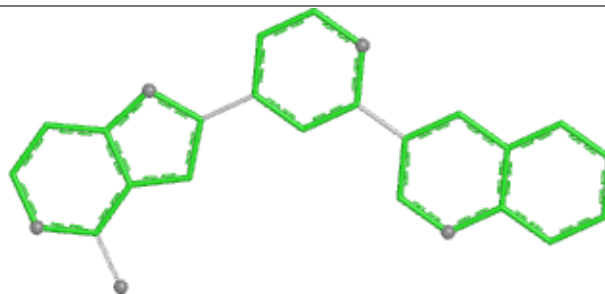
Bond lengths



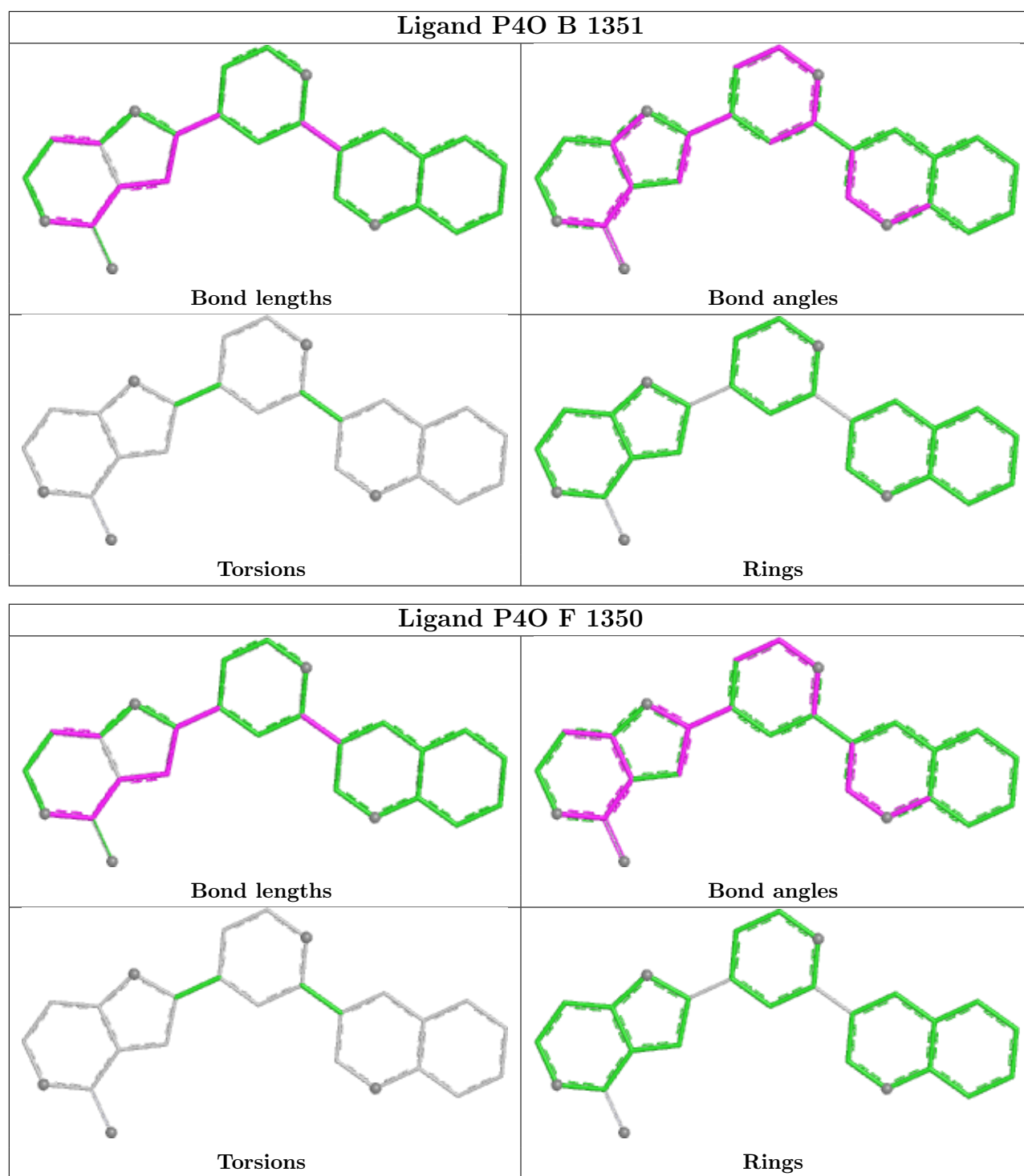
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	283/326 (86%)	-0.75	1 (0%) 88 79	13, 40, 110, 170	0
1	B	290/326 (88%)	-0.65	0 100 100	20, 63, 141, 173	0
1	C	284/326 (87%)	-0.68	2 (0%) 84 70	19, 54, 127, 169	0
1	D	286/326 (87%)	-0.75	2 (0%) 84 70	16, 51, 125, 171	0
1	E	283/326 (86%)	-0.49	0 100 100	33, 81, 140, 174	0
1	F	288/326 (88%)	-0.77	0 100 100	13, 47, 116, 156	0
1	G	288/326 (88%)	-0.54	1 (0%) 90 82	19, 74, 150, 194	0
1	H	283/326 (86%)	-0.52	1 (0%) 88 79	36, 76, 137, 186	0
1	I	289/326 (88%)	-0.47	4 (1%) 73 55	31, 72, 152, 180	0
1	J	225/326 (69%)	-0.20	2 (0%) 81 66	51, 120, 170, 198	0
1	K	265/326 (81%)	-0.10	4 (1%) 72 53	50, 127, 177, 198	0
1	L	268/326 (82%)	-0.33	4 (1%) 72 53	35, 113, 174, 188	0
All	All	3332/3912 (85%)	-0.53	21 (0%) 85 73	13, 73, 157, 198	0

All (21) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	L	147	PHE	4.0
1	J	197	LYS	3.9
1	I	230	VAL	3.4
1	K	257	LEU	3.2
1	H	231	ALA	3.0
1	C	154	GLY	2.6
1	I	76	GLY	2.4
1	A	154	GLY	2.4
1	L	189	PRO	2.4
1	C	228	TYR	2.3
1	D	350	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	J	141	LEU	2.2
1	D	154	GLY	2.2
1	I	229	TYR	2.2
1	L	157	ALA	2.2
1	K	271	ILE	2.2
1	K	317	THR	2.1
1	G	77	LYS	2.1
1	I	235	LEU	2.1
1	K	264	TYR	2.1
1	L	144	GLY	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

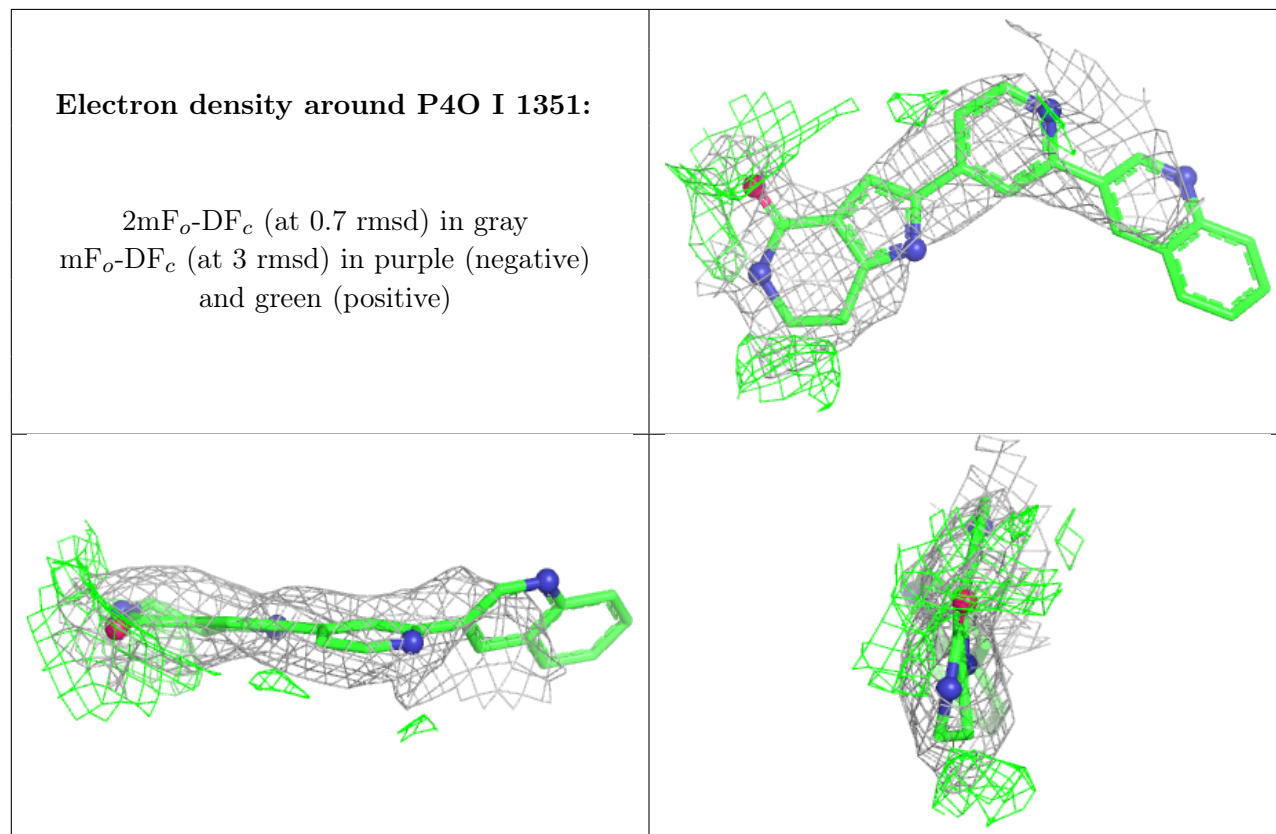
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	P4O	I	1351	26/26	0.86	0.17	117,137,150,162	0
2	P4O	K	1345	26/26	0.87	0.13	133,152,162,171	0
2	P4O	B	1351	26/26	0.88	0.14	54,105,135,142	0
2	P4O	E	1345	26/26	0.88	0.13	79,115,138,145	0
2	P4O	L	1345	26/26	0.88	0.14	125,139,158,161	0
2	P4O	C	1351	26/26	0.91	0.11	55,84,118,136	0
2	P4O	H	1347	26/26	0.92	0.09	37,88,111,116	0
2	P4O	D	1351	26/26	0.93	0.12	42,78,99,104	0
2	P4O	G	1350	26/26	0.94	0.10	39,98,121,130	0
2	P4O	F	1350	26/26	0.95	0.09	28,79,116,121	0
2	P4O	A	1351	26/26	0.97	0.08	25,57,77,89	0

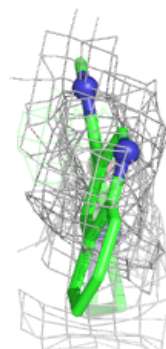
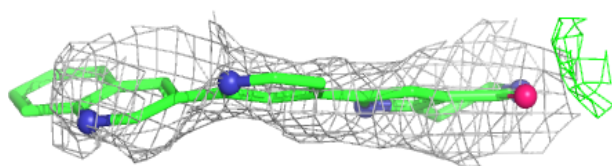
The following is a graphical depiction of the model fit to experimental electron density of all

instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

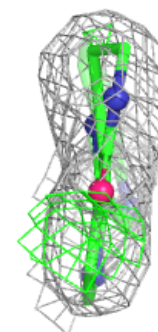
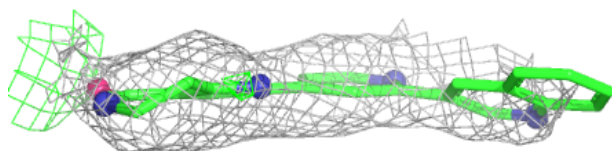
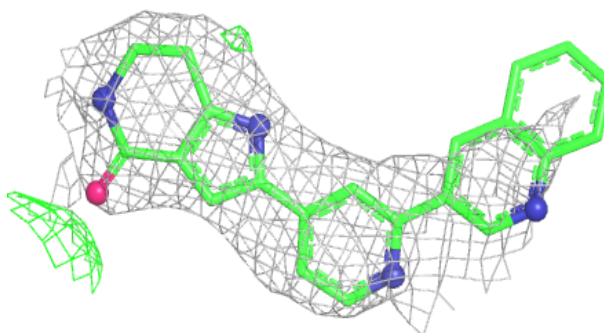


Electron density around P4O K 1345:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

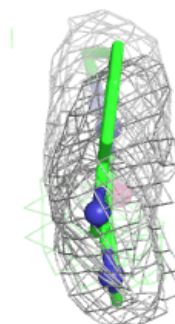
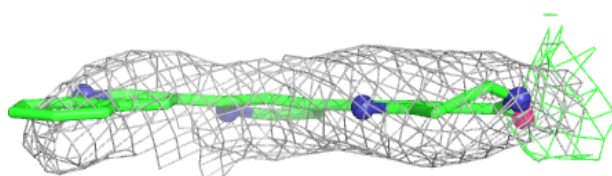
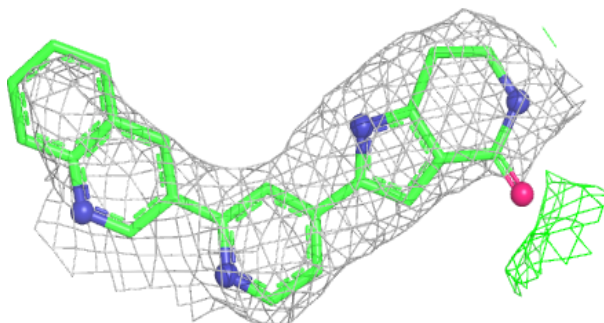
**Electron density around P4O B 1351:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

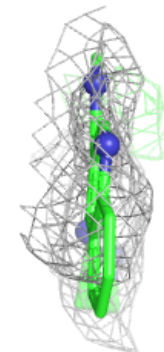
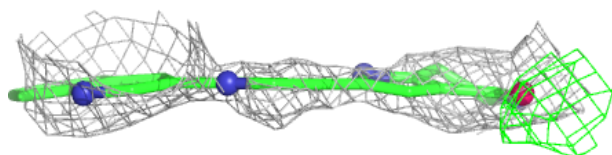
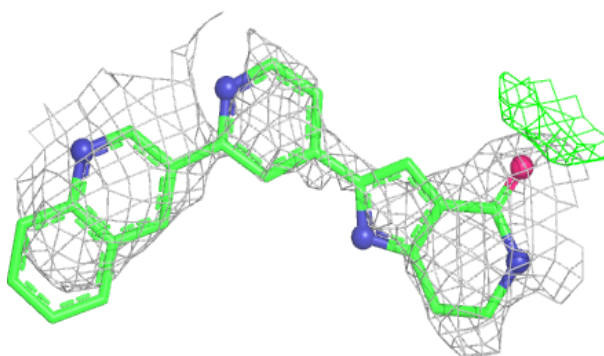


Electron density around P4O E 1345:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

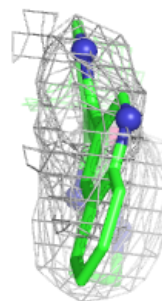
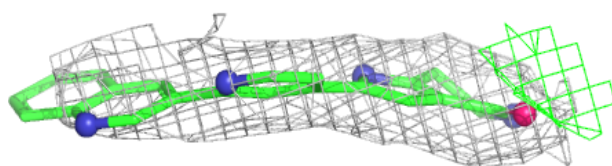
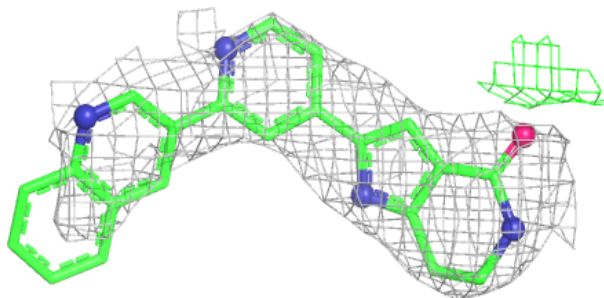
**Electron density around P4O L 1345:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

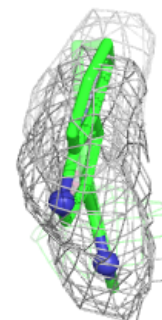
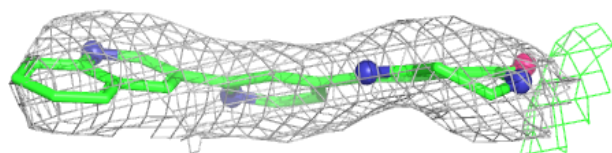
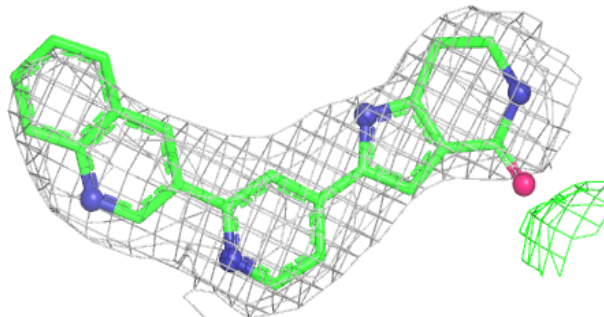


Electron density around P4O C 1351:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

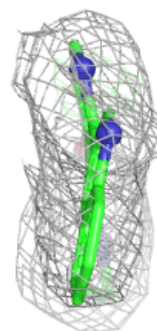
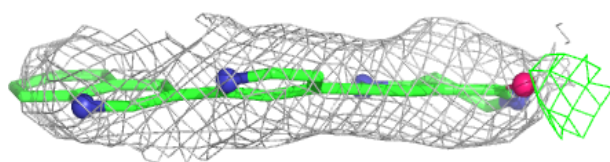
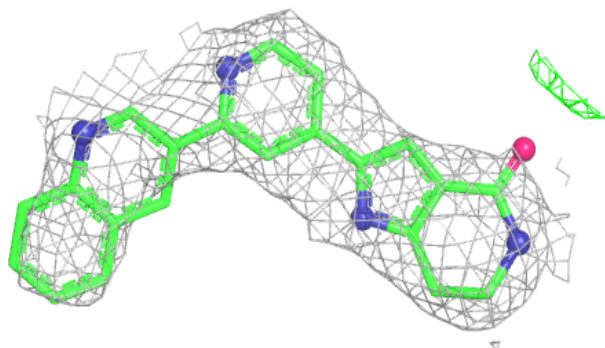
**Electron density around P4O H 1347:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

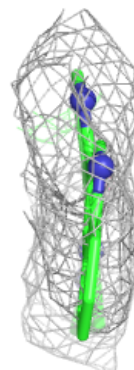
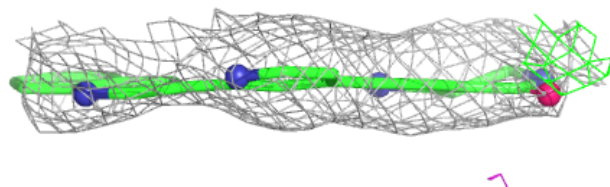
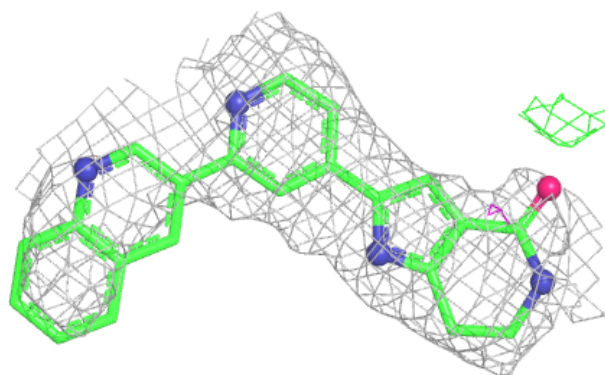


Electron density around P4O D 1351:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

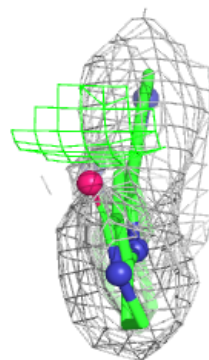
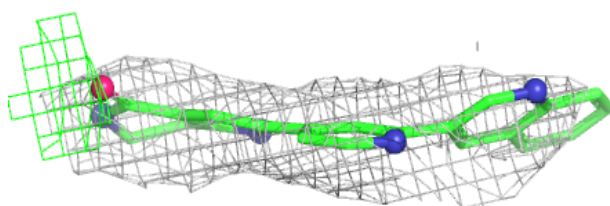
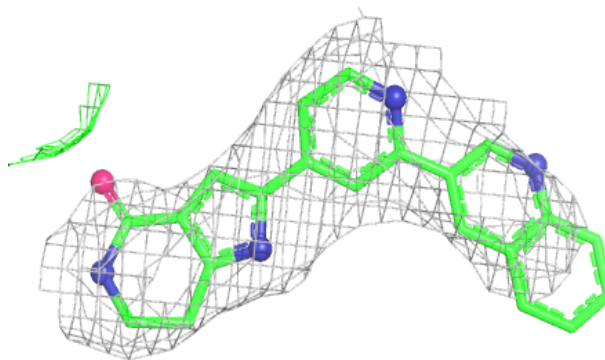
**Electron density around P4O G 1350:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

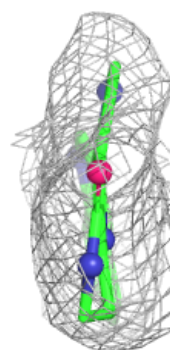
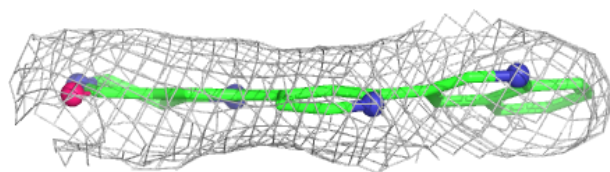
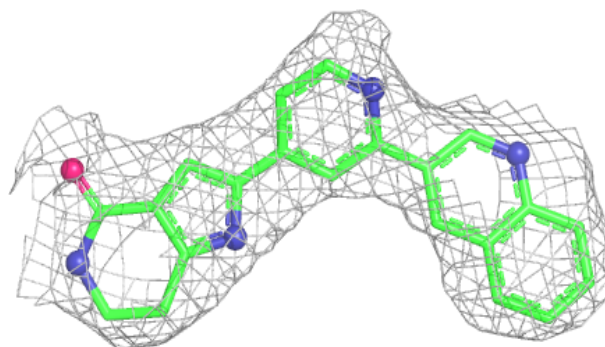


Electron density around P4O F 1350:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

**Electron density around P4O A 1351:**

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers [i](#)

There are no such residues in this entry.