Full wwPDB X-ray Structure Validation Report ⓘ

Jun 17, 2020 – 01:33 am BST

PDB ID	:	3KC3
Title	:	MK2 complexed to inhibitor N4-(7-(benzofuran-2-yl)-1H-indazol-5-yl)pyrimidine-2,4-diamine
Authors	:	Argiriadi, M.A.; Talanian, R.V.; Borhani, D.W.
Deposited on	:	2009-10-20
Resolution	:	2.90 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 following versions of software and data (see references ⓘ) were used in the production of this report:

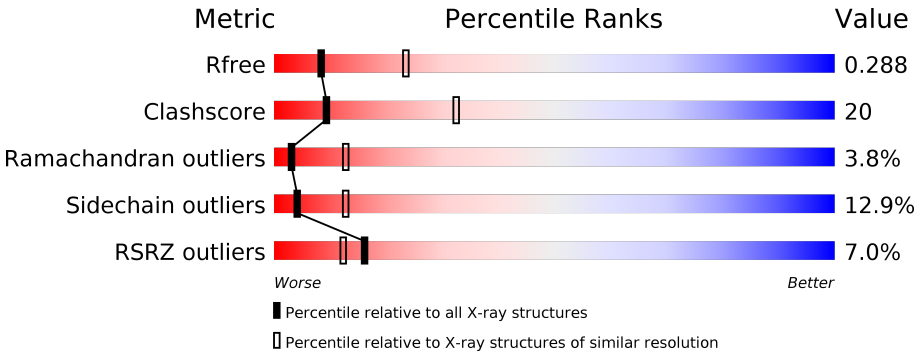
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.90 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}	130704	1957 (2.90-2.90)
Clashscore	141614	2172 (2.90-2.90)
Ramachandran outliers	138981	2115 (2.90-2.90)
Sidechain outliers	138945	2117 (2.90-2.90)
RSRZ outliers	127900	1906 (2.90-2.90)

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 on 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 <=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	324	3% 55% 27% 6% • 11%
1	B	324	2% 52% 28% 10% 10%
1	C	324	6% 50% 30% 7% 13%
1	D	324	10% 50% 27% 6% 17%
1	E	324	2% 53% 28% 6% • 11%
1	F	324	3% 52% 29% 7% • 10%

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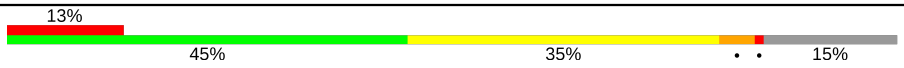
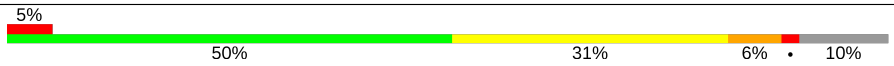
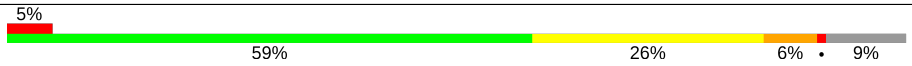
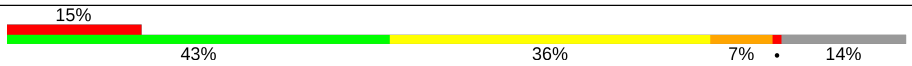
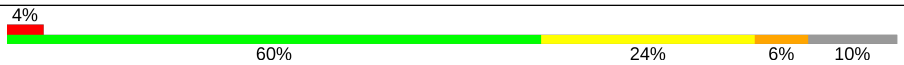
Mol	Chain	Length	Quality of chain
1	G	324	
1	H	324	
1	I	324	
1	J	324	
1	K	324	
1	L	324	

2 Entry composition (i)

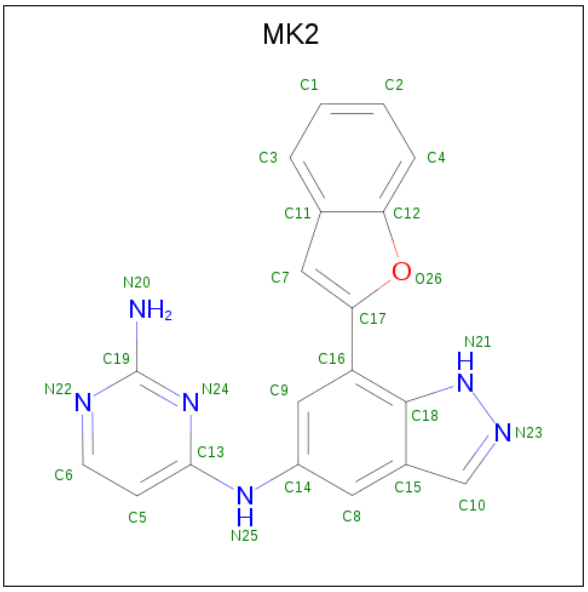
There are 3 unique types of molecules in this entry. The entry contains 28159 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	288	Total	C	N	O	S	0	0	0
			2337	1495	403	422	17			
1	B	290	Total	C	N	O	S	0	0	0
			2361	1510	407	427	17			
1	C	281	Total	C	N	O	S	0	0	0
			2297	1473	394	413	17			
1	D	269	Total	C	N	O	S	0	0	0
			2172	1389	375	391	17			
1	E	287	Total	C	N	O	S	0	0	0
			2326	1486	400	423	17			
1	F	293	Total	C	N	O	S	0	0	0
			2384	1523	413	431	17			
1	G	276	Total	C	N	O	S	0	0	0
			2246	1438	389	402	17			
1	H	290	Total	C	N	O	S	0	0	0
			2355	1503	408	427	17			
1	I	295	Total	C	N	O	S	0	0	0
			2395	1527	414	436	18			
1	J	288	Total	C	N	O	S	0	0	0
			2344	1501	404	422	17			
1	K	280	Total	C	N	O	S	0	0	0
			2269	1448	392	412	17			
1	L	291	Total	C	N	O	S	0	0	0
			2367	1513	408	429	17			

- Molecule 2 is N 4 -[7-(1-benzofuran-2-yl)-1H-indazol-5-yl]pyrimidine-2,4-diamine (three-letter code: MK2) (formula: $C_{19}H_{14}N_6O$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 26 19 6 1	0	0
2	B	1	Total C N O 26 19 6 1	0	0
2	C	1	Total C N O 26 19 6 1	0	0
2	D	1	Total C N O 26 19 6 1	0	0
2	E	1	Total C N O 26 19 6 1	0	0
2	F	1	Total C N O 26 19 6 1	0	0
2	H	1	Total C N O 26 19 6 1	0	0
2	I	1	Total C N O 26 19 6 1	0	0
2	J	1	Total C N O 26 19 6 1	0	0
2	K	1	Total C N O 26 19 6 1	0	0
2	L	1	Total C N O 26 19 6 1	0	0

- Molecule 3 is water.

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

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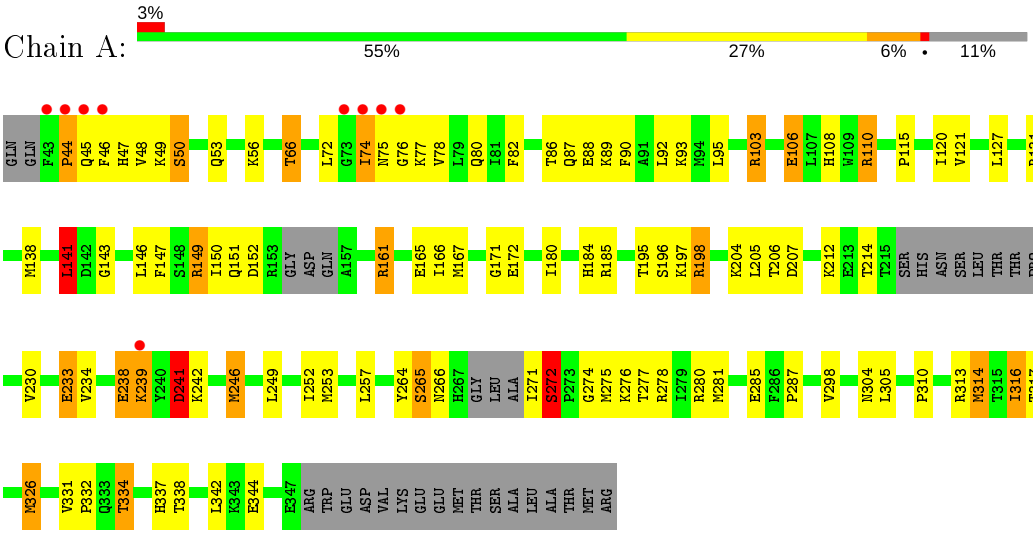
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	5	Total O 5 5	0	0
3	D	1	Total O 1 1	0	0
3	E	3	Total O 3 3	0	0
3	F	3	Total O 3 3	0	0
3	G	1	Total O 1 1	0	0
3	H	1	Total O 1 1	0	0
3	I	2	Total O 2 2	0	0
3	L	1	Total O 1 1	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA 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.

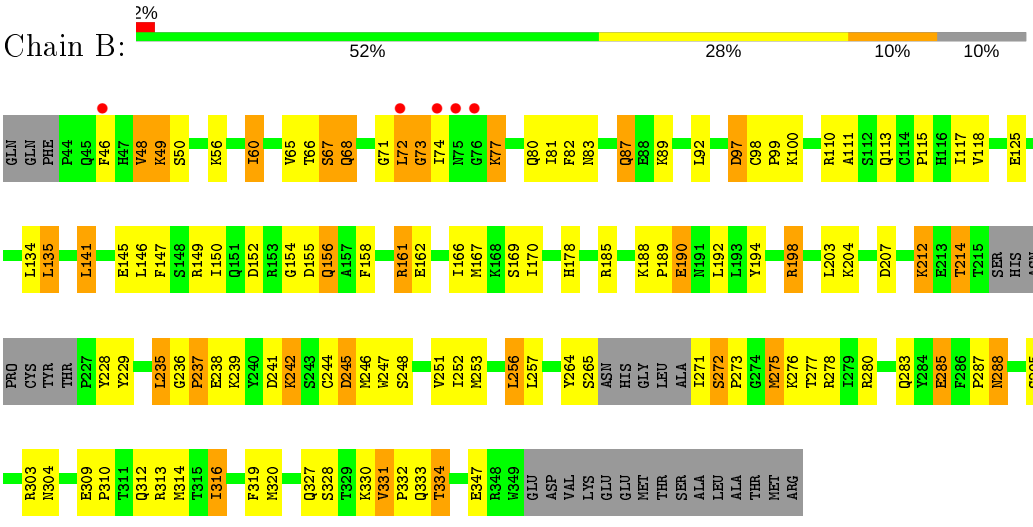
- Molecule 1: MAP kinase-activated protein kinase 2

Chain A:



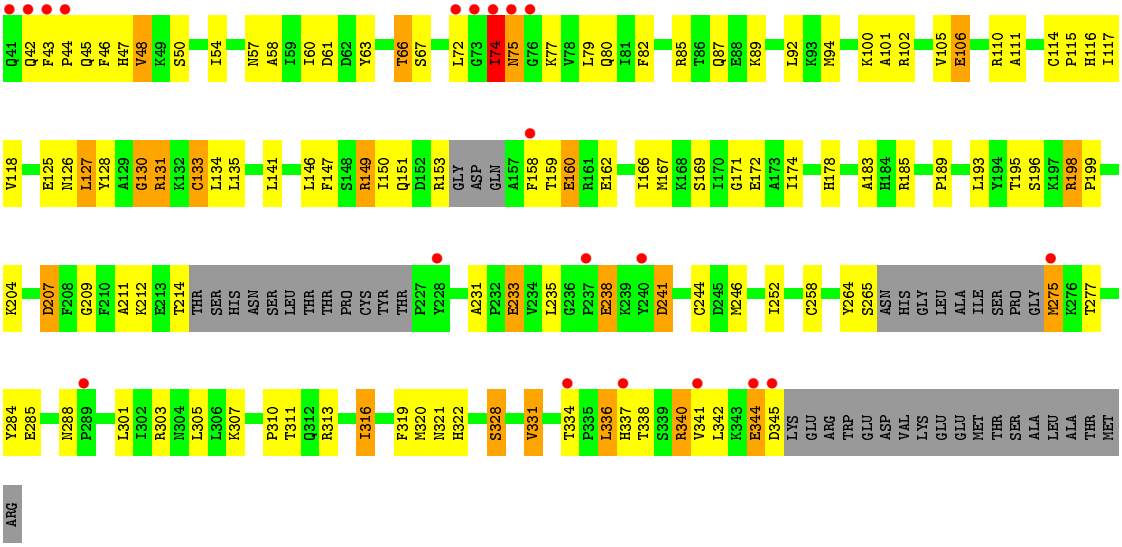
- Molecule 1: MAP kinase-activated protein kinase 2

Chain B:

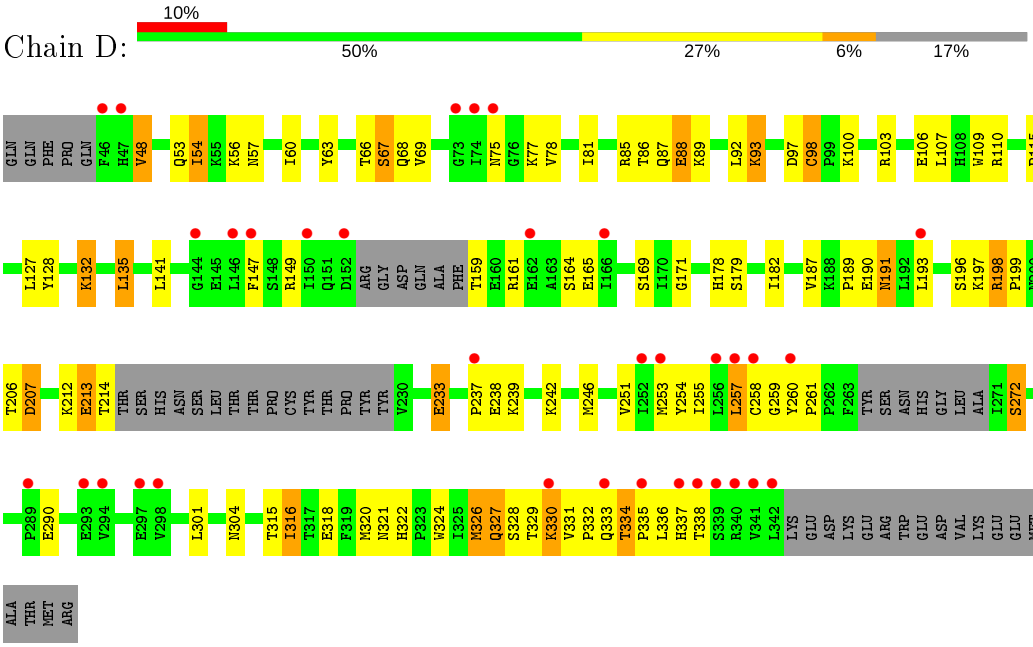


- Molecule 1: MAP kinase-activated protein kinase 2

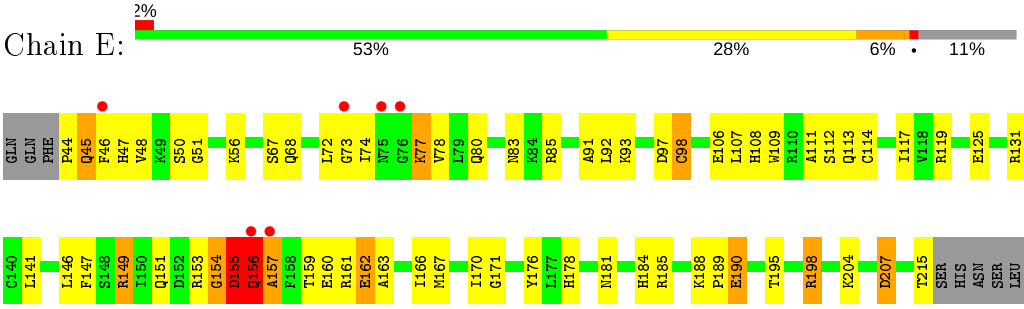
Chain C:

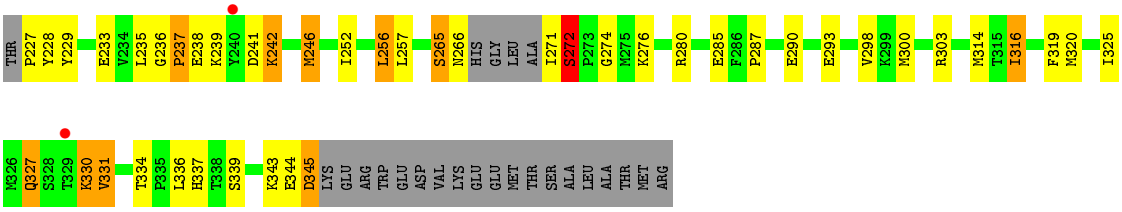


• Molecule 1: MAP kinase-activated protein kinase 2



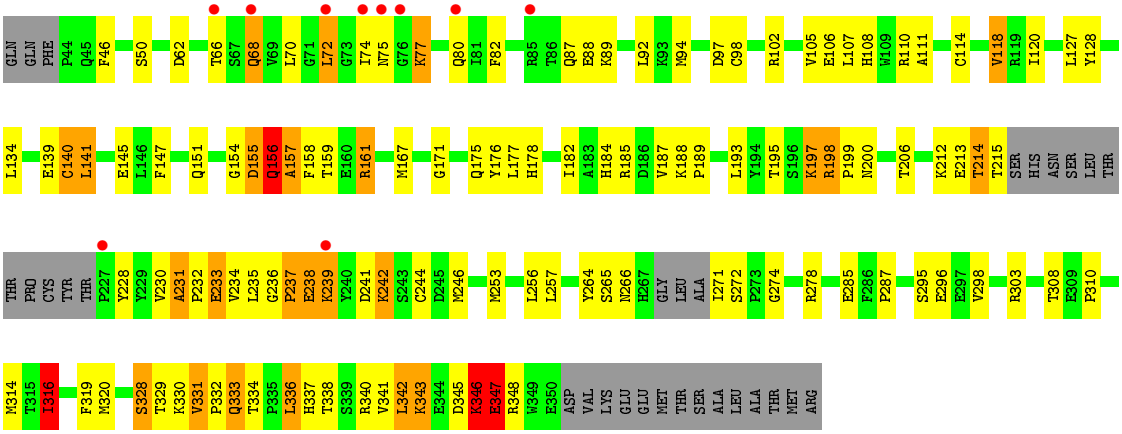
• Molecule 1: MAP kinase-activated protein kinase 2





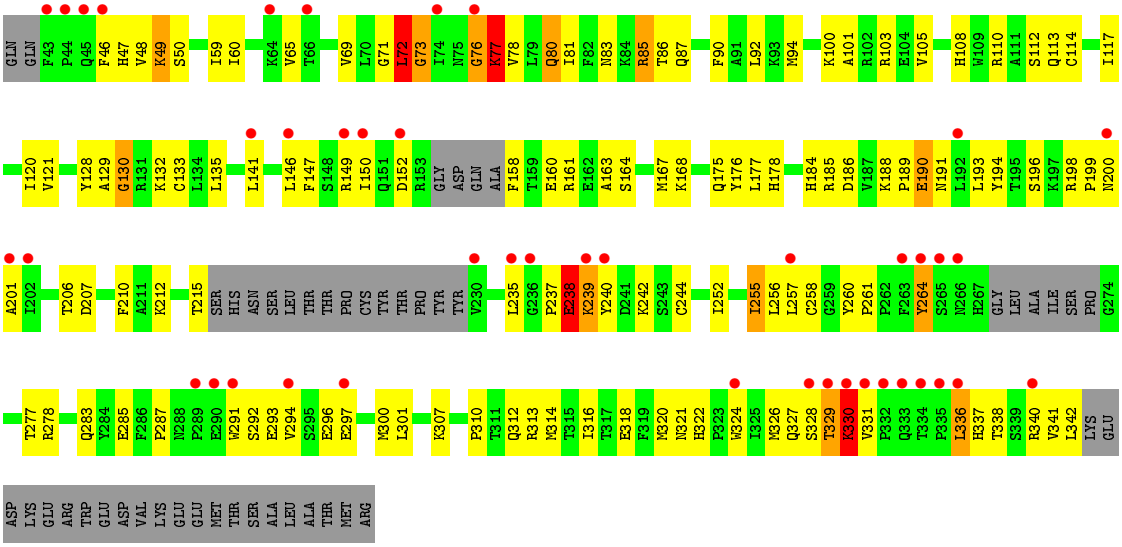
• Molecule 1: MAP kinase-activated protein kinase 2

Chain F:



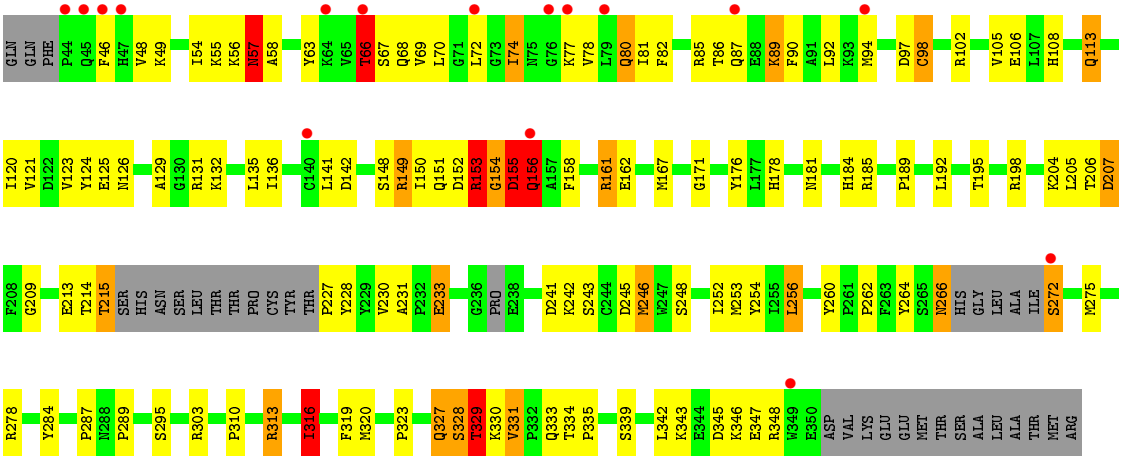
• Molecule 1: MAP kinase-activated protein kinase 2

Chain G:



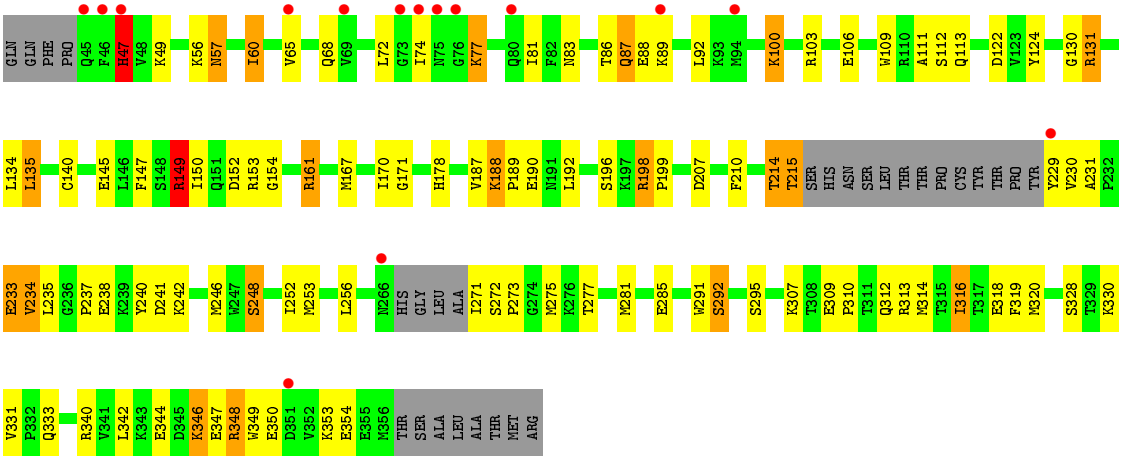
• Molecule 1: MAP kinase-activated protein kinase 2

Chain H:



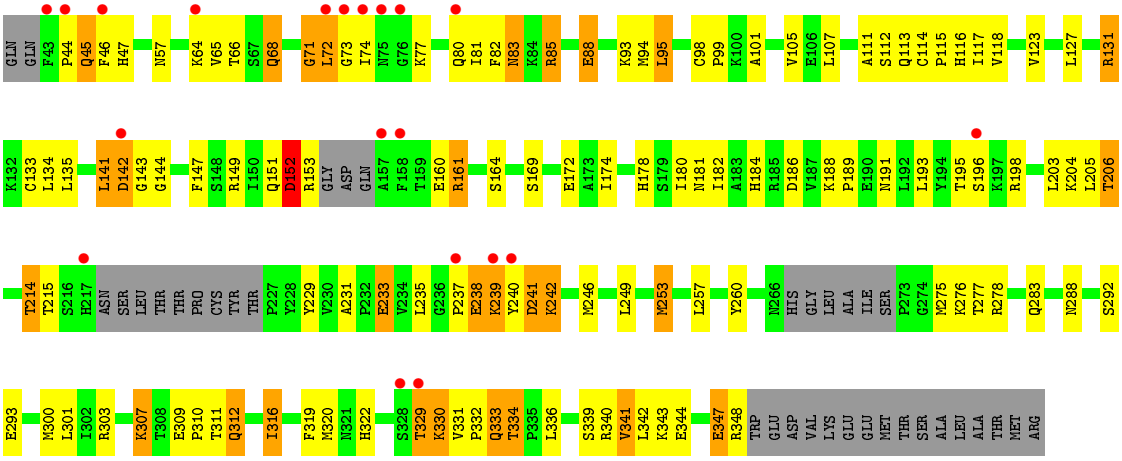
• Molecule 1: MAP kinase-activated protein kinase 2

Chain I:



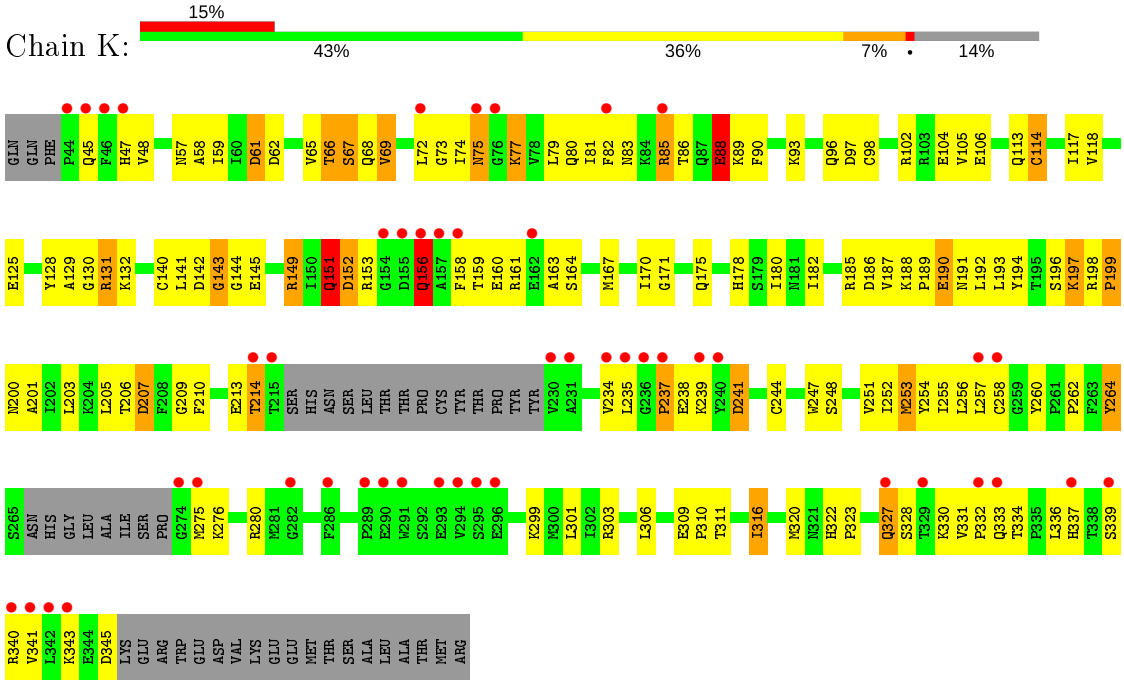
• Molecule 1: MAP kinase-activated protein kinase 2

Chain J:



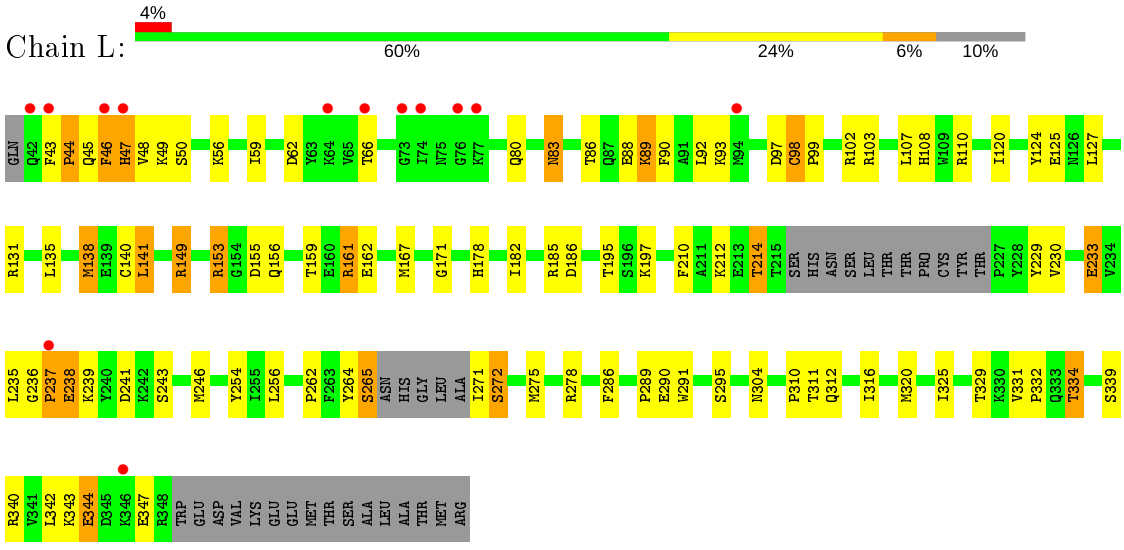
• Molecule 1: MAP kinase-activated protein kinase 2

Chain K:



• Molecule 1: MAP kinase-activated protein kinase 2

Chain L:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	139.35Å 179.79Å 214.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.90 45.44 – 2.90	Depositor EDS
% Data completeness (in resolution range)	97.3 (20.00-2.90) 97.3 (45.44-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	3.98 (at 2.91Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.230 , 0.298 0.219 , 0.288	Depositor DCC
R_{free} test set	5841 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	73.1	Xtriage
Anisotropy	0.105	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 62.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	28159	wwPDB-VP
Average B, all atoms (Å^2)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 1.76% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: MK2

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	1.04	4/2388 (0.2%)	1.05	6/3219 (0.2%)
1	B	1.03	3/2414 (0.1%)	1.03	7/3255 (0.2%)
1	C	0.86	1/2347 (0.0%)	0.93	2/3163 (0.1%)
1	D	0.71	0/2216	0.80	1/2987 (0.0%)
1	E	0.95	2/2377 (0.1%)	0.97	0/3206
1	F	0.95	2/2438 (0.1%)	0.99	4/3288 (0.1%)
1	G	0.62	0/2294	0.72	1/3092 (0.0%)
1	H	0.89	0/2405	0.95	5/3240 (0.2%)
1	I	0.80	0/2445	0.85	1/3295 (0.0%)
1	J	0.80	1/2395 (0.0%)	0.84	2/3227 (0.1%)
1	K	0.63	0/2316	0.74	0/3121
1	L	0.77	0/2419	0.85	0/3261
All	All	0.85	13/28454 (0.0%)	0.90	29/38354 (0.1%)

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	A	0	1
1	B	0	1
1	E	0	1
1	F	0	1
1	H	0	1
1	L	0	1
All	All	0	6

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	106	GLU	CG-CD	8.57	1.64	1.51
1	F	140	CYS	CB-SG	-7.62	1.69	1.82
1	F	244	CYS	CB-SG	-7.05	1.70	1.82
1	A	172	GLU	CD-OE1	7.01	1.33	1.25
1	B	244	CYS	CB-SG	-6.58	1.71	1.82
1	A	106	GLU	CD-OE2	6.36	1.32	1.25
1	A	106	GLU	CD-OE1	6.00	1.32	1.25
1	B	190	GLU	CG-CD	6.00	1.60	1.51
1	E	176	TYR	CD1-CE1	-5.80	1.30	1.39
1	C	106	GLU	CG-CD	5.78	1.60	1.51
1	J	312	GLN	CG-CD	5.49	1.63	1.51
1	B	309	GLU	CD-OE2	5.32	1.31	1.25
1	E	109	TRP	CE3-CZ3	5.26	1.47	1.38

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	161	ARG	NE-CZ-NH2	-9.02	115.79	120.30
1	F	62	ASP	CB-CG-OD1	-7.21	111.81	118.30
1	A	320	MET	CG-SD-CE	-7.10	88.84	100.20
1	F	158	PHE	N-CA-C	-7.09	91.84	111.00
1	B	141	LEU	CA-CB-CG	6.45	130.14	115.30
1	H	161	ARG	NE-CZ-NH2	-6.08	117.26	120.30
1	B	245	ASP	CB-CG-OD1	6.07	123.76	118.30
1	B	97	ASP	CB-CG-OD2	-6.06	112.85	118.30
1	C	127	LEU	CA-CB-CG	6.03	129.17	115.30
1	B	256	LEU	CB-CG-CD1	-5.91	100.95	111.00
1	A	185	ARG	NE-CZ-NH2	-5.80	117.40	120.30
1	H	185	ARG	NE-CZ-NH2	-5.70	117.45	120.30
1	B	97	ASP	CB-CG-OD1	5.69	123.42	118.30
1	G	72	LEU	CA-CB-CG	5.61	128.19	115.30
1	F	316	ILE	CG1-CB-CG2	5.59	123.71	111.40
1	A	141	LEU	CA-CB-CG	5.54	128.04	115.30
1	H	313	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	J	72	LEU	CA-CB-CG	5.45	127.83	115.30
1	B	313	ARG	NE-CZ-NH2	-5.41	117.60	120.30
1	A	241	ASP	CB-CG-OD2	5.37	123.13	118.30
1	I	149	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	D	54	ILE	CB-CA-C	-5.23	101.13	111.60
1	B	72	LEU	CA-CB-CG	5.22	127.32	115.30
1	C	133	CYS	CA-CB-SG	-5.22	104.61	114.00
1	H	256	LEU	CB-CG-CD1	-5.21	102.14	111.00
1	A	133	CYS	CA-CB-SG	-5.14	104.74	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	316	ILE	CG1-CB-CG2	5.14	122.71	111.40
1	J	141	LEU	CA-CB-CG	5.07	126.96	115.30
1	F	161	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

All (6) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	272	SER	Peptide
1	B	272	SER	Peptide
1	E	272	SER	Peptide
1	F	346	LYS	Peptide
1	H	272	SER	Peptide
1	L	272	SER	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	2337	0	2359	114	0
1	B	2361	0	2384	106	0
1	C	2297	0	2326	99	0
1	D	2172	0	2213	69	0
1	E	2326	0	2348	107	1
1	F	2384	0	2399	117	1
1	G	2246	0	2279	92	0
1	H	2355	0	2375	109	0
1	I	2395	0	2412	92	0
1	J	2344	0	2370	86	0
1	K	2269	0	2302	113	0
1	L	2367	0	2390	67	0
2	A	26	0	14	1	0
2	B	26	0	14	2	0
2	C	26	0	14	1	0
2	D	26	0	14	3	0
2	E	26	0	14	3	0
2	F	26	0	14	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	H	26	0	14	3	0
2	I	26	0	14	2	0
2	J	26	0	14	3	0
2	K	26	0	14	3	0
2	L	26	0	14	2	0
3	A	3	0	0	0	0
3	C	5	0	0	0	0
3	D	1	0	0	0	0
3	E	3	0	0	0	0
3	F	3	0	0	0	0
3	G	1	0	0	1	0
3	H	1	0	0	0	0
3	I	2	0	0	0	0
3	L	1	0	0	0	0
All	All	28159	0	28311	1118	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 20.

All (1118) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:316:ILE:CD1	1:C:316:ILE:H	1.53	1.20
1:J:316:ILE:H	1:J:316:ILE:CD1	1.54	1.19
1:I:316:ILE:CD1	1:I:316:ILE:H	1.49	1.18
1:B:316:ILE:CD1	1:B:316:ILE:H	1.56	1.17
1:B:300:MET:HE2	1:B:303:ARG:HE	1.10	1.16
1:A:316:ILE:CD1	1:A:316:ILE:H	1.60	1.14
1:C:316:ILE:HD13	1:C:316:ILE:H	0.97	1.14
1:J:316:ILE:H	1:J:316:ILE:HD12	1.13	1.13
1:E:316:ILE:HD13	1:E:316:ILE:N	1.59	1.12
1:F:214:THR:HG21	1:F:238:GLU:HG3	1.13	1.12
1:E:316:ILE:H	1:E:316:ILE:CD1	1.63	1.10
1:F:316:ILE:HD13	1:F:316:ILE:H	1.15	1.10
1:H:316:ILE:HD13	1:H:316:ILE:H	1.09	1.09
1:I:215:THR:HG21	1:I:237:PRO:HD2	1.33	1.09
1:L:149:ARG:HG2	1:L:149:ARG:HH11	0.94	1.08
1:F:167:MET:CE	1:F:256:LEU:HD12	1.83	1.08
1:B:316:ILE:H	1:B:316:ILE:HD13	1.01	1.08
1:H:167:MET:HE3	1:H:256:LEU:HD12	1.36	1.08
1:K:142:ASP:O	1:K:144:GLY:N	1.88	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:316:ILE:N	1:A:316:ILE:HD13	1.57	1.06
1:H:316:ILE:CD1	1:H:316:ILE:H	1.70	1.04
1:C:316:ILE:HD13	1:C:316:ILE:N	1.71	1.04
1:A:316:ILE:HD13	1:A:316:ILE:H	0.87	1.04
1:F:167:MET:HE2	1:F:256:LEU:HD12	1.34	1.03
1:G:337:HIS:HB3	1:G:340:ARG:HH12	1.16	1.03
1:L:149:ARG:NH1	1:L:149:ARG:HG2	1.67	1.01
1:H:316:ILE:N	1:H:316:ILE:HD13	1.72	1.01
1:A:76:GLY:O	1:A:77:LYS:HG3	1.60	1.00
1:A:75:ASN:HB3	1:A:95:LEU:CD2	1.91	0.99
1:I:149:ARG:HH11	1:I:149:ARG:HG2	1.23	0.99
1:G:90:PHE:CE2	1:G:121:VAL:HG21	1.96	0.99
1:I:316:ILE:H	1:I:316:ILE:HD12	1.23	0.98
1:C:80:GLN:NE2	1:C:89:LYS:HD2	1.77	0.98
1:F:155:ASP:O	1:F:156:GLN:CG	2.11	0.97
1:C:301:LEU:HD13	1:C:322:HIS:CD2	1.99	0.96
1:C:167:MET:HE1	1:C:252:ILE:HG22	1.44	0.96
1:K:323:PRO:O	1:K:327:GLN:HG2	1.63	0.96
1:B:316:ILE:HD13	1:B:316:ILE:N	1.80	0.96
1:B:310:PRO:HG3	1:J:233:GLU:HG2	1.46	0.96
1:I:310:PRO:HG3	1:L:233:GLU:HG2	1.48	0.95
1:H:74:ILE:HD13	1:H:209:GLY:HA3	1.47	0.95
1:G:72:LEU:HB3	1:G:77:LYS:HA	1.49	0.94
1:K:316:ILE:H	1:K:316:ILE:HD12	1.28	0.94
1:G:337:HIS:HB3	1:G:340:ARG:NH1	1.82	0.94
1:C:149:ARG:HG2	1:C:149:ARG:HH11	1.31	0.94
1:E:77:LYS:H	1:E:77:LYS:HD3	1.31	0.94
1:G:72:LEU:HA	1:G:78:VAL:H	1.29	0.94
1:B:198:ARG:HH11	1:B:198:ARG:HG2	1.33	0.92
1:J:288:ASN:OD1	1:J:292:SER:HB3	1.69	0.92
1:E:154:GLY:O	1:E:155:ASP:HB3	1.70	0.92
1:F:185:ARG:NH1	1:F:212:LYS:HD3	1.84	0.92
1:I:316:ILE:N	1:I:316:ILE:CD1	2.28	0.92
1:A:233:GLU:HG2	1:H:310:PRO:HG3	1.52	0.92
1:L:49:LYS:HD3	1:L:50:SER:H	1.34	0.91
1:I:167:MET:HE3	1:I:256:LEU:HD12	1.51	0.91
1:E:316:ILE:HD13	1:E:316:ILE:H	0.76	0.91
1:D:48:VAL:HG23	1:F:128:TYR:HD1	1.34	0.91
1:I:316:ILE:N	1:I:316:ILE:HD12	1.85	0.91
1:C:80:GLN:HE21	1:C:89:LYS:HD2	1.31	0.90
1:E:149:ARG:HG2	1:E:149:ARG:HH11	1.32	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:PRO:HG3	1:I:233:GLU:HG2	1.54	0.89
1:E:149:ARG:HH11	1:E:149:ARG:CG	1.85	0.89
1:H:156:GLN:HA	1:H:156:GLN:NE2	1.87	0.89
1:C:185:ARG:NH1	1:C:212:LYS:HD3	1.88	0.89
1:A:103:ARG:HH21	1:A:103:ARG:CG	1.84	0.88
1:B:300:MET:CE	1:B:303:ARG:HE	1.85	0.88
1:F:214:THR:CG2	1:F:238:GLU:HG3	2.04	0.87
1:E:147:PHE:HE2	1:E:256:LEU:HD23	1.39	0.87
1:H:57:ASN:HD22	1:H:58:ALA:N	1.71	0.87
1:I:316:ILE:HD13	1:I:316:ILE:H	1.39	0.87
1:B:66:THR:HB	1:B:80:GLN:O	1.74	0.87
1:B:77:LYS:HD2	1:B:77:LYS:H	1.38	0.87
1:H:149:ARG:HH11	1:H:149:ARG:HG2	1.39	0.87
1:B:265:SER:HA	1:B:271:ILE:O	1.74	0.86
1:F:155:ASP:O	1:F:156:GLN:CB	2.22	0.86
1:C:258:CYS:O	1:C:338:THR:HA	1.76	0.86
1:I:167:MET:CE	1:I:256:LEU:HD12	2.04	0.86
1:H:74:ILE:CD1	1:H:209:GLY:HA3	2.05	0.86
1:A:103:ARG:HG2	1:A:103:ARG:HH21	1.41	0.85
1:L:149:ARG:CG	1:L:149:ARG:HH11	1.85	0.85
1:I:74:ILE:HD13	1:I:210:PHE:CE2	2.12	0.85
1:J:316:ILE:N	1:J:316:ILE:CD1	2.36	0.85
1:H:74:ILE:HD12	1:H:207:ASP:OD1	1.77	0.84
1:H:149:ARG:HH11	1:H:149:ARG:CG	1.90	0.84
1:E:285:GLU:HB2	1:E:287:PRO:HD3	1.58	0.83
1:H:167:MET:CE	1:H:256:LEU:HD12	2.08	0.83
1:I:167:MET:HE1	1:I:252:ILE:HG22	1.56	0.83
1:J:316:ILE:N	1:J:316:ILE:HD12	1.92	0.83
1:B:167:MET:CE	1:B:256:LEU:HD12	2.09	0.82
1:A:198:ARG:HH11	1:A:198:ARG:HG2	1.42	0.82
1:G:260:TYR:HB2	1:G:261:PRO:CD	2.10	0.82
1:F:310:PRO:HG3	1:H:233:GLU:CG	2.08	0.82
1:E:149:ARG:HG2	1:E:149:ARG:NH1	1.92	0.82
1:F:310:PRO:HG3	1:H:233:GLU:HG3	1.59	0.82
1:A:246:MET:HG2	1:A:314:MET:O	1.78	0.82
1:D:147:PHE:HD2	1:D:189:PRO:HB3	1.45	0.82
1:C:316:ILE:N	1:C:316:ILE:CD1	2.28	0.82
1:F:246:MET:HG2	1:F:314:MET:O	1.78	0.82
1:F:332:PRO:HB2	1:F:334:THR:HG23	1.61	0.81
1:B:316:ILE:CD1	1:B:316:ILE:N	2.37	0.81
1:K:59:ILE:HG22	1:L:48:VAL:HG11	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:LEU:O	1:A:77:LYS:HA	1.81	0.80
1:K:196:SER:HB2	1:K:198:ARG:NH1	1.97	0.79
1:A:76:GLY:C	1:A:77:LYS:HG3	2.04	0.79
1:B:214:THR:HG21	1:B:238:GLU:HG3	1.64	0.79
1:A:167:MET:CE	1:A:252:ILE:HG22	2.13	0.78
1:F:271:ILE:HA	1:F:274:GLY:HA3	1.65	0.78
1:I:167:MET:CE	1:I:252:ILE:HG22	2.13	0.78
1:F:316:ILE:N	1:F:316:ILE:HD13	1.95	0.78
1:J:94:MET:HG2	1:J:135:LEU:HD22	1.65	0.78
1:E:171:GLY:HA3	1:E:320:MET:CE	2.14	0.78
1:G:301:LEU:HD13	1:G:322:HIS:CD2	2.18	0.77
1:E:153:ARG:O	1:E:155:ASP:N	2.16	0.77
1:F:102:ARG:HD2	1:F:134:LEU:HD11	1.67	0.77
1:K:301:LEU:HD13	1:K:322:HIS:CD2	2.20	0.77
1:C:311:THR:O	1:L:312:GLN:NE2	2.16	0.77
1:F:154:GLY:O	1:F:155:ASP:C	2.23	0.77
1:C:147:PHE:HD1	1:C:189:PRO:HB3	1.49	0.77
1:L:98:CYS:HB2	1:L:99:PRO:CD	2.15	0.77
1:B:167:MET:HE3	1:B:256:LEU:HD12	1.65	0.76
1:D:165:GLU:HG2	1:D:328:SER:HB3	1.65	0.76
1:F:198:ARG:HH11	1:F:198:ARG:HG2	1.49	0.76
1:K:327:GLN:HB3	1:K:330:LYS:HB2	1.67	0.76
1:B:300:MET:HE2	1:B:303:ARG:NE	1.95	0.76
1:B:319:PHE:CD2	1:B:320:MET:CE	2.69	0.76
1:E:171:GLY:HA3	1:E:320:MET:HE3	1.66	0.76
1:G:72:LEU:CB	1:G:77:LYS:HA	2.14	0.76
1:H:94:MET:HE2	1:H:135:LEU:HD22	1.68	0.76
1:C:185:ARG:HH12	1:C:212:LYS:HD3	1.49	0.76
1:B:135:LEU:HD23	1:B:135:LEU:N	2.01	0.76
1:A:285:GLU:HG3	1:A:287:PRO:HD3	1.68	0.75
1:I:74:ILE:HD13	1:I:210:PHE:CD2	2.21	0.75
1:C:141:LEU:HD12	1:C:193:LEU:HD12	1.67	0.75
1:G:110:ARG:NH1	1:I:130:GLY:O	2.20	0.74
1:A:75:ASN:HB3	1:A:95:LEU:HD21	1.68	0.74
1:E:272:SER:H	1:E:274:GLY:H	1.32	0.74
1:C:114:CYS:HB3	1:C:117:ILE:HD12	1.69	0.73
1:F:167:MET:HE2	1:F:256:LEU:CD1	2.15	0.73
1:G:260:TYR:HB2	1:G:261:PRO:HD2	1.70	0.73
1:K:316:ILE:H	1:K:316:ILE:CD1	1.99	0.73
1:B:66:THR:HG22	1:B:68:GLN:H	1.53	0.73
1:K:159:THR:HB	1:K:333:GLN:O	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:90:PHE:HE2	1:G:121:VAL:HG21	1.51	0.73
1:B:319:PHE:HD2	1:B:320:MET:CE	2.00	0.73
1:G:114:CYS:HB3	1:G:117:ILE:HD12	1.69	0.73
1:E:343:LYS:C	1:E:345:ASP:H	1.90	0.73
1:C:310:PRO:CG	1:I:233:GLU:HG2	2.19	0.73
1:H:113:GLN:HG2	1:H:176:TYR:CZ	2.24	0.73
1:A:276:LYS:HZ3	1:E:131:ARG:HH12	1.37	0.72
1:I:230:VAL:HG12	1:I:231:ALA:H	1.53	0.72
1:B:167:MET:HE2	1:B:256:LEU:CD1	2.18	0.72
1:D:115:PRO:O	1:D:204:LYS:HE2	1.88	0.72
1:F:185:ARG:NH1	1:F:212:LYS:CD	2.53	0.72
1:A:305:LEU:O	1:A:313:ARG:HD3	1.90	0.71
1:I:149:ARG:NH1	1:I:149:ARG:HG2	1.99	0.71
1:C:167:MET:CE	1:C:252:ILE:HG22	2.18	0.71
1:H:57:ASN:HD22	1:H:57:ASN:C	1.93	0.71
1:I:135:LEU:N	1:I:135:LEU:HD23	2.06	0.71
1:L:167:MET:HE1	1:L:256:LEU:HD12	1.71	0.71
1:K:167:MET:HE3	1:K:253:MET:HA	1.72	0.71
1:F:265:SER:HA	1:F:271:ILE:O	1.91	0.70
1:L:161:ARG:NH1	1:L:331:VAL:O	2.23	0.70
1:F:155:ASP:O	1:F:156:GLN:HG3	1.89	0.70
1:H:57:ASN:C	1:H:57:ASN:ND2	2.42	0.70
1:H:129:ALA:HA	1:I:47:HIS:CE1	2.26	0.70
1:K:114:CYS:SG	1:K:117:ILE:HD12	2.32	0.70
1:K:142:ASP:C	1:K:144:GLY:H	1.94	0.70
1:D:147:PHE:CD2	1:D:189:PRO:HB3	2.27	0.70
1:F:197:LYS:H	1:F:197:LYS:HD2	1.57	0.70
1:A:319:PHE:HD2	1:A:320:MET:HE2	1.56	0.69
1:I:273:PRO:HB2	1:K:131:ARG:HH11	1.55	0.69
1:F:264:TYR:O	1:F:278:ARG:NH1	2.26	0.69
1:A:75:ASN:HB3	1:A:95:LEU:HD22	1.73	0.69
1:F:167:MET:HE3	1:F:256:LEU:HD12	1.74	0.69
1:G:108:HIS:CG	1:G:120:ILE:HD11	2.26	0.69
1:B:92:LEU:HD11	1:B:135:LEU:HB3	1.74	0.68
1:H:149:ARG:NH1	1:H:149:ARG:HG2	2.05	0.68
1:J:231:ALA:HB1	1:J:233:GLU:OE1	1.91	0.68
1:K:67:SER:O	1:K:69:VAL:HG23	1.92	0.68
1:E:178:HIS:ND1	1:E:316:ILE:HD11	2.09	0.68
1:G:50:SER:HB2	1:I:56:LYS:O	1.94	0.68
1:D:315:THR:HG23	1:D:318:GLU:H	1.58	0.68
1:D:97:ASP:O	1:D:98:CYS:HB3	1.92	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:149:ARG:HH11	1:A:149:ARG:HG2	1.59	0.68
1:F:155:ASP:C	1:F:156:GLN:HG3	2.14	0.68
2:L:500:MK2:N24	2:L:500:MK2:H8	2.09	0.68
1:A:167:MET:HE1	1:A:252:ILE:HG22	1.75	0.68
1:C:147:PHE:CD1	1:C:189:PRO:HB3	2.29	0.68
1:F:167:MET:CE	1:F:256:LEU:CD1	2.67	0.67
1:G:255:ILE:HG13	1:G:260:TYR:O	1.94	0.67
1:C:316:ILE:HD12	1:C:316:ILE:H	1.58	0.67
1:J:319:PHE:HD2	1:J:320:MET:CE	2.06	0.67
1:A:88:GLU:HG2	1:A:89:LYS:H	1.59	0.67
1:E:97:ASP:O	1:E:98:CYS:HB3	1.95	0.67
1:K:167:MET:HE1	1:K:252:ILE:HG22	1.75	0.67
1:K:188:LYS:HD2	1:K:190:GLU:OE1	1.95	0.67
1:L:214:THR:HG21	1:L:238:GLU:HG3	1.76	0.67
1:K:299:LYS:O	1:K:303:ARG:HG3	1.95	0.67
1:B:66:THR:CG2	1:B:67:SER:N	2.57	0.67
1:L:161:ARG:HD2	1:L:329:THR:HA	1.76	0.67
1:A:103:ARG:HB3	1:A:103:ARG:NH2	2.10	0.67
1:C:114:CYS:CB	1:C:117:ILE:HD12	2.24	0.67
1:C:319:PHE:HD2	1:C:320:MET:HE2	1.58	0.67
1:E:167:MET:CE	1:E:252:ILE:HG22	2.25	0.67
1:A:143:GLY:HA3	1:A:196:SER:O	1.95	0.67
1:C:319:PHE:HD2	1:C:320:MET:CE	2.08	0.67
1:B:190:GLU:N	1:B:190:GLU:OE1	2.24	0.66
1:C:167:MET:HE1	1:C:252:ILE:CG2	2.21	0.66
1:A:74:ILE:HG12	1:A:75:ASN:H	1.60	0.66
1:J:141:LEU:HD12	1:J:193:LEU:HB2	1.77	0.66
1:F:74:ILE:H	1:F:74:ILE:HD12	1.61	0.66
1:J:83:ASN:HD21	1:J:85:ARG:HD3	1.59	0.66
1:K:66:THR:HG21	1:K:82:PHE:HE1	1.59	0.66
1:A:167:MET:HE1	1:A:252:ILE:CG2	2.25	0.66
1:G:85:ARG:HD3	1:G:85:ARG:H	1.59	0.66
1:C:74:ILE:HD12	1:C:75:ASN:HD22	1.60	0.66
1:E:246:MET:HE1	1:E:316:ILE:HD12	1.77	0.66
1:H:141:LEU:HD23	1:H:195:THR:HG22	1.77	0.66
1:J:319:PHE:HD2	1:J:320:MET:HE2	1.61	0.66
1:E:198:ARG:HG2	1:E:198:ARG:HH11	1.59	0.66
1:B:332:PRO:HB2	1:B:334:THR:CG2	2.26	0.66
1:C:233:GLU:HG2	1:L:310:PRO:HG3	1.76	0.66
1:G:65:VAL:HA	1:G:81:ILE:HG22	1.77	0.66
1:B:170:ILE:HG12	1:B:192:LEU:HD22	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:88:GLU:HG2	1:F:89:LYS:H	1.61	0.65
1:A:75:ASN:CB	1:A:95:LEU:HD21	2.26	0.65
1:H:167:MET:HE1	1:H:252:ILE:HG22	1.78	0.65
1:H:328:SER:O	1:H:330:LYS:N	2.30	0.65
1:H:55:LYS:HD3	1:H:124:TYR:CE2	2.32	0.65
1:A:161:ARG:HD3	1:A:331:VAL:O	1.97	0.65
1:A:276:LYS:HZ1	1:E:131:ARG:HH22	1.44	0.65
1:C:46:PHE:O	1:C:48:VAL:N	2.24	0.65
1:E:327:GLN:HB3	1:E:330:LYS:HD2	1.78	0.65
1:B:319:PHE:CD2	1:B:320:MET:HE2	2.30	0.65
1:L:320:MET:CE	1:L:325:ILE:HG21	2.27	0.65
1:A:103:ARG:HH21	1:A:103:ARG:CB	2.09	0.65
1:B:66:THR:HG22	1:B:67:SER:N	2.10	0.65
1:C:307:LYS:HE2	1:I:318:GLU:OE2	1.97	0.65
1:H:57:ASN:ND2	1:H:58:ALA:N	2.44	0.65
1:I:134:LEU:C	1:I:135:LEU:HD23	2.17	0.65
1:J:319:PHE:CD2	1:J:320:MET:HE2	2.32	0.65
1:B:185:ARG:HH11	1:B:212:LYS:HB2	1.61	0.65
1:G:185:ARG:NH1	1:G:212:LYS:HD3	2.12	0.65
1:I:234:VAL:O	1:I:234:VAL:HG13	1.97	0.65
1:D:48:VAL:HG23	1:F:128:TYR:CD1	2.23	0.64
1:H:141:LEU:HD23	1:H:195:THR:HA	1.80	0.64
1:L:153:ARG:O	1:L:153:ARG:HG2	1.97	0.64
1:I:234:VAL:O	1:I:234:VAL:CG1	2.45	0.64
1:K:118:VAL:HG11	1:K:206:THR:OG1	1.96	0.64
1:B:115:PRO:O	1:B:204:LYS:HE3	1.97	0.64
1:H:227:PRO:O	1:H:230:VAL:HG22	1.98	0.64
1:A:149:ARG:NH1	1:A:149:ARG:HG2	2.12	0.64
1:L:159:THR:OG1	1:L:162:GLU:HG3	1.98	0.64
1:L:49:LYS:HD3	1:L:50:SER:N	2.09	0.64
1:B:167:MET:CE	1:B:256:LEU:CD1	2.74	0.64
1:F:185:ARG:HH12	1:F:212:LYS:CD	2.11	0.64
2:H:500:MK2:N24	2:H:500:MK2:H8	2.13	0.64
1:I:74:ILE:CD1	1:I:210:PHE:CE2	2.80	0.64
1:I:77:LYS:H	1:I:77:LYS:HD3	1.61	0.64
1:F:155:ASP:O	1:F:156:GLN:HB3	1.95	0.63
1:A:80:GLN:NE2	1:A:89:LYS:HG3	2.12	0.63
1:I:277:THR:HG22	1:I:281:MET:HG3	1.80	0.63
1:A:50:SER:HB2	1:C:57:ASN:HA	1.80	0.63
1:C:74:ILE:HD12	1:C:75:ASN:ND2	2.13	0.63
1:G:83:ASN:OD1	1:G:85:ARG:NE	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:167:MET:HE1	1:E:252:ILE:HG22	1.80	0.63
1:F:197:LYS:H	1:F:197:LYS:CD	2.11	0.63
1:I:161:ARG:NH1	1:I:331:VAL:O	2.32	0.63
1:J:161:ARG:HD2	1:J:329:THR:HA	1.81	0.63
1:F:266:ASN:HB2	1:F:271:ILE:CB	2.29	0.62
1:K:192:LEU:HB3	1:K:203:LEU:HD11	1.81	0.62
1:F:178:HIS:CE1	1:F:242:LYS:HG3	2.35	0.62
1:H:156:GLN:CA	1:H:156:GLN:NE2	2.62	0.62
1:B:328:SER:O	1:B:331:VAL:HG13	2.00	0.62
1:E:160:GLU:O	1:E:163:ALA:HB3	1.99	0.62
1:B:332:PRO:HB2	1:B:334:THR:HG22	1.81	0.62
1:C:92:LEU:HD11	1:C:135:LEU:HB3	1.82	0.62
1:E:160:GLU:HA	1:E:336:LEU:HD11	1.80	0.62
1:K:152:ASP:N	1:K:152:ASP:OD2	2.32	0.62
1:K:189:PRO:O	1:K:191:ASN:N	2.31	0.62
1:G:184:HIS:CE1	1:G:186:ASP:O	2.53	0.62
1:C:171:GLY:HA3	1:C:320:MET:HE1	1.80	0.62
1:E:272:SER:H	1:E:274:GLY:N	1.98	0.62
1:I:161:ARG:HA	1:I:331:VAL:HG22	1.81	0.62
2:K:500:MK2:N24	2:K:500:MK2:H8	2.14	0.62
1:J:319:PHE:CD2	1:J:320:MET:CE	2.83	0.62
1:K:178:HIS:HD2	1:K:182:ILE:O	1.83	0.62
1:B:167:MET:HE2	1:B:256:LEU:HD11	1.81	0.61
1:A:110:ARG:NH1	1:C:130:GLY:O	2.32	0.61
1:K:171:GLY:HA3	1:K:320:MET:CE	2.30	0.61
1:I:188:LYS:HG2	1:L:229:TYR:CZ	2.35	0.61
1:C:231:ALA:HB1	1:C:233:GLU:OE1	2.00	0.61
1:J:101:ALA:O	1:J:105:VAL:HG23	2.00	0.61
1:K:156:GLN:OE1	1:K:156:GLN:HA	2.00	0.61
1:E:72:LEU:HD12	1:E:73:GLY:N	2.15	0.61
1:F:235:LEU:HD12	1:F:235:LEU:O	1.99	0.61
1:H:86:THR:O	1:H:87:GLN:HB3	1.99	0.61
1:H:272:SER:HA	1:H:275:MET:H	1.65	0.61
1:K:337:HIS:O	1:K:341:VAL:HG23	2.00	0.61
1:G:314:MET:HA	1:G:318:GLU:OE1	2.00	0.61
1:C:246:MET:CE	1:C:316:ILE:HD12	2.31	0.61
1:E:155:ASP:OD1	1:E:156:GLN:HG3	1.99	0.61
1:H:142:ASP:HA	2:H:500:MK2:H4	1.81	0.61
1:A:198:ARG:NH1	1:A:198:ARG:HG2	2.10	0.61
1:H:323:PRO:O	1:H:327:GLN:HG2	2.01	0.61
1:J:181:ASN:OD1	1:L:131:ARG:NH2	2.33	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:154:GLY:H	1:B:156:GLN:HE21	1.47	0.61
1:G:129:ALA:O	1:G:130:GLY:C	2.40	0.61
1:I:74:ILE:CD1	1:I:210:PHE:HE2	2.14	0.61
1:K:167:MET:CE	1:K:252:ILE:HG22	2.29	0.60
1:E:155:ASP:CG	1:E:156:GLN:HG3	2.21	0.60
1:H:167:MET:CE	1:H:252:ILE:HG22	2.31	0.60
1:J:180:ILE:HG13	1:J:182:ILE:HD12	1.83	0.60
1:K:66:THR:OG1	1:K:67:SER:N	2.32	0.60
1:F:246:MET:HE1	1:F:316:ILE:HD12	1.83	0.60
1:H:153:ARG:O	1:H:155:ASP:N	2.35	0.60
1:J:115:PRO:O	1:J:204:LYS:HE2	2.01	0.60
1:D:258:CYS:O	1:D:338:THR:HA	2.02	0.60
1:F:107:LEU:HD21	1:F:213:GLU:HG2	1.83	0.60
1:F:72:LEU:HA	1:F:77:LYS:HA	1.82	0.60
1:A:196:SER:OG	1:A:198:ARG:HB2	2.01	0.60
1:A:319:PHE:HD2	1:A:320:MET:CE	2.13	0.60
1:B:77:LYS:N	1:B:77:LYS:HD2	2.11	0.60
1:K:193:LEU:O	1:K:203:LEU:HD12	2.00	0.60
1:L:185:ARG:NH1	1:L:210:PHE:O	2.34	0.60
1:B:161:ARG:HD2	1:B:328:SER:O	2.00	0.60
1:E:56:LYS:HE3	1:E:125:GLU:OE1	2.01	0.60
1:F:185:ARG:HH12	1:F:212:LYS:HD3	1.66	0.60
1:F:189:PRO:HG2	1:H:228:TYR:OH	2.02	0.60
1:I:171:GLY:HA3	1:I:320:MET:HE1	1.83	0.60
1:K:58:ALA:O	1:K:61:ASP:HB2	2.02	0.60
1:A:265:SER:O	1:A:266:ASN:HB2	2.02	0.60
1:A:272:SER:H	1:A:274:GLY:H	1.49	0.60
1:G:191:ASN:HD22	1:G:206:THR:HG23	1.67	0.60
1:F:178:HIS:ND1	1:F:316:ILE:CD1	2.65	0.59
1:K:323:PRO:O	1:K:327:GLN:CG	2.45	0.59
1:A:266:ASN:HB2	1:A:271:ILE:CB	2.32	0.59
1:D:141:LEU:HD12	1:D:193:LEU:HB2	1.83	0.59
1:L:98:CYS:HB2	1:L:99:PRO:HD3	1.83	0.59
1:C:149:ARG:CG	1:C:149:ARG:HH11	2.12	0.59
1:C:246:MET:HE1	1:C:316:ILE:HG23	1.84	0.59
1:A:276:LYS:NZ	1:E:131:ARG:HH22	1.99	0.59
1:B:319:PHE:HD2	1:B:320:MET:HE3	1.66	0.59
1:G:72:LEU:HB3	1:G:77:LYS:CA	2.29	0.59
1:L:167:MET:HE1	1:L:256:LEU:CD1	2.33	0.59
1:A:115:PRO:O	1:A:204:LYS:HE3	2.01	0.59
1:F:237:PRO:O	1:F:238:GLU:CB	2.51	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:167:MET:SD	1:H:253:MET:HE2	2.43	0.59
1:I:229:TYR:CD2	1:I:229:TYR:O	2.55	0.59
1:A:103:ARG:CB	1:A:103:ARG:NH2	2.65	0.59
1:C:66:THR:HG21	1:C:82:PHE:HE1	1.67	0.59
1:K:153:ARG:HD3	1:K:158:PHE:HB2	1.83	0.59
1:B:276:LYS:HE2	1:B:280:ARG:HH12	1.68	0.59
1:A:66:THR:HG21	1:A:82:PHE:HE1	1.68	0.59
1:B:66:THR:CG2	1:B:68:GLN:H	2.16	0.59
1:F:230:VAL:O	1:F:231:ALA:CB	2.50	0.59
1:B:198:ARG:HH11	1:B:198:ARG:CG	2.12	0.59
1:H:345:ASP:C	1:H:347:GLU:H	2.06	0.59
1:J:142:ASP:HA	2:J:500:MK2:H4	1.85	0.59
1:I:171:GLY:HA3	1:I:320:MET:CE	2.32	0.58
1:I:271:ILE:O	1:I:275:MET:N	2.34	0.58
1:K:254:TYR:CG	1:K:262:PRO:HG3	2.37	0.58
1:L:246:MET:HE1	1:L:316:ILE:HG23	1.84	0.58
1:E:343:LYS:O	1:E:345:ASP:N	2.33	0.58
1:F:139:GLU:HG3	1:F:141:LEU:HD21	1.84	0.58
1:E:111:ALA:HB1	1:E:117:ILE:HD13	1.84	0.58
1:A:103:ARG:CG	1:A:103:ARG:NH2	2.57	0.58
1:A:171:GLY:HA3	1:A:320:MET:HE1	1.85	0.58
1:D:109:TRP:CH2	1:F:127:LEU:HD22	2.38	0.58
1:C:340:ARG:O	1:C:344:GLU:HG2	2.03	0.58
1:A:184:HIS:CD2	1:A:205:LEU:HD21	2.39	0.58
1:I:74:ILE:HD12	1:I:207:ASP:OD1	2.04	0.58
1:B:312:GLN:NE2	1:J:311:THR:O	2.36	0.58
1:E:227:PRO:HB3	1:E:229:TYR:CE2	2.39	0.58
1:F:230:VAL:O	1:F:231:ALA:HB3	2.03	0.58
2:F:500:MK2:N24	2:F:500:MK2:H8	2.19	0.58
1:G:49:LYS:HG3	1:G:50:SER:O	2.04	0.58
1:B:66:THR:HG22	1:B:68:GLN:N	2.17	0.58
1:D:78:VAL:HG22	1:D:93:LYS:HB2	1.86	0.58
1:F:310:PRO:HG3	1:H:233:GLU:HG2	1.84	0.58
1:J:174:ILE:HG21	1:J:246:MET:CE	2.34	0.58
1:K:199:PRO:O	1:K:201:ALA:N	2.37	0.58
1:B:49:LYS:HG2	1:B:113:GLN:NE2	2.19	0.58
1:E:265:SER:O	1:E:266:ASN:CB	2.51	0.58
1:J:260:TYR:HD2	1:J:341:VAL:HG11	1.68	0.58
1:L:320:MET:HE2	1:L:325:ILE:HG21	1.86	0.58
1:A:304:ASN:OD1	1:A:314:MET:HB3	2.04	0.57
1:D:336:LEU:C	1:D:338:THR:H	2.07	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:154:GLY:O	1:E:155:ASP:CB	2.49	0.57
1:I:150:ILE:O	1:I:153:ARG:HG2	2.04	0.57
1:K:186:ASP:O	1:K:188:LYS:HG3	2.04	0.57
1:A:80:GLN:HE22	1:A:89:LYS:HG3	1.69	0.57
1:D:86:THR:O	1:D:88:GLU:N	2.38	0.57
1:G:90:PHE:CD2	1:G:121:VAL:HG21	2.38	0.57
1:K:104:GLU:HG3	1:K:209:GLY:HA2	1.86	0.57
1:F:171:GLY:HA3	1:F:320:MET:CE	2.34	0.57
1:H:245:ASP:O	1:H:248:SER:HB2	2.05	0.57
1:K:86:THR:C	1:K:88:GLU:H	2.08	0.57
1:D:331:VAL:HB	1:D:332:PRO:HD2	1.87	0.57
1:J:116:HIS:CE1	1:J:169:SER:HB2	2.40	0.57
2:D:500:MK2:N24	2:D:500:MK2:H8	2.19	0.57
1:G:177:LEU:HD12	1:G:184:HIS:HB2	1.86	0.57
1:I:111:ALA:C	1:I:113:GLN:H	2.07	0.57
1:I:240:TYR:O	1:I:242:LYS:N	2.35	0.57
1:K:161:ARG:HG3	1:K:331:VAL:HG23	1.87	0.57
1:J:65:VAL:HB	1:K:45:GLN:HG2	1.85	0.57
1:E:139:GLU:OE2	1:E:204:LYS:HE3	2.05	0.57
1:F:330:LYS:HG2	1:F:330:LYS:O	2.04	0.57
1:B:192:LEU:HD11	1:B:252:ILE:HD13	1.87	0.57
1:H:320:MET:HE2	1:H:320:MET:HA	1.86	0.57
1:I:310:PRO:HG3	1:L:233:GLU:CG	2.30	0.57
1:J:303:ARG:O	1:J:307:LYS:HD3	2.05	0.57
1:F:178:HIS:ND1	1:F:316:ILE:HD11	2.19	0.57
1:F:332:PRO:HB2	1:F:334:THR:CG2	2.33	0.57
1:I:215:THR:CG2	1:I:237:PRO:HD2	2.20	0.57
1:J:114:CYS:HB3	1:J:117:ILE:HG13	1.85	0.57
1:L:80:GLN:HE21	1:L:89:LYS:HG2	1.70	0.57
1:I:328:SER:O	1:I:331:VAL:HG13	2.05	0.56
1:L:46:PHE:CG	1:L:47:HIS:N	2.73	0.56
1:A:47:HIS:O	1:C:128:TYR:HA	2.04	0.56
1:B:134:LEU:C	1:B:135:LEU:HD23	2.25	0.56
1:B:66:THR:CG2	1:B:67:SER:H	2.18	0.56
1:C:183:ALA:O	1:C:211:ALA:HA	2.05	0.56
1:J:149:ARG:NH2	1:J:198:ARG:O	2.38	0.56
1:K:241:ASP:OD2	1:K:241:ASP:N	2.38	0.56
1:A:265:SER:O	1:A:266:ASN:CB	2.53	0.56
1:B:167:MET:HG3	1:B:253:MET:HG3	1.87	0.56
1:C:284:TYR:OH	1:C:303:ARG:HG2	2.04	0.56
1:K:247:TRP:CZ3	1:K:306:LEU:HA	2.39	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:49:LYS:HE3	1:G:113:GLN:HG3	1.88	0.56
1:J:316:ILE:HD13	1:J:316:ILE:H	1.59	0.56
1:K:264:TYR:O	1:K:275:MET:HG2	2.06	0.56
1:C:63:TYR:HA	1:C:82:PHE:O	2.06	0.56
1:J:278:ARG:HG2	1:J:283:GLN:HB2	1.87	0.56
1:K:316:ILE:N	1:K:316:ILE:HD12	2.11	0.56
1:C:141:LEU:HD22	1:C:195:THR:HG22	1.87	0.56
1:D:171:GLY:HA3	1:D:320:MET:HE3	1.86	0.56
1:F:296:GLU:HA	1:F:296:GLU:OE1	2.05	0.56
1:D:116:HIS:O	1:D:204:LYS:HA	2.06	0.56
1:D:92:LEU:HD11	1:D:135:LEU:HB3	1.88	0.56
1:A:103:ARG:HH21	1:A:103:ARG:HB3	1.68	0.56
1:D:301:LEU:HD13	1:D:322:HIS:CD2	2.41	0.56
1:E:161:ARG:HA	1:E:331:VAL:CG2	2.36	0.56
1:H:148:SER:HA	1:H:151:GLN:HG2	1.88	0.56
1:K:189:PRO:HD2	1:K:190:GLU:OE2	2.06	0.56
1:F:155:ASP:O	1:F:156:GLN:HG2	2.05	0.56
1:F:237:PRO:O	1:F:238:GLU:HB2	2.07	0.56
1:K:67:SER:C	1:K:69:VAL:H	2.08	0.55
1:B:82:PHE:CE2	1:B:89:LYS:HG2	2.41	0.55
1:C:185:ARG:HH12	1:C:212:LYS:CD	2.17	0.55
1:H:330:LYS:HG3	1:H:330:LYS:O	2.06	0.55
1:H:92:LEU:HD11	1:H:135:LEU:HB3	1.88	0.55
1:K:128:TYR:HA	1:L:47:HIS:O	2.06	0.55
2:E:500:MK2:H8	2:E:500:MK2:N24	2.20	0.55
1:F:98:CYS:O	1:F:102:ARG:HG2	2.06	0.55
1:A:214:THR:HG21	1:A:242:LYS:HD3	1.89	0.55
1:A:316:ILE:N	1:A:316:ILE:CD1	2.31	0.55
1:E:147:PHE:CE2	1:E:256:LEU:HD23	2.30	0.55
1:F:167:MET:HG3	1:F:253:MET:HG3	1.87	0.55
1:G:69:VAL:CG1	1:G:72:LEU:HG	2.36	0.55
1:H:178:HIS:ND1	1:H:316:ILE:CD1	2.70	0.55
1:D:260:TYR:HB2	1:D:261:PRO:HD2	1.89	0.55
1:F:159:THR:OG1	1:F:333:GLN:NE2	2.38	0.55
1:G:194:TYR:HB3	1:G:201:ALA:HB1	1.88	0.55
1:B:77:LYS:CD	1:B:77:LYS:H	2.17	0.55
1:D:233:GLU:HG2	1:G:310:PRO:HG3	1.89	0.55
1:E:343:LYS:C	1:E:345:ASP:N	2.59	0.55
1:E:56:LYS:O	1:F:50:SER:HB2	2.07	0.55
2:I:500:MK2:H8	2:I:500:MK2:N24	2.22	0.55
1:E:265:SER:O	1:E:266:ASN:HB2	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:329:THR:O	1:G:330:LYS:HG2	2.07	0.55
1:G:72:LEU:O	1:G:73:GLY:C	2.45	0.55
1:G:314:MET:HB2	1:G:318:GLU:HB2	1.89	0.54
1:J:257:LEU:O	1:J:336:LEU:HD22	2.08	0.54
2:J:500:MK2:H8	2:J:500:MK2:N24	2.22	0.54
1:A:171:GLY:HA3	1:A:320:MET:CE	2.37	0.54
1:G:128:TYR:HB3	1:G:133:CYS:SG	2.47	0.54
1:A:151:GLN:HG2	1:A:151:GLN:O	2.07	0.54
1:K:97:ASP:OD1	1:K:98:CYS:N	2.40	0.54
1:C:246:MET:HE3	1:C:316:ILE:HD12	1.88	0.54
1:K:141:LEU:HD12	1:K:193:LEU:HB2	1.89	0.54
1:A:47:HIS:HB2	1:C:128:TYR:CE1	2.43	0.54
1:F:154:GLY:O	1:F:155:ASP:O	2.25	0.54
1:J:301:LEU:HD22	1:J:322:HIS:CD2	2.42	0.54
1:K:175:GLN:HA	1:K:316:ILE:HG21	1.90	0.54
1:L:97:ASP:OD2	1:L:102:ARG:NH1	2.37	0.54
1:E:167:MET:HE1	1:E:252:ILE:CG2	2.38	0.54
1:K:141:LEU:HD12	1:K:193:LEU:HD12	1.90	0.54
1:K:86:THR:OG1	1:K:88:GLU:HB2	2.08	0.54
1:A:167:MET:HE3	1:A:252:ILE:HG22	1.89	0.54
1:H:78:VAL:HA	1:H:92:LEU:O	2.08	0.54
1:G:261:PRO:HG2	1:G:264:TYR:HB3	1.90	0.54
1:B:310:PRO:HG3	1:J:233:GLU:CG	2.28	0.53
1:E:72:LEU:HA	1:E:77:LYS:HA	1.89	0.53
1:I:347:GLU:C	1:I:349:TRP:H	2.11	0.53
1:K:331:VAL:HB	1:K:332:PRO:HD2	1.90	0.53
1:B:130:GLY:O	1:C:110:ARG:NH1	2.38	0.53
1:B:154:GLY:H	1:B:156:GLN:NE2	2.05	0.53
1:D:258:CYS:SG	1:D:259:GLY:N	2.82	0.53
1:G:147:PHE:CE2	1:G:255:ILE:HG21	2.43	0.53
1:C:111:ALA:HB1	1:C:117:ILE:HD13	1.90	0.53
1:B:178:HIS:CE1	1:B:242:LYS:HG3	2.44	0.53
1:K:171:GLY:HA3	1:K:320:MET:HE1	1.89	0.53
1:L:83:ASN:OD1	1:L:86:THR:N	2.38	0.53
1:E:141:LEU:HD22	1:E:195:THR:HG22	1.90	0.53
1:E:77:LYS:HD3	1:E:77:LYS:N	2.13	0.53
1:H:156:GLN:NE2	1:H:339:SER:HB3	2.24	0.53
1:H:63:TYR:CD1	1:H:81:ILE:HD12	2.43	0.53
1:I:319:PHE:CD2	1:I:320:MET:HE2	2.43	0.53
1:J:71:GLY:C	1:J:73:GLY:H	2.09	0.53
1:C:150:ILE:HD12	1:C:153:ARG:HD2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:149:ARG:NH2	1:I:199:PRO:O	2.42	0.53
1:K:141:LEU:CD1	1:K:193:LEU:HB2	2.39	0.53
1:I:312:GLN:HG2	1:L:311:THR:O	2.07	0.53
1:A:319:PHE:CD2	1:A:320:MET:HE2	2.41	0.53
1:B:276:LYS:HE2	1:B:280:ARG:NH1	2.24	0.53
1:D:277:THR:HG21	1:J:131:ARG:NH1	2.24	0.53
1:C:171:GLY:HA3	1:C:320:MET:CE	2.38	0.53
1:D:63:TYR:CD1	1:D:81:ILE:HD12	2.43	0.53
1:E:233:GLU:HG2	1:J:310:PRO:HG3	1.90	0.53
1:F:199:PRO:HG2	1:F:200:ASN:HD22	1.74	0.53
1:K:167:MET:HE1	1:K:253:MET:N	2.24	0.53
1:I:167:MET:HE2	1:I:256:LEU:HD12	1.87	0.53
1:C:101:ALA:O	1:C:105:VAL:HG23	2.09	0.53
1:C:185:ARG:NH1	1:C:212:LYS:CD	2.65	0.53
1:C:328:SER:O	1:C:331:VAL:HG13	2.08	0.53
1:G:196:SER:CB	1:G:198:ARG:HE	2.22	0.53
1:H:161:ARG:HA	1:H:331:VAL:HG22	1.91	0.52
1:I:65:VAL:HA	1:I:81:ILE:HG22	1.91	0.52
1:E:156:GLN:HB3	1:E:339:SER:HB3	1.90	0.52
1:E:78:VAL:HG22	1:E:93:LYS:HB2	1.89	0.52
1:H:231:ALA:HB1	1:H:233:GLU:OE1	2.10	0.52
1:H:264:TYR:O	1:H:278:ARG:NH1	2.39	0.52
1:K:258:CYS:HB2	1:K:260:TYR:CE2	2.43	0.52
1:A:92:LEU:HD11	1:A:135:LEU:HB3	1.92	0.52
1:G:296:GLU:O	1:G:296:GLU:HG3	2.09	0.52
1:G:85:ARG:N	1:G:85:ARG:HD3	2.25	0.52
1:D:327:GLN:HB2	1:D:330:LYS:HB3	1.92	0.52
1:B:167:MET:HE2	1:B:256:LEU:HD12	1.80	0.52
1:B:83:ASN:O	1:B:87:GLN:HA	2.09	0.52
1:C:60:ILE:HD12	1:C:60:ILE:C	2.30	0.52
1:H:108:HIS:CG	1:H:120:ILE:HD11	2.45	0.52
1:K:151:GLN:O	1:K:339:SER:HA	2.09	0.52
2:A:500:MK2:N24	2:A:500:MK2:H8	2.25	0.52
1:E:171:GLY:HA3	1:E:320:MET:HE1	1.90	0.52
1:K:118:VAL:HG13	1:K:118:VAL:O	2.09	0.52
1:D:332:PRO:HG2	1:D:334:THR:HG22	1.92	0.52
1:E:178:HIS:ND1	1:E:316:ILE:CD1	2.73	0.52
1:H:97:ASP:O	1:H:98:CYS:HB3	2.10	0.52
1:A:74:ILE:HG23	1:A:75:ASN:OD1	2.11	0.51
1:H:87:GLN:O	1:H:87:GLN:HG3	2.10	0.51
1:A:161:ARG:HA	1:A:331:VAL:CG2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:GLN:O	1:A:47:HIS:N	2.43	0.51
1:H:74:ILE:HD12	1:H:209:GLY:HA3	1.90	0.51
1:B:167:MET:HE1	1:B:252:ILE:HG22	1.92	0.51
1:D:56:LYS:O	1:E:51:GLY:N	2.40	0.51
2:H:500:MK2:N24	2:H:500:MK2:C8	2.73	0.51
1:I:92:LEU:HD11	1:I:135:LEU:HB3	1.92	0.51
1:L:320:MET:HE1	1:L:325:ILE:HG21	1.91	0.51
1:D:100:LYS:NZ	1:D:103:ARG:HH22	2.08	0.51
1:F:171:GLY:HA3	1:F:320:MET:HE3	1.93	0.51
1:G:69:VAL:HG13	1:G:72:LEU:HG	1.92	0.51
1:I:135:LEU:CD2	1:I:135:LEU:N	2.74	0.51
1:B:257:LEU:CD1	1:B:298:VAL:HG11	2.40	0.51
1:E:153:ARG:NH2	1:E:162:GLU:OE1	2.43	0.51
1:G:291:TRP:C	1:G:293:GLU:H	2.14	0.51
1:H:74:ILE:HD13	1:H:209:GLY:CA	2.31	0.51
1:L:320:MET:HA	1:L:320:MET:HE2	1.91	0.51
1:A:149:ARG:HH11	1:A:149:ARG:CG	2.23	0.51
1:L:186:ASP:HB2	1:L:210:PHE:HD2	1.76	0.51
1:B:246:MET:HG2	1:B:314:MET:O	2.11	0.51
1:D:178:HIS:CG	1:D:242:LYS:HD2	2.46	0.51
1:J:127:LEU:O	1:K:48:VAL:HA	2.11	0.51
1:J:340:ARG:O	1:J:342:LEU:N	2.44	0.51
1:B:147:PHE:CD1	1:B:189:PRO:HB3	2.46	0.51
1:B:247:TRP:O	1:B:251:VAL:HG23	2.11	0.51
1:G:238:GLU:HG3	1:G:239:LYS:O	2.10	0.51
1:G:72:LEU:HA	1:G:78:VAL:N	2.12	0.51
1:G:141:LEU:CD1	1:G:193:LEU:HB2	2.41	0.51
1:G:337:HIS:O	1:G:341:VAL:HG23	2.11	0.51
1:G:240:TYR:CE2	1:K:309:GLU:OE2	2.65	0.51
1:E:178:HIS:CE1	1:E:242:LYS:HG2	2.46	0.50
1:E:285:GLU:CB	1:E:287:PRO:HD3	2.35	0.50
1:E:319:PHE:CE2	1:E:320:MET:CE	2.94	0.50
1:L:141:LEU:HD23	1:L:195:THR:HG22	1.92	0.50
1:L:289:PRO:HD2	1:L:290:GLU:OE1	2.11	0.50
1:C:94:MET:HB3	1:C:135:LEU:HD23	1.92	0.50
1:K:251:VAL:O	1:K:255:ILE:HG13	2.10	0.50
1:C:337:HIS:O	1:C:341:VAL:HG23	2.11	0.50
1:H:264:TYR:HA	1:H:275:MET:CE	2.41	0.50
1:L:108:HIS:CG	1:L:120:ILE:HD11	2.46	0.50
1:F:70:LEU:HD11	1:F:140:CYS:SG	2.51	0.50
1:B:146:LEU:HD11	1:B:166:ILE:HD13	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:66:THR:O	1:C:79:LEU:HD13	2.12	0.50
1:E:316:ILE:N	1:E:316:ILE:CD1	2.37	0.50
1:F:184:HIS:O	1:F:185:ARG:HB2	2.11	0.50
1:H:206:THR:OG1	1:H:207:ASP:N	2.44	0.50
1:K:167:MET:CE	1:K:253:MET:HA	2.42	0.50
1:D:321:ASN:HA	1:D:326:MET:HG3	1.93	0.50
1:K:197:LYS:HB2	1:K:198:ARG:HH21	1.77	0.50
1:A:272:SER:N	1:A:274:GLY:H	2.10	0.50
1:B:56:LYS:O	1:C:50:SER:HB2	2.11	0.50
1:F:141:LEU:HB3	1:F:195:THR:HA	1.93	0.50
1:F:257:LEU:HD23	1:F:336:LEU:HD21	1.94	0.50
1:K:66:THR:HG21	1:K:82:PHE:CE1	2.43	0.50
1:L:93:LYS:HB2	1:L:138:MET:CE	2.42	0.50
1:A:151:GLN:HG3	1:A:342:LEU:HB3	1.94	0.50
1:B:190:GLU:CD	1:B:190:GLU:H	2.14	0.50
1:B:288:ASN:N	1:B:288:ASN:OD1	2.45	0.50
1:E:161:ARG:HD3	1:E:331:VAL:O	2.12	0.50
1:G:114:CYS:CB	1:G:117:ILE:HD12	2.40	0.50
1:K:74:ILE:O	1:K:75:ASN:HB2	2.11	0.50
1:K:80:GLN:NE2	1:K:89:LYS:HE3	2.27	0.50
1:A:141:LEU:HD13	1:A:195:THR:HA	1.94	0.49
1:A:90:PHE:HE2	1:A:121:VAL:HG21	1.77	0.49
1:B:194:TYR:CZ	1:B:203:LEU:HD13	2.47	0.49
1:G:90:PHE:HE2	1:G:121:VAL:CG2	2.23	0.49
1:J:340:ARG:HB3	1:J:340:ARG:NH1	2.27	0.49
1:E:290:GLU:HA	1:E:337:HIS:CD2	2.47	0.49
1:H:141:LEU:CD2	1:H:195:THR:HG22	2.42	0.49
1:K:74:ILE:HD12	1:K:74:ILE:O	2.11	0.49
1:F:345:ASP:O	1:F:346:LYS:CG	2.61	0.49
1:C:319:PHE:CD2	1:C:320:MET:CE	2.94	0.49
1:F:337:HIS:O	1:F:341:VAL:HG23	2.12	0.49
1:G:146:LEU:O	1:G:150:ILE:HG12	2.12	0.49
1:H:178:HIS:ND1	1:H:316:ILE:HD12	2.27	0.49
1:K:143:GLY:HA3	1:K:194:TYR:HB3	1.94	0.49
1:A:143:GLY:HA2	1:A:197:LYS:HG3	1.94	0.49
1:F:296:GLU:OE2	1:F:303:ARG:NH2	2.45	0.49
1:E:181:ASN:ND2	1:E:215:THR:HG23	2.28	0.49
1:J:131:ARG:NH2	1:K:180:ILE:HG22	2.27	0.49
1:K:189:PRO:C	1:K:191:ASN:H	2.16	0.49
1:D:191:ASN:HB3	1:D:206:THR:HG23	1.95	0.49
1:E:265:SER:OG	1:E:266:ASN:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:161:ARG:HG3	1:K:331:VAL:CG2	2.42	0.49
1:E:153:ARG:NH1	1:E:157:ALA:O	2.45	0.49
1:J:193:LEU:O	1:J:203:LEU:HA	2.12	0.49
1:K:65:VAL:HA	1:K:81:ILE:HG22	1.95	0.49
1:K:74:ILE:CG1	1:K:207:ASP:OD2	2.61	0.49
1:B:278:ARG:HG2	1:B:283:GLN:CB	2.43	0.48
1:F:161:ARG:HD3	1:F:331:VAL:O	2.13	0.48
1:C:115:PRO:O	1:C:204:LYS:HE2	2.12	0.48
1:H:254:TYR:CD1	1:H:262:PRO:HD3	2.48	0.48
1:I:170:ILE:HG12	1:I:192:LEU:HD22	1.94	0.48
1:G:49:LYS:HD3	3:G:3:HOH:O	2.13	0.48
1:L:167:MET:CE	1:L:256:LEU:HD12	2.42	0.48
1:C:149:ARG:NH1	1:C:149:ARG:HG2	2.10	0.48
1:C:66:THR:HG21	1:C:82:PHE:CE1	2.47	0.48
1:G:258:CYS:HB3	1:G:291:TRP:NE1	2.29	0.48
1:G:297:GLU:O	1:G:300:MET:N	2.47	0.48
1:G:48:VAL:HB	1:I:60:ILE:HD13	1.95	0.48
1:F:97:ASP:OD1	1:F:102:ARG:HD3	2.14	0.48
1:K:149:ARG:HG2	1:K:194:TYR:CD2	2.48	0.48
1:L:286:PHE:HB3	1:L:291:TRP:CG	2.48	0.48
1:A:141:LEU:HD11	1:A:204:LYS:HB2	1.95	0.48
1:A:146:LEU:O	1:A:150:ILE:HG12	2.14	0.48
1:D:109:TRP:HA	1:D:120:ILE:HD12	1.95	0.48
1:E:167:MET:HE3	1:E:252:ILE:HG22	1.94	0.48
1:I:187:VAL:O	1:I:248:SER:OG	2.25	0.48
1:K:129:ALA:H	1:L:47:HIS:HB3	1.78	0.48
1:A:238:GLU:O	1:A:239:LYS:O	2.32	0.48
1:F:234:VAL:O	1:F:234:VAL:HG12	2.13	0.48
1:G:185:ARG:HH12	1:G:212:LYS:HD3	1.78	0.48
1:G:328:SER:O	1:G:331:VAL:HG22	2.13	0.48
1:H:141:LEU:HD21	1:H:204:LYS:HD2	1.95	0.48
1:H:158:PHE:HA	1:H:162:GLU:OE2	2.13	0.48
1:H:156:GLN:HE22	1:H:339:SER:CB	2.27	0.48
1:I:291:TRP:O	1:I:292:SER:C	2.52	0.48
1:I:72:LEU:HA	1:I:77:LYS:HA	1.96	0.48
1:E:167:MET:HE1	1:E:170:ILE:HD12	1.94	0.48
1:G:257:LEU:HD23	1:G:336:LEU:HD21	1.96	0.48
1:H:153:ARG:O	1:H:154:GLY:C	2.51	0.48
1:A:90:PHE:CE2	1:A:121:VAL:HG21	2.48	0.48
1:A:206:THR:OG1	1:A:207:ASP:N	2.47	0.48
1:F:161:ARG:HD2	1:F:328:SER:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:125:GLU:C	1:H:126:ASN:HD22	2.17	0.48
1:J:307:LYS:HG3	1:J:312:GLN:HB3	1.95	0.48
1:C:233:GLU:CG	1:L:310:PRO:HG3	2.43	0.48
1:B:300:MET:CE	1:B:303:ARG:NE	2.67	0.48
1:E:300:MET:CE	1:E:303:ARG:HE	2.26	0.48
1:F:106:GLU:O	1:F:110:ARG:HG3	2.13	0.48
1:J:332:PRO:HB2	1:J:334:THR:HG22	1.96	0.48
1:K:205:LEU:HD12	1:K:206:THR:H	1.78	0.48
1:L:265:SER:HA	1:L:271:ILE:O	2.14	0.48
1:A:180:ILE:HG13	1:A:180:ILE:O	2.14	0.47
1:B:257:LEU:HD13	1:B:298:VAL:HG11	1.96	0.47
1:C:159:THR:O	1:C:162:GLU:HB2	2.14	0.47
1:C:74:ILE:HG12	1:C:207:ASP:OD1	2.13	0.47
1:G:132:LYS:HB2	1:G:132:LYS:HE3	1.58	0.47
1:J:178:HIS:CE1	1:J:242:LYS:HG3	2.49	0.47
1:E:114:CYS:HB3	1:E:117:ILE:HD12	1.96	0.47
1:J:184:HIS:CD2	1:J:205:LEU:HD21	2.50	0.47
1:L:92:LEU:HD11	1:L:135:LEU:HB3	1.96	0.47
1:B:60:ILE:HD13	1:C:48:VAL:HG12	1.97	0.47
1:F:198:ARG:NH1	1:F:198:ARG:HG2	2.26	0.47
1:J:161:ARG:HA	1:J:331:VAL:HG22	1.96	0.47
1:A:45:GLN:C	1:A:47:HIS:H	2.18	0.47
1:E:91:ALA:HB3	1:E:138:MET:HB2	1.97	0.47
1:H:319:PHE:CD2	1:H:320:MET:CE	2.97	0.47
1:I:246:MET:HG2	1:I:314:MET:O	2.14	0.47
1:J:161:ARG:HA	1:J:331:VAL:CG2	2.44	0.47
1:E:233:GLU:CG	1:J:310:PRO:HG3	2.45	0.47
1:K:213:GLU:O	1:K:214:THR:HG23	2.15	0.47
1:A:66:THR:HG21	1:A:82:PHE:CE1	2.47	0.47
1:H:171:GLY:HA3	1:H:320:MET:HE3	1.97	0.47
1:A:147:PHE:O	1:A:151:GLN:HB2	2.15	0.47
1:B:192:LEU:HD11	1:B:252:ILE:CD1	2.44	0.47
1:E:44:PRO:O	1:E:45:GLN:CB	2.62	0.47
1:F:102:ARG:CD	1:F:134:LEU:HD11	2.42	0.47
1:B:278:ARG:HG2	1:B:283:GLN:HB3	1.97	0.47
1:B:319:PHE:CE2	1:B:320:MET:CE	2.97	0.47
1:H:178:HIS:HE1	1:H:246:MET:CE	2.28	0.47
1:H:246:MET:CE	1:H:316:ILE:HD12	2.45	0.47
1:I:109:TRP:O	1:I:112:SER:HB3	2.15	0.47
1:J:93:LYS:HE2	1:J:95:LEU:HD21	1.97	0.47
1:K:74:ILE:HG12	1:K:207:ASP:OD2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:LEU:HD22	1:E:276:LYS:HD3	1.97	0.47
1:D:128:TYR:OH	1:E:44:PRO:HB3	2.14	0.47
1:G:185:ARG:HB2	1:G:210:PHE:O	2.15	0.47
1:J:239:LYS:HB3	1:J:240:TYR:H	1.61	0.47
1:A:48:VAL:HG12	1:C:58:ALA:HB1	1.96	0.47
1:F:198:ARG:HH11	1:F:198:ARG:CG	2.24	0.47
1:F:308:THR:O	1:F:310:PRO:HD3	2.15	0.47
1:G:114:CYS:HB2	1:G:176:TYR:CD2	2.50	0.47
1:D:179:SER:O	1:G:277:THR:HG23	2.15	0.46
1:I:122:ASP:HB3	1:I:124:TYR:HE1	1.79	0.46
1:A:115:PRO:O	1:A:204:LYS:CE	2.63	0.46
1:C:246:MET:HE1	1:C:316:ILE:HD12	1.96	0.46
1:E:56:LYS:CE	1:E:125:GLU:OE1	2.64	0.46
1:G:103:ARG:HA	1:G:103:ARG:HD3	1.78	0.46
1:H:189:PRO:HA	1:H:192:LEU:HD12	1.97	0.46
1:I:131:ARG:NH2	1:K:276:LYS:NZ	2.63	0.46
1:I:281:MET:HA	1:I:281:MET:CE	2.45	0.46
1:K:189:PRO:C	1:K:191:ASN:N	2.69	0.46
1:E:343:LYS:HB2	1:E:343:LYS:HE2	1.59	0.46
1:G:188:LYS:HD2	1:G:190:GLU:OE1	2.15	0.46
1:H:74:ILE:CD1	1:H:207:ASP:OD1	2.58	0.46
1:L:167:MET:CE	1:L:256:LEU:CD1	2.93	0.46
1:A:272:SER:HA	1:A:275:MET:H	1.81	0.46
1:C:146:LEU:HD11	1:C:166:ILE:HD13	1.97	0.46
1:G:261:PRO:CG	1:G:264:TYR:HB3	2.45	0.46
1:H:161:ARG:HD3	1:H:331:VAL:O	2.16	0.46
1:H:246:MET:HE1	1:H:316:ILE:HD12	1.97	0.46
1:K:185:ARG:HD3	1:K:210:PHE:O	2.16	0.46
1:A:253:MET:HE3	1:A:305:LEU:HD12	1.97	0.46
1:D:164:SER:OG	1:D:324:TRP:O	2.33	0.46
1:E:146:LEU:HD11	1:E:166:ILE:HD13	1.96	0.46
1:F:134:LEU:HA	1:F:134:LEU:HD23	1.73	0.46
1:C:60:ILE:HD12	1:C:61:ASP:N	2.30	0.46
1:G:196:SER:HB2	1:G:198:ARG:HE	1.79	0.46
1:H:149:ARG:NH1	1:H:149:ARG:CG	2.60	0.46
1:A:319:PHE:CD2	1:A:320:MET:CE	2.97	0.46
1:C:158:PHE:CE1	1:C:162:GLU:HB3	2.51	0.46
1:D:161:ARG:HE	1:D:329:THR:HG22	1.81	0.46
1:A:233:GLU:CD	1:H:313:ARG:HH12	2.19	0.46
1:I:307:LYS:HB2	1:I:313:ARG:HG3	1.98	0.46
1:J:152:ASP:O	1:J:153:ARG:HB2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:LYS:O	1:B:50:SER:HB2	2.16	0.46
1:B:198:ARG:NH1	1:B:198:ARG:HG2	2.14	0.46
1:C:74:ILE:HD13	1:C:209:GLY:HA3	1.98	0.46
1:E:246:MET:HB2	1:E:246:MET:HE3	1.52	0.46
1:F:285:GLU:O	1:F:287:PRO:HD3	2.15	0.46
1:I:319:PHE:CD2	1:I:320:MET:CE	2.99	0.46
1:D:277:THR:HG21	1:J:131:ARG:HH12	1.81	0.46
1:K:197:LYS:HD3	1:K:198:ARG:NH2	2.31	0.46
1:A:332:PRO:HB2	1:A:334:THR:HG22	1.96	0.46
2:B:500:MK2:H8	2:B:500:MK2:N24	2.30	0.46
1:C:149:ARG:NH1	1:C:149:ARG:CG	2.78	0.46
1:D:86:THR:C	1:D:88:GLU:H	2.18	0.46
1:D:97:ASP:O	1:D:98:CYS:CB	2.64	0.46
1:F:151:GLN:HE21	1:F:342:LEU:HB3	1.81	0.46
1:J:186:ASP:OD2	1:J:188:LYS:HE2	2.16	0.46
1:K:199:PRO:C	1:K:201:ALA:H	2.19	0.46
1:B:147:PHE:CE1	1:B:189:PRO:HB3	2.51	0.45
1:A:165:GLU:O	1:A:166:ILE:C	2.54	0.45
1:D:109:TRP:CA	1:D:120:ILE:HD12	2.47	0.45
1:F:338:THR:HG22	1:F:342:LEU:HD22	1.97	0.45
1:G:240:TYR:HE2	1:K:309:GLU:OE2	2.00	0.45
1:H:150:ILE:HG22	1:H:342:LEU:HD12	1.98	0.45
1:H:260:TYR:OH	1:H:287:PRO:HG2	2.16	0.45
1:D:251:VAL:O	1:D:255:ILE:HG13	2.15	0.45
1:G:164:SER:HB2	1:G:324:TRP:CE2	2.51	0.45
1:J:134:LEU:HD23	1:J:134:LEU:HA	1.80	0.45
1:K:102:ARG:O	1:K:106:GLU:HB3	2.15	0.45
1:K:171:GLY:HA3	1:K:320:MET:HE3	1.97	0.45
1:D:57:ASN:HA	1:E:50:SER:HB2	1.97	0.45
1:E:319:PHE:CE2	1:E:320:MET:HE2	2.52	0.45
1:F:118:VAL:HG11	1:F:206:THR:HB	1.99	0.45
1:G:59:ILE:HG22	1:H:48:VAL:HG11	1.98	0.45
1:G:92:LEU:HD11	1:G:135:LEU:HB3	1.98	0.45
1:I:131:ARG:HH22	1:K:276:LYS:NZ	2.14	0.45
1:A:257:LEU:HA	1:A:257:LEU:HD23	1.87	0.45
2:C:500:MK2:N24	2:C:500:MK2:H8	2.32	0.45
1:J:151:GLN:HG3	1:J:151:GLN:O	2.16	0.45
1:J:141:LEU:HD22	1:J:195:THR:HG22	1.99	0.45
1:K:160:GLU:O	1:K:163:ALA:HB3	2.15	0.45
1:K:83:ASN:HD21	1:K:85:ARG:CZ	2.30	0.45
1:C:131:ARG:HB2	1:C:131:ARG:HE	1.38	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:83:ASN:HB3	1:I:87:GLN:H	1.82	0.45
1:B:188:LYS:HD3	1:J:229:TYR:CZ	2.51	0.45
1:C:54:ILE:O	1:C:54:ILE:HG22	2.17	0.45
1:F:80:GLN:HE21	1:F:89:LYS:HG2	1.82	0.45
1:F:80:GLN:HE21	1:F:89:LYS:CG	2.29	0.45
1:H:56:LYS:HE3	1:H:125:GLU:OE1	2.17	0.45
1:K:185:ARG:HB2	1:K:210:PHE:O	2.17	0.45
2:K:500:MK2:N24	2:K:500:MK2:C8	2.80	0.45
1:L:316:ILE:O	1:L:320:MET:N	2.48	0.45
1:L:332:PRO:HB2	1:L:334:THR:HG22	1.97	0.45
1:A:338:THR:O	1:A:342:LEU:HG	2.16	0.45
1:B:188:LYS:HD3	1:J:229:TYR:OH	2.17	0.45
1:D:198:ARG:HG3	1:D:199:PRO:HD2	1.98	0.45
1:F:236:GLY:O	1:F:237:PRO:O	2.34	0.45
1:H:264:TYR:HA	1:H:275:MET:HE2	1.97	0.45
1:H:92:LEU:HG	1:H:94:MET:HE3	1.99	0.45
1:K:257:LEU:HD23	1:K:336:LEU:HD21	1.99	0.45
1:B:178:HIS:ND1	1:B:316:ILE:CD1	2.79	0.45
1:A:280:ARG:HD2	1:F:235:LEU:HD11	1.99	0.45
1:G:178:HIS:CE1	1:G:242:LYS:HG3	2.52	0.45
1:H:105:VAL:HG22	1:H:136:ILE:HD11	1.99	0.45
1:A:78:VAL:HG22	1:A:93:LYS:HB2	1.99	0.44
1:A:88:GLU:HG2	1:A:89:LYS:N	2.29	0.44
1:B:129:ALA:C	1:B:131:ARG:H	2.21	0.44
2:E:500:MK2:C8	2:E:500:MK2:N24	2.80	0.44
1:F:108:HIS:CG	1:F:120:ILE:HD11	2.52	0.44
1:F:316:ILE:N	1:F:316:ILE:CD1	2.72	0.44
1:F:87:GLN:OE1	1:F:87:GLN:HA	2.17	0.44
1:I:214:THR:HG21	1:I:238:GLU:HG3	2.00	0.44
2:J:500:MK2:C8	2:J:500:MK2:N24	2.80	0.44
1:K:82:PHE:CE2	1:K:89:LYS:HG3	2.52	0.44
1:A:305:LEU:HD23	1:A:305:LEU:HA	1.77	0.44
1:B:273:PRO:O	1:B:277:THR:OG1	2.35	0.44
1:B:161:ARG:HD3	1:B:331:VAL:O	2.17	0.44
1:C:160:GLU:HA	1:C:336:LEU:HD21	1.98	0.44
1:E:92:LEU:HD12	1:E:93:LYS:N	2.33	0.44
1:H:178:HIS:CE1	1:H:246:MET:CE	2.99	0.44
1:J:249:LEU:HD12	1:J:249:LEU:HA	1.64	0.44
1:J:309:GLU:HB2	1:J:312:GLN:HE21	1.81	0.44
1:K:105:VAL:HG12	1:K:106:GLU:N	2.32	0.44
1:K:170:ILE:HG12	1:K:192:LEU:CD1	2.47	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:301:LEU:HD13	1:K:322:HIS:HD2	1.79	0.44
1:F:175:GLN:HA	1:F:316:ILE:HG13	2.00	0.44
1:G:80:GLN:HG3	1:G:81:ILE:N	2.33	0.44
1:C:74:ILE:HD12	1:C:75:ASN:H	1.82	0.44
1:D:207:ASP:C	1:D:207:ASP:OD1	2.56	0.44
2:D:500:MK2:N24	2:D:500:MK2:C8	2.81	0.44
1:I:256:LEU:HA	1:I:256:LEU:HD23	1.85	0.44
1:J:329:THR:O	1:J:330:LYS:HB2	2.17	0.44
1:K:151:GLN:HB3	1:K:152:ASP:H	1.70	0.44
1:L:127:LEU:HD12	1:L:127:LEU:HA	1.61	0.44
1:L:56:LYS:HD3	1:L:125:GLU:HB3	2.00	0.44
1:B:135:LEU:CD2	1:B:135:LEU:N	2.72	0.44
1:C:125:GLU:HA	1:C:133:CYS:O	2.18	0.44
1:E:141:LEU:HB3	1:E:195:THR:HA	1.98	0.44
1:H:80:GLN:OE1	1:H:89:LYS:CG	2.65	0.44
1:I:196:SER:OG	1:I:198:ARG:HB2	2.17	0.44
1:K:167:MET:HE3	1:K:256:LEU:HD23	1.99	0.44
1:B:236:GLY:HA2	1:B:237:PRO:HD2	1.67	0.44
1:E:271:ILE:O	1:E:272:SER:HB2	2.18	0.44
1:F:68:GLN:HB3	1:F:68:GLN:HE21	1.66	0.44
1:G:190:GLU:OE2	1:G:190:GLU:N	2.51	0.44
1:C:319:PHE:CD2	1:C:320:MET:HE1	2.53	0.44
1:G:76:GLY:O	1:G:77:LYS:C	2.55	0.44
1:H:66:THR:HG21	1:H:82:PHE:HE1	1.83	0.44
1:I:246:MET:HE2	1:I:246:MET:CA	2.47	0.44
1:D:132:LYS:HE2	1:E:106:GLU:OE1	2.17	0.44
1:F:178:HIS:ND1	1:F:316:ILE:HD12	2.31	0.44
1:A:337:HIS:O	1:A:338:THR:C	2.55	0.44
1:B:285:GLU:O	1:B:287:PRO:HD3	2.18	0.44
1:D:327:GLN:HE21	1:D:330:LYS:HD3	1.83	0.44
1:F:319:PHE:CD2	1:F:320:MET:HE3	2.53	0.44
1:F:328:SER:O	1:F:331:VAL:HG13	2.18	0.44
1:F:66:THR:HG21	1:F:82:PHE:HE1	1.83	0.44
1:G:149:ARG:NH2	1:G:198:ARG:O	2.50	0.44
1:G:188:LYS:HB2	1:G:189:PRO:CD	2.47	0.44
1:G:85:ARG:CD	1:G:85:ARG:H	2.29	0.44
1:J:105:VAL:HG11	1:J:123:VAL:HG11	1.99	0.44
1:L:343:LYS:O	1:L:344:GLU:C	2.56	0.44
1:B:178:HIS:ND1	1:B:316:ILE:HD11	2.33	0.43
1:B:66:THR:HG23	1:B:67:SER:H	1.83	0.43
1:B:71:GLY:C	1:B:73:GLY:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:128:TYR:HB2	1:C:48:VAL:HG23	2.00	0.43
1:C:58:ALA:HA	1:C:126:ASN:OD1	2.17	0.43
1:G:141:LEU:HD13	1:G:193:LEU:HB2	2.00	0.43
1:F:147:PHE:CD1	1:F:189:PRO:HB3	2.53	0.43
1:I:189:PRO:HA	1:I:192:LEU:HD12	1.99	0.43
1:I:350:GLU:HA	1:I:353:LYS:HE3	2.00	0.43
1:J:133:CYS:HB3	1:J:135:LEU:HD21	1.99	0.43
1:E:246:MET:HG2	1:E:314:MET:O	2.17	0.43
1:E:83:ASN:HD21	1:E:85:ARG:HH12	1.66	0.43
1:F:193:LEU:HD11	1:F:206:THR:HG21	2.00	0.43
1:H:94:MET:HA	1:H:94:MET:HE2	2.00	0.43
1:I:149:ARG:NH1	1:I:149:ARG:CG	2.75	0.43
1:I:246:MET:N	1:I:246:MET:HE2	2.33	0.43
1:C:116:HIS:O	1:C:204:LYS:HA	2.19	0.43
1:D:276:LYS:CE	1:D:280:ARG:HH22	2.32	0.43
1:E:257:LEU:HD13	1:E:298:VAL:HG11	2.00	0.43
1:G:158:PHE:HE1	1:G:163:ALA:HB2	1.83	0.43
1:G:199:PRO:C	1:G:201:ALA:H	2.22	0.43
1:J:82:PHE:HA	1:J:88:GLU:O	2.19	0.43
1:K:237:PRO:O	1:K:238:GLU:HB3	2.19	0.43
1:A:344:GLU:OE1	1:A:344:GLU:HA	2.19	0.43
1:E:44:PRO:O	1:E:45:GLN:HG2	2.18	0.43
1:I:100:LYS:HE2	1:I:103:ARG:NH2	2.32	0.43
1:I:65:VAL:HG22	1:I:81:ILE:HG21	2.00	0.43
1:K:130:GLY:O	1:L:110:ARG:NH1	2.50	0.43
1:D:149:ARG:HG2	1:D:149:ARG:O	2.18	0.43
1:E:320:MET:HE2	1:E:325:ILE:HG21	2.00	0.43
1:F:235:LEU:CD1	1:F:235:LEU:O	2.65	0.43
1:H:54:ILE:HG23	1:H:123:VAL:O	2.18	0.43
2:I:500:MK2:C8	2:I:500:MK2:N24	2.80	0.43
1:K:327:GLN:O	1:K:328:SER:C	2.57	0.43
1:L:171:GLY:HA3	1:L:320:MET:HE3	2.00	0.43
1:E:190:GLU:H	1:E:190:GLU:CD	2.22	0.43
1:E:319:PHE:CD2	1:E:320:MET:HE2	2.54	0.43
1:J:160:GLU:HB2	1:J:334:THR:HG23	2.01	0.43
1:A:108:HIS:CD2	1:A:120:ILE:HG13	2.54	0.43
1:F:107:LEU:HD22	1:F:182:ILE:HG12	2.00	0.43
1:H:161:ARG:HA	1:H:331:VAL:CG2	2.48	0.43
1:I:178:HIS:ND1	1:I:316:ILE:HD11	2.34	0.43
1:J:147:PHE:CE1	1:J:189:PRO:HB3	2.54	0.43
1:K:276:LYS:HE2	1:K:280:ARG:HH12	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:67:SER:C	1:K:69:VAL:N	2.72	0.43
1:C:214:THR:HG21	1:C:238:GLU:HG3	2.00	0.43
1:C:178:HIS:ND1	1:C:316:ILE:HD11	2.34	0.43
1:F:197:LYS:N	1:F:197:LYS:HD2	2.31	0.43
1:H:181:ASN:O	1:H:213:GLU:HA	2.17	0.43
1:H:319:PHE:HD2	1:H:320:MET:CE	2.32	0.43
1:D:119:ARG:HG2	1:D:119:ARG:HH11	1.84	0.42
1:F:171:GLY:HA3	1:F:320:MET:HE1	2.01	0.42
1:I:147:PHE:CE1	1:I:189:PRO:CG	3.02	0.42
1:I:309:GLU:HA	1:I:310:PRO:HD2	1.90	0.42
1:I:346:LYS:HB3	1:I:349:TRP:CD1	2.53	0.42
1:L:347:GLU:H	1:L:347:GLU:CD	2.22	0.42
1:A:149:ARG:CG	1:A:149:ARG:NH1	2.82	0.42
1:B:207:ASP:OD1	1:B:207:ASP:C	2.56	0.42
1:B:245:ASP:O	1:B:248:SER:HB2	2.19	0.42
1:D:196:SER:H	1:D:201:ALA:HB1	1.83	0.42
1:J:111:ALA:O	1:J:113:GLN:N	2.52	0.42
1:J:45:GLN:HG3	1:J:46:PHE:CD1	2.54	0.42
1:C:174:ILE:HG21	1:C:246:MET:HE2	2.01	0.42
1:C:185:ARG:HH11	1:C:212:LYS:HD3	1.77	0.42
1:G:307:LYS:O	1:G:313:ARG:NE	2.46	0.42
1:K:69:VAL:HG22	1:K:79:LEU:HD23	2.01	0.42
1:L:178:HIS:CE1	1:L:246:MET:HE3	2.55	0.42
1:L:340:ARG:O	1:L:343:LYS:HB3	2.20	0.42
1:B:264:TYR:HA	1:B:275:MET:CE	2.49	0.42
1:E:147:PHE:CD1	1:E:189:PRO:HB3	2.55	0.42
1:J:275:MET:O	1:J:276:LYS:C	2.56	0.42
1:K:332:PRO:HB2	1:K:334:THR:HG23	2.01	0.42
2:L:500:MK2:C8	2:L:500:MK2:N24	2.74	0.42
1:A:49:LYS:HA	1:A:49:LYS:HD2	1.82	0.42
1:B:203:LEU:HA	1:B:203:LEU:HD12	1.89	0.42
1:B:178:HIS:CE1	1:B:246:MET:HE1	2.54	0.42
1:C:105:VAL:HG21	1:C:134:LEU:HD13	2.01	0.42
1:G:101:ALA:O	1:G:105:VAL:HG23	2.18	0.42
1:G:158:PHE:CZ	1:G:256:LEU:HD22	2.54	0.42
1:D:246:MET:SD	1:D:316:ILE:HG23	2.59	0.42
1:F:343:LYS:HE3	1:F:343:LYS:HB2	1.77	0.42
1:G:108:HIS:CD2	1:G:120:ILE:HD11	2.55	0.42
1:H:334:THR:HG22	1:H:335:PRO:O	2.19	0.42
1:L:107:LEU:O	1:L:108:HIS:C	2.57	0.42
1:B:111:ALA:HB1	1:B:117:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:129:ALA:O	1:B:131:ARG:N	2.51	0.42
2:B:500:MK2:HN21	2:B:500:MK2:H7	1.84	0.42
1:E:184:HIS:NE2	1:E:207:ASP:O	2.52	0.42
2:E:500:MK2:H7	2:E:500:MK2:HN21	1.84	0.42
1:G:260:TYR:OH	1:G:287:PRO:HG2	2.19	0.42
1:G:69:VAL:HG11	1:G:72:LEU:HG	2.01	0.42
1:H:90:PHE:HE2	1:H:121:VAL:HG21	1.84	0.42
1:H:184:HIS:CD2	1:H:205:LEU:HD21	2.55	0.42
1:H:319:PHE:CD2	1:H:320:MET:HE2	2.55	0.42
1:I:190:GLU:N	1:I:190:GLU:OE2	2.52	0.42
1:J:196:SER:OG	1:J:198:ARG:HB2	2.19	0.42
1:A:238:GLU:C	1:A:239:LYS:O	2.58	0.42
1:A:257:LEU:CD1	1:A:298:VAL:HG11	2.49	0.42
1:B:319:PHE:CD2	1:B:320:MET:HE3	2.46	0.42
1:D:198:ARG:HE	1:D:198:ARG:HB2	1.73	0.42
1:D:60:ILE:HG21	1:E:45:GLN:O	2.19	0.42
1:E:319:PHE:HE2	1:E:320:MET:CE	2.32	0.42
1:D:110:ARG:HG2	1:F:127:LEU:HD21	2.02	0.42
1:F:319:PHE:CE2	1:F:320:MET:CE	3.02	0.42
1:G:129:ALA:O	1:G:130:GLY:O	2.37	0.42
1:H:161:ARG:NH2	1:H:333:GLN:OE1	2.53	0.42
1:A:239:LYS:HB2	1:A:241:ASP:OD2	2.19	0.42
1:C:87:GLN:HG3	1:C:87:GLN:O	2.20	0.42
1:F:111:ALA:HB1	1:F:177:LEU:HD21	2.01	0.42
2:F:500:MK2:N24	2:F:500:MK2:C8	2.82	0.42
1:H:214:THR:O	1:H:215:THR:HG23	2.20	0.42
1:J:118:VAL:HG11	1:J:206:THR:OG1	2.20	0.42
1:L:236:GLY:HA2	1:L:237:PRO:HD2	1.90	0.42
1:C:185:ARG:HD2	1:C:241:ASP:HB3	2.02	0.42
1:C:44:PRO:HA	1:C:45:GLN:OE1	2.20	0.42
1:I:347:GLU:O	1:I:349:TRP:N	2.45	0.42
1:J:107:LEU:HD22	1:J:182:ILE:HG12	2.02	0.42
1:C:303:ARG:O	1:C:307:LYS:HG2	2.19	0.41
1:D:93:LYS:HE3	2:D:500:MK2:C6	2.50	0.41
1:E:46:PHE:C	1:E:48:VAL:H	2.24	0.41
1:G:278:ARG:HG2	1:G:283:GLN:HB3	2.02	0.41
1:I:122:ASP:HB3	1:I:124:TYR:CE1	2.55	0.41
1:J:300:MET:CE	1:J:303:ARG:HE	2.33	0.41
1:J:65:VAL:HA	1:J:81:ILE:HG22	2.02	0.41
1:J:131:ARG:HH22	1:K:180:ILE:HG22	1.85	0.41
1:A:230:VAL:HG22	1:A:234:VAL:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:ASN:CB	1:A:95:LEU:CD2	2.75	0.41
1:B:65:VAL:HA	1:B:81:ILE:HG22	2.01	0.41
1:D:161:ARG:HB3	1:D:333:GLN:HE21	1.85	0.41
1:F:114:CYS:HB2	1:F:176:TYR:CG	2.55	0.41
1:H:171:GLY:HA3	1:H:320:MET:CE	2.50	0.41
1:J:191:ASN:HB3	1:J:206:THR:HG22	2.02	0.41
1:J:347:GLU:HB3	1:J:348:ARG:H	1.60	0.41
1:L:90:PHE:HA	1:L:140:CYS:HB2	2.02	0.41
1:C:158:PHE:O	1:C:336:LEU:HD22	2.20	0.41
1:C:275:MET:HG2	1:C:275:MET:O	2.20	0.41
1:C:305:LEU:O	1:C:313:ARG:HD3	2.19	0.41
1:D:161:ARG:HB2	1:D:333:GLN:HA	2.02	0.41
1:E:167:MET:CE	1:E:170:ILE:HD12	2.50	0.41
1:E:300:MET:HE2	1:E:303:ARG:HH21	1.85	0.41
1:G:189:PRO:C	1:G:191:ASN:N	2.74	0.41
1:L:264:TYR:O	1:L:278:ARG:NH1	2.53	0.41
1:E:68:GLN:HB3	1:E:80:GLN:HB3	2.01	0.41
1:F:347:GLU:HG2	1:F:347:GLU:O	2.19	0.41
1:G:163:ALA:O	1:G:167:MET:HG2	2.20	0.41
1:H:284:TYR:OH	1:H:303:ARG:HG2	2.20	0.41
1:I:178:HIS:CE1	1:I:246:MET:HE1	2.55	0.41
1:L:156:GLN:HG3	1:L:339:SER:OG	2.20	0.41
1:L:107:LEU:HD13	1:L:182:ILE:HG23	2.01	0.41
1:B:332:PRO:HB2	1:B:334:THR:HG23	2.02	0.41
1:D:89:LYS:HB3	1:D:89:LYS:HE2	1.89	0.41
1:G:147:PHE:CZ	1:G:255:ILE:HG21	2.55	0.41
1:I:161:ARG:HD3	1:I:331:VAL:O	2.20	0.41
1:F:257:LEU:HD13	1:F:298:VAL:HG11	2.01	0.41
1:H:266:ASN:HA	1:H:266:ASN:HD22	1.63	0.41
1:H:161:ARG:HD2	1:H:329:THR:HA	2.02	0.41
1:K:90:PHE:HA	1:K:140:CYS:HB2	2.02	0.41
1:L:254:TYR:CG	1:L:262:PRO:HG3	2.56	0.41
1:L:43:PHE:CD2	1:L:44:PRO:HD2	2.55	0.41
1:L:46:PHE:CE2	1:L:47:HIS:HB2	2.56	0.41
1:A:277:THR:HG22	1:A:281:MET:HG3	2.01	0.41
1:A:310:PRO:HG3	1:F:233:GLU:HG2	2.02	0.41
1:D:213:GLU:HG2	1:D:213:GLU:H	1.67	0.41
1:D:253:MET:O	1:D:257:LEU:HB2	2.20	0.41
1:E:319:PHE:CD2	1:E:320:MET:CE	3.04	0.41
1:I:167:MET:CE	1:I:253:MET:HA	2.51	0.41
1:I:57:ASN:C	1:I:57:ASN:ND2	2.74	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:PRO:HB3	1:A:47:HIS:CD2	2.55	0.41
1:A:74:ILE:HG12	1:A:75:ASN:N	2.31	0.41
1:A:87:GLN:OE1	1:A:87:GLN:HA	2.15	0.41
1:D:178:HIS:CE1	1:D:242:LYS:HG3	2.56	0.41
1:D:329:THR:O	1:D:330:LYS:HB2	2.20	0.41
1:H:102:ARG:O	1:H:106:GLU:HB2	2.21	0.41
1:I:111:ALA:C	1:I:113:GLN:N	2.72	0.41
1:A:316:ILE:O	1:A:317:THR:C	2.58	0.41
1:B:190:GLU:N	1:B:190:GLU:CD	2.74	0.41
1:C:158:PHE:HE1	1:C:162:GLU:HB3	1.86	0.41
1:D:333:GLN:CG	1:D:333:GLN:O	2.69	0.41
1:D:334:THR:HA	1:D:335:PRO:HD3	1.85	0.41
1:D:66:THR:O	1:D:68:GLN:N	2.54	0.41
1:G:161:ARG:HA	1:G:331:VAL:HG23	2.02	0.41
1:H:70:LEU:HD23	1:H:70:LEU:HA	1.82	0.41
1:E:107:LEU:O	1:E:108:HIS:C	2.56	0.41
1:G:175:GLN:NE2	1:G:320:MET:HG3	2.36	0.41
1:J:214:THR:HG21	1:J:238:GLU:HG3	2.03	0.41
1:J:249:LEU:O	1:J:253:MET:HB2	2.21	0.41
1:J:307:LYS:HD2	1:J:307:LYS:HA	1.67	0.41
1:B:161:ARG:O	1:B:162:GLU:C	2.59	0.41
1:B:56:LYS:HD3	1:B:125:GLU:HB3	2.03	0.41
1:E:256:LEU:HD23	1:E:256:LEU:HA	1.63	0.41
1:E:156:GLN:CB	1:E:339:SER:HB3	2.51	0.41
1:F:231:ALA:HA	1:F:232:PRO:HD3	1.97	0.41
1:H:55:LYS:HD3	1:H:124:TYR:CZ	2.56	0.41
1:I:57:ASN:C	1:I:57:ASN:HD22	2.25	0.41
1:K:309:GLU:HA	1:K:310:PRO:HD2	1.78	0.41
1:B:150:ILE:HD12	1:B:158:PHE:CE1	2.56	0.40
1:B:228:TYR:CE1	1:B:229:TYR:HD2	2.38	0.40
1:D:290:GLU:HA	1:D:337:HIS:CD2	2.56	0.40
1:I:235:LEU:HD12	1:I:235:LEU:C	2.42	0.40
1:J:98:CYS:HB2	1:J:99:PRO:HD2	2.03	0.40
1:K:85:ARG:HG2	1:K:86:THR:HG23	2.03	0.40
1:K:93:LYS:HD2	2:K:500:MK2:N22	2.36	0.40
1:A:320:MET:O	1:A:326:MET:HG3	2.21	0.40
1:E:119:ARG:HH11	1:E:119:ARG:CB	2.35	0.40
1:E:236:GLY:HA2	1:E:237:PRO:HD3	1.89	0.40
1:E:178:HIS:CE1	1:E:246:MET:HE1	2.56	0.40
1:F:105:VAL:HG21	1:F:134:LEU:HD13	2.03	0.40
1:F:187:VAL:HG12	1:F:187:VAL:O	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:319:PHE:CD2	1:F:320:MET:CE	3.04	0.40
1:H:80:GLN:OE1	1:H:89:LYS:HG2	2.21	0.40
1:C:189:PRO:HD3	1:I:229:TYR:OH	2.22	0.40
1:D:277:THR:CG2	1:J:131:ARG:NH1	2.84	0.40
1:J:340:ARG:O	1:J:343:LYS:N	2.55	0.40
1:J:85:ARG:HG2	1:J:85:ARG:O	2.20	0.40
1:K:86:THR:O	1:K:88:GLU:N	2.54	0.40
1:A:86:THR:O	1:A:87:GLN:HB2	2.20	0.40
1:C:198:ARG:O	1:C:199:PRO:C	2.57	0.40
1:E:92:LEU:HD11	1:E:135:LEU:HB3	2.02	0.40
1:E:151:GLN:HB2	1:E:151:GLN:HE21	1.64	0.40
1:F:156:GLN:O	1:F:157:ALA:HB3	2.21	0.40
1:H:167:MET:CE	1:H:256:LEU:CD1	2.92	0.40
1:B:46:PHE:CE2	1:B:48:VAL:HG21	2.55	0.40
1:D:107:LEU:HD22	1:D:182:ILE:HG12	2.02	0.40
1:H:86:THR:O	1:H:87:GLN:CB	2.68	0.40
1:K:73:GLY:H	1:K:77:LYS:HA	1.86	0.40
1:L:178:HIS:CE1	1:L:246:MET:CE	3.04	0.40
1:A:227:PRO:O	1:A:230:VAL:HG12	2.21	0.40
1:A:271:ILE:HA	1:A:278:ARG:HH22	1.86	0.40
1:A:321:ASN:O	1:A:326:MET:HE2	2.21	0.40
1:D:254:TYR:CD1	1:D:254:TYR:C	2.95	0.40
1:E:188:LYS:NZ	1:E:190:GLU:HB2	2.37	0.40
1:F:295:SER:OG	1:F:298:VAL:HG23	2.20	0.40
1:F:346:LYS:C	1:F:348:ARG:N	2.75	0.40
1:H:178:HIS:ND1	1:H:316:ILE:HD11	2.37	0.40
1:H:345:ASP:C	1:H:347:GLU:N	2.73	0.40
1:J:142:ASP:O	1:J:144:GLY:N	2.54	0.40
1:J:68:GLN:HE21	1:J:68:GLN:HB3	1.66	0.40
1:K:180:ILE:HG13	1:K:182:ILE:HG13	2.03	0.40
1:K:337:HIS:HB3	1:K:340:ARG:NH1	2.36	0.40
1:L:59:ILE:HG13	1:L:124:TYR:CE1	2.57	0.40
1:L:127:LEU:HD12	1:L:131:ARG:O	2.22	0.40

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

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:293:GLU:OE2	1:F:156:GLN:NE2[4_555]	2.07	0.13

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	280/324 (86%)	250 (89%)	25 (9%)	5 (2%)	8 29
1	B	284/324 (88%)	251 (88%)	26 (9%)	7 (2%)	5 21
1	C	273/324 (84%)	239 (88%)	27 (10%)	7 (3%)	5 20
1	D	261/324 (81%)	224 (86%)	27 (10%)	10 (4%)	3 13
1	E	281/324 (87%)	245 (87%)	22 (8%)	14 (5%)	2 7
1	F	287/324 (89%)	248 (86%)	30 (10%)	9 (3%)	4 16
1	G	268/324 (83%)	221 (82%)	32 (12%)	15 (6%)	2 5
1	H	282/324 (87%)	242 (86%)	26 (9%)	14 (5%)	2 7
1	I	289/324 (89%)	245 (85%)	39 (14%)	5 (2%)	9 31
1	J	280/324 (86%)	234 (84%)	29 (10%)	17 (6%)	1 4
1	K	274/324 (85%)	214 (78%)	42 (15%)	18 (7%)	1 3
1	L	285/324 (88%)	251 (88%)	27 (10%)	7 (2%)	5 21
All	All	3344/3888 (86%)	2864 (86%)	352 (10%)	128 (4%)	3 13

All (128) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	239	LYS
1	A	272	SER
1	B	272	SER
1	C	47	HIS
1	D	67	SER
1	D	75	ASN
1	D	87	GLN
1	D	330	LYS
1	E	98	CYS
1	E	155	ASP
1	E	156	GLN
1	E	272	SER

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Mol	Chain	Res	Type
1	F	155	ASP
1	F	156	GLN
1	F	231	ALA
1	F	237	PRO
1	F	238	GLU
1	F	346	LYS
1	F	347	GLU
1	G	238	GLU
1	G	239	LYS
1	G	330	LYS
1	H	98	CYS
1	H	156	GLN
1	H	329	THR
1	J	45	GLN
1	J	74	ILE
1	J	143	GLY
1	J	215	THR
1	J	239	LYS
1	J	330	LYS
1	K	67	SER
1	K	69	VAL
1	K	88	GLU
1	K	143	GLY
1	K	151	GLN
1	K	187	VAL
1	K	190	GLU
1	K	200	ASN
1	K	207	ASP
1	K	214	THR
1	L	46	PHE
1	L	272	SER
1	B	48	VAL
1	C	74	ILE
1	C	344	GLU
1	D	88	GLU
1	D	272	SER
1	E	45	GLN
1	E	154	GLY
1	E	228	TYR
1	E	238	GLU
1	E	344	GLU
1	F	157	ALA

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Mol	Chain	Res	Type
1	G	46	PHE
1	G	72	LEU
1	G	73	GLY
1	G	77	LYS
1	G	130	GLY
1	G	160	GLU
1	G	200	ASN
1	G	207	ASP
1	G	237	PRO
1	H	66	THR
1	H	74	ILE
1	H	154	GLY
1	H	328	SER
1	I	348	ARG
1	J	238	GLU
1	J	241	ASP
1	J	341	VAL
1	J	347	GLU
1	K	75	ASN
1	K	145	GLU
1	K	199	PRO
1	K	237	PRO
1	K	239	LYS
1	L	98	CYS
1	L	239	LYS
1	A	44	PRO
1	A	46	PHE
1	B	130	GLY
1	B	239	LYS
1	C	207	ASP
1	D	237	PRO
1	E	207	ASP
1	F	239	LYS
1	G	292	SER
1	H	207	ASP
1	I	47	HIS
1	I	241	ASP
1	K	68	GLN
1	K	156	GLN
1	B	237	PRO
1	C	238	GLU
1	D	187	VAL

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Mol	Chain	Res	Type
1	D	207	ASP
1	E	157	ALA
1	E	237	PRO
1	E	239	LYS
1	H	57	ASN
1	H	68	GLN
1	H	155	ASP
1	I	292	SER
1	J	44	PRO
1	J	152	ASP
1	K	66	THR
1	A	265	SER
1	B	73	GLY
1	D	98	CYS
1	E	47	HIS
1	G	71	GLY
1	H	153	ARG
1	I	154	GLY
1	J	72	LEU
1	J	333	GLN
1	J	344	GLU
1	L	238	GLU
1	C	43	PHE
1	G	76	GLY
1	H	346	LYS
1	J	237	PRO
1	C	130	GLY
1	L	237	PRO
1	B	99	PRO
1	L	44	PRO
1	J	71	GLY
1	H	289	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	260/293 (89%)	235 (90%)	25 (10%)	8 25
1	B	262/293 (89%)	221 (84%)	41 (16%)	2 8
1	C	256/293 (87%)	215 (84%)	41 (16%)	2 7
1	D	243/293 (83%)	211 (87%)	32 (13%)	4 12
1	E	259/293 (88%)	233 (90%)	26 (10%)	7 23
1	F	264/293 (90%)	231 (88%)	33 (12%)	4 14
1	G	251/293 (86%)	217 (86%)	34 (14%)	4 11
1	H	261/293 (89%)	227 (87%)	34 (13%)	4 12
1	I	265/293 (90%)	227 (86%)	38 (14%)	3 10
1	J	260/293 (89%)	227 (87%)	33 (13%)	4 13
1	K	253/293 (86%)	221 (87%)	32 (13%)	4 13
1	L	263/293 (90%)	234 (89%)	29 (11%)	6 19
All	All	3097/3516 (88%)	2699 (87%)	398 (13%)	4 13

All (398) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	SER
1	A	53	GLN
1	A	66	THR
1	A	74	ILE
1	A	103	ARG
1	A	106	GLU
1	A	110	ARG
1	A	127	LEU
1	A	131	ARG
1	A	138	MET
1	A	141	LEU
1	A	149	ARG
1	A	152	ASP
1	A	198	ARG
1	A	212	LYS
1	A	233	GLU
1	A	238	GLU
1	A	241	ASP
1	A	246	MET
1	A	249	LEU
1	A	264	TYR
1	A	314	MET

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Mol	Chain	Res	Type
1	A	316	ILE
1	A	326	MET
1	A	334	THR
1	B	49	LYS
1	B	60	ILE
1	B	67	SER
1	B	68	GLN
1	B	72	LEU
1	B	74	ILE
1	B	77	LYS
1	B	87	GLN
1	B	97	ASP
1	B	98	CYS
1	B	100	LYS
1	B	110	ARG
1	B	118	VAL
1	B	131	ARG
1	B	135	LEU
1	B	141	LEU
1	B	145	GLU
1	B	149	ARG
1	B	152	ASP
1	B	155	ASP
1	B	156	GLN
1	B	161	ARG
1	B	169	SER
1	B	198	ARG
1	B	212	LYS
1	B	214	THR
1	B	235	LEU
1	B	241	ASP
1	B	242	LYS
1	B	275	MET
1	B	285	GLU
1	B	288	ASN
1	B	295	SER
1	B	304	ASN
1	B	316	ILE
1	B	327	GLN
1	B	330	LYS
1	B	331	VAL
1	B	333	GLN

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Mol	Chain	Res	Type
1	B	334	THR
1	B	347	GLU
1	C	42	GLN
1	C	48	VAL
1	C	66	THR
1	C	67	SER
1	C	72	LEU
1	C	74	ILE
1	C	75	ASN
1	C	77	LYS
1	C	85	ARG
1	C	100	LYS
1	C	102	ARG
1	C	106	GLU
1	C	118	VAL
1	C	127	LEU
1	C	131	ARG
1	C	149	ARG
1	C	151	GLN
1	C	160	GLU
1	C	169	SER
1	C	172	GLU
1	C	196	SER
1	C	198	ARG
1	C	233	GLU
1	C	235	LEU
1	C	241	ASP
1	C	244	CYS
1	C	264	TYR
1	C	265	SER
1	C	275	MET
1	C	277	THR
1	C	285	GLU
1	C	288	ASN
1	C	316	ILE
1	C	321	ASN
1	C	328	SER
1	C	331	VAL
1	C	334	THR
1	C	336	LEU
1	C	340	ARG
1	C	342	LEU

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Mol	Chain	Res	Type
1	C	345	ASP
1	D	48	VAL
1	D	53	GLN
1	D	54	ILE
1	D	67	SER
1	D	69	VAL
1	D	77	LYS
1	D	85	ARG
1	D	93	LYS
1	D	106	GLU
1	D	127	LEU
1	D	132	LYS
1	D	135	LEU
1	D	159	THR
1	D	169	SER
1	D	190	GLU
1	D	191	ASN
1	D	197	LYS
1	D	198	ARG
1	D	212	LYS
1	D	213	GLU
1	D	214	THR
1	D	233	GLU
1	D	238	GLU
1	D	239	LYS
1	D	257	LEU
1	D	272	SER
1	D	277	THR
1	D	304	ASN
1	D	316	ILE
1	D	326	MET
1	D	327	GLN
1	D	334	THR
1	E	67	SER
1	E	74	ILE
1	E	77	LYS
1	E	112	SER
1	E	113	GLN
1	E	149	ARG
1	E	155	ASP
1	E	156	GLN
1	E	159	THR

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Mol	Chain	Res	Type
1	E	162	GLU
1	E	185	ARG
1	E	190	GLU
1	E	198	ARG
1	E	235	LEU
1	E	241	ASP
1	E	242	LYS
1	E	246	MET
1	E	256	LEU
1	E	265	SER
1	E	280	ARG
1	E	316	ILE
1	E	327	GLN
1	E	330	LYS
1	E	331	VAL
1	E	334	THR
1	E	345	ASP
1	F	46	PHE
1	F	68	GLN
1	F	72	LEU
1	F	75	ASN
1	F	77	LYS
1	F	92	LEU
1	F	94	MET
1	F	118	VAL
1	F	141	LEU
1	F	145	GLU
1	F	156	GLN
1	F	188	LYS
1	F	197	LYS
1	F	198	ARG
1	F	214	THR
1	F	215	THR
1	F	228	TYR
1	F	233	GLU
1	F	239	LYS
1	F	241	ASP
1	F	242	LYS
1	F	272	SER
1	F	316	ILE
1	F	328	SER
1	F	329	THR

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Mol	Chain	Res	Type
1	F	331	VAL
1	F	333	GLN
1	F	336	LEU
1	F	340	ARG
1	F	342	LEU
1	F	343	LYS
1	F	346	LYS
1	F	347	GLU
1	G	47	HIS
1	G	49	LYS
1	G	60	ILE
1	G	72	LEU
1	G	77	LYS
1	G	80	GLN
1	G	85	ARG
1	G	86	THR
1	G	87	GLN
1	G	94	MET
1	G	100	LYS
1	G	112	SER
1	G	152	ASP
1	G	168	LYS
1	G	190	GLU
1	G	215	THR
1	G	235	LEU
1	G	238	GLU
1	G	244	CYS
1	G	252	ILE
1	G	255	ILE
1	G	264	TYR
1	G	285	GLU
1	G	294	VAL
1	G	312	GLN
1	G	316	ILE
1	G	321	ASN
1	G	326	MET
1	G	327	GLN
1	G	329	THR
1	G	330	LYS
1	G	336	LEU
1	G	338	THR
1	G	342	LEU

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Mol	Chain	Res	Type
1	H	46	PHE
1	H	49	LYS
1	H	57	ASN
1	H	66	THR
1	H	67	SER
1	H	69	VAL
1	H	72	LEU
1	H	77	LYS
1	H	80	GLN
1	H	85	ARG
1	H	89	LYS
1	H	113	GLN
1	H	131	ARG
1	H	132	LYS
1	H	149	ARG
1	H	152	ASP
1	H	153	ARG
1	H	155	ASP
1	H	156	GLN
1	H	198	ARG
1	H	215	THR
1	H	233	GLU
1	H	241	ASP
1	H	242	LYS
1	H	243	SER
1	H	246	MET
1	H	266	ASN
1	H	295	SER
1	H	316	ILE
1	H	327	GLN
1	H	329	THR
1	H	331	VAL
1	H	343	LYS
1	H	348	ARG
1	I	47	HIS
1	I	49	LYS
1	I	57	ASN
1	I	60	ILE
1	I	68	GLN
1	I	77	LYS
1	I	86	THR
1	I	87	GLN

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Mol	Chain	Res	Type
1	I	88	GLU
1	I	89	LYS
1	I	100	LYS
1	I	106	GLU
1	I	131	ARG
1	I	135	LEU
1	I	140	CYS
1	I	145	GLU
1	I	149	ARG
1	I	152	ASP
1	I	161	ARG
1	I	188	LYS
1	I	198	ARG
1	I	214	THR
1	I	215	THR
1	I	233	GLU
1	I	234	VAL
1	I	248	SER
1	I	272	SER
1	I	285	GLU
1	I	295	SER
1	I	316	ILE
1	I	330	LYS
1	I	333	GLN
1	I	340	ARG
1	I	342	LEU
1	I	344	GLU
1	I	346	LYS
1	I	348	ARG
1	I	354	GLU
1	J	47	HIS
1	J	57	ASN
1	J	64	LYS
1	J	66	THR
1	J	68	GLN
1	J	77	LYS
1	J	80	GLN
1	J	83	ASN
1	J	85	ARG
1	J	88	GLU
1	J	95	LEU
1	J	112	SER

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Mol	Chain	Res	Type
1	J	131	ARG
1	J	142	ASP
1	J	152	ASP
1	J	161	ARG
1	J	164	SER
1	J	172	GLU
1	J	206	THR
1	J	214	THR
1	J	233	GLU
1	J	235	LEU
1	J	241	ASP
1	J	242	LYS
1	J	253	MET
1	J	277	THR
1	J	293	GLU
1	J	307	LYS
1	J	316	ILE
1	J	329	THR
1	J	333	GLN
1	J	334	THR
1	J	339	SER
1	K	47	HIS
1	K	57	ASN
1	K	61	ASP
1	K	62	ASP
1	K	72	LEU
1	K	77	LYS
1	K	85	ARG
1	K	88	GLU
1	K	96	GLN
1	K	113	GLN
1	K	114	CYS
1	K	125	GLU
1	K	131	ARG
1	K	132	LYS
1	K	149	ARG
1	K	151	GLN
1	K	152	ASP
1	K	156	GLN
1	K	164	SER
1	K	197	LYS
1	K	234	VAL

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Mol	Chain	Res	Type
1	K	235	LEU
1	K	241	ASP
1	K	244	CYS
1	K	248	SER
1	K	253	MET
1	K	264	TYR
1	K	311	THR
1	K	316	ILE
1	K	327	GLN
1	K	343	LYS
1	K	345	ASP
1	L	45	GLN
1	L	47	HIS
1	L	62	ASP
1	L	66	THR
1	L	83	ASN
1	L	88	GLU
1	L	89	LYS
1	L	103	ARG
1	L	138	MET
1	L	141	LEU
1	L	149	ARG
1	L	153	ARG
1	L	155	ASP
1	L	161	ARG
1	L	197	LYS
1	L	212	LYS
1	L	214	THR
1	L	230	VAL
1	L	233	GLU
1	L	235	LEU
1	L	241	ASP
1	L	243	SER
1	L	265	SER
1	L	275	MET
1	L	295	SER
1	L	304	ASN
1	L	334	THR
1	L	342	LEU
1	L	344	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (82) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	68	GLN
1	A	80	GLN
1	A	113	GLN
1	A	181	ASN
1	A	191	ASN
1	A	266	ASN
1	A	283	GLN
1	A	321	ASN
1	B	47	HIS
1	B	75	ASN
1	B	80	GLN
1	B	113	GLN
1	B	156	GLN
1	B	191	ASN
1	B	321	ASN
1	B	333	GLN
1	B	337	HIS
1	C	42	GLN
1	C	75	ASN
1	C	80	GLN
1	C	87	GLN
1	C	191	ASN
1	C	200	ASN
1	C	304	ASN
1	D	80	GLN
1	D	151	GLN
1	D	191	ASN
1	D	321	ASN
1	D	333	GLN
1	D	337	HIS
1	E	47	HIS
1	E	68	GLN
1	E	75	ASN
1	E	80	GLN
1	E	151	GLN
1	E	327	GLN
1	F	53	GLN
1	F	68	GLN
1	F	75	ASN
1	F	151	GLN
1	F	191	ASN
1	F	200	ASN
1	F	267	HIS

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Mol	Chain	Res	Type
1	F	327	GLN
1	F	333	GLN
1	G	80	GLN
1	G	175	GLN
1	G	191	ASN
1	G	304	ASN
1	G	321	ASN
1	G	327	GLN
1	G	337	HIS
1	H	45	GLN
1	H	57	ASN
1	H	96	GLN
1	H	156	GLN
1	H	191	ASN
1	H	266	ASN
1	H	321	ASN
1	H	327	GLN
1	I	57	ASN
1	I	191	ASN
1	J	45	GLN
1	J	57	ASN
1	J	68	GLN
1	J	75	ASN
1	J	87	GLN
1	J	304	ASN
1	J	337	HIS
1	K	57	ASN
1	K	80	GLN
1	K	113	GLN
1	K	151	GLN
1	K	181	ASN
1	K	333	GLN
1	L	42	GLN
1	L	45	GLN
1	L	57	ASN
1	L	80	GLN
1	L	96	GLN
1	L	283	GLN
1	L	321	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry

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	MK2	F	500	-	26,30,30	1.36	4 (15%)	26,43,43	2.15	8 (30%)
2	MK2	D	500	-	26,30,30	1.31	3 (11%)	26,43,43	1.98	7 (26%)
2	MK2	K	500	-	26,30,30	1.27	3 (11%)	26,43,43	2.11	8 (30%)
2	MK2	E	500	-	26,30,30	1.38	4 (15%)	26,43,43	2.47	9 (34%)
2	MK2	C	500	-	26,30,30	1.33	4 (15%)	26,43,43	1.93	6 (23%)
2	MK2	I	500	-	26,30,30	1.41	3 (11%)	26,43,43	2.15	10 (38%)
2	MK2	J	500	-	26,30,30	1.25	3 (11%)	26,43,43	2.21	7 (26%)
2	MK2	H	500	-	26,30,30	1.15	3 (11%)	26,43,43	2.57	10 (38%)
2	MK2	A	500	-	26,30,30	1.23	2 (7%)	26,43,43	2.49	9 (34%)
2	MK2	L	500	-	26,30,30	1.31	4 (15%)	26,43,43	2.63	8 (30%)
2	MK2	B	500	-	26,30,30	1.39	5 (19%)	26,43,43	2.33	10 (38%)

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	MK2	F	500	-	-	0/5/8/8	0/5/5/5
2	MK2	D	500	-	-	0/5/8/8	0/5/5/5
2	MK2	K	500	-	-	2/5/8/8	0/5/5/5
2	MK2	E	500	-	-	1/5/8/8	0/5/5/5
2	MK2	C	500	-	-	0/5/8/8	0/5/5/5
2	MK2	I	500	-	-	0/5/8/8	0/5/5/5
2	MK2	J	500	-	-	1/5/8/8	0/5/5/5
2	MK2	H	500	-	-	1/5/8/8	0/5/5/5
2	MK2	A	500	-	-	0/5/8/8	0/5/5/5
2	MK2	L	500	-	-	0/5/8/8	0/5/5/5
2	MK2	B	500	-	-	1/5/8/8	0/5/5/5

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	500	MK2	C19-N20	3.75	1.41	1.33
2	L	500	MK2	C19-N20	3.70	1.41	1.33
2	B	500	MK2	C19-N20	3.60	1.41	1.33
2	J	500	MK2	C19-N20	3.45	1.40	1.33
2	A	500	MK2	C19-N20	3.40	1.40	1.33
2	I	500	MK2	C16-C18	-3.34	1.38	1.43
2	E	500	MK2	C16-C18	-3.30	1.38	1.43
2	C	500	MK2	C19-N20	3.20	1.40	1.33
2	K	500	MK2	C16-C18	-3.20	1.38	1.43
2	A	500	MK2	C16-C18	-3.09	1.38	1.43
2	H	500	MK2	C19-N20	2.99	1.39	1.33
2	I	500	MK2	C19-N20	2.98	1.39	1.33
2	F	500	MK2	C16-C18	-2.93	1.38	1.43
2	F	500	MK2	C19-N20	2.92	1.39	1.33
2	B	500	MK2	C16-C18	-2.90	1.38	1.43
2	H	500	MK2	C16-C18	-2.89	1.38	1.43
2	C	500	MK2	C16-C18	-2.84	1.38	1.43
2	J	500	MK2	C16-C18	-2.74	1.38	1.43
2	K	500	MK2	C19-N20	2.64	1.39	1.33
2	D	500	MK2	C16-C18	-2.61	1.39	1.43
2	E	500	MK2	C19-N20	2.60	1.39	1.33
2	F	500	MK2	C13-N25	2.39	1.42	1.38
2	F	500	MK2	C11-C12	-2.38	1.38	1.43
2	L	500	MK2	C11-C12	-2.36	1.38	1.43
2	L	500	MK2	C16-C18	-2.36	1.39	1.43
2	C	500	MK2	C11-C12	-2.35	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	500	MK2	C11-C12	-2.29	1.38	1.43
2	D	500	MK2	C11-C12	-2.27	1.38	1.43
2	J	500	MK2	C11-C12	-2.23	1.38	1.43
2	I	500	MK2	C11-C12	-2.19	1.38	1.43
2	C	500	MK2	C16-C17	-2.16	1.42	1.46
2	L	500	MK2	C8-C15	-2.15	1.37	1.42
2	H	500	MK2	C11-C12	-2.14	1.39	1.43
2	E	500	MK2	C11-C12	-2.10	1.39	1.43
2	E	500	MK2	C10-C15	-2.08	1.36	1.40
2	B	500	MK2	C13-N25	2.08	1.42	1.38
2	B	500	MK2	C8-C15	-2.08	1.37	1.42
2	K	500	MK2	C13-N25	2.01	1.42	1.38

All (92) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	500	MK2	C14-C8-C15	-7.75	108.93	120.29
2	H	500	MK2	C14-C8-C15	-7.54	109.25	120.29
2	E	500	MK2	C14-C8-C15	-7.09	109.89	120.29
2	I	500	MK2	C14-C8-C15	-6.52	110.73	120.29
2	J	500	MK2	C14-C8-C15	-6.40	110.92	120.29
2	A	500	MK2	C14-C8-C15	-6.26	111.12	120.29
2	B	500	MK2	C14-C8-C15	-5.97	111.54	120.29
2	D	500	MK2	C14-C8-C15	-5.80	111.80	120.29
2	L	500	MK2	C9-C16-C18	-5.77	112.05	118.46
2	E	500	MK2	C9-C16-C17	5.69	127.78	120.39
2	F	500	MK2	C14-C8-C15	-5.62	112.06	120.29
2	B	500	MK2	C9-C16-C17	5.49	127.53	120.39
2	K	500	MK2	C14-C8-C15	-5.46	112.29	120.29
2	A	500	MK2	C9-C16-C17	5.43	127.45	120.39
2	C	500	MK2	C14-C8-C15	-5.31	112.51	120.29
2	H	500	MK2	C9-C16-C18	-5.24	112.64	118.46
2	H	500	MK2	C16-C9-C14	4.63	126.49	119.43
2	F	500	MK2	C16-C9-C14	4.57	126.39	119.43
2	K	500	MK2	C16-C9-C14	4.46	126.23	119.43
2	A	500	MK2	C16-C9-C14	4.39	126.11	119.43
2	J	500	MK2	C16-C9-C14	4.31	126.00	119.43
2	C	500	MK2	C16-C9-C14	4.21	125.83	119.43
2	A	500	MK2	C9-C16-C18	-4.18	113.81	118.46
2	F	500	MK2	C9-C16-C18	-4.01	114.01	118.46
2	J	500	MK2	C9-C16-C18	-3.95	114.07	118.46
2	K	500	MK2	C9-C16-C18	-3.83	114.20	118.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	L	500	MK2	C8-C14-C9	3.81	124.67	119.57
2	L	500	MK2	C16-C9-C14	3.75	125.15	119.43
2	E	500	MK2	C9-C16-C18	-3.71	114.34	118.46
2	H	500	MK2	N20-C19-N22	3.53	121.02	117.44
2	I	500	MK2	C16-C9-C14	3.47	124.72	119.43
2	I	500	MK2	C9-C16-C18	-3.44	114.64	118.46
2	D	500	MK2	C16-C9-C14	3.44	124.67	119.43
2	B	500	MK2	C9-C16-C18	-3.41	114.67	118.46
2	J	500	MK2	C1-C3-C11	-3.40	115.13	120.44
2	E	500	MK2	C1-C3-C11	-3.35	115.21	120.44
2	L	500	MK2	C15-C10-N23	-3.31	102.83	111.30
2	E	500	MK2	C16-C9-C14	3.25	124.38	119.43
2	D	500	MK2	C9-C16-C18	-3.25	114.85	118.46
2	B	500	MK2	C16-C9-C14	3.18	124.28	119.43
2	A	500	MK2	N25-C13-N24	3.11	125.72	116.95
2	L	500	MK2	C1-C3-C11	-3.08	115.63	120.44
2	E	500	MK2	C1-C2-C4	2.97	124.61	120.44
2	H	500	MK2	N20-C19-N24	-2.95	112.66	117.25
2	D	500	MK2	C1-C3-C11	-2.93	115.86	120.44
2	K	500	MK2	C1-C3-C11	-2.91	115.89	120.44
2	H	500	MK2	C15-C10-N23	-2.90	103.88	111.30
2	C	500	MK2	C9-C16-C18	-2.86	115.28	118.46
2	J	500	MK2	C15-C10-N23	-2.85	104.00	111.30
2	F	500	MK2	C9-C16-C17	2.82	124.06	120.39
2	K	500	MK2	C15-C10-N23	-2.77	104.21	111.30
2	H	500	MK2	C8-C14-C9	2.73	123.22	119.57
2	B	500	MK2	C15-C10-N23	-2.72	104.34	111.30
2	L	500	MK2	C9-C16-C17	2.72	123.92	120.39
2	I	500	MK2	C1-C3-C11	-2.69	116.23	120.44
2	D	500	MK2	C15-C10-N23	-2.68	104.44	111.30
2	E	500	MK2	C8-C14-C9	2.65	123.11	119.57
2	C	500	MK2	C15-C10-N23	-2.64	104.54	111.30
2	A	500	MK2	C15-C10-N23	-2.58	104.69	111.30
2	I	500	MK2	C15-C10-N23	-2.54	104.79	111.30
2	K	500	MK2	C9-C16-C17	2.53	123.67	120.39
2	B	500	MK2	C1-C3-C11	-2.52	116.50	120.44
2	C	500	MK2	C1-C3-C11	-2.51	116.52	120.44
2	I	500	MK2	C8-C14-C9	2.49	122.91	119.57
2	H	500	MK2	C1-C2-C4	2.49	123.93	120.44
2	F	500	MK2	C1-C3-C11	-2.45	116.61	120.44
2	F	500	MK2	C5-C13-N24	-2.44	119.04	123.16
2	A	500	MK2	C1-C3-C11	-2.43	116.65	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	H	500	MK2	C1-C3-C11	-2.41	116.68	120.44
2	B	500	MK2	C8-C14-C9	2.38	122.75	119.57
2	L	500	MK2	N25-C13-N24	2.36	123.61	116.95
2	J	500	MK2	C17-C16-C18	2.35	125.18	121.38
2	F	500	MK2	C15-C10-N23	-2.35	105.28	111.30
2	E	500	MK2	C15-C10-N23	-2.35	105.29	111.30
2	I	500	MK2	C2-C1-C3	2.32	123.69	120.44
2	I	500	MK2	C9-C16-C17	2.30	123.38	120.39
2	F	500	MK2	C19-N24-C13	2.28	119.87	114.68
2	A	500	MK2	N20-C19-N22	-2.24	115.17	117.44
2	B	500	MK2	C17-C16-C18	-2.23	117.79	121.38
2	A	500	MK2	C6-N22-C19	-2.19	114.00	116.24
2	B	500	MK2	C1-C2-C4	2.19	123.51	120.44
2	B	500	MK2	N25-C13-N24	2.19	123.13	116.95
2	E	500	MK2	C17-C16-C18	-2.18	117.87	121.38
2	I	500	MK2	N25-C13-N24	2.17	123.07	116.95
2	D	500	MK2	C9-C16-C17	2.12	123.14	120.39
2	C	500	MK2	N20-C19-N22	2.10	119.57	117.44
2	I	500	MK2	C9-C14-N25	-2.06	113.35	120.32
2	K	500	MK2	C5-C13-N24	-2.05	119.71	123.16
2	D	500	MK2	C8-C14-C9	2.03	122.29	119.57
2	K	500	MK2	C19-N24-C13	2.02	119.27	114.68
2	H	500	MK2	C17-C16-C18	2.01	124.63	121.38
2	J	500	MK2	C1-C2-C4	2.01	123.26	120.44

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	500	MK2	C9-C16-C17-C7
2	J	500	MK2	C9-C16-C17-C7
2	B	500	MK2	C9-C16-C17-C7
2	K	500	MK2	N24-C13-N25-C14
2	K	500	MK2	C5-C13-N25-C14
2	H	500	MK2	C9-C16-C17-C7

There are no ring outliers.

11 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	500	MK2	2	0

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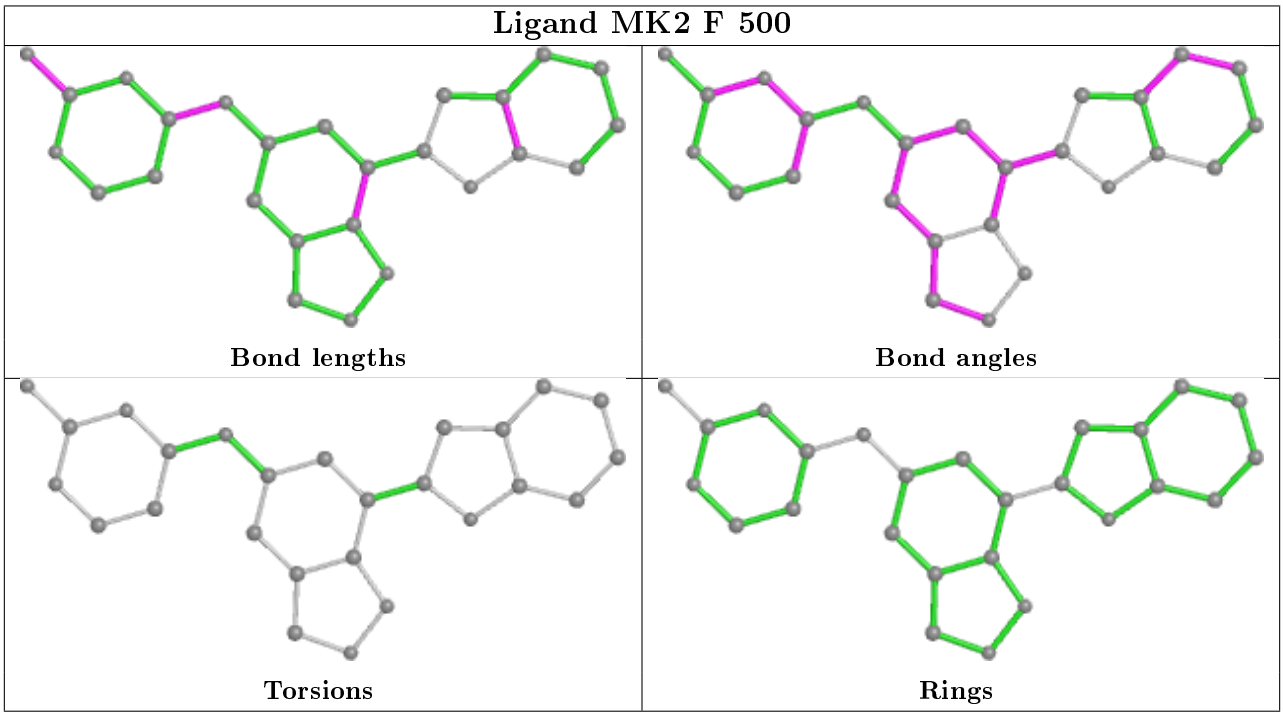
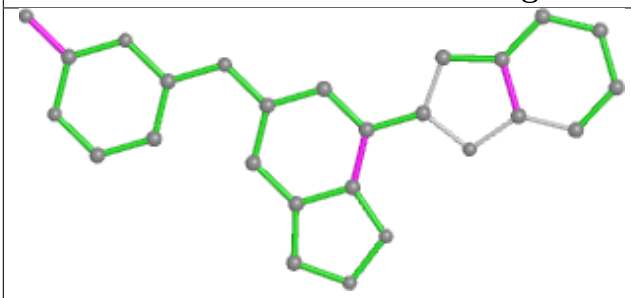
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	500	MK2	3	0
2	K	500	MK2	3	0
2	E	500	MK2	3	0
2	C	500	MK2	1	0
2	I	500	MK2	2	0
2	J	500	MK2	3	0
2	H	500	MK2	3	0
2	A	500	MK2	1	0
2	L	500	MK2	2	0
2	B	500	MK2	2	0

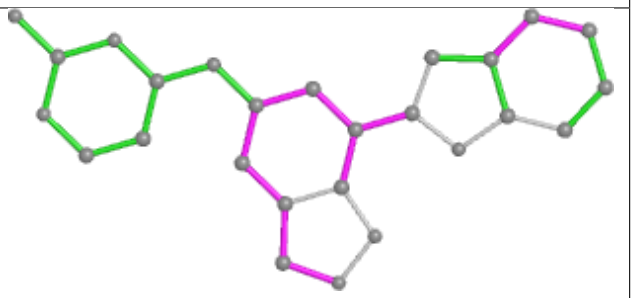
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



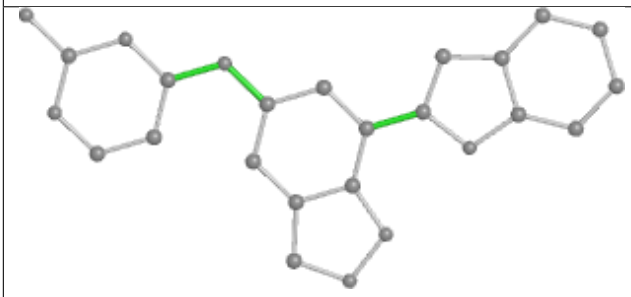
Ligand MK2 D 500



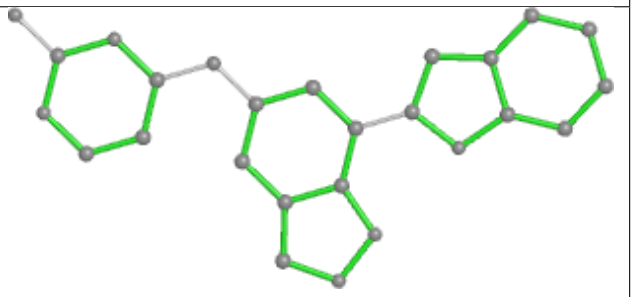
Bond lengths



Bond angles

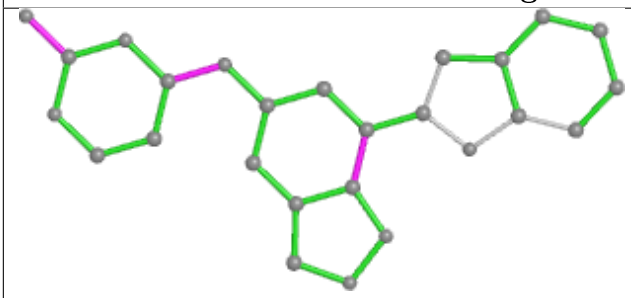


Torsions

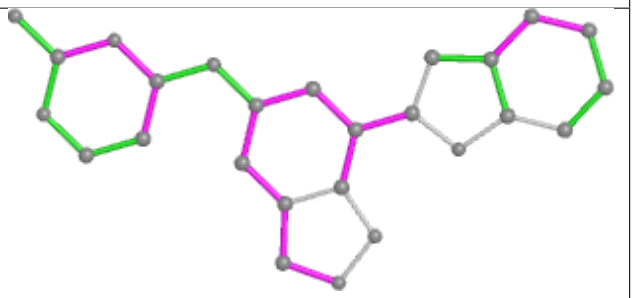


Rings

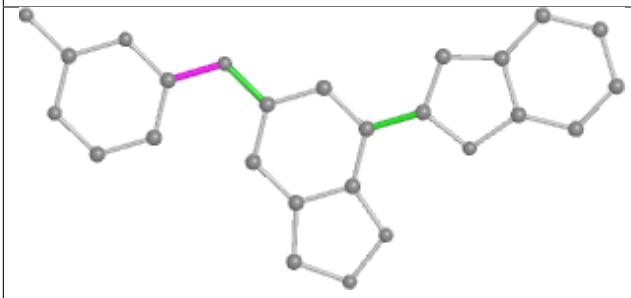
Ligand MK2 K 500



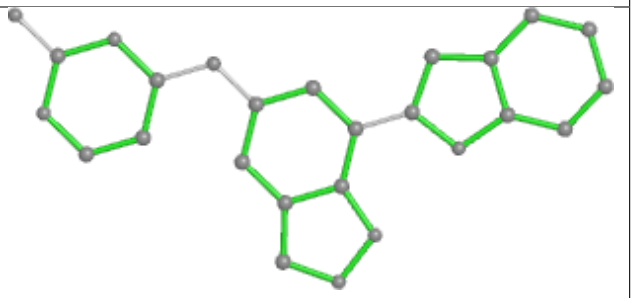
Bond lengths



Bond angles

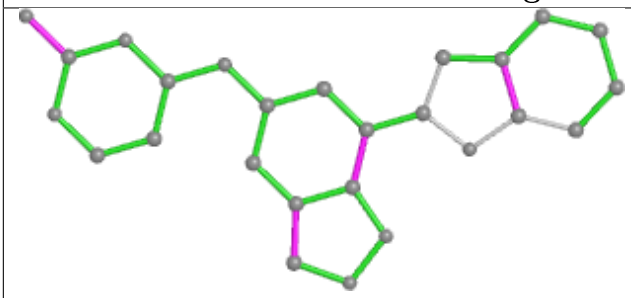


Torsions

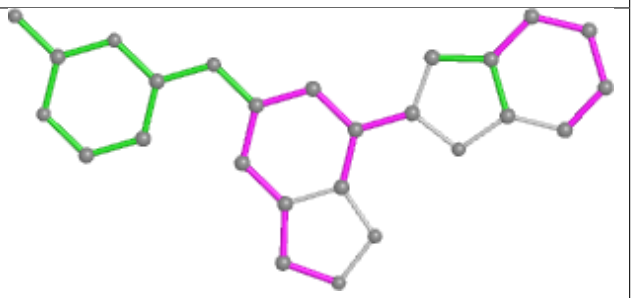


Rings

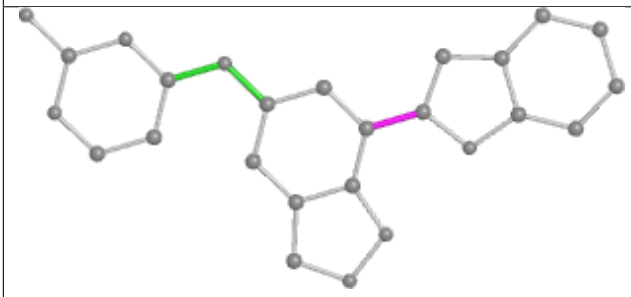
Ligand MK2 E 500



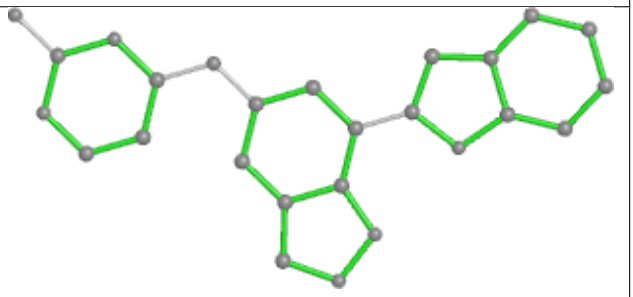
Bond lengths



Bond angles

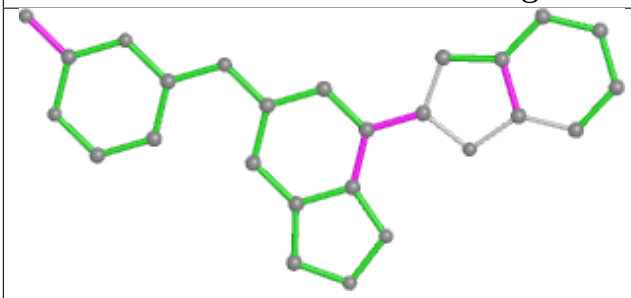


Torsions

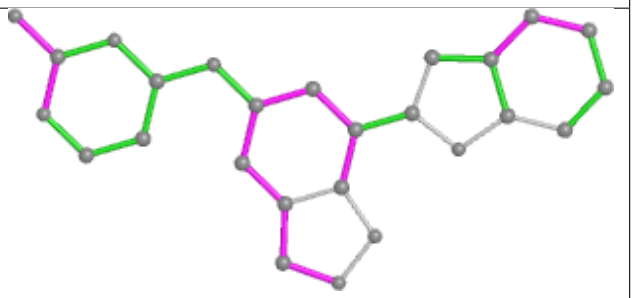


Rings

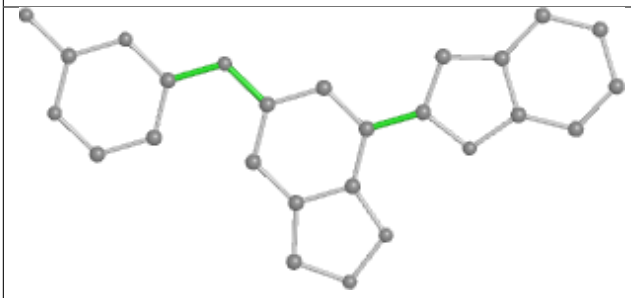
Ligand MK2 C 500



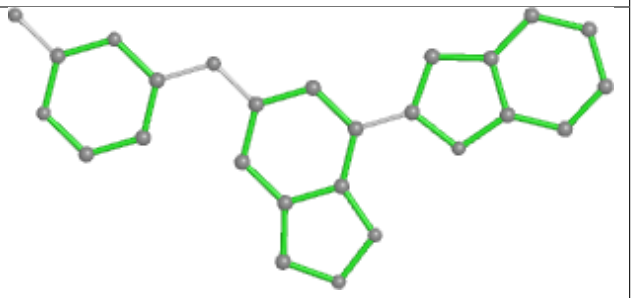
Bond lengths



Bond angles

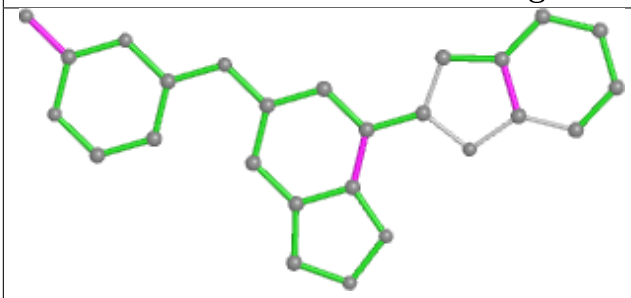


Torsions

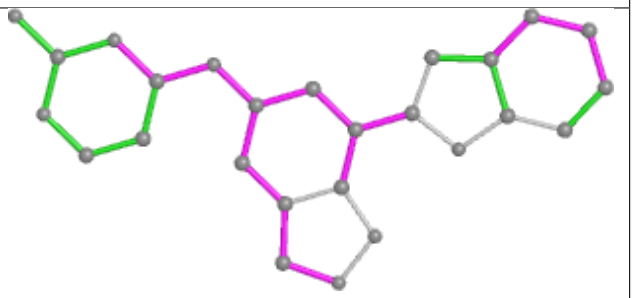


Rings

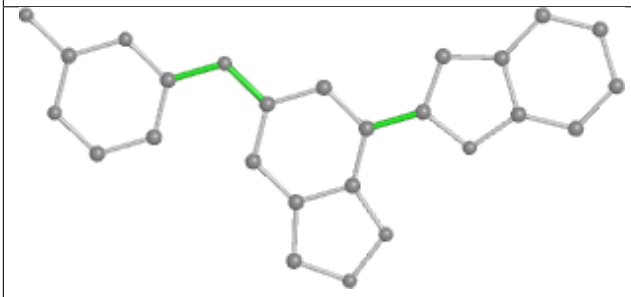
Ligand MK2 I 500



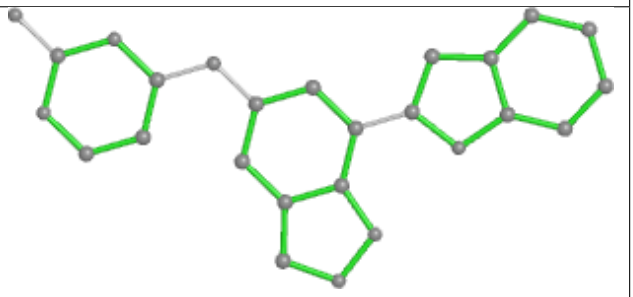
Bond lengths



Bond angles

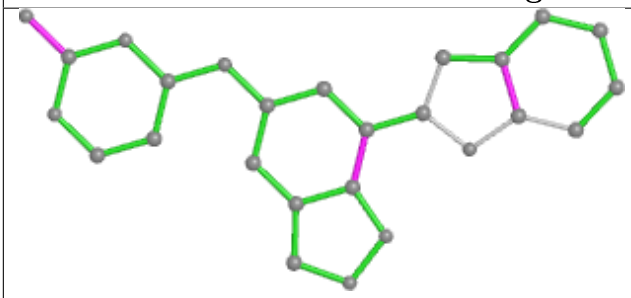


Torsions

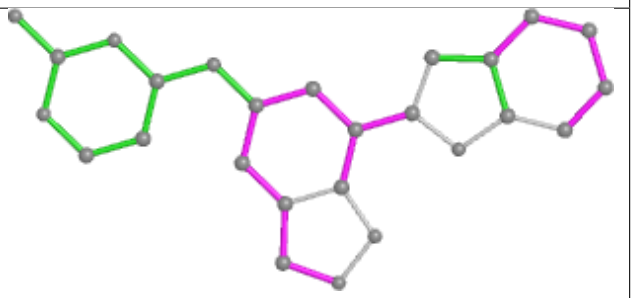


Rings

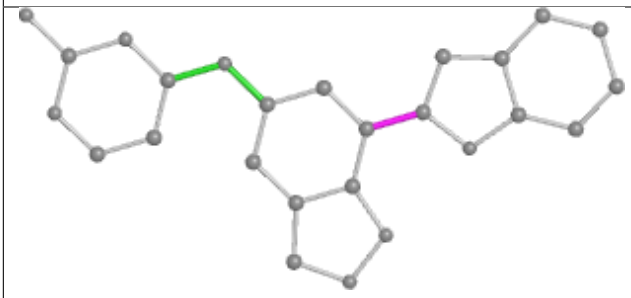
Ligand MK2 J 500



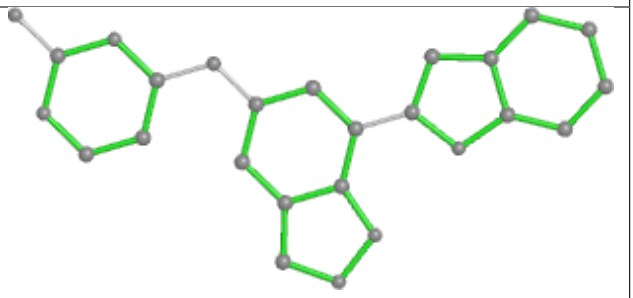
Bond lengths



Bond angles

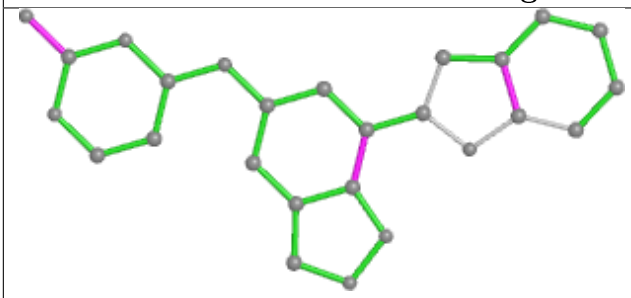


Torsions

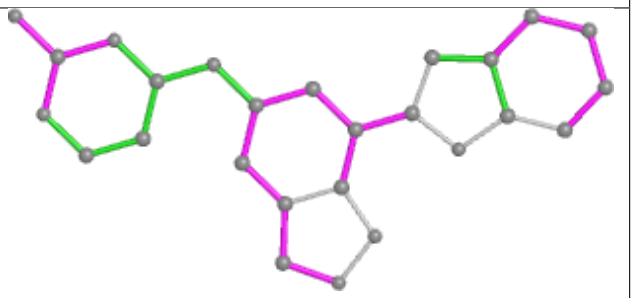


Rings

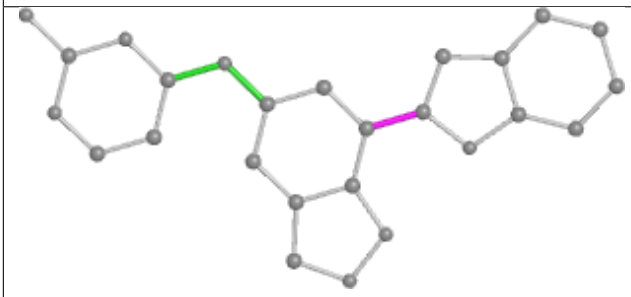
Ligand MK2 H 500



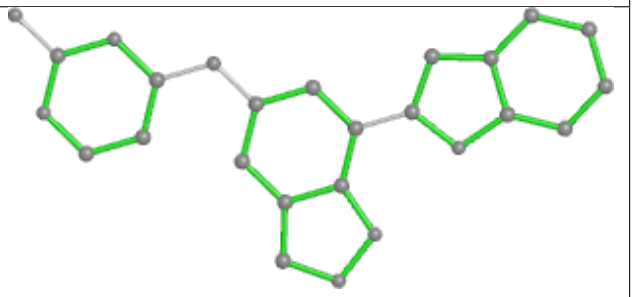
Bond lengths



Bond angles

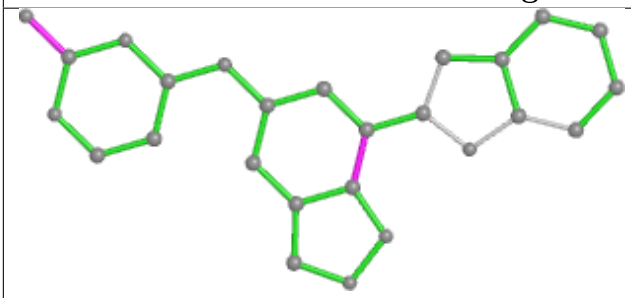


Torsions

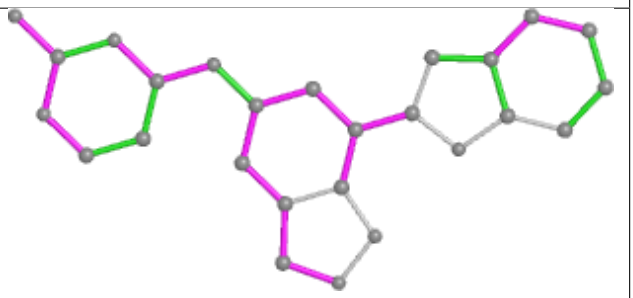


Rings

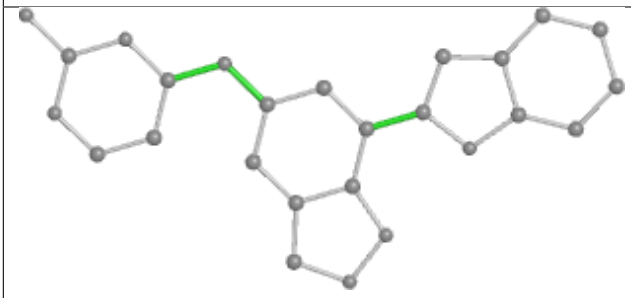
Ligand MK2 A 500



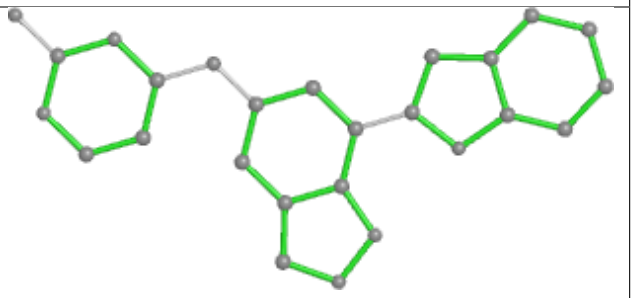
Bond lengths



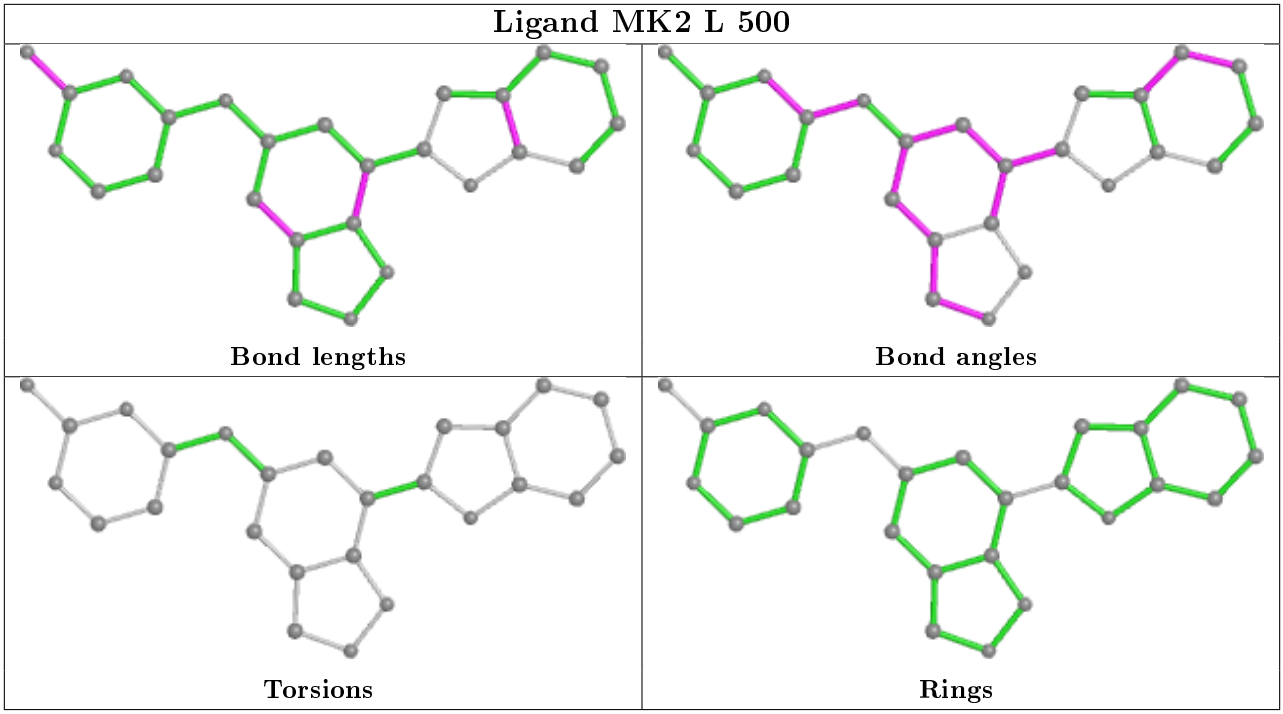
Bond angles

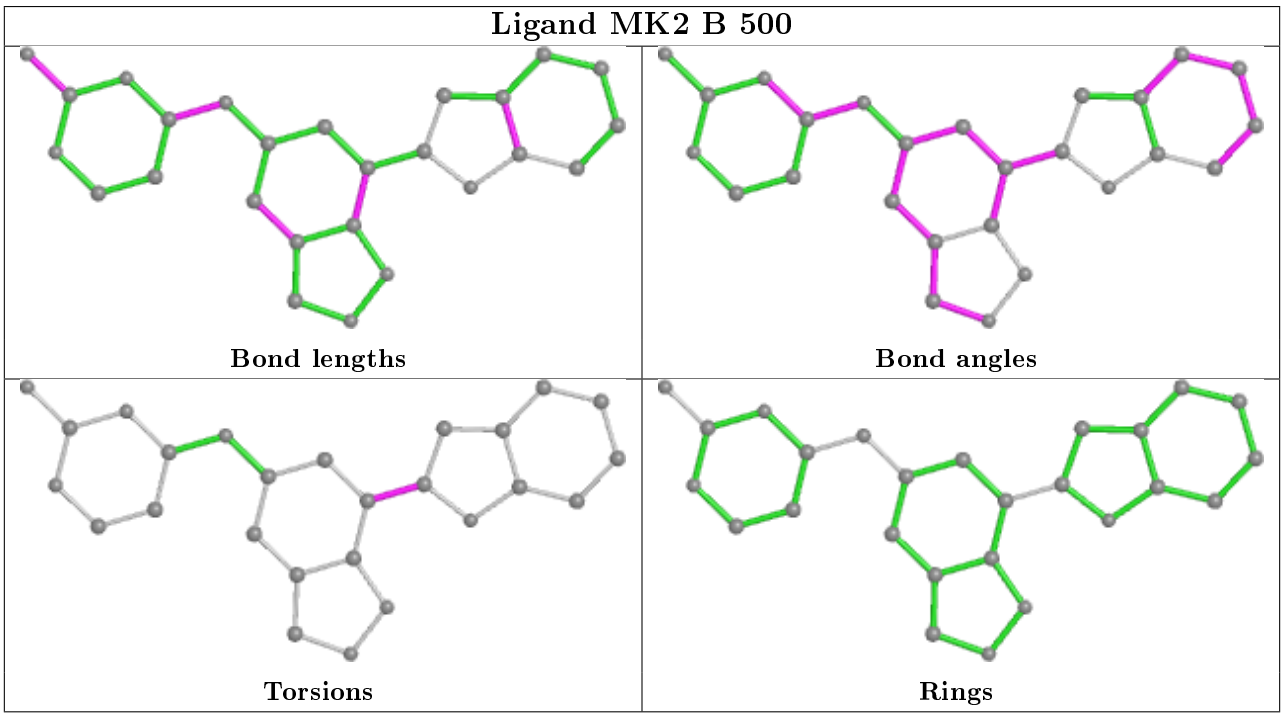


Torsions



Rings





5.7 Other polymers

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, 95^{th} 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	288/324 (88%)	0.15	9 (3%) 49 44	32, 48, 86, 115	0
1	B	290/324 (89%)	0.11	5 (1%) 70 69	33, 51, 85, 104	0
1	C	281/324 (86%)	0.31	20 (7%) 16 12	42, 62, 93, 121	0
1	D	269/324 (83%)	0.69	34 (12%) 3 3	48, 77, 108, 114	0
1	E	287/324 (88%)	0.16	8 (2%) 53 49	38, 52, 86, 100	0
1	F	293/324 (90%)	0.15	10 (3%) 45 40	36, 52, 88, 98	0
1	G	276/324 (85%)	0.77	43 (15%) 2 1	52, 87, 113, 122	0
1	H	290/324 (89%)	0.15	16 (5%) 25 21	36, 55, 92, 128	0
1	I	295/324 (91%)	0.25	15 (5%) 28 24	35, 59, 99, 121	0
1	J	288/324 (88%)	0.41	20 (6%) 16 13	44, 69, 98, 116	0
1	K	280/324 (86%)	0.87	48 (17%) 1 1	61, 85, 113, 121	0
1	L	291/324 (89%)	0.29	13 (4%) 33 29	43, 64, 99, 122	0
All	All	3428/3888 (88%)	0.35	241 (7%) 16 12	32, 63, 104, 128	0

All (241) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	74	ILE	10.7
1	C	75	ASN	7.2
1	J	217	HIS	7.0
1	A	74	ILE	6.8
1	K	294	VAL	6.7
1	I	65	VAL	6.4
1	A	75	ASN	6.3
1	I	74	ILE	6.2
1	G	150	ILE	6.0
1	G	43	PHE	6.0
1	E	75	ASN	6.0

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Mol	Chain	Res	Type	RSRZ
1	B	74	ILE	5.9
1	A	76	GLY	5.8
1	J	72	LEU	5.6
1	C	76	GLY	5.6
1	I	47	HIS	5.5
1	C	41	GLN	5.2
1	D	73	GLY	5.1
1	K	236	GLY	5.1
1	K	155	ASP	5.1
1	K	291	TRP	5.0
1	K	293	GLU	4.8
1	H	76	GLY	4.8
1	L	73	GLY	4.8
1	D	294	VAL	4.8
1	D	150	ILE	4.7
1	G	201	ALA	4.7
1	K	157	ALA	4.7
1	I	75	ASN	4.6
1	B	76	GLY	4.6
1	F	76	GLY	4.6
1	J	328	SER	4.6
1	C	289	PRO	4.5
1	J	43	PHE	4.4
1	I	89	LYS	4.3
1	A	73	GLY	4.2
1	D	340	ARG	4.2
1	G	333	GLN	4.2
1	G	291	TRP	4.2
1	K	230	VAL	4.2
1	G	44	PRO	4.2
1	G	76	GLY	4.2
1	J	73	GLY	4.2
1	K	154	GLY	4.1
1	J	46	PHE	4.1
1	G	45	GLN	4.1
1	K	340	ARG	4.0
1	C	73	GLY	4.0
1	J	157	ALA	4.0
1	D	237	PRO	3.9
1	B	75	ASN	3.9
1	G	289	PRO	3.9
1	J	158	PHE	3.9

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Mol	Chain	Res	Type	RSRZ
1	J	329	THR	3.9
1	K	332	PRO	3.9
1	K	289	PRO	3.9
1	L	74	ILE	3.8
1	G	329	THR	3.7
1	K	257	LEU	3.7
1	G	335	PRO	3.7
1	L	76	GLY	3.7
1	D	337	HIS	3.7
1	A	43	PHE	3.7
1	K	329	THR	3.5
1	K	75	ASN	3.5
1	K	85	ARG	3.5
1	G	264	TYR	3.5
1	L	66	THR	3.5
1	K	295	SER	3.5
1	G	257	LEU	3.5
1	D	333	GLN	3.5
1	C	43	PHE	3.4
1	I	69	VAL	3.4
1	G	297	GLU	3.4
1	G	240	TYR	3.4
1	K	45	GLN	3.4
1	K	231	ALA	3.4
1	L	77	LYS	3.3
1	H	349	TRP	3.3
1	C	74	ILE	3.3
1	D	162	GLU	3.3
1	B	72	LEU	3.3
1	D	75	ASN	3.3
1	G	141	LEU	3.3
1	K	240	TYR	3.3
1	K	337	HIS	3.3
1	G	266	ASN	3.3
1	C	44	PRO	3.2
1	G	152	ASP	3.2
1	G	74	ILE	3.2
1	K	343	LYS	3.2
1	K	234	VAL	3.2
1	K	44	PRO	3.2
1	K	76	GLY	3.2
1	I	73	GLY	3.1

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Mol	Chain	Res	Type	RSRZ
1	G	294	VAL	3.1
1	L	47	HIS	3.1
1	K	290	GLU	3.1
1	K	286	PHE	3.1
1	G	230	VAL	3.1
1	F	85	ARG	3.1
1	K	237	PRO	3.1
1	E	240	TYR	3.1
1	F	239	LYS	3.1
1	I	80	GLN	3.1
1	G	200	ASN	3.1
1	G	202	ILE	3.0
1	D	289	PRO	3.0
1	D	253	MET	3.0
1	J	74	ILE	3.0
1	G	332	PRO	3.0
1	G	66	THR	3.0
1	K	327	GLN	3.0
1	A	45	GLN	2.9
1	E	329	THR	2.9
1	K	239	LYS	2.9
1	J	76	GLY	2.9
1	A	46	PHE	2.9
1	I	45	GLN	2.9
1	G	328	SER	2.9
1	H	94	MET	2.9
1	D	46	PHE	2.9
1	G	192	LEU	2.9
1	K	72	LEU	2.9
1	D	297	GLU	2.8
1	F	75	ASN	2.8
1	B	46	PHE	2.8
1	D	260	TYR	2.8
1	K	274	GLY	2.8
1	D	342	LEU	2.8
1	C	344	GLU	2.8
1	D	339	SER	2.8
1	A	239	LYS	2.8
1	C	228	TYR	2.8
1	D	341	VAL	2.8
1	C	42	GLN	2.8
1	F	68	GLN	2.8

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Mol	Chain	Res	Type	RSRZ
1	G	263	PHE	2.8
1	L	43	PHE	2.8
1	K	162	GLU	2.8
1	C	345	ASP	2.8
1	H	45	GLN	2.8
1	I	76	GLY	2.7
1	K	215	THR	2.7
1	I	46	PHE	2.7
1	L	46	PHE	2.7
1	H	46	PHE	2.7
1	H	72	LEU	2.7
1	K	258	CYS	2.7
1	J	240	TYR	2.6
1	F	72	LEU	2.6
1	F	66	THR	2.6
1	K	339	SER	2.6
1	L	94	MET	2.6
1	D	152	ASP	2.6
1	L	42	GLN	2.5
1	D	147	PHE	2.5
1	J	64	LYS	2.5
1	K	82	PHE	2.5
1	D	257	LEU	2.5
1	G	331	VAL	2.5
1	G	46	PHE	2.5
1	E	76	GLY	2.5
1	K	342	LEU	2.5
1	H	47	HIS	2.5
1	G	340	ARG	2.5
1	K	296	GLU	2.5
1	I	351	ASP	2.5
1	J	80	GLN	2.5
1	I	229	TYR	2.5
1	C	334	THR	2.4
1	A	44	PRO	2.4
1	G	330	LYS	2.4
1	K	275	MET	2.4
1	F	227	PRO	2.4
1	D	252	ILE	2.4
1	K	235	LEU	2.4
1	C	158	PHE	2.4
1	D	144	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	K	214	THR	2.4
1	C	240	TYR	2.3
1	J	142	ASP	2.3
1	G	334	THR	2.3
1	H	77	LYS	2.3
1	K	341	VAL	2.3
1	G	336	LEU	2.3
1	K	46	PHE	2.3
1	K	333	GLN	2.3
1	G	265	SER	2.2
1	I	266	ASN	2.2
1	J	44	PRO	2.2
1	F	80	GLN	2.2
1	H	44	PRO	2.2
1	E	156	GLN	2.2
1	G	149	ARG	2.2
1	D	256	LEU	2.2
1	D	338	THR	2.2
1	E	157	ALA	2.2
1	C	275	MET	2.2
1	C	337	HIS	2.2
1	D	47	HIS	2.2
1	D	335	PRO	2.2
1	H	272	SER	2.2
1	D	298	VAL	2.2
1	H	156	GLN	2.1
1	G	239	LYS	2.1
1	F	74	ILE	2.1
1	G	290	GLU	2.1
1	J	75	ASN	2.1
1	H	64	LYS	2.1
1	H	66	THR	2.1
1	K	156	GLN	2.1
1	J	237	PRO	2.1
1	L	237	PRO	2.1
1	C	72	LEU	2.1
1	D	146	LEU	2.1
1	G	236	GLY	2.1
1	H	140	CYS	2.1
1	K	47	HIS	2.1
1	D	193	LEU	2.1
1	G	235	LEU	2.1

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Mol	Chain	Res	Type	RSRZ
1	J	239	LYS	2.1
1	L	346	LYS	2.1
1	I	94	MET	2.1
1	L	64	LYS	2.1
1	H	79	LEU	2.0
1	K	158	PHE	2.1
1	G	324	TRP	2.0
1	E	73	GLY	2.0
1	G	64	LYS	2.0
1	D	293	GLU	2.0
1	J	196	SER	2.0
1	K	282	GLY	2.0
1	C	341	VAL	2.0
1	C	237	PRO	2.0
1	E	46	PHE	2.0
1	D	258	CYS	2.0
1	D	330	LYS	2.0
1	D	166	ILE	2.0
1	G	146	LEU	2.0
1	H	87	GLN	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 carbohydrates 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, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MK2	K	500	26/26	0.89	0.30	89,100,111,111	0
2	MK2	J	500	26/26	0.92	0.28	76,83,95,96	0
2	MK2	I	500	26/26	0.93	0.29	73,75,79,80	0

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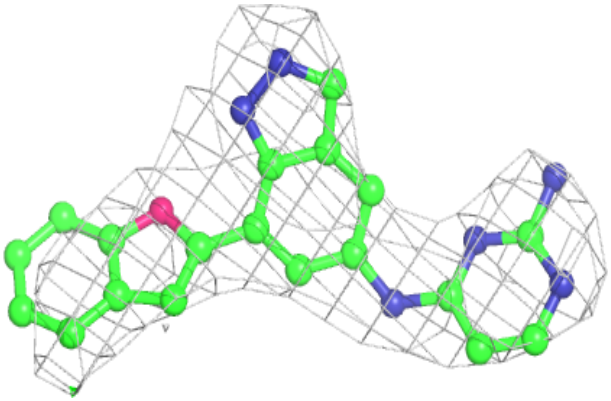
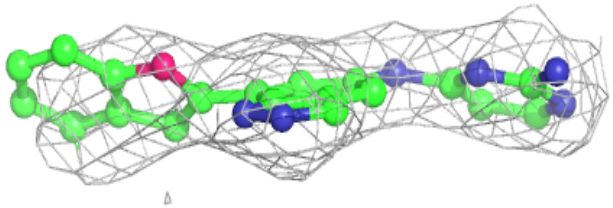
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	MK2	H	500	26/26	0.94	0.25	58,64,75,76	0
2	MK2	L	500	26/26	0.94	0.20	67,72,75,75	0
2	MK2	D	500	26/26	0.95	0.28	77,81,87,87	0
2	MK2	E	500	26/26	0.96	0.26	49,52,61,61	0
2	MK2	C	500	26/26	0.96	0.26	50,57,67,68	0
2	MK2	F	500	26/26	0.96	0.23	49,54,58,60	0
2	MK2	A	500	26/26	0.97	0.18	32,46,56,58	0
2	MK2	B	500	26/26	0.98	0.15	47,51,58,58	0

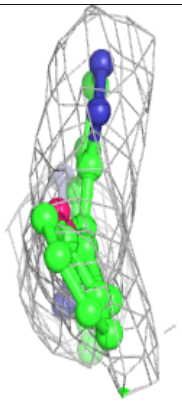
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around MK2 K 500:

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

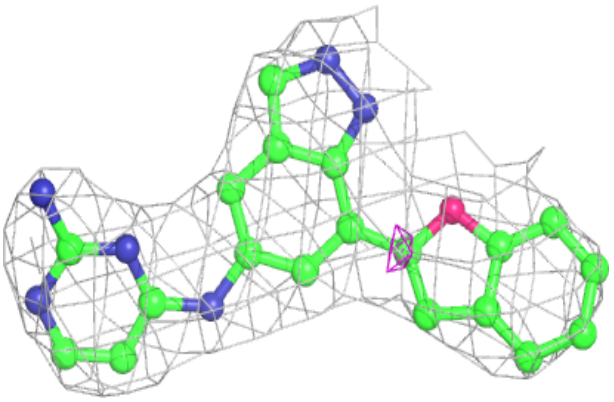


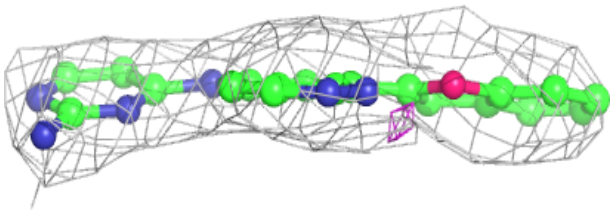


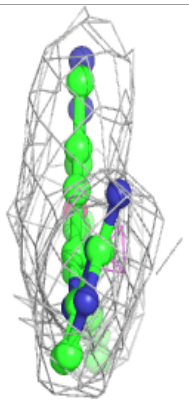


Electron density around MK2 J 500:

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

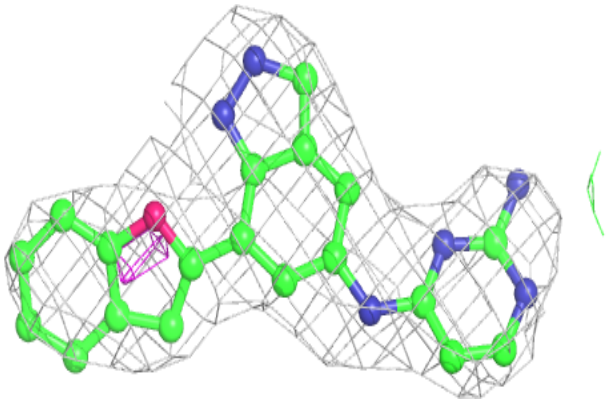


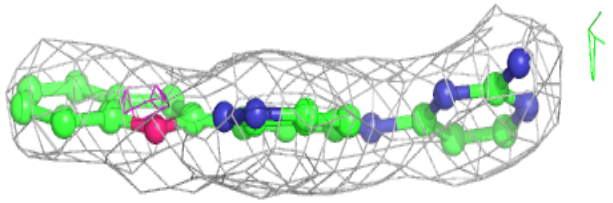


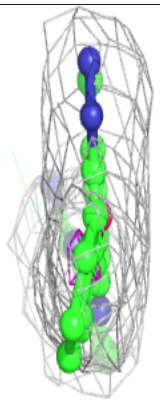


Electron density around MK2 I 500:

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

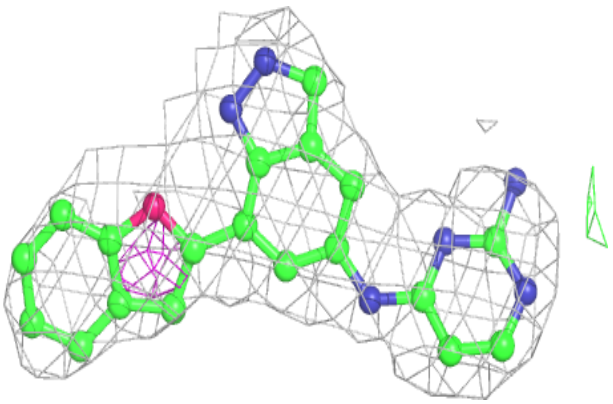


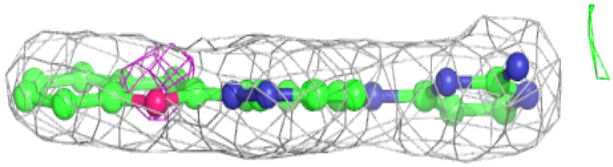


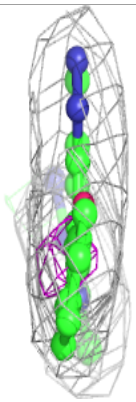


Electron density around MK2 H 500:

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

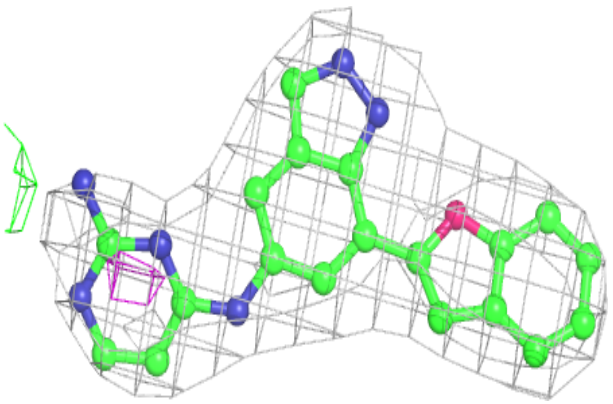


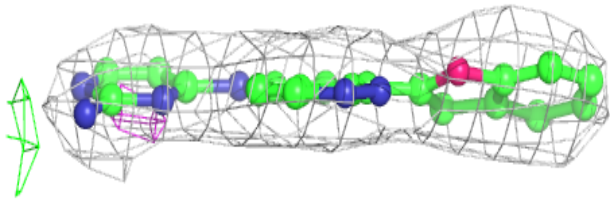


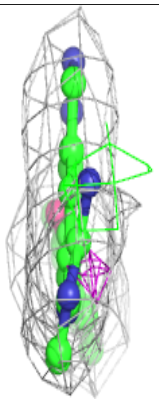


Electron density around MK2 L 500:

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

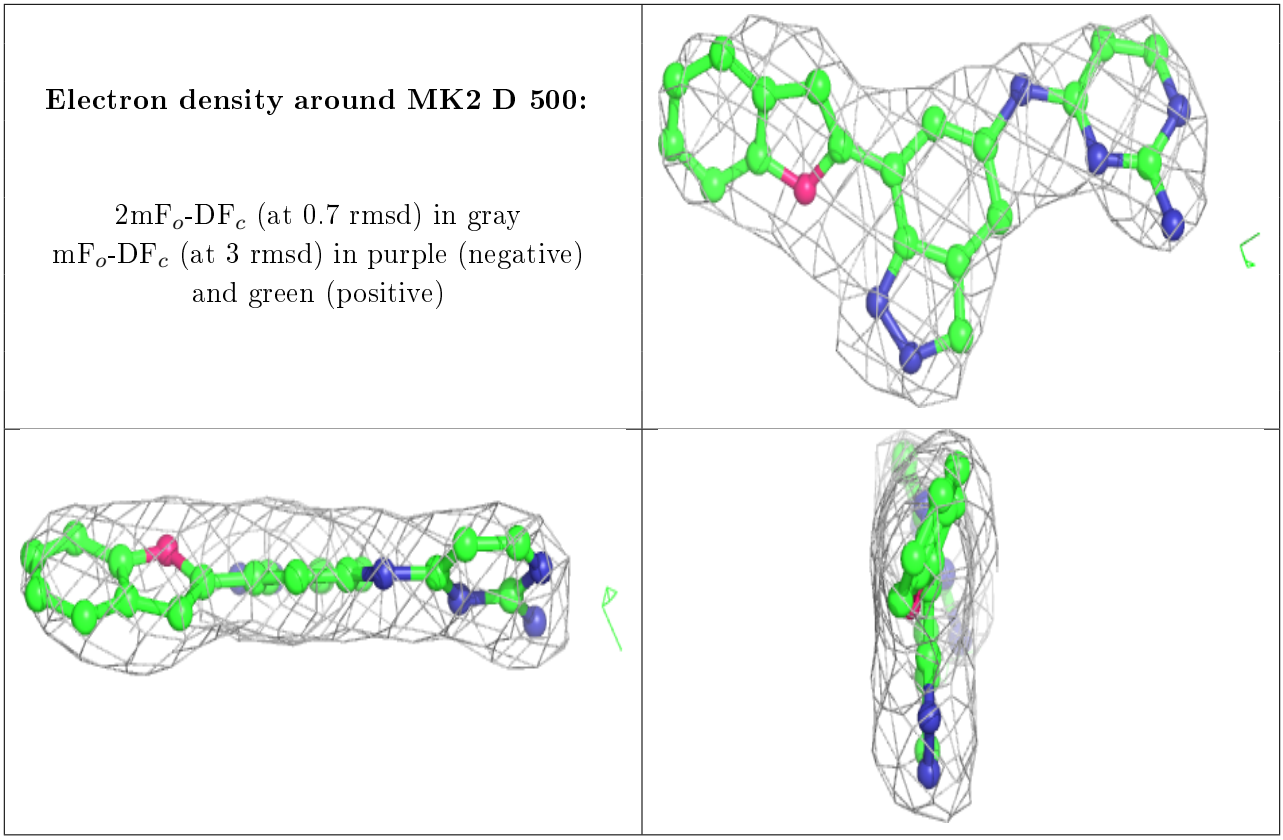






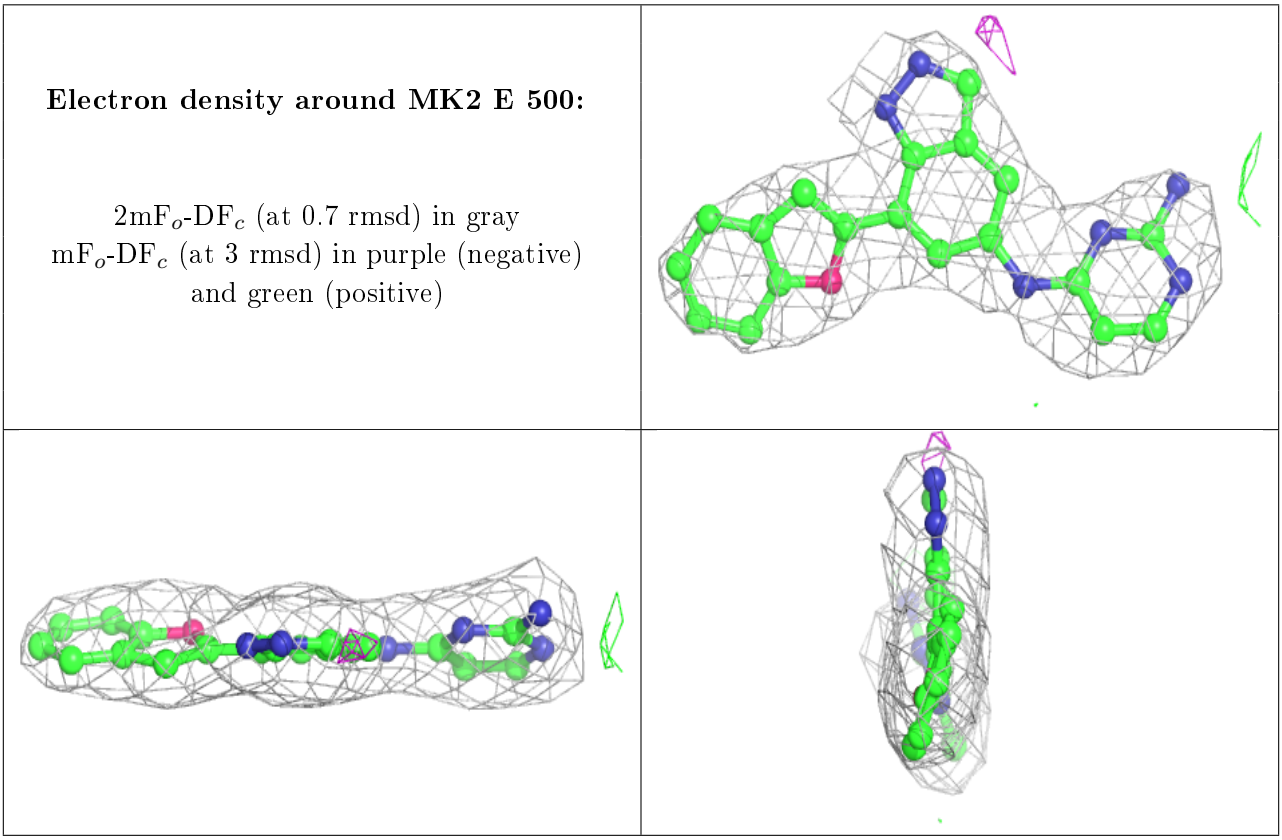
Electron density around MK2 D 500:

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



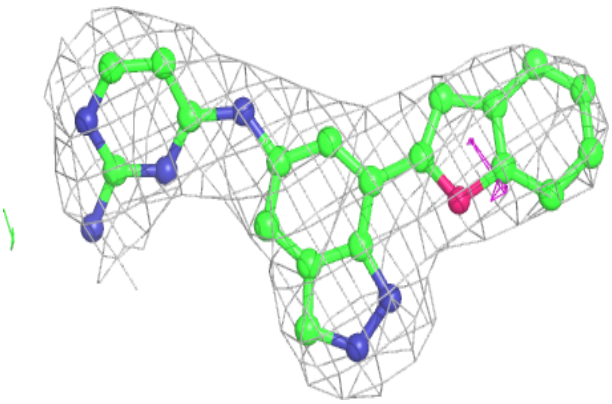
Electron density around MK2 E 500:

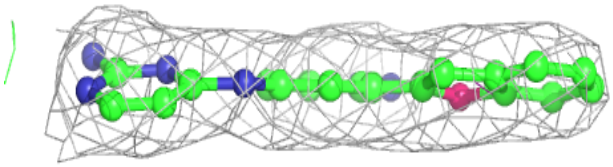
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

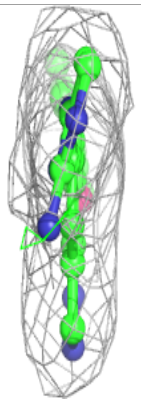


Electron density around MK2 C 500:

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

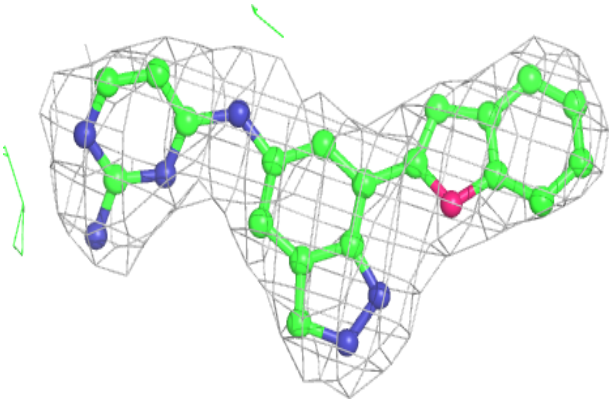


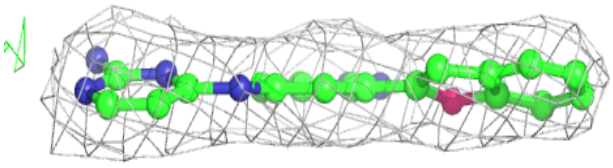


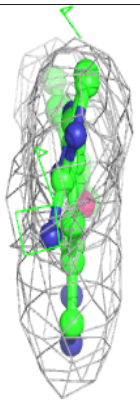


Electron density around MK2 F 500:

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

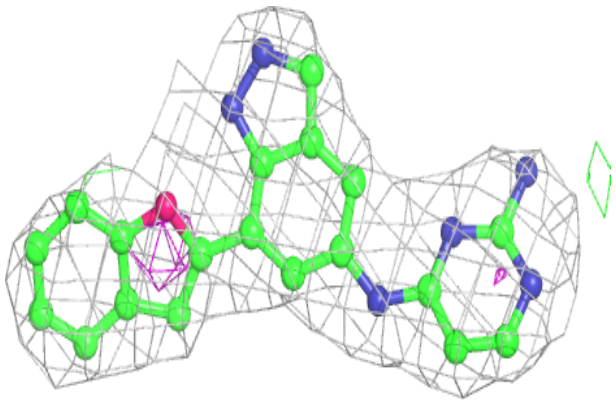


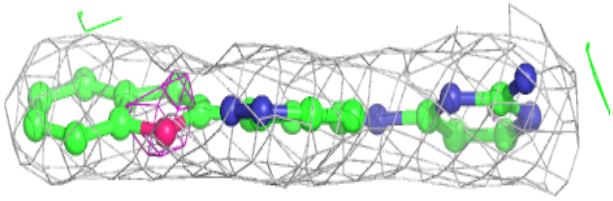


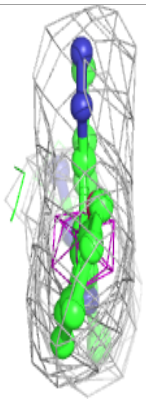


Electron density around MK2 A 500:

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

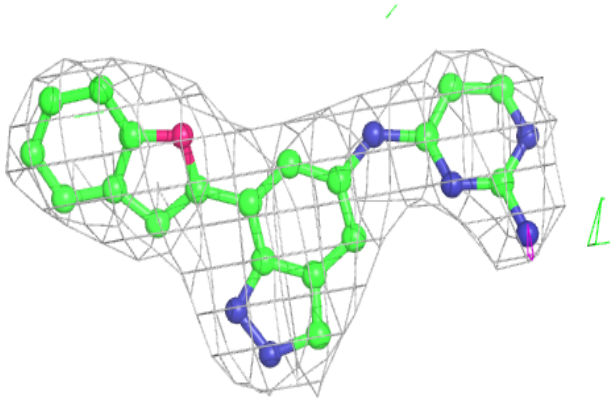


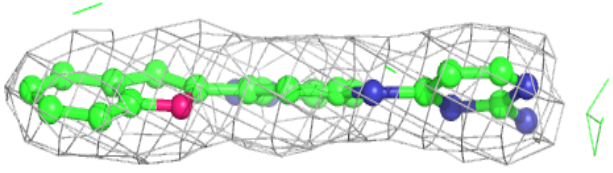


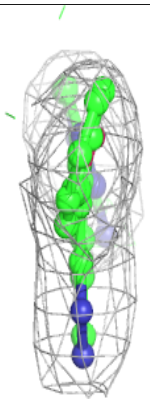


Electron density around MK2 B 500:

$2mF_o$-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.