



# Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 03:18 AM UTC

PDB ID : 9M1Z / pdb\_00009m1z  
Title : Crystal Structure of MAP2K6 complexed with 5Z-7-oxozeaenol  
Authors : Yumura, S.; Kinoshita, T.  
Deposited on : 2025-02-26  
Resolution : 3.00 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

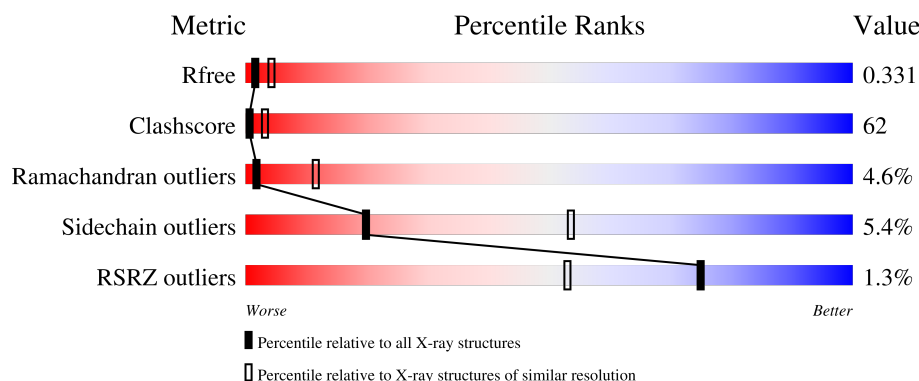
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	340	
1	B	340	
1	C	340	
1	D	340	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	1FM	D	401	-	X	-	-

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9384 atoms, of which 88 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 Dual specificity mitogen-activated protein kinase kinase 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	D	289	Total	C	N	O	S	0	0	0
			2282	1459	381	425	17			
1	A	288	Total	C	N	O	S	0	0	0
			2275	1455	380	423	17			
1	B	287	Total	C	N	O	S	0	0	0
			2267	1451	379	420	17			
1	C	289	Total	C	N	O	S	0	0	0
			2287	1464	381	425	17			

There are 24 discrepancies between the modelled and reference sequences:

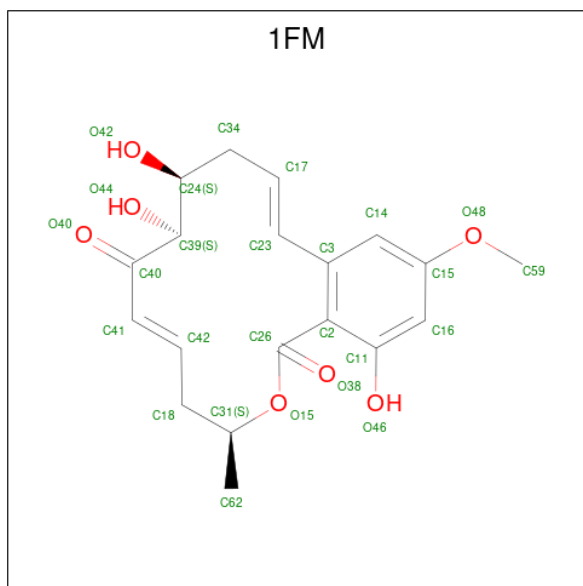
Chain	Residue	Modelled	Actual	Comment	Reference
D	335	HIS	-	expression tag	UNP P52564
D	336	HIS	-	expression tag	UNP P52564
D	337	HIS	-	expression tag	UNP P52564
D	338	HIS	-	expression tag	UNP P52564
D	339	HIS	-	expression tag	UNP P52564
D	340	HIS	-	expression tag	UNP P52564
A	335	HIS	-	expression tag	UNP P52564
A	336	HIS	-	expression tag	UNP P52564
A	337	HIS	-	expression tag	UNP P52564
A	338	HIS	-	expression tag	UNP P52564
A	339	HIS	-	expression tag	UNP P52564
A	340	HIS	-	expression tag	UNP P52564
B	335	HIS	-	expression tag	UNP P52564
B	336	HIS	-	expression tag	UNP P52564
B	337	HIS	-	expression tag	UNP P52564
B	338	HIS	-	expression tag	UNP P52564
B	339	HIS	-	expression tag	UNP P52564
B	340	HIS	-	expression tag	UNP P52564
C	335	HIS	-	expression tag	UNP P52564
C	336	HIS	-	expression tag	UNP P52564
C	337	HIS	-	expression tag	UNP P52564

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Chain	Residue	Modelled	Actual	Comment	Reference
C	338	HIS	-	expression tag	UNP P52564
C	339	HIS	-	expression tag	UNP P52564
C	340	HIS	-	expression tag	UNP P52564

- Molecule 2 is (3S,5Z,8S,9S,11E)-8,9,16-trihydroxy-14-methoxy-3-methyl-3,4,9,10-tetrahydro-1H-2-benzoxacyclotetradecine-1,7(8H)-dione (CCD ID: 1FM) (formula: C<sub>19</sub>H<sub>22</sub>O<sub>7</sub>) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	D	1	Total	C	H	O	0	0
			48	19	22	7		
2	A	1	Total	C	H	O	0	0
			48	19	22	7		
2	B	1	Total	C	H	O	0	0
			48	19	22	7		
2	C	1	Total	C	H	O	0	0
			48	19	22	7		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	31	Total	O	0	0
			31	31		
3	A	29	Total	O	0	0
			29	29		
3	B	8	Total	O	0	0
			8	8		

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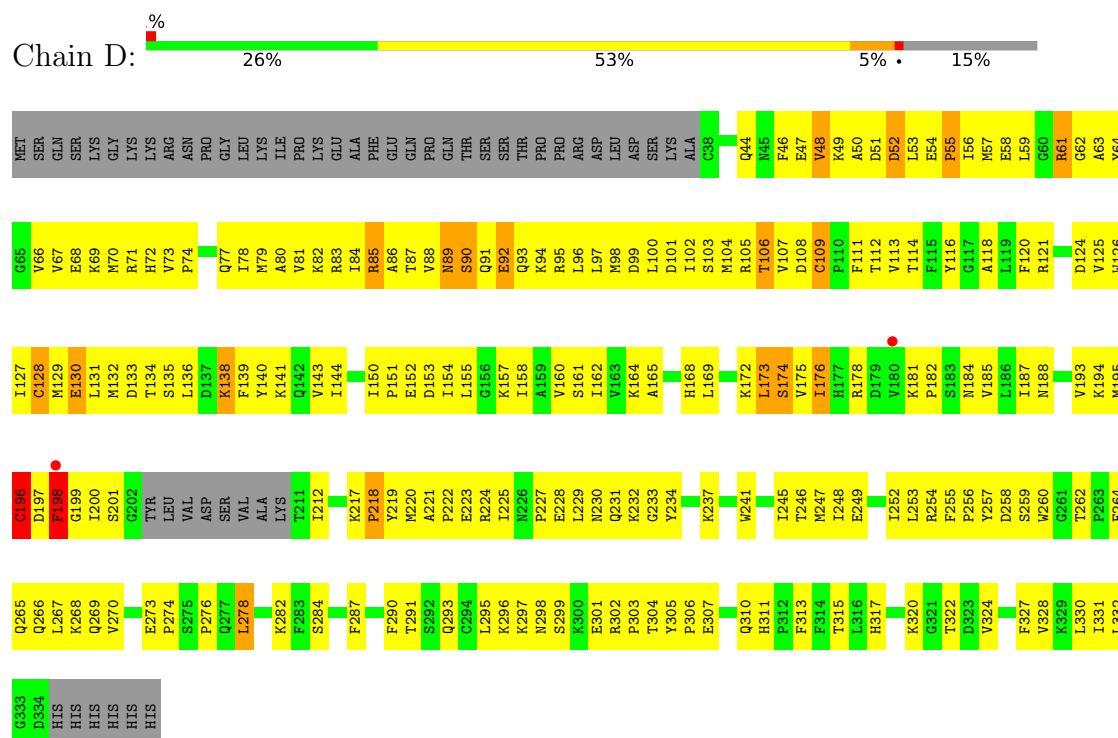
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	13	Total	O	0	0
			13	13		

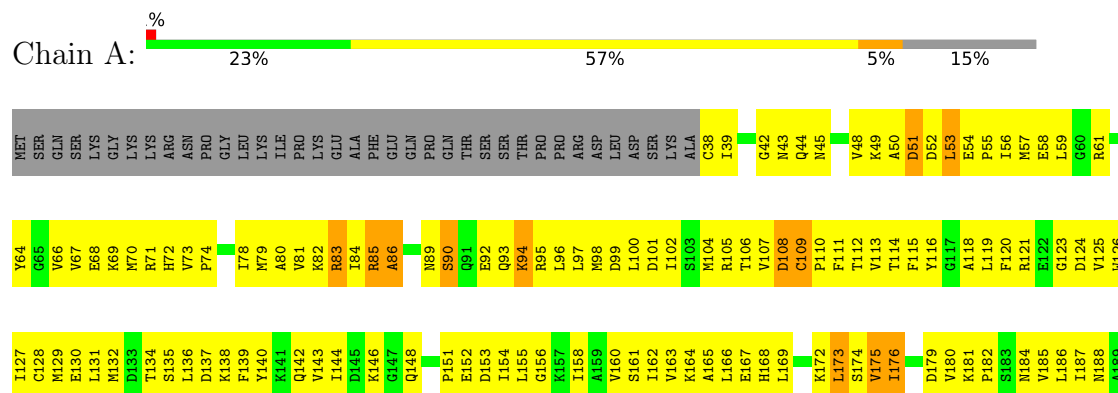
### 3 Residue-property plots

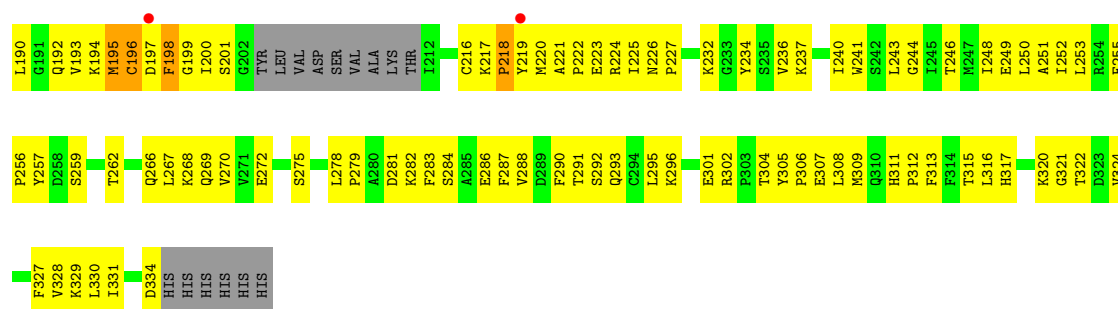
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

- Molecule 1: Dual specificity mitogen-activated protein kinase kinase 6

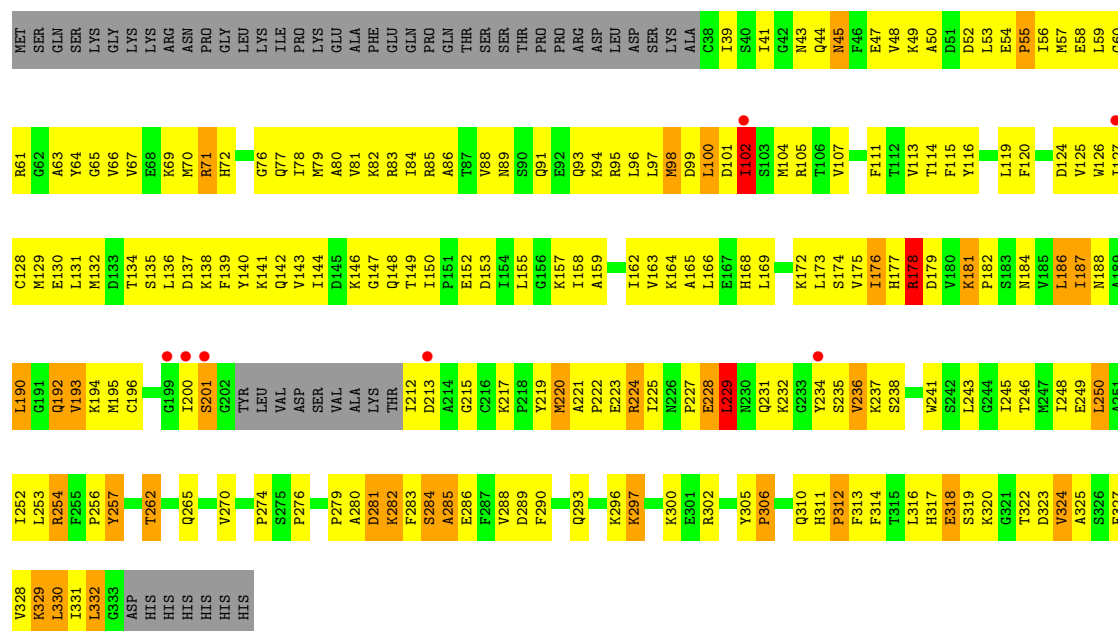


- Molecule 1: Dual specificity mitogen-activated protein kinase kinase 6

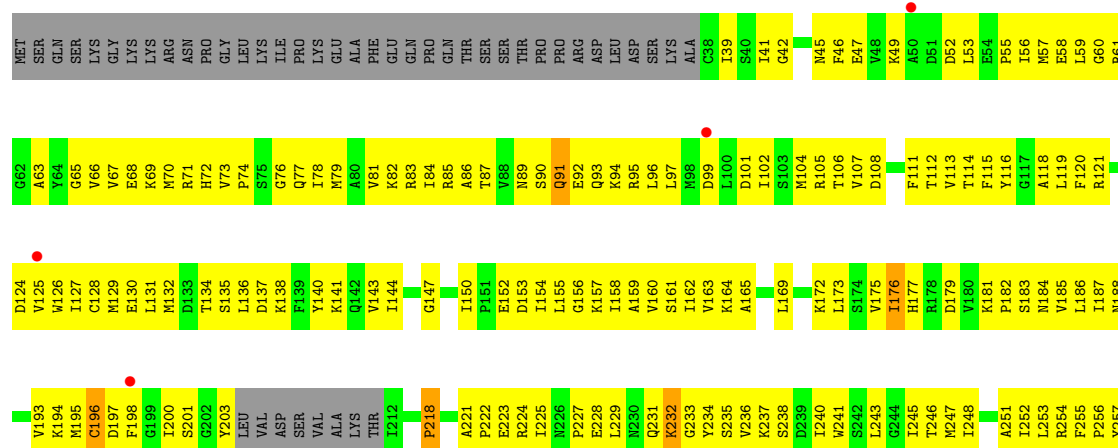
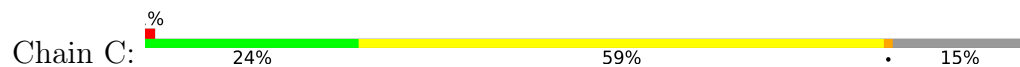




- Molecule 1: Dual specificity mitogen-activated protein kinase kinase 6



- Molecule 1: Dual specificity mitogen-activated protein kinase kinase 6







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.35Å 120.16Å 106.32Å 90.00° 101.01° 90.00°	Depositor
Resolution (Å)	47.86 – 3.00 47.86 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.8 (47.86-3.00) 91.8 (47.86-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.04 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.274 , 0.332 0.283 , 0.331	Depositor DCC
$R_{free}$ test set	1715 reflections (4.83%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	98.5	Xtriage
Anisotropy	0.489	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 122.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.44$ , $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9384	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	119.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.08% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 1FM

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.25	0/2322	0.45	0/3135
1	B	0.70	0/2314	0.96	4/3124 (0.1%)
1	C	0.24	0/2335	0.44	1/3153 (0.0%)
1	D	0.33	0/2329	0.50	1/3145 (0.0%)
All	All	0.42	0/9300	0.62	6/12557 (0.0%)

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	3
All	All	0	4

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	63	ALA	CB-CA-C	-8.60	106.66	116.63
1	D	198	PHE	CA-CB-CG	8.21	122.01	113.80
1	B	219	TYR	N-CA-C	-6.51	105.30	112.72
1	B	257	TYR	N-CA-CB	-5.96	101.22	110.46
1	B	283	PHE	CB-CA-C	5.21	120.80	110.42
1	B	310	GLN	N-CA-C	-5.12	106.44	113.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	83	ARG	Sidechain
1	B	178	ARG	Sidechain
1	B	224	ARG	Sidechain
1	B	71	ARG	Sidechain

## 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	2275	0	2296	306	1
1	B	2267	0	2292	228	0
1	C	2287	0	2304	330	1
1	D	2282	0	2302	289	0
2	A	26	22	22	6	0
2	B	26	22	21	6	0
2	C	26	22	21	6	0
2	D	26	22	20	2	0
3	A	29	0	0	6	0
3	B	8	0	0	0	0
3	C	13	0	0	2	0
3	D	31	0	0	4	0
All	All	9296	88	9278	1146	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 62.

All (1146) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:LYS:HE3	1:A:84:ILE:HD11	1.23	1.14
1:A:96:LEU:HA	1:A:100:LEU:HB2	1.29	1.12
1:C:169:LEU:HG	1:C:176:ILE:HD13	1.14	1.12
1:D:229:LEU:HD23	1:C:297:LYS:HG3	1.10	1.09
1:C:224:ARG:HD2	1:C:238:SER:HB2	1.27	1.08
1:A:83:ARG:HG2	1:A:124:ASP:HB2	1.33	1.08
1:C:132:MET:HB2	1:C:186:LEU:HD23	1.30	1.07
1:C:162:ILE:HG21	1:C:243:LEU:HD13	1.36	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:155:LEU:HA	1:D:158:ILE:HD12	1.37	1.04
1:A:180:VAL:HG22	1:A:195:MET:HE1	1.35	1.03
1:C:58:GLU:HG3	1:C:61:ARG:HB3	1.39	1.01
1:C:252:ILE:HD12	1:C:254:ARG:HG3	1.43	1.00
1:A:304:THR:HG22	1:A:307:GLU:HB2	1.41	0.99
1:C:181:LYS:HE3	1:C:183:SER:HB2	1.44	0.99
1:C:86:ALA:HB3	1:C:124:ASP:HA	1.44	0.99
1:C:93:GLN:O	1:C:95:ARG:NH2	1.96	0.98
1:B:55:PRO:HB3	1:B:70:MET:HB3	1.47	0.97
1:C:55:PRO:HA	1:C:70:MET:HB3	1.47	0.96
1:A:69:LYS:HG2	1:A:131:LEU:HD11	1.50	0.93
1:D:140:TYR:HE1	1:D:253:LEU:HA	1.35	0.92
1:C:152:GLU:HA	1:C:155:LEU:HD12	1.51	0.92
1:A:113:VAL:HG12	1:A:196:CYS:HA	1.52	0.92
1:C:221:ALA:H	1:C:224:ARG:HD3	1.35	0.91
1:A:84:ILE:H	1:A:125:VAL:HG12	1.33	0.91
1:C:59:LEU:HD21	1:C:69:LYS:HG2	1.50	0.91
1:C:73:VAL:HG23	1:C:74:PRO:HD3	1.53	0.90
1:D:114:THR:H	1:D:130:GLU:HG2	1.36	0.90
1:A:296:LYS:HE3	1:A:301:GLU:HB3	1.54	0.90
1:D:157:LYS:HZ1	1:D:320:LYS:HE3	1.36	0.89
1:A:51:ASP:HA	1:A:121:ARG:NH2	1.86	0.89
1:A:140:TYR:HE1	1:A:253:LEU:HA	1.35	0.89
1:D:229:LEU:CD2	1:C:297:LYS:HG3	2.01	0.89
1:B:95:ARG:NH1	1:B:120:PHE:HB2	1.88	0.88
1:B:66:VAL:CG1	1:B:83:ARG:HB3	2.03	0.88
1:C:58:GLU:OE2	1:C:61:ARG:HD2	1.72	0.88
1:C:179:ASP:OD1	1:C:224:ARG:NH2	2.06	0.88
1:D:49:LYS:HE3	1:D:49:LYS:HA	1.54	0.88
1:D:93:GLN:HG2	1:D:94:LYS:HG3	1.55	0.88
1:A:93:GLN:HE22	1:A:97:LEU:HB3	1.37	0.88
1:A:188:ASN:HD21	1:A:190:LEU:HB2	1.39	0.88
1:D:157:LYS:NZ	1:D:320:LYS:HE3	1.88	0.88
1:A:55:PRO:HA	1:A:70:MET:HB3	1.55	0.88
1:C:173:LEU:HD23	1:C:173:LEU:H	1.38	0.88
1:C:102:ILE:HG23	1:C:175:VAL:HG12	1.56	0.87
1:C:152:GLU:OE2	1:C:284:SER:OG	1.92	0.87
1:A:268:LYS:HG3	1:A:272:GLU:OE1	1.74	0.87
1:C:172:LYS:HG3	1:C:173:LEU:HD23	1.56	0.87
1:A:287:PHE:O	1:A:291:THR:HG23	1.75	0.86
1:C:90:SER:O	1:C:95:ARG:NH2	2.08	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:96:LEU:HD13	1:D:100:LEU:HB3	1.58	0.85
1:A:69:LYS:CG	1:A:131:LEU:HD11	2.06	0.85
1:B:172:LYS:HE3	1:B:172:LYS:HA	1.58	0.85
1:C:132:MET:CB	1:C:186:LEU:HD23	2.06	0.85
1:A:50:ALA:HB1	1:A:119:LEU:HD22	1.59	0.85
1:D:61:ARG:HH21	1:D:63:ALA:HA	1.38	0.85
1:C:90:SER:HB3	1:C:95:ARG:NH1	1.92	0.84
1:C:42:GLY:O	1:C:45:ASN:ND2	2.09	0.84
1:A:93:GLN:NE2	1:A:97:LEU:HB3	1.93	0.84
1:A:101:ASP:O	1:A:105:ARG:HG2	1.77	0.84
1:B:119:LEU:HG	1:B:126:TRP:HB2	1.59	0.83
1:C:105:ARG:CB	1:C:173:LEU:HD21	2.09	0.83
1:D:198:PHE:HD1	1:D:199:GLY:H	1.27	0.82
1:A:330:LEU:HD12	1:A:331:ILE:HD13	1.62	0.82
1:C:181:LYS:HG3	1:C:184:ASN:H	1.44	0.82
1:D:154:ILE:HG13	1:D:324:VAL:HG22	1.61	0.82
1:C:223:GLU:OE1	1:C:302:ARG:NH2	2.12	0.82
1:D:71:ARG:HH12	1:D:73:VAL:HG22	1.45	0.82
1:B:173:LEU:HG	1:B:175:VAL:H	1.44	0.81
1:A:146:LYS:HE3	1:A:334:ASP:HB3	1.62	0.81
1:B:173:LEU:HD12	1:B:175:VAL:HB	1.60	0.81
1:C:317:HIS:HA	1:C:320:LYS:HZ2	1.45	0.81
1:A:96:LEU:HA	1:A:100:LEU:CB	2.11	0.81
1:B:44:GLN:HE22	1:B:116:TYR:HA	1.45	0.81
1:D:132:MET:HE3	1:D:188:ASN:HB3	1.61	0.81
1:C:39:ILE:HD13	1:C:41:ILE:HG12	1.62	0.81
1:C:172:LYS:HG3	1:C:173:LEU:CD2	2.11	0.81
1:B:55:PRO:HA	1:B:70:MET:HA	1.62	0.80
1:B:93:GLN:HG2	1:B:94:LYS:HG3	1.61	0.80
1:C:105:ARG:HB3	1:C:173:LEU:HD21	1.62	0.80
1:D:94:LYS:HE2	1:D:97:LEU:HD13	1.62	0.80
1:C:104:MET:HE3	1:C:104:MET:HA	1.61	0.80
1:C:322:THR:OG1	1:C:324:VAL:HG23	1.82	0.80
1:C:90:SER:HB3	1:C:95:ARG:HH12	1.44	0.80
1:C:105:ARG:CG	1:C:173:LEU:HD21	2.12	0.80
1:A:92:GLU:O	1:A:95:ARG:NH2	2.15	0.80
1:C:278:LEU:HD22	1:C:291:THR:HG21	1.63	0.80
1:C:304:THR:HG23	1:C:306:PRO:HD2	1.64	0.80
1:D:96:LEU:HD11	1:D:104:MET:SD	2.21	0.79
1:A:67:VAL:HB	1:A:82:LYS:HB2	1.64	0.79
1:B:81:VAL:HA	1:B:127:ILE:O	1.82	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:84:ILE:O	1:C:124:ASP:HB2	1.82	0.79
1:C:157:LYS:HZ1	1:C:320:LYS:HG2	1.45	0.79
1:B:142:GLN:O	1:B:146:LYS:HG2	1.83	0.79
1:A:82:LYS:CE	1:A:84:ILE:HD11	2.10	0.79
1:C:317:HIS:HA	1:C:320:LYS:NZ	1.97	0.79
1:C:312:PRO:O	1:C:316:LEU:HD12	1.82	0.79
1:D:229:LEU:HD13	1:D:230:ASN:N	1.98	0.79
1:C:140:TYR:HE1	1:C:253:LEU:HA	1.45	0.79
1:C:143:VAL:HG11	1:C:150:ILE:HD11	1.64	0.78
1:C:105:ARG:HA	1:C:172:LYS:HE3	1.64	0.78
1:B:94:LYS:O	1:B:97:LEU:HG	1.83	0.78
1:C:228:GLU:O	1:C:229:LEU:HD22	1.84	0.78
1:D:229:LEU:HD23	1:C:297:LYS:CG	2.03	0.78
1:A:58:GLU:HA	1:A:68:GLU:HA	1.65	0.78
1:B:67:VAL:HG22	1:B:82:LYS:CD	2.12	0.78
1:A:119:LEU:HD12	1:A:120:PHE:H	1.46	0.78
1:C:254:ARG:HD3	3:C:504:HOH:O	1.83	0.78
1:B:61:ARG:HH11	1:B:63:ALA:HB3	1.47	0.78
1:A:70:MET:HE3	1:A:81:VAL:HB	1.64	0.77
1:A:100:LEU:O	1:A:104:MET:HG3	1.82	0.77
1:C:143:VAL:HG12	1:C:331:ILE:HD12	1.66	0.77
1:A:59:LEU:HD23	1:A:69:LYS:HG3	1.67	0.77
1:A:67:VAL:HA	1:A:82:LYS:HA	1.67	0.77
1:A:223:GLU:OE1	1:A:302:ARG:NH2	2.17	0.77
1:A:70:MET:HE1	1:A:126:TRP:CZ3	2.20	0.77
1:B:60:GLY:HA3	1:B:67:VAL:H	1.50	0.77
1:C:231:GLN:O	1:C:232:LYS:HB2	1.83	0.76
1:B:69:LYS:HG3	1:B:131:LEU:CD1	2.16	0.76
1:C:101:ASP:O	1:C:105:ARG:HG2	1.85	0.76
1:D:98:MET:O	1:D:201:SER:HB3	1.85	0.76
1:D:224:ARG:HD3	1:D:234:TYR:CE1	2.20	0.76
1:C:95:ARG:HB2	1:C:96:LEU:HG	1.67	0.76
1:A:83:ARG:HH12	1:A:85:ARG:HG2	1.51	0.76
1:A:248:ILE:HG12	1:A:278:LEU:HG	1.67	0.76
1:A:82:LYS:HE3	1:A:84:ILE:CD1	2.12	0.76
1:A:139:PHE:O	1:A:143:VAL:HG23	1.85	0.76
1:D:311:HIS:O	1:D:315:THR:HG23	1.84	0.76
1:C:159:ALA:HB2	1:C:247:MET:HE2	1.68	0.76
1:D:80:ALA:HB2	1:D:131:LEU:CD2	2.16	0.75
1:A:70:MET:HE1	1:A:126:TRP:HZ3	1.51	0.75
1:A:244:GLY:HA3	1:A:295:LEU:HD21	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:GLU:OE2	1:A:284:SER:N	2.20	0.75
1:D:61:ARG:NH2	1:D:63:ALA:HA	2.02	0.74
1:A:311:HIS:O	1:A:315:THR:HG23	1.87	0.74
1:B:66:VAL:HG13	1:B:83:ARG:HB3	1.69	0.74
1:D:82:LYS:HD3	1:D:198:PHE:HE2	1.51	0.74
1:B:83:ARG:HD3	1:B:124:ASP:OD2	1.88	0.74
1:B:107:VAL:HB	1:B:168:HIS:NE2	2.03	0.74
1:D:132:MET:CE	1:D:188:ASN:HB3	2.18	0.73
1:A:83:ARG:HA	1:A:125:VAL:O	1.88	0.73
1:A:259:SER:HB3	1:A:266:GLN:HE21	1.51	0.73
1:D:79:MET:HE2	1:D:128:CYS:HB3	1.69	0.73
1:D:218:PRO:HA	1:D:220:MET:CE	2.17	0.73
1:A:93:GLN:O	1:A:95:ARG:NE	2.14	0.73
1:A:180:VAL:CG2	1:A:195:MET:HE1	2.17	0.73
1:A:259:SER:HB3	1:A:266:GLN:NE2	2.04	0.73
1:A:237:LYS:HA	1:A:240:ILE:HD12	1.69	0.73
1:C:236:VAL:HG13	1:C:305:TYR:CE2	2.22	0.73
1:A:107:VAL:HG13	1:A:108:ASP:OD1	1.88	0.73
1:A:113:VAL:HG23	1:A:130:GLU:HG3	1.71	0.73
1:D:80:ALA:HB2	1:D:131:LEU:HD21	1.71	0.73
1:D:305:TYR:HB2	1:D:306:PRO:HD3	1.70	0.73
1:A:50:ALA:CB	1:A:119:LEU:HD22	2.19	0.73
1:D:181:LYS:HG2	1:D:219:TYR:CG	2.24	0.72
1:A:255:PHE:CE1	1:A:257:TYR:HB2	2.24	0.72
1:B:132:MET:HG3	1:B:186:LEU:HB3	1.71	0.72
1:C:73:VAL:CG2	1:C:74:PRO:HD3	2.19	0.72
1:D:85:ARG:HG3	1:D:85:ARG:HH11	1.53	0.72
1:D:225:ILE:O	1:D:227:PRO:HD3	1.90	0.72
1:C:292:SER:O	1:C:296:LYS:HG2	1.89	0.72
1:D:96:LEU:HD12	1:D:96:LEU:O	1.88	0.72
1:A:113:VAL:HG23	1:A:130:GLU:CG	2.19	0.72
1:D:299:SER:HA	1:D:302:ARG:NH1	2.04	0.72
1:A:176:ILE:HG23	1:A:199:GLY:CA	2.20	0.72
1:C:135:SER:HB3	1:C:138:LYS:HG2	1.70	0.72
1:D:61:ARG:O	1:D:66:VAL:HA	1.90	0.72
1:C:143:VAL:HG12	1:C:331:ILE:CD1	2.20	0.72
1:C:86:ALA:HB2	1:C:125:VAL:HG23	1.71	0.71
1:D:71:ARG:CB	1:D:78:ILE:HA	2.20	0.71
1:D:218:PRO:HA	1:D:220:MET:HE3	1.72	0.71
1:A:281:ASP:HB3	1:B:93:GLN:NE2	2.04	0.71
1:D:108:ASP:O	1:D:112:THR:OG1	2.08	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:71:ARG:HH22	1:B:76:GLY:HA2	1.55	0.71
1:D:218:PRO:HB3	1:D:267:LEU:CD2	2.21	0.71
1:A:72:HIS:CD2	1:A:74:PRO:HD2	2.24	0.71
1:D:255:PHE:HE1	1:D:257:TYR:HB2	1.55	0.71
1:D:94:LYS:CE	1:D:97:LEU:HD13	2.20	0.71
1:D:231:GLN:HG3	1:D:232:LYS:N	2.05	0.71
1:D:138:LYS:HE3	3:D:504:HOH:O	1.90	0.71
1:C:67:VAL:HG12	1:C:82:LYS:HB2	1.73	0.71
1:C:79:MET:SD	1:C:128:CYS:HB3	2.31	0.70
1:D:161:SER:HB2	1:D:193:VAL:HG23	1.73	0.70
1:A:130:GLU:HG3	1:A:132:MET:HE3	1.72	0.70
1:B:67:VAL:HG22	1:B:82:LYS:HD2	1.73	0.70
1:C:105:ARG:HB3	1:C:173:LEU:CD2	2.21	0.70
1:C:173:LEU:HD23	1:C:173:LEU:N	2.07	0.70
1:C:248:ILE:HG12	1:C:278:LEU:CD1	2.22	0.70
1:B:55:PRO:CB	1:B:70:MET:HB3	2.21	0.70
1:B:142:GLN:HG3	1:B:146:LYS:HE3	1.74	0.70
1:C:177:HIS:NE2	1:C:179:ASP:HB2	2.07	0.70
1:C:252:ILE:CD1	1:C:254:ARG:HG3	2.22	0.70
1:C:182:PRO:HG3	1:C:246:THR:HG23	1.72	0.70
1:A:96:LEU:HD12	1:A:96:LEU:H	1.56	0.69
1:A:221:ALA:HA	1:A:241:TRP:CD1	2.27	0.69
1:D:118:ALA:HA	1:D:126:TRP:O	1.92	0.69
1:C:298:ASN:HB3	1:C:301:GLU:HG3	1.73	0.69
1:C:175:VAL:HG23	1:C:176:ILE:HD12	1.75	0.69
1:A:151:PRO:HD3	1:A:327:PHE:CZ	2.27	0.69
1:D:58:GLU:HB3	1:D:68:GLU:CD	2.18	0.69
1:D:327:PHE:HA	1:D:330:LEU:CD2	2.22	0.69
1:C:84:ILE:HB	1:C:125:VAL:HB	1.74	0.69
1:B:153:ASP:HB3	1:B:322:THR:HG22	1.75	0.69
1:B:181:LYS:HG3	1:B:184:ASN:HB2	1.74	0.69
1:C:234:TYR:CD2	1:C:236:VAL:HB	2.28	0.69
1:C:329:LYS:HE2	1:C:329:LYS:HA	1.75	0.69
1:A:185:VAL:O	1:A:186:LEU:HD23	1.93	0.68
1:C:53:LEU:HG	1:C:72:HIS:CA	2.22	0.68
1:A:96:LEU:CA	1:A:100:LEU:HB2	2.18	0.68
1:B:50:ALA:O	1:B:53:LEU:HG	1.91	0.68
1:C:94:LYS:HD2	1:C:97:LEU:CD1	2.24	0.68
1:D:132:MET:HB3	1:D:187:ILE:O	1.93	0.68
1:B:57:MET:HG2	1:B:58:GLU:N	2.08	0.68
1:B:41:ILE:HG22	1:B:44:GLN:HB3	1.74	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:61:ARG:NH1	1:B:63:ALA:HB3	2.06	0.68
1:D:85:ARG:O	1:D:87:THR:HG23	1.93	0.68
1:A:84:ILE:N	1:A:125:VAL:HG12	2.07	0.68
1:C:78:ILE:HD11	1:C:131:LEU:HD13	1.75	0.68
1:A:296:LYS:CE	1:A:301:GLU:HB3	2.23	0.68
1:B:95:ARG:HB3	1:B:100:LEU:HD22	1.75	0.68
1:B:173:LEU:HD11	1:B:176:ILE:HD12	1.75	0.68
1:C:39:ILE:CD1	1:C:41:ILE:HG12	2.24	0.68
1:D:96:LEU:HD11	1:D:104:MET:CE	2.24	0.68
1:B:58:GLU:OE2	1:B:66:VAL:HG23	1.93	0.68
1:B:140:TYR:CE1	1:B:253:LEU:HA	2.29	0.68
1:C:269:GLN:O	1:C:273:GLU:HB2	1.94	0.68
1:A:144:ILE:HG12	1:A:253:LEU:HD13	1.76	0.67
1:C:61:ARG:HA	1:C:66:VAL:HA	1.76	0.67
1:D:99:ASP:HA	1:D:201:SER:CB	2.25	0.67
1:C:113:VAL:HA	1:C:194:LYS:HD3	1.77	0.67
1:A:248:ILE:HD12	1:A:295:LEU:CD1	2.25	0.67
1:A:113:VAL:CG1	1:A:196:CYS:HA	2.23	0.67
1:A:174:SER:HB3	1:A:234:TYR:HE1	1.58	0.67
1:A:304:THR:HG23	1:A:307:GLU:H	1.59	0.67
1:D:78:ILE:O	1:D:131:LEU:HD12	1.95	0.67
1:B:41:ILE:HG22	1:B:44:GLN:HG2	1.77	0.67
1:B:111:PHE:CE2	1:B:164:LYS:HD2	2.29	0.67
1:C:71:ARG:NH2	1:C:76:GLY:HA2	2.09	0.67
1:D:59:LEU:H	1:D:69:LYS:HZ3	1.40	0.67
1:B:41:ILE:HG22	1:B:44:GLN:CG	2.24	0.67
1:C:81:VAL:HA	1:C:127:ILE:O	1.94	0.67
1:D:120:PHE:CZ	1:D:125:VAL:HG22	2.30	0.67
1:A:131:LEU:C	1:A:132:MET:HE2	2.20	0.66
1:B:95:ARG:HH11	1:B:120:PHE:HB2	1.57	0.66
1:B:188:ASN:HD21	1:B:192:GLN:HB2	1.60	0.66
1:D:92:GLU:HG3	1:D:92:GLU:O	1.93	0.66
1:A:320:LYS:HG2	1:A:322:THR:HG23	1.76	0.66
1:A:54:GLU:OE1	1:A:56:ILE:HG23	1.94	0.66
1:D:95:ARG:HG3	1:D:96:LEU:H	1.60	0.66
1:A:255:PHE:HE1	1:A:257:TYR:HB2	1.60	0.66
1:D:138:LYS:CE	3:D:504:HOH:O	2.43	0.66
1:D:233:GLY:O	1:D:234:TYR:HB2	1.96	0.66
1:A:51:ASP:HA	1:A:121:ARG:HH21	1.57	0.66
1:A:132:MET:HG3	1:A:186:LEU:HB3	1.78	0.66
1:C:169:LEU:CG	1:C:176:ILE:HD13	2.09	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:140:TYR:O	1:B:143:VAL:HG12	1.96	0.66
1:C:77:GLN:NE2	1:C:78:ILE:O	2.29	0.66
1:C:132:MET:HG3	1:C:186:LEU:HB3	1.78	0.66
1:D:113:VAL:HA	1:D:194:LYS:HE2	1.77	0.66
1:C:290:PHE:HD2	1:C:313:PHE:HB3	1.60	0.66
1:D:54:GLU:O	1:D:56:ILE:N	2.28	0.65
1:D:53:LEU:HD13	1:D:126:TRP:CZ3	2.30	0.65
1:D:56:ILE:HG22	1:D:57:MET:H	1.61	0.65
1:A:262:THR:O	1:A:266:GLN:HG3	1.96	0.65
1:A:187:ILE:HD13	1:A:193:VAL:HG12	1.78	0.65
1:B:173:LEU:HG	1:B:175:VAL:N	2.11	0.65
1:A:57:MET:O	1:A:69:LYS:N	2.29	0.65
1:B:143:VAL:HG22	1:B:148:GLN:O	1.97	0.65
1:A:143:VAL:HG12	1:A:148:GLN:O	1.96	0.65
1:A:53:LEU:H	1:A:72:HIS:CD2	2.14	0.65
1:A:257:TYR:CE2	1:A:270:VAL:HG12	2.32	0.65
1:C:52:ASP:O	1:C:53:LEU:HB2	1.97	0.65
1:C:66:VAL:O	1:C:82:LYS:HA	1.96	0.65
1:D:99:ASP:HA	1:D:201:SER:HB3	1.79	0.65
1:C:94:LYS:CB	1:C:97:LEU:HB2	2.27	0.65
1:D:181:LYS:HG2	1:D:219:TYR:CD1	2.31	0.65
1:D:83:ARG:HH12	1:D:124:ASP:CG	2.04	0.65
1:A:102:ILE:HA	1:A:105:ARG:HG3	1.79	0.65
1:B:70:MET:HG3	1:B:81:VAL:HG21	1.79	0.65
1:D:237:LYS:HD2	1:D:302:ARG:HB3	1.79	0.64
1:A:82:LYS:HD3	1:A:198:PHE:HE2	1.61	0.64
1:A:84:ILE:H	1:A:125:VAL:CG1	2.07	0.64
1:B:53:LEU:HD11	1:B:119:LEU:HD21	1.79	0.64
1:C:78:ILE:HG12	1:C:131:LEU:HD22	1.79	0.64
1:C:198:PHE:HD2	1:C:200:ILE:HB	1.62	0.64
1:D:182:PRO:HG3	1:D:249:GLU:OE1	1.98	0.64
1:D:273:GLU:HG2	1:D:274:PRO:HD2	1.77	0.64
1:A:39:ILE:CG2	1:A:110:PRO:HB3	2.27	0.64
1:B:237:LYS:HD2	1:B:302:ARG:HB3	1.77	0.64
1:A:58:GLU:OE2	1:A:61:ARG:NE	2.30	0.64
1:C:78:ILE:HD12	1:C:79:MET:H	1.62	0.64
1:D:92:GLU:OE1	1:D:95:ARG:NH1	2.30	0.64
1:C:105:ARG:HG3	1:C:173:LEU:HD21	1.79	0.64
1:C:162:ILE:HD12	1:C:195:MET:HE2	1.79	0.64
1:A:102:ILE:HA	1:A:105:ARG:CG	2.28	0.64
1:C:318:GLU:OE2	1:C:319:SER:OG	2.16	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:VAL:HA	1:A:127:ILE:O	1.97	0.64
1:C:300:LYS:HD3	1:C:300:LYS:N	2.12	0.64
1:D:47:GLU:OE2	1:D:72:HIS:ND1	2.28	0.64
1:A:83:ARG:HH12	1:A:85:ARG:CG	2.11	0.64
1:B:105:ARG:HD3	1:B:176:ILE:HD11	1.77	0.64
1:D:116:TYR:CE2	1:D:130:GLU:HA	2.32	0.64
1:A:153:ASP:HA	1:A:317:HIS:NE2	2.13	0.64
1:A:241:TRP:HB2	1:A:302:ARG:NH1	2.13	0.64
1:C:153:ASP:HA	1:C:317:HIS:CE1	2.33	0.64
1:C:181:LYS:CE	1:C:183:SER:HB2	2.24	0.64
1:C:141:LYS:HA	1:C:144:ILE:HD12	1.80	0.63
1:D:141:LYS:HA	1:D:144:ILE:HD12	1.80	0.63
1:B:84:ILE:O	1:B:124:ASP:HB2	1.98	0.63
1:C:58:GLU:HA	1:C:68:GLU:HA	1.80	0.63
1:B:190:LEU:HD22	1:B:190:LEU:H	1.62	0.63
1:D:248:ILE:HD12	1:D:295:LEU:HD11	1.81	0.63
1:B:69:LYS:HG3	1:B:131:LEU:HD11	1.80	0.63
1:C:52:ASP:HA	3:C:506:HOH:O	1.98	0.63
1:D:59:LEU:H	1:D:69:LYS:NZ	1.95	0.63
1:A:182:PRO:HG3	1:A:246:THR:HG23	1.80	0.63
1:D:105:ARG:HH11	1:D:105:ARG:HG2	1.63	0.63
1:D:310:GLN:HA	1:D:310:GLN:OE1	1.98	0.63
1:A:83:ARG:CG	1:A:124:ASP:HB2	2.18	0.63
1:D:70:MET:CE	1:D:81:VAL:HG11	2.29	0.62
1:A:38:CYS:C	1:A:39:ILE:HD12	2.24	0.62
1:A:108:ASP:O	1:A:109:CYS:HB3	1.99	0.62
1:A:248:ILE:HD12	1:A:295:LEU:HD11	1.81	0.62
1:C:61:ARG:H	1:C:61:ARG:HD3	1.64	0.62
1:D:229:LEU:HD22	1:D:230:ASN:H	1.63	0.62
1:A:163:VAL:HG12	1:A:309:MET:HE2	1.81	0.62
1:B:152:GLU:HA	1:B:155:LEU:HD12	1.81	0.62
1:C:67:VAL:HG21	2:C:401:1FM:C23	2.30	0.62
1:D:48:VAL:HG23	1:D:48:VAL:O	1.97	0.62
1:B:84:ILE:CG1	1:B:125:VAL:HB	2.30	0.62
1:B:172:LYS:HA	1:B:172:LYS:CE	2.24	0.62
1:D:135:SER:H	2:D:401:1FM:H59B	1.64	0.62
1:A:104:MET:HE2	3:A:526:HOH:O	1.99	0.62
1:A:153:ASP:HA	1:A:317:HIS:CD2	2.34	0.62
1:C:221:ALA:N	1:C:224:ARG:HD3	2.12	0.62
1:C:287:PHE:O	1:C:291:THR:HG23	1.99	0.62
1:A:55:PRO:HA	1:A:70:MET:CB	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:56:ILE:HG13	1:D:70:MET:HA	1.82	0.62
1:D:61:ARG:HH21	1:D:63:ALA:CA	2.12	0.62
1:B:60:GLY:HA2	1:B:67:VAL:HG23	1.81	0.62
1:B:93:GLN:C	1:B:94:LYS:HG3	2.24	0.62
1:C:59:LEU:HD21	1:C:69:LYS:CG	2.26	0.62
1:C:162:ILE:CG2	1:C:243:LEU:HD13	2.23	0.62
1:D:157:LYS:HZ2	1:D:317:HIS:CA	2.12	0.62
1:D:155:LEU:CA	1:D:158:ILE:HD12	2.24	0.62
1:A:179:ASP:O	1:A:184:ASN:ND2	2.33	0.62
1:D:97:LEU:O	1:D:101:ASP:HB3	2.00	0.61
1:A:134:THR:HG22	1:A:135:SER:O	1.99	0.61
1:B:53:LEU:HD11	1:B:119:LEU:CD2	2.30	0.61
1:C:285:ALA:O	1:C:288:VAL:HG22	1.99	0.61
1:A:330:LEU:HD12	1:A:331:ILE:CD1	2.30	0.61
1:D:52:ASP:HB2	1:D:72:HIS:CD2	2.35	0.61
1:A:181:LYS:HG2	1:A:219:TYR:CG	2.36	0.61
1:C:248:ILE:HG12	1:C:278:LEU:HD13	1.82	0.61
1:D:221:ALA:HA	1:D:241:TRP:CD1	2.36	0.61
1:D:248:ILE:HD12	1:D:295:LEU:CD1	2.31	0.61
1:A:70:MET:HE3	1:A:81:VAL:CB	2.31	0.61
1:C:252:ILE:HG13	1:C:254:ARG:H	1.65	0.61
1:C:279:PRO:HB2	1:C:282:LYS:HB2	1.82	0.61
1:B:70:MET:HG3	1:B:81:VAL:CG2	2.31	0.61
1:B:135:SER:H	2:B:401:1FM:H59B	1.64	0.61
1:A:188:ASN:ND2	1:A:190:LEU:HB2	2.14	0.61
1:A:132:MET:HE2	1:A:132:MET:N	2.16	0.61
1:A:146:LYS:CE	1:A:334:ASP:HB3	2.30	0.61
1:C:96:LEU:HD13	1:C:118:ALA:HB3	1.83	0.61
1:A:248:ILE:O	1:A:252:ILE:HG12	2.01	0.60
1:D:327:PHE:HA	1:D:330:LEU:HD21	1.83	0.60
1:A:115:PHE:HB2	1:A:129:MET:HE2	1.83	0.60
1:C:137:ASP:OD2	1:C:138:LYS:HD3	2.01	0.60
1:D:97:LEU:HA	1:D:101:ASP:CB	2.30	0.60
1:D:299:SER:HA	1:D:302:ARG:HH12	1.64	0.60
1:A:58:GLU:HB3	1:A:68:GLU:HG2	1.83	0.60
1:D:50:ALA:O	1:D:121:ARG:HG3	2.01	0.60
1:C:162:ILE:HD12	1:C:195:MET:CE	2.32	0.60
1:D:114:THR:N	1:D:130:GLU:HG2	2.12	0.60
1:A:143:VAL:HG22	1:A:331:ILE:HG13	1.83	0.60
1:B:105:ARG:HB3	1:B:173:LEU:HD13	1.83	0.60
1:C:158:ILE:HG23	1:C:193:VAL:HG11	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:LYS:HD3	1:D:198:PHE:CE2	2.34	0.60
1:B:182:PRO:HG3	1:B:246:THR:HG23	1.84	0.60
1:C:111:PHE:CE2	1:C:164:LYS:HD3	2.37	0.60
1:D:139:PHE:O	1:D:143:VAL:HG23	2.01	0.60
1:A:161:SER:CB	1:A:193:VAL:HG23	2.32	0.60
1:A:292:SER:O	1:A:296:LYS:HG3	2.01	0.60
1:C:240:ILE:HD13	1:C:303:PRO:O	2.02	0.60
1:C:255:PHE:HE2	1:C:257:TYR:HB2	1.67	0.59
1:C:327:PHE:HA	1:C:330:LEU:HD12	1.84	0.59
1:A:180:VAL:HA	1:A:195:MET:CE	2.32	0.59
1:A:248:ILE:HG12	1:A:278:LEU:CG	2.31	0.59
1:A:241:TRP:HB2	1:A:302:ARG:HH11	1.67	0.59
1:B:66:VAL:HG13	1:B:83:ARG:CB	2.32	0.59
1:B:173:LEU:CD1	1:B:175:VAL:HB	2.30	0.59
1:D:106:THR:HG21	1:D:169:LEU:HD21	1.84	0.59
1:C:285:ALA:HA	1:C:288:VAL:HG22	1.85	0.59
1:A:269:GLN:HB3	3:A:501:HOH:O	2.00	0.59
1:C:61:ARG:CB	1:C:66:VAL:HG23	2.32	0.59
1:C:68:GLU:HB2	1:C:70:MET:HE3	1.84	0.59
1:C:185:VAL:O	1:C:186:LEU:HD12	2.02	0.59
1:C:279:PRO:HB2	1:C:282:LYS:HG3	1.83	0.59
1:C:304:THR:CG2	1:C:306:PRO:HD2	2.32	0.59
1:D:102:ILE:CD1	1:D:175:VAL:HG21	2.33	0.59
1:B:41:ILE:CG2	1:B:44:GLN:HB3	2.33	0.59
1:C:140:TYR:CE1	1:C:253:LEU:HA	2.34	0.59
1:C:156:GLY:HA3	1:C:317:HIS:CG	2.37	0.59
1:D:67:VAL:HG22	1:D:82:LYS:HB2	1.84	0.59
1:D:103:SER:HB2	1:D:176:ILE:HG13	1.83	0.59
1:B:140:TYR:HE1	1:B:253:LEU:HA	1.67	0.59
1:D:273:GLU:HG2	1:D:274:PRO:CD	2.32	0.59
1:C:262:THR:OG1	1:C:265:GLN:HG3	2.03	0.59
1:A:222:PRO:HD3	1:A:241:TRP:CE2	2.38	0.59
1:B:125:VAL:HG12	1:B:127:ILE:CD1	2.33	0.59
1:A:66:VAL:CG1	1:A:83:ARG:HH21	2.15	0.59
1:D:157:LYS:HZ2	1:D:317:HIS:CB	2.16	0.58
1:D:249:GLU:HG3	1:D:255:PHE:HA	1.85	0.58
1:B:111:PHE:O	1:B:194:LYS:HA	2.02	0.58
1:C:58:GLU:N	1:C:58:GLU:OE1	2.36	0.58
1:C:252:ILE:HD11	1:C:254:ARG:O	2.03	0.58
1:A:82:LYS:CD	1:A:198:PHE:HE2	2.15	0.58
1:A:106:THR:HG21	1:A:169:LEU:HD23	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:251:ALA:HB1	1:A:283:PHE:CZ	2.38	0.58
1:B:45:ASN:HA	1:B:116:TYR:O	2.02	0.58
1:C:231:GLN:CD	1:C:233:GLY:H	2.11	0.58
1:C:241:TRP:HB2	1:C:302:ARG:NH1	2.18	0.58
1:D:228:GLU:O	1:C:297:LYS:HD2	2.03	0.58
1:A:69:LYS:HG2	1:A:131:LEU:CD1	2.31	0.58
1:C:94:LYS:HD2	1:C:97:LEU:CB	2.34	0.58
1:A:187:ILE:HD12	1:A:188:ASN:H	1.68	0.58
1:A:218:PRO:HA	1:A:220:MET:HE2	1.84	0.58
1:D:140:TYR:CE1	1:D:253:LEU:HA	2.25	0.58
1:A:101:ASP:HA	1:A:104:MET:SD	2.44	0.58
1:B:71:ARG:HH22	1:B:76:GLY:CA	2.17	0.58
1:C:65:GLY:HA3	1:C:82:LYS:CE	2.34	0.58
1:C:102:ILE:HD12	1:C:175:VAL:HG12	1.84	0.58
1:D:176:ILE:HD12	1:D:199:GLY:HA3	1.86	0.58
1:A:176:ILE:HD12	1:A:199:GLY:CA	2.33	0.58
1:B:41:ILE:HG22	1:B:44:GLN:CB	2.33	0.58
1:C:56:ILE:HG12	1:C:70:MET:HA	1.86	0.58
1:C:104:MET:HE2	1:C:107:VAL:HG22	1.86	0.58
1:B:158:ILE:HA	1:B:193:VAL:HG21	1.84	0.58
1:C:198:PHE:CD2	1:C:200:ILE:HB	2.39	0.58
1:A:304:THR:CG2	1:A:307:GLU:H	2.16	0.58
1:B:53:LEU:CD1	1:B:119:LEU:HD21	2.34	0.58
1:B:71:ARG:HH12	1:B:72:HIS:C	2.12	0.58
1:D:140:TYR:HE1	1:D:253:LEU:CA	2.14	0.57
1:B:120:PHE:HE1	1:B:125:VAL:HG22	1.69	0.57
1:A:84:ILE:HB	1:A:125:VAL:HG12	1.86	0.57
1:B:137:ASP:OD2	1:B:138:LYS:HD3	2.03	0.57
1:C:234:TYR:CE2	1:C:236:VAL:HB	2.39	0.57
1:D:97:LEU:HA	1:D:101:ASP:HB3	1.85	0.57
1:C:132:MET:HB2	1:C:186:LEU:CD2	2.21	0.57
1:C:222:PRO:HD3	1:C:241:TRP:CE2	2.39	0.57
1:D:52:ASP:OD2	1:D:74:PRO:HD3	2.05	0.57
1:D:151:PRO:HD3	1:D:327:PHE:CE1	2.40	0.57
1:A:59:LEU:CD2	1:A:69:LYS:HG3	2.34	0.57
1:A:162:ILE:HG21	1:A:243:LEU:HD13	1.86	0.57
1:B:60:GLY:HA2	1:B:67:VAL:CG2	2.34	0.57
1:C:241:TRP:HB2	1:C:302:ARG:HH11	1.69	0.57
1:D:55:PRO:HA	1:D:70:MET:HB3	1.84	0.57
1:D:68:GLU:HB3	1:D:70:MET:HG2	1.86	0.57
1:A:79:MET:SD	1:A:128:CYS:HB3	2.44	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:185:VAL:C	1:A:186:LEU:HD23	2.30	0.57
1:C:105:ARG:HD3	1:C:172:LYS:HZ1	1.68	0.57
1:C:267:LEU:O	1:C:270:VAL:HG12	2.05	0.57
1:D:218:PRO:HB3	1:D:267:LEU:HD23	1.87	0.57
1:D:248:ILE:O	1:D:252:ILE:HG12	2.05	0.57
1:B:43:ASN:OD1	1:B:47:GLU:HG3	2.05	0.57
1:C:132:MET:SD	1:C:188:ASN:HB2	2.45	0.57
1:C:113:VAL:CG2	1:C:194:LYS:HB3	2.34	0.57
1:D:67:VAL:HG22	1:D:82:LYS:CB	2.34	0.57
1:D:252:ILE:HD12	1:D:254:ARG:HG3	1.87	0.57
1:A:311:HIS:CD2	1:A:312:PRO:HD2	2.40	0.57
1:A:136:LEU:O	1:A:140:TYR:HB3	2.05	0.56
1:A:142:GLN:NE2	3:A:503:HOH:O	2.37	0.56
1:C:96:LEU:HD13	1:C:118:ALA:C	2.29	0.56
1:A:71:ARG:HG2	1:A:78:ILE:HD12	1.88	0.56
1:B:169:LEU:O	1:B:174:SER:HA	2.05	0.56
1:C:108:ASP:HA	1:C:112:THR:CG2	2.36	0.56
1:D:54:GLU:O	1:D:56:ILE:HG13	2.05	0.56
1:A:59:LEU:HD12	1:A:67:VAL:HG13	1.87	0.56
1:A:244:GLY:CA	1:A:295:LEU:HD21	2.36	0.56
1:C:94:LYS:HD2	1:C:97:LEU:HD12	1.87	0.56
1:C:251:ALA:HB1	1:C:283:PHE:CZ	2.40	0.56
1:D:56:ILE:HG22	1:D:57:MET:N	2.20	0.56
1:A:85:ARG:HA	1:A:123:GLY:O	2.06	0.56
1:A:305:TYR:HB2	1:A:306:PRO:HD3	1.87	0.56
1:D:256:PRO:HB2	1:D:276:PRO:HG2	1.87	0.56
1:A:244:GLY:HA3	1:A:295:LEU:CD2	2.35	0.56
1:B:60:GLY:HA2	1:B:67:VAL:HB	1.88	0.56
1:C:85:ARG:NH2	1:C:124:ASP:OD2	2.39	0.56
1:D:91:GLN:HE22	1:D:93:GLN:HA	1.71	0.56
1:A:79:MET:HE3	1:A:81:VAL:HG22	1.88	0.56
1:A:80:ALA:HB3	2:A:401:1FM:H62B	1.88	0.56
1:C:99:ASP:N	1:C:99:ASP:OD1	2.38	0.56
1:C:85:ARG:HG3	1:C:87:THR:OG1	2.05	0.56
1:D:121:ARG:HD3	1:D:126:TRP:CZ2	2.41	0.56
1:B:65:GLY:C	1:B:82:LYS:HE2	2.29	0.56
1:B:96:LEU:HD21	1:B:201:SER:OG	2.06	0.56
1:C:68:GLU:OE1	1:C:70:MET:HE2	2.05	0.56
1:C:105:ARG:HB2	1:C:175:VAL:HG11	1.88	0.56
1:C:154:ILE:HD11	1:C:327:PHE:CD2	2.41	0.56
1:D:151:PRO:HD3	1:D:327:PHE:CZ	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:156:GLY:HA3	1:C:317:HIS:ND1	2.21	0.56
1:B:50:ALA:HB2	1:B:119:LEU:HD22	1.88	0.56
1:C:114:THR:HB	1:C:130:GLU:HB3	1.88	0.56
1:A:172:LYS:HE3	1:A:172:LYS:HA	1.88	0.55
1:C:187:ILE:HD13	1:C:193:VAL:HG22	1.89	0.55
1:A:322:THR:OG1	1:A:324:VAL:HG23	2.06	0.55
1:C:114:THR:HB	1:C:130:GLU:CB	2.36	0.55
1:C:289:ASP:O	1:C:293:GLN:HG2	2.06	0.55
1:D:70:MET:HE3	1:D:81:VAL:HG11	1.88	0.55
1:D:136:LEU:O	1:D:140:TYR:HB3	2.06	0.55
1:B:102:ILE:HA	1:B:105:ARG:HG3	1.87	0.55
1:C:175:VAL:CG2	1:C:176:ILE:HD12	2.35	0.55
1:D:101:ASP:HA	1:D:104:MET:SD	2.46	0.55
1:A:293:GLN:HA	1:A:296:LYS:HD3	1.87	0.55
1:D:262:THR:O	1:D:266:GLN:HG3	2.06	0.55
1:B:66:VAL:HG12	1:B:85:ARG:HH12	1.71	0.55
1:B:113:VAL:HG13	1:B:130:GLU:HG3	1.87	0.55
1:C:120:PHE:O	1:C:121:ARG:HB3	2.05	0.55
1:C:157:LYS:O	1:C:160:VAL:HG22	2.07	0.55
1:B:119:LEU:HG	1:B:126:TRP:CB	2.33	0.55
1:D:256:PRO:HB2	1:D:276:PRO:CG	2.36	0.55
1:D:259:SER:HB3	1:D:266:GLN:OE1	2.07	0.55
1:B:105:ARG:CB	1:B:173:LEU:HD13	2.36	0.55
1:C:270:VAL:O	1:C:297:LYS:NZ	2.35	0.55
1:D:132:MET:HE3	1:D:187:ILE:C	2.33	0.54
1:D:139:PHE:HD2	1:D:332:LEU:HD21	1.71	0.54
1:C:53:LEU:HG	1:C:72:HIS:CB	2.37	0.54
1:C:218:PRO:HD2	1:C:255:PHE:CZ	2.43	0.54
1:D:153:ASP:HA	1:D:317:HIS:CD2	2.41	0.54
1:A:84:ILE:HB	1:A:125:VAL:CG1	2.38	0.54
1:D:98:MET:C	1:D:201:SER:HB3	2.33	0.54
1:D:257:TYR:CE2	1:D:270:VAL:HG12	2.43	0.54
1:D:269:GLN:O	1:D:273:GLU:HB3	2.07	0.54
1:B:59:LEU:HD13	2:B:401:1FM:C14	2.38	0.54
1:A:134:THR:CG2	1:A:138:LYS:HB2	2.38	0.54
1:D:52:ASP:HB2	1:D:72:HIS:NE2	2.23	0.54
1:A:71:ARG:HG2	1:A:78:ILE:CD1	2.37	0.54
1:C:78:ILE:CG1	1:C:131:LEU:HD22	2.38	0.54
1:D:276:PRO:HD2	1:D:295:LEU:HD13	1.89	0.54
1:D:138:LYS:NZ	3:D:504:HOH:O	2.38	0.54
1:D:153:ASP:HA	1:D:317:HIS:NE2	2.22	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:221:ALA:O	1:D:224:ARG:HB2	2.07	0.54
1:D:273:GLU:CG	1:D:274:PRO:HD2	2.38	0.54
1:A:196:CYS:SG	2:A:401:1FM:H42	2.47	0.54
1:B:91:GLN:CD	1:B:91:GLN:H	2.16	0.54
1:C:56:ILE:HB	1:C:69:LYS:HB2	1.88	0.54
1:C:90:SER:C	1:C:95:ARG:HH22	2.08	0.54
1:D:161:SER:CB	1:D:193:VAL:HG23	2.37	0.54
1:C:248:ILE:HG12	1:C:278:LEU:HD11	1.89	0.54
1:D:79:MET:HE2	1:D:128:CYS:CB	2.38	0.53
1:D:249:GLU:HB2	1:D:256:PRO:HD3	1.88	0.53
1:D:297:LYS:HE2	1:D:297:LYS:H	1.74	0.53
1:D:176:ILE:HG23	1:D:199:GLY:HA3	1.91	0.53
1:C:304:THR:HG23	1:C:306:PRO:CD	2.37	0.53
1:D:157:LYS:HZ2	1:D:317:HIS:HA	1.71	0.53
1:A:151:PRO:HD2	1:A:154:ILE:HB	1.90	0.53
1:A:196:CYS:SG	2:A:401:1FM:C42	2.97	0.53
1:B:61:ARG:HG3	1:B:63:ALA:H	1.73	0.53
1:B:187:ILE:HD11	1:B:328:VAL:HG21	1.89	0.53
1:D:129:MET:HE3	1:D:198:PHE:HB3	1.90	0.53
1:A:176:ILE:HG23	1:A:199:GLY:HA2	1.89	0.53
1:B:57:MET:HG2	1:B:58:GLU:H	1.71	0.53
1:C:120:PHE:CE1	1:C:125:VAL:HG22	2.44	0.53
1:C:293:GLN:HA	1:C:296:LYS:CG	2.39	0.53
1:D:56:ILE:HD11	1:D:71:ARG:HD2	1.89	0.53
1:A:320:LYS:HG2	1:A:322:THR:CG2	2.38	0.53
1:D:112:THR:HG22	1:D:165:ALA:HB1	1.91	0.53
1:A:53:LEU:O	1:A:55:PRO:HD3	2.08	0.53
1:A:59:LEU:HD22	2:A:401:1FM:C16	2.39	0.53
1:D:173:LEU:HD22	1:D:175:VAL:HG23	1.91	0.53
1:A:153:ASP:HB3	1:A:322:THR:HG22	1.89	0.53
1:B:65:GLY:HA3	1:B:82:LYS:NZ	2.24	0.53
1:D:327:PHE:HA	1:D:330:LEU:HD23	1.90	0.53
1:A:132:MET:HG3	1:A:186:LEU:CB	2.38	0.53
1:B:235:SER:O	1:B:236:VAL:C	2.52	0.53
1:C:60:GLY:O	1:C:66:VAL:HA	2.09	0.53
1:A:111:PHE:C	1:A:194:LYS:HG3	2.34	0.52
1:A:179:ASP:OD1	1:A:224:ARG:NH2	2.42	0.52
1:D:157:LYS:O	1:D:160:VAL:HG22	2.09	0.52
1:A:248:ILE:HG12	1:A:278:LEU:CD2	2.40	0.52
1:A:83:ARG:NH1	1:A:85:ARG:HG2	2.22	0.52
1:A:236:VAL:HB	1:A:305:TYR:CE1	2.45	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:PRO:HD3	1:A:327:PHE:CE1	2.44	0.52
1:C:173:LEU:HG	1:C:175:VAL:HG13	1.90	0.52
1:C:279:PRO:HG2	1:C:282:LYS:HD2	1.89	0.52
1:C:120:PHE:HE1	1:C:125:VAL:CG2	2.22	0.52
1:D:71:ARG:HB3	1:D:78:ILE:HA	1.90	0.52
1:B:60:GLY:HA2	1:B:67:VAL:CB	2.39	0.52
1:B:84:ILE:HG12	1:B:125:VAL:HB	1.90	0.52
1:B:134:THR:HG21	1:B:332:LEU:HD21	1.92	0.52
1:C:276:PRO:HD2	1:C:295:LEU:HD13	1.92	0.52
1:D:152:GLU:HG2	1:D:153:ASP:N	2.25	0.52
1:A:67:VAL:HG23	1:A:81:VAL:C	2.34	0.52
1:A:278:LEU:HD13	1:A:283:PHE:CD2	2.44	0.52
1:A:320:LYS:HG3	1:A:321:GLY:N	2.25	0.52
1:B:115:PHE:HA	1:B:129:MET:HG2	1.90	0.52
1:B:120:PHE:CE1	1:B:125:VAL:HG22	2.45	0.52
1:C:53:LEU:HG	1:C:72:HIS:HA	1.92	0.52
1:C:163:VAL:HB	1:C:314:PHE:HE2	1.75	0.52
1:C:252:ILE:O	1:C:253:LEU:HB2	2.09	0.52
1:D:102:ILE:HD13	1:D:175:VAL:HG21	1.91	0.52
1:A:279:PRO:HG2	1:A:282:LYS:HG3	1.92	0.52
1:C:234:TYR:HD2	1:C:236:VAL:HB	1.71	0.52
1:D:157:LYS:HD2	1:D:157:LYS:N	2.25	0.52
1:A:112:THR:HG23	1:A:165:ALA:HB1	1.92	0.52
1:D:105:ARG:HG2	1:D:105:ARG:NH1	2.24	0.51
1:B:71:ARG:NH1	1:B:72:HIS:C	2.69	0.51
1:D:61:ARG:HG3	1:D:62:GLY:N	2.25	0.51
1:C:96:LEU:HA	1:C:99:ASP:OD1	2.10	0.51
1:C:144:ILE:HG13	1:C:253:LEU:HD23	1.93	0.51
1:D:96:LEU:HB2	1:D:100:LEU:HB3	1.92	0.51
1:D:96:LEU:HA	1:D:99:ASP:OD1	2.10	0.51
1:D:225:ILE:HD12	1:D:270:VAL:CG2	2.40	0.51
1:D:227:PRO:O	1:C:274:PRO:HD3	2.09	0.51
1:A:140:TYR:CE1	1:A:253:LEU:HA	2.28	0.51
1:A:166:LEU:HB3	1:A:305:TYR:OH	2.10	0.51
1:A:180:VAL:HA	1:A:195:MET:HE1	1.91	0.51
1:A:248:ILE:HD12	1:A:295:LEU:HD12	1.91	0.51
1:D:104:MET:HB2	1:D:105:ARG:HH12	1.75	0.51
1:A:225:ILE:O	1:A:227:PRO:HD3	2.10	0.51
1:C:71:ARG:CZ	1:C:76:GLY:HA2	2.41	0.51
1:C:252:ILE:HD12	1:C:254:ARG:CG	2.30	0.51
1:D:71:ARG:HG3	1:D:78:ILE:HA	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:262:THR:OG1	1:D:265:GLN:HG3	2.10	0.51
1:D:278:LEU:HD22	1:D:291:THR:HG21	1.91	0.51
1:A:71:ARG:HB3	1:A:78:ILE:HA	1.92	0.51
1:A:161:SER:HB2	1:A:193:VAL:HG23	1.91	0.51
1:C:91:GLN:HG3	1:C:92:GLU:N	2.26	0.51
1:D:91:GLN:NE2	1:D:92:GLU:O	2.42	0.51
1:B:50:ALA:C	1:B:53:LEU:HG	2.36	0.51
1:B:82:LYS:HB3	1:B:127:ILE:HB	1.92	0.51
1:C:290:PHE:CD2	1:C:313:PHE:HB3	2.43	0.51
1:D:231:GLN:HG3	1:D:232:LYS:H	1.72	0.51
1:A:66:VAL:HG12	1:A:83:ARG:HH21	1.75	0.51
1:A:329:LYS:NZ	3:A:505:HOH:O	2.44	0.51
1:A:134:THR:HG23	1:A:138:LYS:HB2	1.93	0.51
1:C:104:MET:CE	1:C:107:VAL:HG22	2.41	0.51
1:C:224:ARG:HD2	1:C:238:SER:CB	2.20	0.51
1:C:311:HIS:O	1:C:315:THR:HG23	2.11	0.51
1:D:47:GLU:CD	1:D:72:HIS:HD1	2.16	0.51
1:A:52:ASP:O	1:A:53:LEU:HB2	2.10	0.51
1:B:173:LEU:O	1:B:174:SER:OG	2.23	0.51
1:B:235:SER:O	1:B:238:SER:N	2.44	0.51
1:D:113:VAL:HG13	1:D:195:MET:O	2.11	0.50
1:D:298:ASN:HB3	1:D:301:GLU:HG3	1.93	0.50
1:A:174:SER:O	1:A:175:VAL:CG2	2.60	0.50
1:A:252:ILE:O	1:A:253:LEU:HB2	2.11	0.50
1:C:240:ILE:CG2	1:C:294:CYS:HA	2.41	0.50
1:D:71:ARG:HB2	1:D:79:MET:H	1.76	0.50
1:D:152:GLU:HG2	1:D:153:ASP:H	1.76	0.50
1:B:41:ILE:CG2	1:B:44:GLN:HG2	2.42	0.50
1:B:317:HIS:O	1:B:318:GLU:C	2.53	0.50
1:C:187:ILE:HD12	1:C:188:ASN:H	1.77	0.50
1:C:248:ILE:HA	1:C:278:LEU:HD11	1.93	0.50
1:A:153:ASP:HA	1:A:317:HIS:HE2	1.76	0.50
1:B:56:ILE:HG22	1:B:69:LYS:HB3	1.94	0.50
1:B:125:VAL:HG12	1:B:127:ILE:HD13	1.92	0.50
1:C:304:THR:HG23	1:C:307:GLU:H	1.76	0.50
1:D:241:TRP:CZ2	1:D:245:ILE:HD11	2.46	0.50
1:D:267:LEU:O	1:D:270:VAL:HG22	2.12	0.50
1:B:235:SER:C	1:B:237:LYS:N	2.68	0.50
1:D:96:LEU:HD11	1:D:104:MET:HE3	1.94	0.50
1:A:73:VAL:HB	1:A:74:PRO:HD3	1.93	0.50
1:A:107:VAL:O	1:A:108:ASP:C	2.55	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:121:ARG:HG3	1:A:126:TRP:CE2	2.46	0.50
1:B:71:ARG:NH2	1:B:76:GLY:HA2	2.24	0.50
1:B:119:LEU:O	1:B:126:TRP:N	2.44	0.50
1:B:132:MET:HE3	1:B:187:ILE:C	2.36	0.50
1:C:90:SER:CB	1:C:95:ARG:HH12	2.17	0.50
1:C:105:ARG:CA	1:C:172:LYS:HE3	2.37	0.50
1:D:85:ARG:HG2	1:D:86:ALA:N	2.25	0.50
1:A:56:ILE:HD11	1:A:69:LYS:HZ2	1.76	0.50
1:A:316:LEU:HD11	1:A:317:HIS:CE1	2.47	0.50
1:C:251:ALA:HB1	1:C:283:PHE:CE2	2.46	0.50
1:B:105:ARG:O	1:B:173:LEU:HD22	2.11	0.50
2:C:401:1FM:O15	2:C:401:1FM:H23	2.11	0.50
1:D:278:LEU:CD2	1:D:291:THR:HG21	2.42	0.49
1:A:53:LEU:HB3	1:A:70:MET:SD	2.51	0.49
1:B:136:LEU:HD21	1:B:193:VAL:HG12	1.93	0.49
1:D:44:GLN:HA	1:D:44:GLN:OE1	2.12	0.49
1:A:82:LYS:HD3	1:A:198:PHE:CE2	2.44	0.49
1:A:100:LEU:HD21	1:A:118:ALA:CB	2.42	0.49
1:A:176:ILE:HG23	1:A:199:GLY:HA3	1.92	0.49
1:C:140:TYR:HE1	1:C:253:LEU:CA	2.21	0.49
1:C:136:LEU:O	1:C:140:TYR:HB3	2.12	0.49
1:A:100:LEU:HD21	1:A:118:ALA:HB3	1.93	0.49
1:B:135:SER:HA	1:B:186:LEU:HD23	1.93	0.49
1:C:156:GLY:HA2	1:C:313:PHE:CE2	2.46	0.49
1:C:278:LEU:CD2	1:C:291:THR:HG21	2.38	0.49
1:C:300:LYS:N	1:C:300:LYS:CD	2.75	0.49
1:D:102:ILE:HD13	1:D:175:VAL:HG11	1.93	0.49
1:A:119:LEU:HB3	1:A:126:TRP:HB2	1.94	0.49
1:D:88:VAL:O	1:D:89:ASN:C	2.55	0.49
1:D:178:ARG:CG	1:D:197:ASP:HA	2.43	0.49
1:A:121:ARG:HG3	1:A:126:TRP:CZ2	2.48	0.49
1:B:120:PHE:HE1	1:B:125:VAL:CG2	2.25	0.49
1:B:155:LEU:HA	1:B:158:ILE:HD12	1.94	0.49
1:C:65:GLY:HA3	1:C:82:LYS:HE2	1.94	0.49
1:C:155:LEU:HD13	1:C:287:PHE:HE2	1.78	0.49
1:C:269:GLN:HA	1:C:273:GLU:OE1	2.12	0.49
1:D:304:THR:HG23	1:D:307:GLU:H	1.78	0.49
1:A:112:THR:CG2	1:A:165:ALA:HB1	2.42	0.49
1:A:132:MET:CG	1:A:186:LEU:HB3	2.43	0.49
1:B:101:ASP:O	1:B:102:ILE:C	2.55	0.49
1:B:102:ILE:CA	1:B:105:ARG:HG3	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:ALA:HB3	1:C:224:ARG:HD2	1.94	0.49
1:C:94:LYS:HB2	1:C:97:LEU:HB2	1.93	0.49
1:C:157:LYS:HE2	1:C:322:THR:HG23	1.94	0.49
1:D:89:ASN:O	1:D:90:SER:C	2.55	0.49
1:D:134:THR:O	1:D:187:ILE:HG22	2.13	0.49
1:D:290:PHE:HD2	1:D:313:PHE:CD2	2.31	0.49
1:D:304:THR:HG23	1:D:306:PRO:HD2	1.94	0.49
1:A:220:MET:HB2	1:A:225:ILE:HD11	1.93	0.49
1:A:304:THR:HG23	1:A:306:PRO:HD2	1.95	0.49
1:B:48:VAL:O	1:B:49:LYS:HE2	2.11	0.49
1:C:60:GLY:H	1:C:67:VAL:HG22	1.78	0.49
1:C:105:ARG:HB3	1:C:172:LYS:CG	2.42	0.49
1:B:59:LEU:HD11	1:B:67:VAL:CG1	2.42	0.49
1:B:284:SER:O	1:B:286:GLU:N	2.46	0.49
1:C:79:MET:HE2	1:C:116:TYR:CD2	2.47	0.49
1:A:173:LEU:HG	1:A:175:VAL:HG22	1.95	0.48
1:B:136:LEU:HD22	1:B:187:ILE:HG22	1.94	0.48
1:C:65:GLY:HA3	1:C:82:LYS:NZ	2.27	0.48
1:C:293:GLN:HB3	1:C:303:PRO:HD3	1.94	0.48
1:D:97:LEU:HA	1:D:101:ASP:HB2	1.95	0.48
1:A:334:ASP:OD1	1:A:334:ASP:N	2.46	0.48
1:B:132:MET:HG3	1:B:186:LEU:CB	2.42	0.48
1:B:153:ASP:HB3	1:B:322:THR:CG2	2.43	0.48
1:D:260:TRP:NE1	1:A:39:ILE:HG12	2.28	0.48
1:A:290:PHE:HD2	1:A:313:PHE:CD2	2.31	0.48
1:B:175:VAL:HG12	1:B:176:ILE:N	2.28	0.48
1:D:46:PHE:C	1:D:48:VAL:H	2.21	0.48
1:D:48:VAL:O	1:D:48:VAL:CG2	2.61	0.48
1:D:121:ARG:HD3	1:D:126:TRP:CH2	2.49	0.48
1:A:180:VAL:HG22	1:A:195:MET:CE	2.26	0.48
1:B:186:LEU:HD21	2:B:401:1FM:C3	2.42	0.48
1:B:317:HIS:O	1:B:320:LYS:N	2.46	0.48
1:D:77:GLN:NE2	1:D:78:ILE:O	2.45	0.48
1:D:290:PHE:CD2	1:D:313:PHE:HD2	2.31	0.48
1:A:66:VAL:HG13	1:A:66:VAL:O	2.14	0.48
1:A:180:VAL:HA	1:A:195:MET:HE3	1.96	0.48
1:C:279:PRO:HB2	1:C:282:LYS:CG	2.43	0.48
1:C:61:ARG:HA	1:C:66:VAL:HG23	1.95	0.48
1:D:255:PHE:CE1	1:D:257:TYR:HB2	2.43	0.48
1:C:120:PHE:HE1	1:C:125:VAL:HG22	1.77	0.48
1:C:173:LEU:CD2	1:C:173:LEU:N	2.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:258:ASP:OD1	1:D:258:ASP:O	2.31	0.48
1:C:59:LEU:HB2	1:C:67:VAL:HG23	1.95	0.48
1:C:73:VAL:HG23	1:C:74:PRO:CD	2.33	0.48
1:A:304:THR:CG2	1:A:307:GLU:HB2	2.29	0.47
1:D:80:ALA:HB2	1:D:131:LEU:CG	2.45	0.47
1:A:187:ILE:HD13	1:A:193:VAL:CG1	2.42	0.47
1:B:105:ARG:HB3	1:B:173:LEU:CD1	2.44	0.47
1:D:71:ARG:HH12	1:D:73:VAL:CG2	2.21	0.47
1:D:71:ARG:NH1	1:D:73:VAL:HG22	2.21	0.47
1:A:42:GLY:O	1:A:43:ASN:HB3	2.14	0.47
1:B:84:ILE:HB	1:B:125:VAL:HB	1.96	0.47
1:C:96:LEU:HD22	1:C:118:ALA:CB	2.44	0.47
1:C:154:ILE:HD11	1:C:327:PHE:CE2	2.49	0.47
1:C:279:PRO:HB2	1:C:282:LYS:CB	2.44	0.47
1:D:320:LYS:HD2	1:D:322:THR:HG22	1.95	0.47
1:A:93:GLN:HE22	1:A:97:LEU:CB	2.20	0.47
1:C:251:ALA:O	1:C:253:LEU:HD12	2.14	0.47
1:A:168:HIS:O	1:A:172:LYS:HG2	2.14	0.47
1:B:97:LEU:HA	1:B:100:LEU:HB3	1.96	0.47
1:C:158:ILE:O	1:C:162:ILE:HG12	2.14	0.47
1:C:221:ALA:HB3	1:C:224:ARG:CD	2.44	0.47
1:D:100:LEU:CD2	1:D:118:ALA:HB2	2.44	0.47
1:D:106:THR:HG21	1:D:169:LEU:CD2	2.43	0.47
1:A:114:THR:OG1	1:A:130:GLU:OE1	2.30	0.47
1:A:237:LYS:NZ	1:A:302:ARG:O	2.48	0.47
1:B:59:LEU:HD11	1:B:67:VAL:HG11	1.95	0.47
1:D:96:LEU:HD22	1:D:100:LEU:HD23	1.95	0.47
1:A:290:PHE:HB2	1:A:311:HIS:CE1	2.49	0.47
1:B:125:VAL:HG12	1:B:127:ILE:HD11	1.97	0.47
1:B:135:SER:H	2:B:401:1FM:C59	2.27	0.47
1:B:163:VAL:HB	1:B:314:PHE:HE2	1.80	0.47
1:B:175:VAL:O	1:B:176:ILE:HB	2.15	0.47
1:A:54:GLU:O	1:A:70:MET:HB2	2.14	0.47
1:A:257:TYR:CZ	1:A:270:VAL:HG12	2.49	0.47
1:B:71:ARG:NH2	1:B:76:GLY:C	2.73	0.47
1:C:47:GLU:HB3	1:C:49:LYS:HG3	1.96	0.47
1:A:121:ARG:HB2	1:A:126:TRP:HE1	1.79	0.47
1:B:158:ILE:O	1:B:162:ILE:HG12	2.14	0.47
1:C:61:ARG:CA	1:C:66:VAL:HG23	2.45	0.47
1:C:113:VAL:HG23	1:C:194:LYS:HB3	1.96	0.47
1:D:199:GLY:O	1:D:200:ILE:HG12	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:290:PHE:HD2	1:D:313:PHE:HD2	1.62	0.47
1:A:108:ASP:CG	1:A:109:CYS:H	2.23	0.47
1:A:121:ARG:HB2	1:A:124:ASP:OD1	2.15	0.47
1:B:89:ASN:ND2	1:B:91:GLN:HG2	2.30	0.47
1:C:154:ILE:HG13	1:C:324:VAL:HG22	1.97	0.47
1:D:158:ILE:O	1:D:162:ILE:HG13	2.14	0.46
1:A:39:ILE:HG21	1:A:110:PRO:HB3	1.97	0.46
1:B:52:ASP:OD2	1:B:54:GLU:HG2	2.15	0.46
1:B:195:MET:HE2	1:B:195:MET:HB3	1.64	0.46
1:D:53:LEU:HA	1:D:71:ARG:O	2.15	0.46
1:A:64:TYR:HD2	1:A:84:ILE:HD12	1.81	0.46
1:B:305:TYR:HB2	1:B:306:PRO:HD3	1.97	0.46
1:C:96:LEU:HD13	1:C:118:ALA:CB	2.46	0.46
1:C:300:LYS:HD3	1:C:300:LYS:H	1.77	0.46
1:D:220:MET:O	1:D:241:TRP:NE1	2.48	0.46
1:A:58:GLU:HB3	1:A:68:GLU:CG	2.45	0.46
1:C:67:VAL:HG21	2:C:401:1FM:C3	2.45	0.46
1:B:59:LEU:HD13	2:B:401:1FM:C15	2.45	0.46
1:B:86:ALA:HB2	1:B:124:ASP:HB3	1.97	0.46
1:D:71:ARG:CG	1:D:78:ILE:HA	2.44	0.46
1:D:97:LEU:N	1:D:99:ASP:OD1	2.48	0.46
1:D:102:ILE:HD11	1:D:175:VAL:HG21	1.97	0.46
1:D:109:CYS:HB2	1:D:168:HIS:CD2	2.50	0.46
1:A:195:MET:O	1:A:196:CYS:HB2	2.15	0.46
1:B:140:TYR:CD1	1:B:250:LEU:HA	2.49	0.46
1:B:311:HIS:O	1:B:312:PRO:C	2.59	0.46
1:B:50:ALA:HA	1:B:53:LEU:HG	1.96	0.46
1:B:84:ILE:HD13	1:B:84:ILE:N	2.31	0.46
1:B:119:LEU:HD12	1:B:120:PHE:N	2.31	0.46
1:C:57:MET:C	1:C:57:MET:SD	2.99	0.46
1:C:71:ARG:HH22	1:C:76:GLY:HA2	1.80	0.46
1:A:152:GLU:OE1	1:A:284:SER:OG	2.32	0.46
1:B:61:ARG:CG	1:B:63:ALA:H	2.29	0.46
1:B:71:ARG:NH2	1:B:76:GLY:CA	2.79	0.46
1:B:141:LYS:HD3	1:B:144:ILE:HD12	1.96	0.46
1:B:254:ARG:HE	1:B:254:ARG:HB2	1.63	0.46
1:C:222:PRO:HD3	1:C:241:TRP:CD2	2.51	0.46
1:C:231:GLN:HG2	1:C:233:GLY:H	1.79	0.46
1:D:157:LYS:HZ2	1:D:317:HIS:HB3	1.80	0.46
1:A:64:TYR:CD2	1:A:84:ILE:HD12	2.50	0.46
1:A:99:ASP:HB3	1:A:201:SER:HB3	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:THR:O	1:A:187:ILE:HG22	2.16	0.46
1:A:188:ASN:ND2	1:A:192:GLN:HE21	2.14	0.46
1:B:50:ALA:CA	1:B:53:LEU:HG	2.45	0.46
1:B:61:ARG:HD3	1:B:64:TYR:CD1	2.51	0.46
1:C:95:ARG:HD3	1:C:120:PHE:CD2	2.51	0.46
1:C:160:VAL:HA	1:C:314:PHE:CE2	2.50	0.46
1:A:249:GLU:HB2	1:A:256:PRO:HD3	1.98	0.45
1:B:55:PRO:HB3	1:B:70:MET:HE2	1.98	0.45
1:B:59:LEU:O	1:B:59:LEU:HD12	2.16	0.45
1:B:71:ARG:HB2	1:B:78:ILE:HA	1.98	0.45
1:B:165:ALA:O	1:B:169:LEU:HD23	2.16	0.45
1:B:285:ALA:O	1:B:286:GLU:C	2.59	0.45
1:B:327:PHE:O	1:B:328:VAL:C	2.58	0.45
1:D:90:SER:O	1:D:91:GLN:C	2.59	0.45
1:A:176:ILE:HD12	1:A:199:GLY:HA3	1.97	0.45
1:C:218:PRO:HB3	1:C:267:LEU:HD21	1.98	0.45
1:D:153:ASP:HB3	1:D:322:THR:CG2	2.47	0.45
1:D:287:PHE:O	1:D:291:THR:HG23	2.15	0.45
1:A:196:CYS:O	1:A:197:ASP:HB2	2.17	0.45
1:B:80:ALA:O	1:B:128:CYS:HA	2.16	0.45
1:B:157:LYS:NZ	1:B:322:THR:HG23	2.32	0.45
1:C:94:LYS:HB3	1:C:97:LEU:HB2	1.95	0.45
1:C:175:VAL:O	1:C:176:ILE:HB	2.15	0.45
1:D:70:MET:HE2	1:D:81:VAL:HG11	1.97	0.45
1:D:260:TRP:CE2	1:A:39:ILE:HG12	2.52	0.45
1:A:56:ILE:HG12	1:A:70:MET:HA	1.97	0.45
1:B:101:ASP:O	1:B:104:MET:N	2.49	0.45
1:C:56:ILE:HG22	1:C:57:MET:N	2.31	0.45
1:C:107:VAL:O	1:C:112:THR:HG21	2.17	0.45
1:C:221:ALA:O	1:C:224:ARG:N	2.49	0.45
1:A:96:LEU:HA	1:A:100:LEU:CG	2.46	0.45
1:A:140:TYR:HE1	1:A:253:LEU:CA	2.18	0.45
1:B:111:PHE:CD2	1:B:164:LYS:CB	2.99	0.45
1:D:229:LEU:HD11	1:D:230:ASN:OD1	2.16	0.45
1:A:53:LEU:H	1:A:72:HIS:HD2	1.58	0.45
1:C:47:GLU:CG	1:C:49:LYS:HG3	2.47	0.45
1:A:316:LEU:HD11	3:A:513:HOH:O	2.16	0.45
1:B:89:ASN:HD22	1:B:91:GLN:HE21	1.64	0.45
1:B:97:LEU:O	1:B:98:MET:C	2.60	0.45
1:B:249:GLU:HB2	1:B:256:PRO:HD3	1.99	0.45
1:C:104:MET:HA	1:C:104:MET:CE	2.40	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:143:VAL:HG11	1:C:150:ILE:CD1	2.43	0.45
1:D:253:LEU:N	1:D:253:LEU:HD22	2.31	0.45
1:B:284:SER:O	1:B:285:ALA:C	2.60	0.45
1:C:157:LYS:HE3	1:C:320:LYS:O	2.17	0.45
1:C:304:THR:CG2	1:C:307:GLU:H	2.30	0.45
1:D:113:VAL:HG22	1:D:196:CYS:O	2.17	0.45
1:A:188:ASN:OD1	1:A:192:GLN:N	2.50	0.45
1:B:55:PRO:HA	1:B:70:MET:CA	2.39	0.45
1:B:225:ILE:O	1:B:227:PRO:HD3	2.17	0.45
1:B:289:ASP:O	1:B:290:PHE:C	2.59	0.45
1:D:96:LEU:CD1	1:D:104:MET:SD	3.00	0.45
1:D:173:LEU:O	1:D:174:SER:HB2	2.17	0.45
1:B:173:LEU:CD1	1:B:176:ILE:HD12	2.47	0.45
1:C:186:LEU:HD21	2:C:401:1FM:C11	2.46	0.45
1:D:225:ILE:C	1:D:227:PRO:HD3	2.41	0.44
1:A:59:LEU:HD13	2:A:401:1FM:C14	2.47	0.44
1:A:160:VAL:O	1:A:164:LYS:HG2	2.17	0.44
1:A:311:HIS:CG	1:A:312:PRO:HD2	2.52	0.44
1:B:241:TRP:CZ2	1:B:245:ILE:HD11	2.52	0.44
1:C:47:GLU:HG2	1:C:49:LYS:HG3	1.99	0.44
1:C:86:ALA:CB	1:C:125:VAL:HG23	2.45	0.44
1:A:139:PHE:CE2	1:A:328:VAL:HA	2.51	0.44
1:A:155:LEU:O	1:A:158:ILE:HB	2.17	0.44
1:B:71:ARG:NH1	1:B:72:HIS:O	2.43	0.44
1:B:107:VAL:H	1:B:168:HIS:CE1	2.36	0.44
1:B:280:ALA:O	1:B:281:ASP:C	2.59	0.44
1:C:59:LEU:HB2	1:C:67:VAL:CG2	2.47	0.44
1:C:78:ILE:HD12	1:C:79:MET:N	2.29	0.44
1:C:95:ARG:N	1:C:95:ARG:HE	2.15	0.44
1:D:157:LYS:HD2	1:D:157:LYS:H	1.82	0.44
1:D:229:LEU:CD1	1:D:230:ASN:OD1	2.65	0.44
1:A:93:GLN:O	1:A:94:LYS:C	2.59	0.44
1:B:279:PRO:O	1:B:280:ALA:C	2.60	0.44
1:D:107:VAL:HB	1:D:168:HIS:NE2	2.32	0.44
1:A:100:LEU:C	1:A:104:MET:HG3	2.42	0.44
1:A:236:VAL:HB	1:A:305:TYR:CZ	2.52	0.44
1:B:71:ARG:HG3	1:B:71:ARG:HH11	1.81	0.44
1:B:111:PHE:HE2	1:B:164:LYS:HD2	1.77	0.44
1:C:69:LYS:HB3	1:C:69:LYS:HE3	1.73	0.44
1:C:134:THR:HA	2:C:401:1FM:O48	2.17	0.44
1:D:107:VAL:HB	1:D:168:HIS:HE2	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:148:GLN:NE2	3:A:504:HOH:O	2.38	0.44
1:B:77:GLN:O	1:B:79:MET:HE3	2.18	0.44
1:B:223:GLU:HG2	1:B:224:ARG:N	2.32	0.44
1:C:106:THR:OG1	1:C:176:ILE:HD11	2.17	0.44
1:C:222:PRO:HA	1:C:225:ILE:HD12	1.99	0.44
1:D:302:ARG:HG2	1:D:303:PRO:HD2	1.99	0.44
1:B:125:VAL:CG1	1:B:127:ILE:HD11	2.48	0.44
1:B:262:THR:H	1:B:265:GLN:HE21	1.65	0.44
1:C:116:TYR:CZ	1:C:130:GLU:HA	2.53	0.44
1:C:196:CYS:O	1:C:197:ASP:HB2	2.17	0.44
1:D:71:ARG:CB	1:D:79:MET:H	2.30	0.44
1:A:71:ARG:HB3	1:A:78:ILE:HD12	1.99	0.44
1:B:234:TYR:O	1:B:235:SER:C	2.60	0.44
1:C:56:ILE:HG22	1:C:57:MET:H	1.82	0.44
1:D:96:LEU:HD13	1:D:100:LEU:C	2.43	0.44
1:D:221:ALA:HB1	1:D:223:GLU:OE1	2.17	0.44
1:A:69:LYS:HG3	1:A:131:LEU:HD11	1.95	0.44
1:C:72:HIS:CG	1:C:74:PRO:HD2	2.52	0.44
1:D:151:PRO:HD2	1:D:154:ILE:HB	1.98	0.44
1:D:264:PHE:O	1:D:268:LYS:HB2	2.17	0.44
1:A:136:LEU:HD23	1:A:185:VAL:HG12	2.00	0.44
1:C:47:GLU:HG2	1:C:49:LYS:H	1.83	0.44
1:C:115:PHE:HD1	1:C:129:MET:SD	2.41	0.44
1:C:201:SER:HB2	1:C:203:TYR:CE1	2.53	0.44
1:C:326:SER:O	1:C:330:LEU:HG	2.17	0.44
1:A:101:ASP:OD1	1:A:102:ILE:N	2.50	0.43
1:A:113:VAL:HG23	1:A:130:GLU:HG2	1.96	0.43
1:B:114:THR:HB	1:B:130:GLU:HG2	2.00	0.43
1:C:154:ILE:O	1:C:158:ILE:HG13	2.18	0.43
1:C:234:TYR:OH	1:C:237:LYS:HG2	2.18	0.43
1:C:237:LYS:NZ	1:C:304:THR:HA	2.33	0.43
1:A:67:VAL:HG23	1:A:82:LYS:N	2.34	0.43
1:A:198:PHE:HD1	1:A:198:PHE:HA	1.70	0.43
1:B:134:THR:HA	2:B:401:1FM:H59B	2.00	0.43
1:C:83:ARG:NH2	1:C:126:TRP:HZ2	2.16	0.43
1:C:152:GLU:O	1:C:155:LEU:HB2	2.18	0.43
1:C:255:PHE:CE2	1:C:257:TYR:HB2	2.50	0.43
1:C:299:SER:HA	1:C:302:ARG:HE	1.83	0.43
1:A:137:ASP:CG	1:A:138:LYS:N	2.76	0.43
1:A:148:GLN:OE1	1:A:148:GLN:HA	2.18	0.43
1:A:153:ASP:HB3	1:A:322:THR:CG2	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:119:LEU:C	1:C:119:LEU:HD12	2.44	0.43
1:D:139:PHE:HD2	1:D:332:LEU:CD2	2.30	0.43
1:C:57:MET:O	1:C:69:LYS:HG3	2.18	0.43
1:D:52:ASP:CB	1:D:72:HIS:CD2	3.02	0.43
1:A:284:SER:O	1:A:288:VAL:HG23	2.19	0.43
1:B:297:LYS:O	1:B:302:ARG:NH2	2.51	0.43
1:C:152:GLU:O	1:C:155:LEU:N	2.51	0.43
1:C:157:LYS:NZ	1:C:317:HIS:O	2.42	0.43
1:D:61:ARG:CG	1:D:62:GLY:N	2.82	0.43
1:D:84:ILE:O	1:D:84:ILE:HG13	2.18	0.43
1:D:114:THR:H	1:D:130:GLU:CG	2.18	0.43
1:A:79:MET:HE3	1:A:128:CYS:SG	2.58	0.43
1:A:81:VAL:HG11	1:A:126:TRP:HE3	1.83	0.43
1:A:82:LYS:HB3	1:A:198:PHE:HZ	1.83	0.43
1:B:293:GLN:HA	1:B:296:LYS:HG2	1.99	0.43
1:C:68:GLU:HB2	1:C:70:MET:CE	2.47	0.43
1:C:305:TYR:O	1:C:309:MET:HG3	2.18	0.43
1:D:111:PHE:CE2	1:D:164:LYS:HD3	2.52	0.43
1:B:99:ASP:C	1:B:101:ASP:H	2.27	0.43
1:C:96:LEU:HD11	1:C:119:LEU:CA	2.49	0.43
1:D:157:LYS:HD3	1:D:322:THR:OG1	2.19	0.43
1:A:71:ARG:CG	1:A:78:ILE:HD12	2.48	0.43
1:B:312:PRO:O	1:B:313:PHE:C	2.60	0.43
1:C:95:ARG:O	1:C:96:LEU:HD23	2.18	0.43
1:C:108:ASP:CG	1:C:115:PHE:H	2.26	0.43
1:C:223:GLU:OE1	1:C:299:SER:HB2	2.18	0.43
1:D:49:LYS:HA	1:D:49:LYS:CE	2.31	0.43
1:A:89:ASN:O	1:A:90:SER:C	2.61	0.43
1:B:84:ILE:CB	1:B:125:VAL:HB	2.49	0.43
1:C:279:PRO:CB	1:C:282:LYS:HG3	2.48	0.43
1:D:68:GLU:OE1	1:D:68:GLU:HA	2.18	0.43
1:D:99:ASP:HA	1:D:201:SER:OG	2.18	0.43
1:D:257:TYR:CD2	1:D:270:VAL:HG12	2.53	0.43
1:A:116:TYR:N	1:A:128:CYS:O	2.50	0.43
1:C:113:VAL:HG22	1:C:194:LYS:HB3	2.00	0.43
1:D:80:ALA:H	1:D:131:LEU:HG	1.84	0.42
1:D:222:PRO:HD3	1:D:241:TRP:CE2	2.54	0.42
1:A:59:LEU:CD1	1:A:67:VAL:HG13	2.49	0.42
1:B:228:GLU:HB2	1:B:229:LEU:HD23	2.01	0.42
1:B:279:PRO:HB2	1:B:282:LYS:HB2	2.00	0.42
1:C:231:GLN:CG	1:C:233:GLY:H	2.31	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:241:TRP:CZ2	1:C:245:ILE:HD11	2.54	0.42
1:D:173:LEU:HD22	1:D:175:VAL:H	1.84	0.42
1:A:102:ILE:HG13	1:A:176:ILE:HD11	2.01	0.42
1:C:78:ILE:CD1	1:C:131:LEU:HD13	2.45	0.42
1:D:47:GLU:O	1:D:49:LYS:HG2	2.19	0.42
1:B:82:LYS:HB3	1:B:127:ILE:CG1	2.49	0.42
1:B:119:LEU:HD12	1:B:119:LEU:C	2.44	0.42
1:C:53:LEU:HG	1:C:72:HIS:N	2.33	0.42
1:C:61:ARG:HB3	1:C:66:VAL:HG23	1.99	0.42
1:C:235:SER:HB3	1:C:238:SER:OG	2.20	0.42
1:C:252:ILE:CD1	1:C:254:ARG:O	2.66	0.42
1:C:290:PHE:CD1	1:C:290:PHE:C	2.97	0.42
1:D:221:ALA:HB3	1:D:224:ARG:HG3	2.00	0.42
1:D:264:PHE:CD1	1:D:264:PHE:C	2.97	0.42
1:A:251:ALA:HB1	1:A:283:PHE:CE1	2.55	0.42
1:B:60:GLY:CA	1:B:67:VAL:H	2.24	0.42
1:B:221:ALA:O	1:B:222:PRO:C	2.61	0.42
1:D:67:VAL:HA	1:D:81:VAL:O	2.19	0.42
1:D:85:ARG:HG3	1:D:85:ARG:NH1	2.24	0.42
1:D:97:LEU:C	1:D:97:LEU:HD23	2.44	0.42
1:D:184:ASN:HA	2:D:401:1FM:O44	2.19	0.42
1:D:196:CYS:HB3	1:D:197:ASP:H	1.67	0.42
1:D:217:LYS:HE2	1:D:259:SER:HB2	2.02	0.42
1:B:55:PRO:CA	1:B:70:MET:HB3	2.50	0.42
1:B:173:LEU:HG	1:B:174:SER:N	2.35	0.42
1:B:178:ARG:HD2	1:B:234:TYR:HA	2.01	0.42
1:C:185:VAL:HG12	1:C:186:LEU:N	2.34	0.42
1:A:79:MET:HE3	1:A:81:VAL:CG2	2.48	0.42
1:A:102:ILE:HA	1:A:105:ARG:HG2	1.98	0.42
1:B:192:GLN:HB2	1:B:194:LYS:HE3	2.00	0.42
1:D:80:ALA:HB2	1:D:131:LEU:HG	2.00	0.42
1:A:68:GLU:C	1:A:70:MET:H	2.27	0.42
1:A:193:VAL:HG23	1:A:193:VAL:O	2.20	0.42
1:B:43:ASN:OD1	1:B:43:ASN:C	2.62	0.42
1:C:160:VAL:HG23	1:C:161:SER:N	2.34	0.42
1:C:237:LYS:HG3	1:C:299:SER:O	2.19	0.42
1:D:187:ILE:HD11	1:D:328:VAL:HG21	2.02	0.42
1:B:111:PHE:CD2	1:B:164:LYS:HB3	2.55	0.42
1:B:252:ILE:HG13	1:B:254:ARG:HG3	2.02	0.42
1:C:89:ASN:OD1	1:C:89:ASN:C	2.62	0.42
1:C:105:ARG:CB	1:C:172:LYS:HE3	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:225:ILE:HD13	1:C:270:VAL:CG1	2.50	0.42
1:D:69:LYS:HA	1:D:69:LYS:HD3	1.64	0.42
1:D:95:ARG:CG	1:D:96:LEU:N	2.82	0.42
1:D:253:LEU:HD21	3:D:510:HOH:O	2.19	0.42
1:A:241:TRP:CH2	1:A:275:SER:HB2	2.54	0.42
1:B:55:PRO:HB3	1:B:70:MET:CE	2.50	0.42
1:B:132:MET:HB3	1:B:187:ILE:O	2.20	0.42
1:C:79:MET:HG3	1:C:116:TYR:HD2	1.85	0.42
1:C:105:ARG:HB3	1:C:172:LYS:HG3	2.01	0.42
1:C:165:ALA:O	1:C:169:LEU:HD13	2.20	0.42
1:C:224:ARG:CD	1:C:238:SER:HB2	2.20	0.42
1:A:85:ARG:O	1:A:86:ALA:C	2.63	0.42
1:A:100:LEU:O	1:A:101:ASP:C	2.62	0.42
1:A:111:PHE:CD2	1:A:164:LYS:HB3	2.55	0.42
1:A:114:THR:CB	1:A:130:GLU:OE1	2.68	0.42
1:A:200:ILE:HG23	1:A:200:ILE:O	2.20	0.42
1:B:97:LEU:HD23	1:B:100:LEU:HB3	2.01	0.42
1:D:136:LEU:HD12	1:D:185:VAL:HB	2.01	0.41
1:A:49:LYS:O	1:A:50:ALA:HB3	2.20	0.41
1:A:176:ILE:HG22	1:A:197:ASP:HB3	2.02	0.41
1:A:304:THR:O	1:A:308:LEU:HD12	2.20	0.41
1:C:304:THR:HG22	1:C:307:GLU:HB2	2.02	0.41
1:A:93:GLN:OE1	1:A:98:MET:SD	2.78	0.41
1:A:248:ILE:HG23	1:A:278:LEU:CD2	2.50	0.41
1:B:71:ARG:HH11	1:B:71:ARG:CG	2.33	0.41
1:B:166:LEU:HB3	1:B:305:TYR:CZ	2.55	0.41
1:A:44:GLN:HG2	1:A:45:ASN:N	2.36	0.41
1:B:50:ALA:HB1	1:B:53:LEU:HD12	2.02	0.41
1:B:114:THR:H	1:B:130:GLU:HG2	1.85	0.41
1:C:58:GLU:HB2	1:C:67:VAL:O	2.20	0.41
1:D:143:VAL:HG22	1:D:331:ILE:HG21	2.02	0.41
1:A:113:VAL:CG2	1:A:130:GLU:HG2	2.50	0.41
1:A:146:LYS:NZ	1:A:334:ASP:HB3	2.36	0.41
1:A:156:GLY:HA3	1:A:317:HIS:CG	2.55	0.41
1:A:246:THR:O	1:A:250:LEU:HD23	2.21	0.41
1:A:313:PHE:HA	1:A:316:LEU:CD2	2.50	0.41
1:C:94:LYS:HD2	1:C:97:LEU:HB2	2.00	0.41
1:C:97:LEU:HD23	1:C:97:LEU:HA	1.88	0.41
1:C:114:THR:HB	1:C:130:GLU:HB2	2.03	0.41
1:D:91:GLN:NE2	1:D:93:GLN:HA	2.32	0.41
1:D:172:LYS:O	1:D:173:LEU:HB2	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:229:LEU:HD13	1:D:230:ASN:H	1.80	0.41
1:A:71:ARG:HD2	1:A:71:ARG:O	2.21	0.41
1:B:58:GLU:HG3	1:B:67:VAL:O	2.20	0.41
1:D:125:VAL:HG12	1:D:127:ILE:CD1	2.51	0.41
1:D:248:ILE:HD12	1:D:295:LEU:HD12	2.03	0.41
1:A:84:ILE:CB	1:A:125:VAL:HG12	2.51	0.41
1:A:248:ILE:HG23	1:A:278:LEU:HD21	2.02	0.41
1:C:129:MET:HG3	2:C:401:1FM:H62	2.03	0.41
1:C:136:LEU:HB2	1:C:182:PRO:O	2.21	0.41
1:C:245:ILE:N	1:C:295:LEU:HD21	2.36	0.41
1:D:104:MET:HB2	1:D:105:ARG:NH1	2.36	0.41
1:A:52:ASP:O	1:A:53:LEU:CB	2.69	0.41
1:A:167:GLU:OE2	1:A:305:TYR:HB3	2.21	0.41
1:B:235:SER:O	1:B:237:LYS:N	2.53	0.41
1:C:46:PHE:O	1:C:46:PHE:CD1	2.73	0.41
1:C:85:ARG:O	1:C:124:ASP:HB3	2.20	0.41
1:C:94:LYS:HB2	1:C:94:LYS:HE3	1.75	0.41
1:D:54:GLU:O	1:D:55:PRO:C	2.63	0.41
1:D:133:ASP:HB2	1:D:188:ASN:HA	2.02	0.41
1:D:152:GLU:OE1	1:D:152:GLU:N	2.50	0.41
1:D:181:LYS:HB3	1:D:182:PRO:HD2	2.01	0.41
1:D:196:CYS:O	1:D:197:ASP:HB2	2.21	0.41
1:D:293:GLN:O	1:D:296:LYS:HG3	2.20	0.41
1:A:53:LEU:HD13	1:A:126:TRP:CE3	2.55	0.41
1:A:155:LEU:HD23	1:A:155:LEU:HA	1.81	0.41
1:A:217:LYS:NZ	1:A:259:SER:HB2	2.36	0.41
1:A:217:LYS:HZ3	1:A:259:SER:CB	2.32	0.41
1:A:267:LEU:O	1:A:270:VAL:HG22	2.21	0.41
1:B:139:PHE:CE1	1:B:331:ILE:HB	2.56	0.41
1:B:159:ALA:O	1:B:163:VAL:HG23	2.20	0.41
1:B:257:TYR:OH	1:B:276:PRO:HD3	2.21	0.41
1:C:126:TRP:C	1:C:127:ILE:HD13	2.45	0.41
1:C:157:LYS:NZ	1:C:322:THR:HG23	2.36	0.41
1:C:228:GLU:C	1:C:229:LEU:HD22	2.45	0.41
1:D:64:TYR:O	1:D:84:ILE:HG22	2.20	0.41
1:D:150:ILE:HD13	1:D:327:PHE:CE2	2.56	0.41
1:D:246:THR:O	1:D:247:MET:C	2.64	0.41
1:A:120:PHE:HA	1:A:126:TRP:HD1	1.86	0.41
1:B:57:MET:CG	1:B:58:GLU:N	2.81	0.41
1:B:324:VAL:O	1:B:325:ALA:C	2.64	0.41
1:B:329:LYS:O	1:B:330:LEU:C	2.64	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:67:VAL:HA	1:C:81:VAL:O	2.21	0.41
1:C:111:PHE:O	1:C:194:LYS:HA	2.21	0.41
1:D:169:LEU:HA	1:D:169:LEU:HD23	1.80	0.40
1:D:224:ARG:HD3	1:D:234:TYR:CZ	2.54	0.40
1:A:67:VAL:HG13	1:A:67:VAL:O	2.21	0.40
1:A:70:MET:HE3	1:A:81:VAL:CG1	2.52	0.40
1:B:65:GLY:HA3	1:B:82:LYS:HE2	2.02	0.40
1:B:69:LYS:CD	1:B:131:LEU:HD11	2.51	0.40
1:D:50:ALA:HB1	1:D:120:PHE:O	2.22	0.40
1:D:95:ARG:HE	1:D:96:LEU:N	2.19	0.40
1:D:150:ILE:HD13	1:D:327:PHE:CZ	2.56	0.40
1:A:58:GLU:CA	1:A:68:GLU:HA	2.45	0.40
1:A:174:SER:C	1:A:175:VAL:O	2.64	0.40
2:A:401:IFM:H18	2:A:401:IFM:H23	2.03	0.40
1:B:136:LEU:HD23	1:B:186:LEU:CA	2.51	0.40
1:B:157:LYS:HZ2	1:B:322:THR:HG23	1.86	0.40
1:B:245:ILE:HG23	1:B:256:PRO:HG2	2.02	0.40
1:C:255:PHE:HA	1:C:256:PRO:HD3	1.97	0.40
1:C:327:PHE:N	1:C:327:PHE:CD1	2.89	0.40
1:D:47:GLU:OE1	1:D:74:PRO:HB2	2.21	0.40
1:B:220:MET:HB3	1:B:220:MET:HE3	1.54	0.40
1:C:296:LYS:HE3	1:C:296:LYS:HB3	1.87	0.40
1:B:165:ALA:O	1:B:169:LEU:CD2	2.68	0.40
1:C:237:LYS:HE3	1:C:302:ARG:O	2.22	0.40
1:D:73:VAL:HB	1:D:74:PRO:HD3	2.03	0.40
1:D:99:ASP:HA	1:D:201:SER:H	1.87	0.40
1:D:187:ILE:CD1	1:D:328:VAL:HG21	2.52	0.40
1:D:290:PHE:CD2	1:D:313:PHE:CD2	3.08	0.40
1:A:286:GLU:HG3	1:A:313:PHE:HD1	1.87	0.40
1:B:147:GLY:HA3	1:C:147:GLY:HA3	2.03	0.40
1:C:111:PHE:CZ	1:C:164:LYS:HD2	2.56	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:A:226:ASN:OD1	1:C:265:GLN:NE2[2_645]	2.02	0.18



## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	284/340 (84%)	239 (84%)	28 (10%)	17 (6%)	1	7
1	B	283/340 (83%)	234 (83%)	38 (13%)	11 (4%)	2	14
1	C	285/340 (84%)	267 (94%)	13 (5%)	5 (2%)	6	31
1	D	285/340 (84%)	228 (80%)	38 (13%)	19 (7%)	1	5
All	All	1137/1360 (84%)	968 (85%)	117 (10%)	52 (5%)	2	11

All (52) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	55	PRO
1	D	61	ARG
1	D	173	LEU
1	D	174	SER
1	D	196	CYS
1	A	108	ASP
1	A	175	VAL
1	A	196	CYS
1	C	176	ILE
1	D	48	VAL
1	D	90	SER
1	D	212	ILE
1	A	51	ASP
1	A	85	ARG
1	A	90	SER
1	A	195	MET
1	B	285	ALA
1	C	91	GLN
1	D	85	ARG
1	D	109	CYS
1	D	130	GLU
1	A	86	ALA

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Mol	Chain	Res	Type
1	A	94	LYS
1	A	173	LEU
1	B	45	ASN
1	C	232	LYS
1	D	89	ASN
1	D	92	GLU
1	D	128	CYS
1	A	109	CYS
1	B	39	ILE
1	B	229	LEU
1	C	218	PRO
1	D	52	ASP
1	D	106	THR
1	D	218	PRO
1	A	216	CYS
1	A	232	LYS
1	B	176	ILE
1	C	227	PRO
1	D	51	ASP
1	D	176	ILE
1	A	53	LEU
1	A	218	PRO
1	B	88	VAL
1	B	102	ILE
1	A	176	ILE
1	B	55	PRO
1	A	48	VAL
1	B	215	GLY
1	B	236	VAL
1	B	274	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	256/303 (84%)	255 (100%)	1 (0%)	84 90

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	255/303 (84%)	208 (82%)	47 (18%)	1	9
1	C	257/303 (85%)	256 (100%)	1 (0%)	84	90
1	D	257/303 (85%)	251 (98%)	6 (2%)	44	74
All	All	1025/1212 (85%)	970 (95%)	55 (5%)	20	53

All (55) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	138	LYS
1	D	196	CYS
1	D	198	PHE
1	D	278	LEU
1	D	282	LYS
1	D	284	SER
1	A	198	PHE
1	B	98	MET
1	B	100	LEU
1	B	102	ILE
1	B	149	THR
1	B	150	ILE
1	B	177	HIS
1	B	178	ARG
1	B	179	ASP
1	B	181	LYS
1	B	186	LEU
1	B	187	ILE
1	B	190	LEU
1	B	192	GLN
1	B	193	VAL
1	B	196	CYS
1	B	200	ILE
1	B	201	SER
1	B	212	ILE
1	B	213	ASP
1	B	217	LYS
1	B	220	MET
1	B	228	GLU
1	B	229	LEU
1	B	231	GLN
1	B	232	LYS
1	B	243	LEU

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Mol	Chain	Res	Type
1	B	248	ILE
1	B	250	LEU
1	B	254	ARG
1	B	262	THR
1	B	270	VAL
1	B	281	ASP
1	B	282	LYS
1	B	284	SER
1	B	288	VAL
1	B	297	LYS
1	B	300	LYS
1	B	306	PRO
1	B	312	PRO
1	B	316	LEU
1	B	318	GLU
1	B	319	SER
1	B	323	ASP
1	B	324	VAL
1	B	329	LYS
1	B	330	LEU
1	B	332	LEU
1	C	196	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	D	91	GLN
1	D	184	ASN
1	D	188	ASN
1	D	226	ASN
1	D	298	ASN
1	D	317	HIS
1	A	91	GLN
1	A	184	ASN
1	A	192	GLN
1	A	311	HIS
1	B	89	ASN
1	B	93	GLN
1	B	148	GLN
1	B	170	HIS
1	B	231	GLN
1	B	265	GLN

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Mol	Chain	Res	Type
1	C	43	ASN
1	C	44	GLN
1	C	91	GLN
1	C	230	ASN
1	C	265	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 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	1FM	B	401	-	27,27,27	2.98	12 (44%)	33,37,37	2.21	10 (30%)
2	1FM	A	401	-	27,27,27	3.37	12 (44%)	33,37,37	2.60	10 (30%)
2	1FM	D	401	1	27,27,27	3.56	10 (37%)	33,37,37	3.16	15 (45%)
2	1FM	C	401	1	27,27,27	3.00	12 (44%)	33,37,37	2.52	11 (33%)

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	1FM	B	401	-	-	16/30/30/30	0/1/2/2
2	1FM	A	401	-	-	15/30/30/30	0/1/2/2
2	1FM	D	401	1	-	14/30/30/30	0/1/2/2
2	1FM	C	401	1	-	9/30/30/30	0/1/2/2

All (46) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	401	1FM	C41-C42	12.53	1.66	1.32
2	C	401	1FM	C41-C42	8.92	1.56	1.32
2	B	401	1FM	C41-C42	8.37	1.55	1.32
2	A	401	1FM	C41-C42	8.31	1.55	1.32
2	C	401	1FM	O48-C59	7.10	1.62	1.42
2	D	401	1FM	C24-C39	6.56	1.61	1.53
2	B	401	1FM	O48-C59	6.32	1.60	1.42
2	A	401	1FM	O48-C59	6.15	1.60	1.42
2	A	401	1FM	C39-C40	5.89	1.59	1.53
2	A	401	1FM	C24-C39	5.85	1.60	1.53
2	D	401	1FM	C34-C24	5.56	1.62	1.53
2	A	401	1FM	C3-C23	5.03	1.55	1.47
2	B	401	1FM	C3-C23	4.99	1.55	1.47
2	D	401	1FM	C18-C42	4.87	1.64	1.50
2	D	401	1FM	O46-C11	-4.67	1.26	1.36
2	A	401	1FM	O48-C15	4.60	1.46	1.37
2	B	401	1FM	O48-C15	4.54	1.46	1.37
2	D	401	1FM	C2-C26	4.01	1.59	1.50
2	B	401	1FM	C24-C39	3.95	1.57	1.53
2	C	401	1FM	C3-C23	3.87	1.53	1.47
2	C	401	1FM	O44-C39	3.86	1.49	1.42
2	A	401	1FM	C16-C11	3.80	1.44	1.38
2	B	401	1FM	C16-C11	3.73	1.44	1.38
2	A	401	1FM	C2-C26	3.72	1.59	1.50
2	C	401	1FM	C18-C42	3.39	1.59	1.50
2	C	401	1FM	O15-C26	3.37	1.41	1.34
2	D	401	1FM	O40-C40	-3.34	1.18	1.22
2	A	401	1FM	C14-C15	3.28	1.44	1.39
2	C	401	1FM	C16-C11	3.08	1.43	1.38
2	C	401	1FM	O15-C31	-3.04	1.41	1.47
2	C	401	1FM	C34-C17	2.96	1.58	1.50
2	B	401	1FM	C2-C26	2.95	1.57	1.50
2	A	401	1FM	O15-C26	2.83	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	401	1FM	O40-C40	-2.82	1.18	1.22
2	C	401	1FM	C2-C26	2.73	1.56	1.50
2	D	401	1FM	C2-C11	-2.71	1.37	1.41
2	B	401	1FM	C39-C40	2.43	1.55	1.53
2	D	401	1FM	O44-C39	-2.42	1.37	1.42
2	C	401	1FM	O48-C15	2.38	1.42	1.37
2	B	401	1FM	C18-C42	2.37	1.57	1.50
2	B	401	1FM	C16-C15	2.35	1.42	1.39
2	A	401	1FM	C34-C17	2.33	1.56	1.50
2	B	401	1FM	C34-C17	2.31	1.56	1.50
2	C	401	1FM	C16-C15	2.30	1.42	1.39
2	B	401	1FM	C14-C15	2.21	1.42	1.39
2	D	401	1FM	C16-C15	-2.17	1.35	1.39

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	1FM	C18-C42-C41	-11.82	100.36	125.93
2	A	401	1FM	C62-C31-C18	-8.58	97.78	113.26
2	C	401	1FM	C18-C42-C41	-6.83	111.16	125.93
2	D	401	1FM	C34-C17-C23	6.83	133.12	124.31
2	A	401	1FM	C18-C42-C41	-5.68	113.64	125.93
2	B	401	1FM	C18-C42-C41	-5.65	113.71	125.93
2	C	401	1FM	C62-C31-C18	-5.54	103.27	113.26
2	A	401	1FM	C42-C41-C40	-5.47	114.25	124.40
2	C	401	1FM	C31-O15-C26	-5.42	107.56	117.67
2	C	401	1FM	C34-C17-C23	4.98	130.74	124.31
2	B	401	1FM	C34-C17-C23	4.51	130.13	124.31
2	B	401	1FM	C59-O48-C15	4.49	127.13	117.50
2	B	401	1FM	C42-C41-C40	-4.46	116.11	124.40
2	D	401	1FM	C16-C11-C2	4.29	125.72	120.92
2	A	401	1FM	C31-O15-C26	-3.99	110.23	117.67
2	B	401	1FM	O15-C31-C62	-3.87	99.30	107.96
2	A	401	1FM	C34-C17-C23	3.86	129.28	124.31
2	D	401	1FM	O44-C39-C40	-3.82	102.26	109.25
2	D	401	1FM	C24-C34-C17	-3.71	107.06	112.88
2	B	401	1FM	C62-C31-C18	-3.37	107.19	113.26
2	D	401	1FM	C62-C31-C18	-3.28	107.34	113.26
2	C	401	1FM	C59-O48-C15	3.26	124.48	117.50
2	A	401	1FM	C31-C18-C42	3.24	120.51	114.11
2	C	401	1FM	O44-C39-C24	-3.16	101.41	109.46
2	D	401	1FM	C2-C3-C23	3.13	126.65	121.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	401	1FM	C42-C41-C40	-3.03	118.77	124.40
2	C	401	1FM	O44-C39-C40	-2.96	103.83	109.25
2	D	401	1FM	O42-C24-C34	2.87	115.84	109.24
2	C	401	1FM	O15-C31-C18	2.70	114.11	107.09
2	A	401	1FM	C59-O48-C15	2.62	123.12	117.50
2	D	401	1FM	C3-C2-C11	-2.61	116.08	118.73
2	C	401	1FM	C42-C41-C40	-2.59	119.59	124.40
2	A	401	1FM	C3-C14-C15	2.58	123.39	120.46
2	B	401	1FM	C3-C14-C15	2.57	123.37	120.46
2	D	401	1FM	C31-O15-C26	-2.53	112.95	117.67
2	C	401	1FM	C31-C18-C42	2.44	118.92	114.11
2	D	401	1FM	C31-C18-C42	2.35	118.73	114.11
2	A	401	1FM	O44-C39-C40	-2.34	104.98	109.25
2	D	401	1FM	C14-C3-C23	-2.30	114.76	120.66
2	B	401	1FM	C31-C18-C42	2.23	118.52	114.11
2	B	401	1FM	C3-C23-C17	2.22	130.23	125.55
2	D	401	1FM	C16-C15-C14	-2.16	117.71	120.98
2	A	401	1FM	C16-C15-C14	-2.08	117.83	120.98
2	C	401	1FM	C24-C34-C17	2.05	116.10	112.88
2	B	401	1FM	C24-C34-C17	2.03	116.07	112.88
2	D	401	1FM	C3-C14-C15	2.02	122.75	120.46

There are no chirality outliers.

All (54) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	401	1FM	C39-C24-C34-C17
2	D	401	1FM	O42-C24-C34-C17
2	D	401	1FM	C34-C24-C39-C40
2	D	401	1FM	O42-C24-C39-O44
2	D	401	1FM	C24-C39-C40-C41
2	D	401	1FM	O44-C39-C40-C41
2	D	401	1FM	C40-C41-C42-C18
2	A	401	1FM	C2-C26-O15-C31
2	A	401	1FM	C42-C18-C31-O15
2	A	401	1FM	C42-C18-C31-C62
2	A	401	1FM	C34-C24-C39-C40
2	A	401	1FM	C34-C24-C39-O44
2	A	401	1FM	C39-C40-C41-C42
2	A	401	1FM	O40-C40-C41-C42
2	A	401	1FM	C40-C41-C42-C18
2	B	401	1FM	C42-C18-C31-O15

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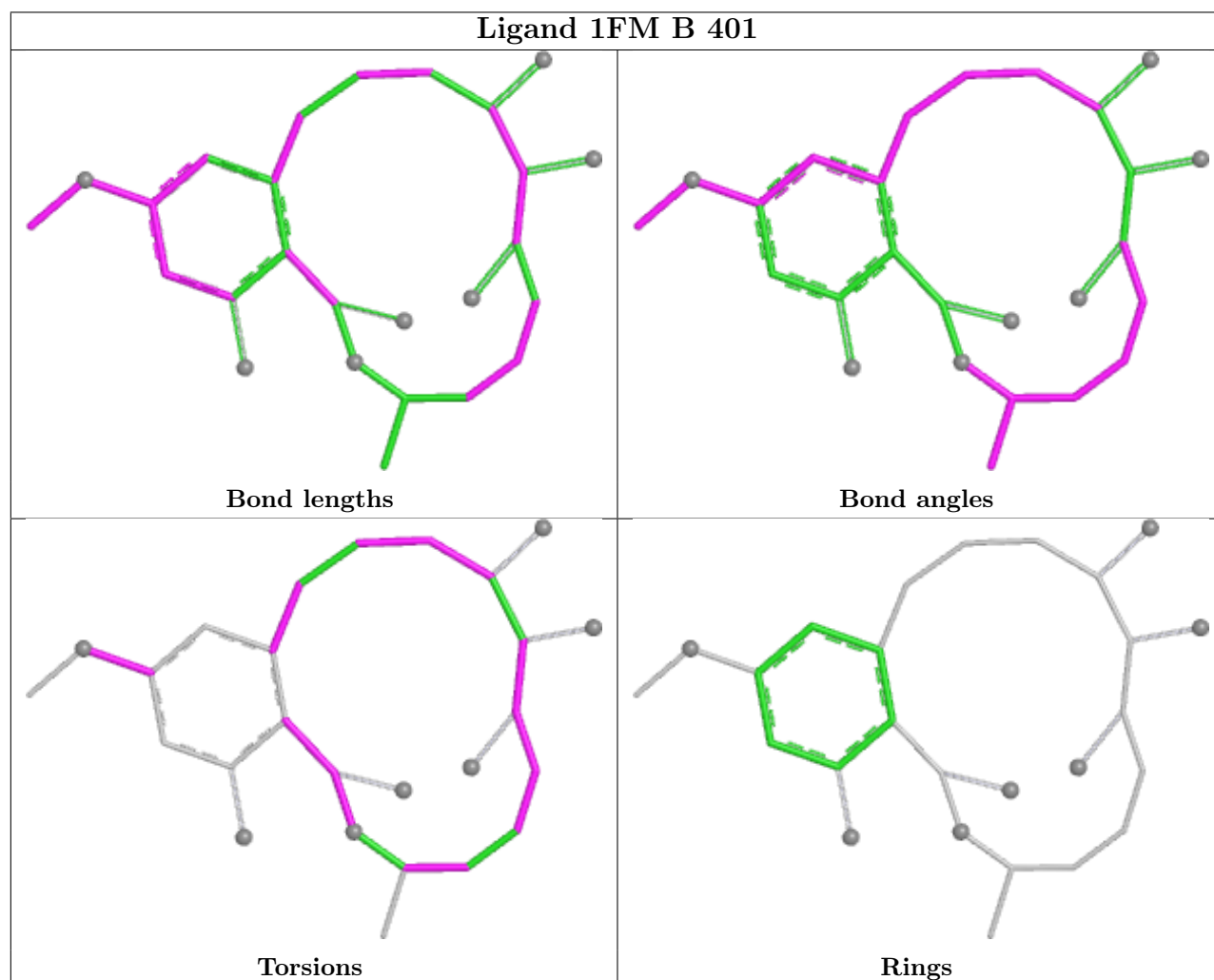
Mol	Chain	Res	Type	Atoms
2	B	401	1FM	C42-C18-C31-C62
2	B	401	1FM	C39-C24-C34-C17
2	B	401	1FM	O42-C24-C34-C17
2	B	401	1FM	C24-C39-C40-C41
2	B	401	1FM	C39-C40-C41-C42
2	B	401	1FM	O40-C40-C41-C42
2	B	401	1FM	C40-C41-C42-C18
2	C	401	1FM	O42-C24-C34-C17
2	C	401	1FM	O42-C24-C39-C40
2	C	401	1FM	C2-C26-O15-C31
2	B	401	1FM	C14-C15-O48-C59
2	B	401	1FM	C16-C15-O48-C59
2	C	401	1FM	C14-C15-O48-C59
2	C	401	1FM	C16-C15-O48-C59
2	A	401	1FM	O38-C26-O15-C31
2	C	401	1FM	O38-C26-O15-C31
2	B	401	1FM	C2-C26-O15-C31
2	B	401	1FM	O38-C26-O15-C31
2	B	401	1FM	C23-C17-C34-C24
2	A	401	1FM	C14-C15-O48-C59
2	A	401	1FM	C16-C15-O48-C59
2	D	401	1FM	C17-C23-C3-C2
2	D	401	1FM	C14-C15-O48-C59
2	A	401	1FM	C39-C24-C34-C17
2	C	401	1FM	C39-C24-C34-C17
2	D	401	1FM	C17-C23-C3-C14
2	D	401	1FM	C16-C15-O48-C59
2	C	401	1FM	C34-C24-C39-C40
2	D	401	1FM	C23-C17-C34-C24
2	A	401	1FM	C3-C2-C26-O38
2	D	401	1FM	O44-C39-C40-O40
2	B	401	1FM	C17-C23-C3-C14
2	D	401	1FM	C31-C18-C42-C41
2	C	401	1FM	C34-C24-C39-O44
2	A	401	1FM	O42-C24-C34-C17
2	A	401	1FM	C3-C2-C26-O15
2	B	401	1FM	C17-C23-C3-C2
2	B	401	1FM	C11-C2-C26-O38

There are no ring outliers.

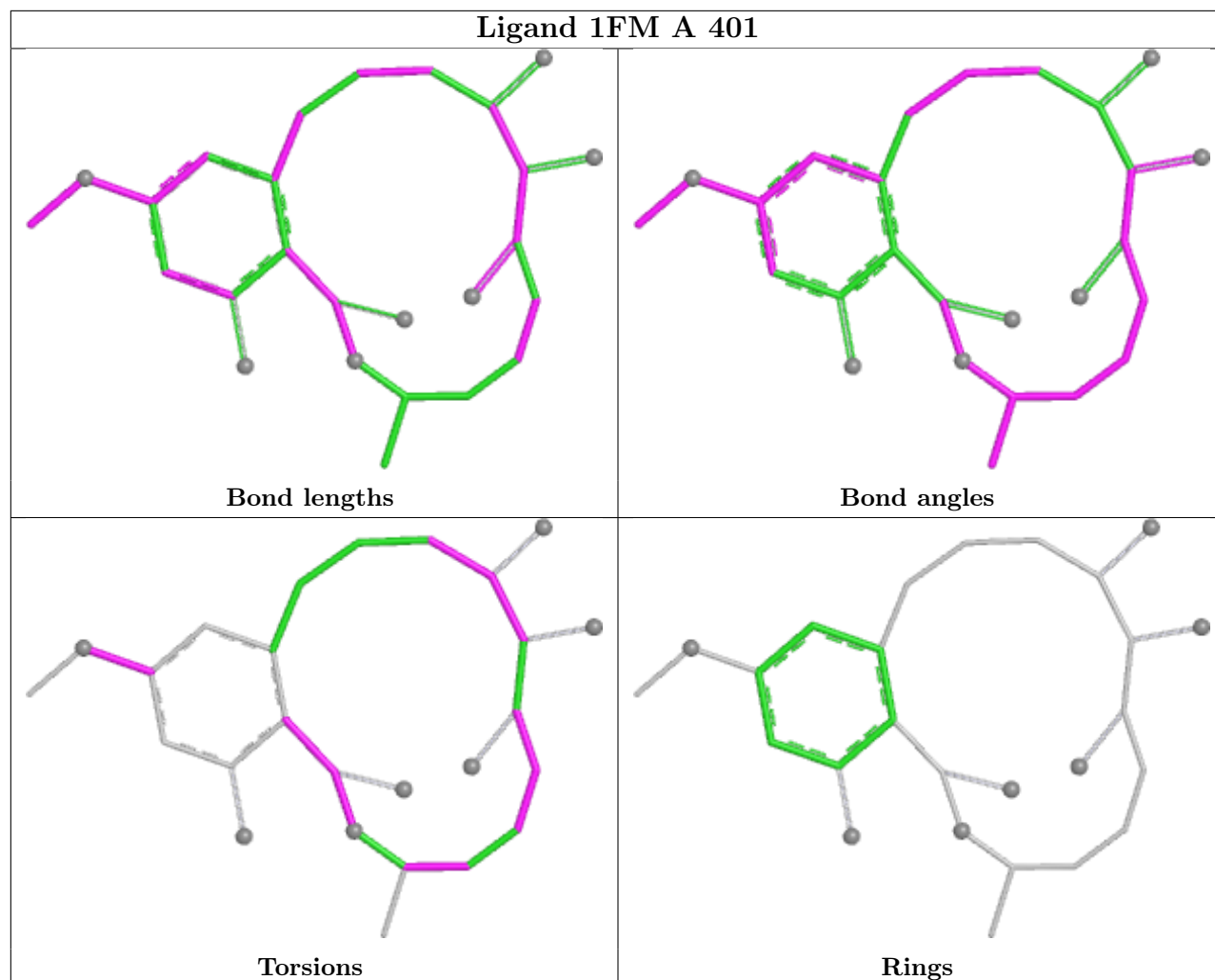
4 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	401	1FM	6	0
2	A	401	1FM	6	0
2	D	401	1FM	2	0
2	C	401	1FM	6	0

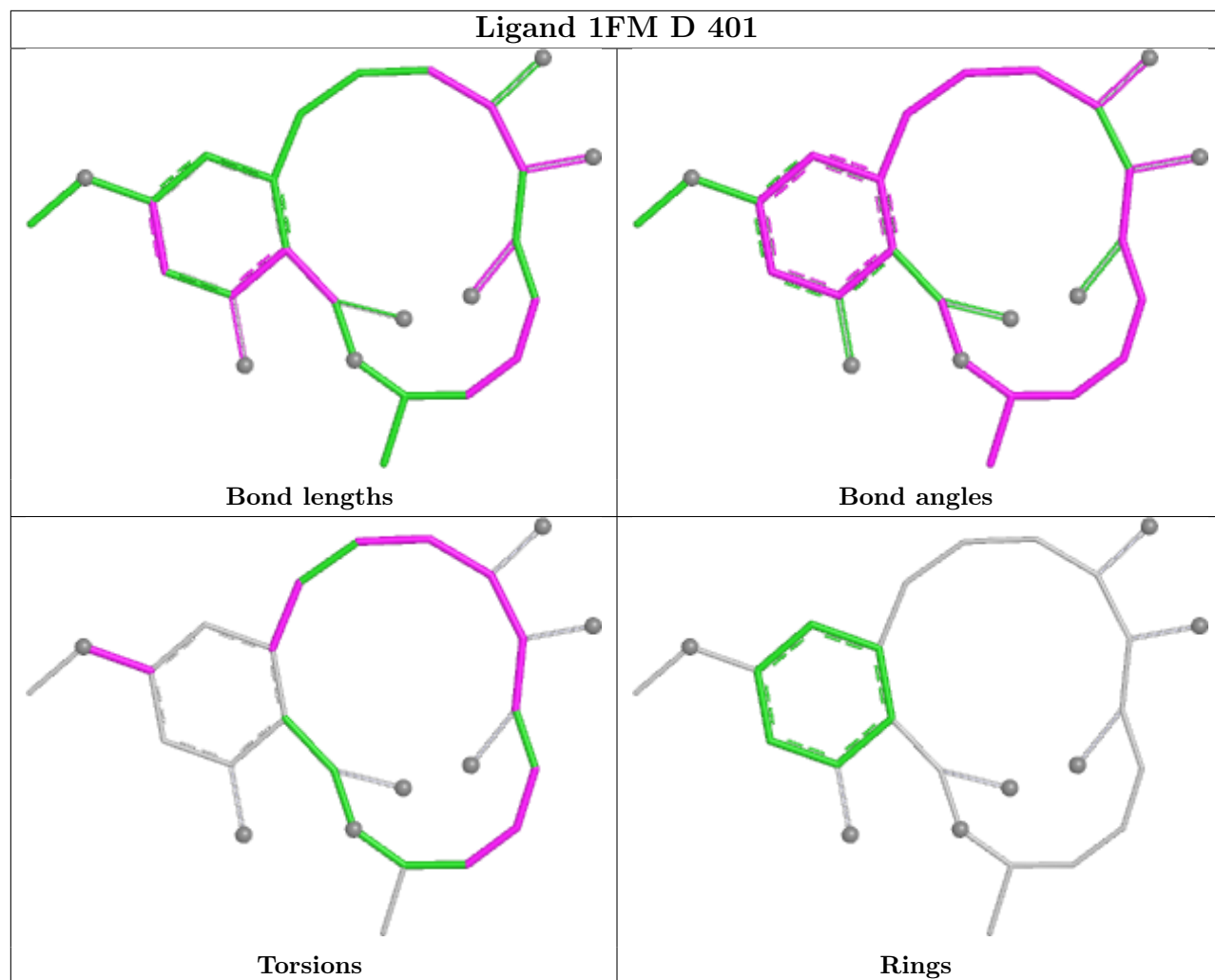
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

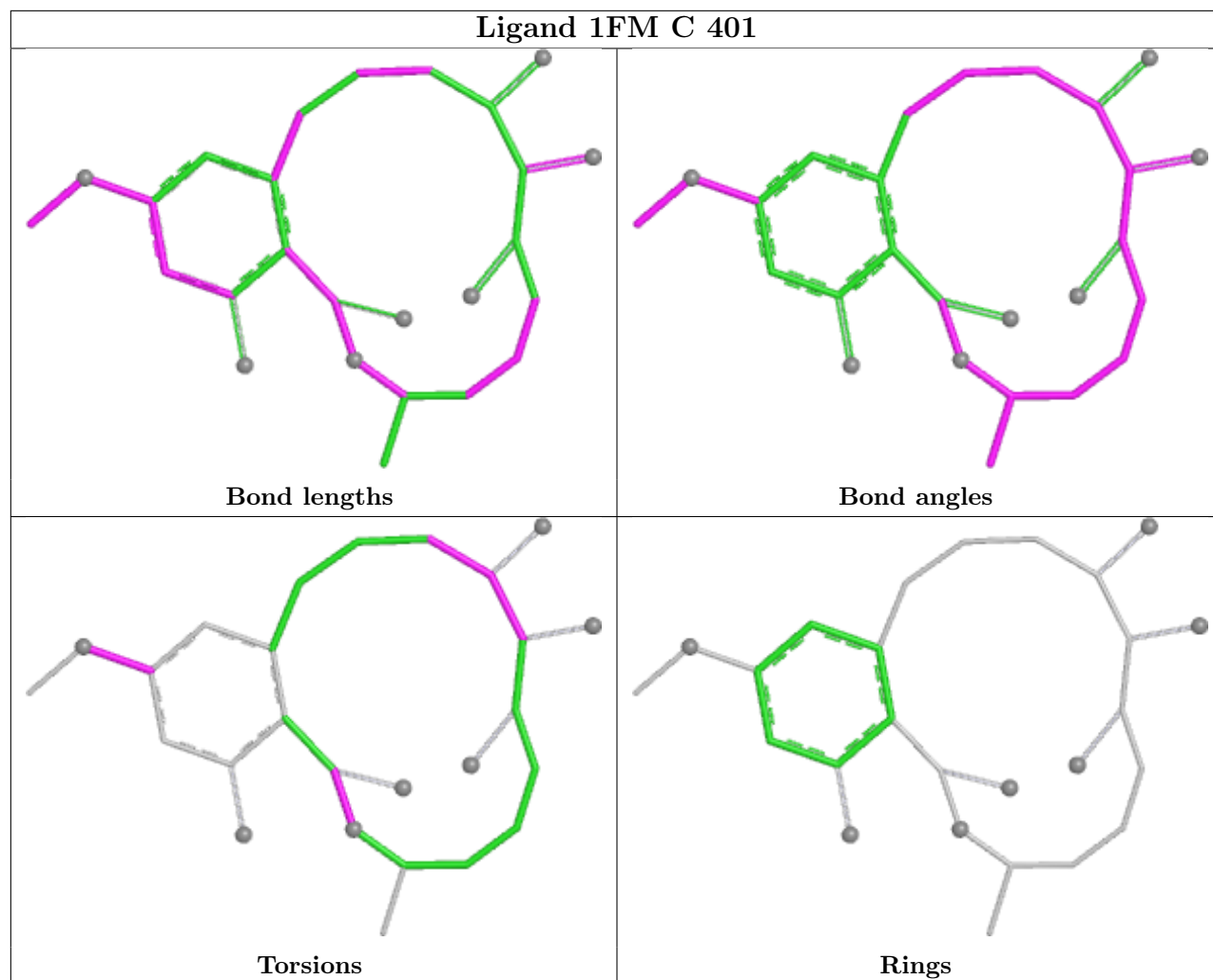


## Ligand 1FM A 401



## Ligand 1FM D 401





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

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

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

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	288/340 (84%)	-0.15	2 (0%) 84 66	57, 99, 194, 229	0
1	B	287/340 (84%)	0.10	7 (2%) 59 36	30, 109, 211, 245	0
1	C	289/340 (85%)	-0.10	4 (1%) 73 51	55, 106, 206, 236	0
1	D	289/340 (85%)	-0.09	2 (0%) 84 66	46, 98, 185, 247	0
All	All	1153/1360 (84%)	-0.06	15 (1%) 75 53	30, 104, 204, 247	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	201	SER	5.2
1	B	199	GLY	4.9
1	B	200	ILE	3.5
1	B	213	ASP	3.4
1	A	197	ASP	3.2
1	B	102	ILE	2.9
1	C	99	ASP	2.7
1	C	50	ALA	2.4
1	D	180	VAL	2.3
1	D	198	PHE	2.2
1	B	234	TYR	2.2
1	C	125	VAL	2.1
1	A	219	TYR	2.0
1	C	198	PHE	2.0
1	B	127	ILE	2.0

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

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

## 6.3 Carbohydrates [i](#)

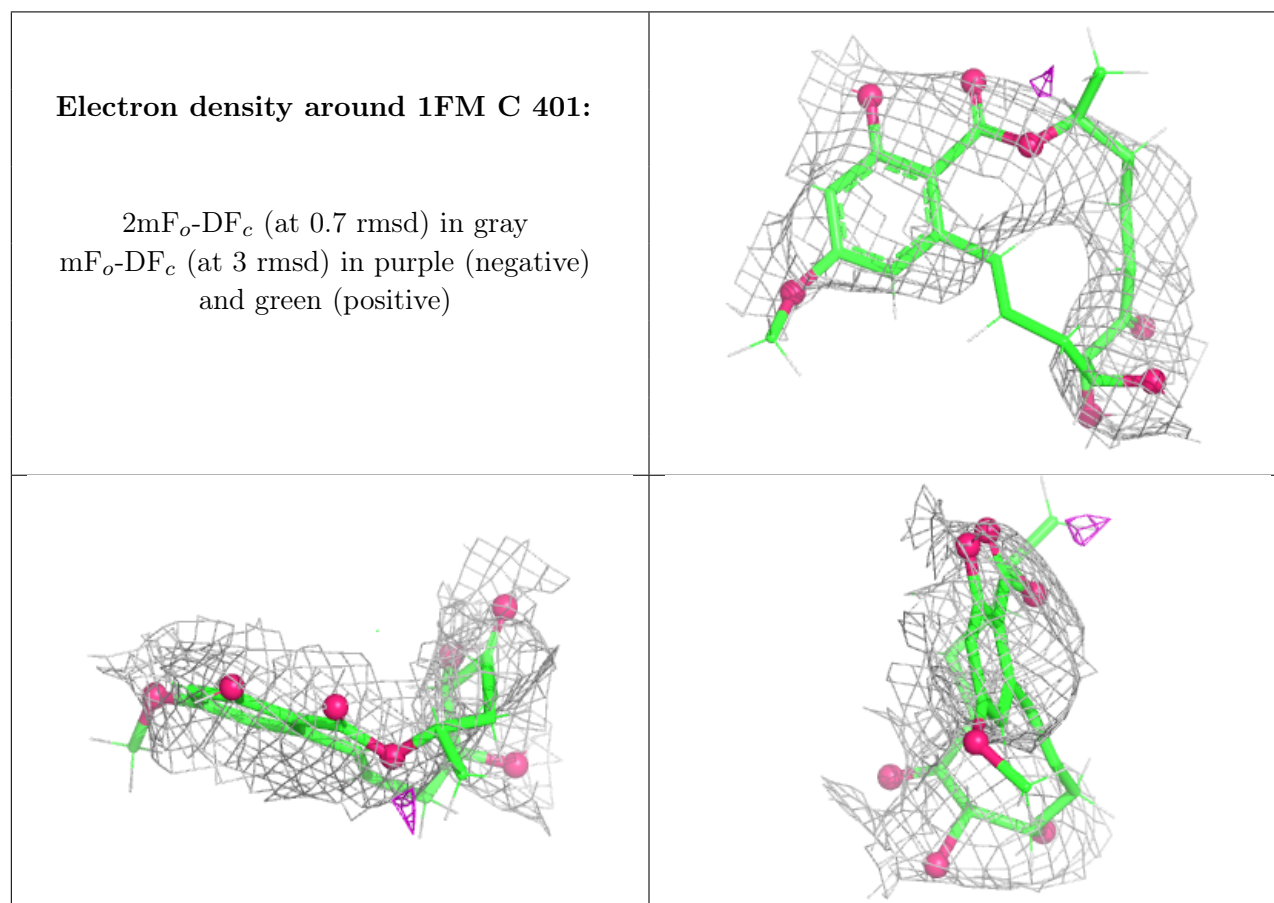
There are no oligosaccharides in this entry.

## 6.4 Ligands [i](#)

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

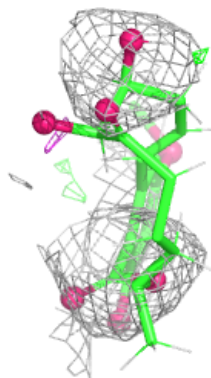
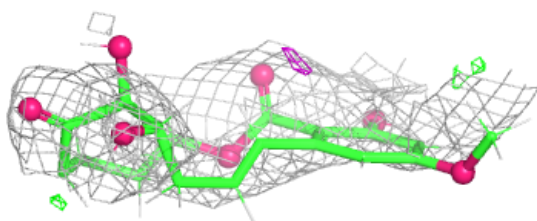
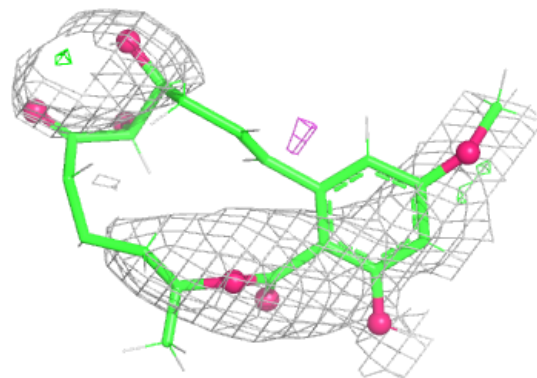
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	1FM	C	401	26/26	0.80	0.12	113,144,181,193	0
2	1FM	B	401	26/26	0.81	0.14	117,163,184,207	0
2	1FM	D	401	26/26	0.82	0.14	89,125,149,157	0
2	1FM	A	401	26/26	0.90	0.09	107,136,162,175	0

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 1FM B 401:**

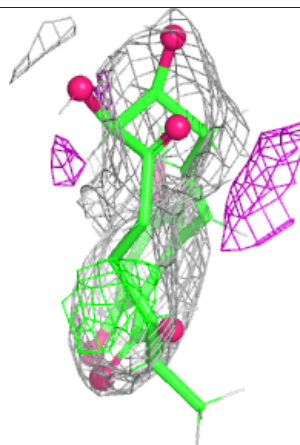
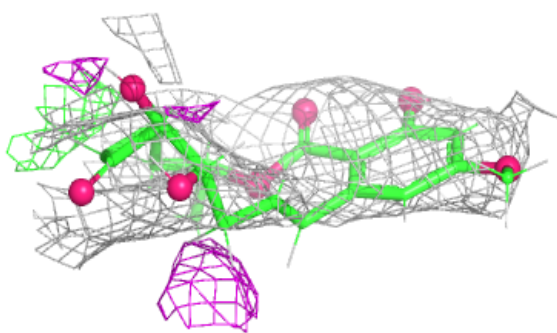
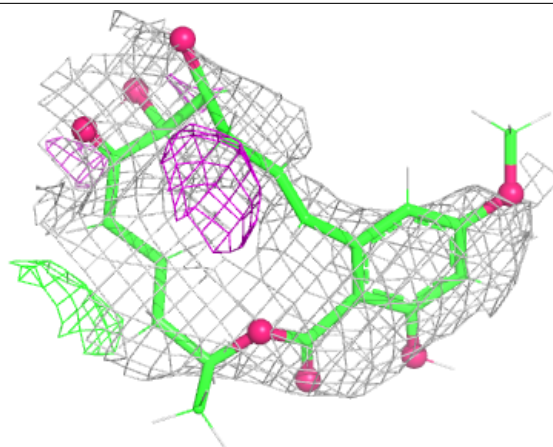
$2mF_o - DF_c$  (at 0.7 rmsd) in gray  
 $mF_o - DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)

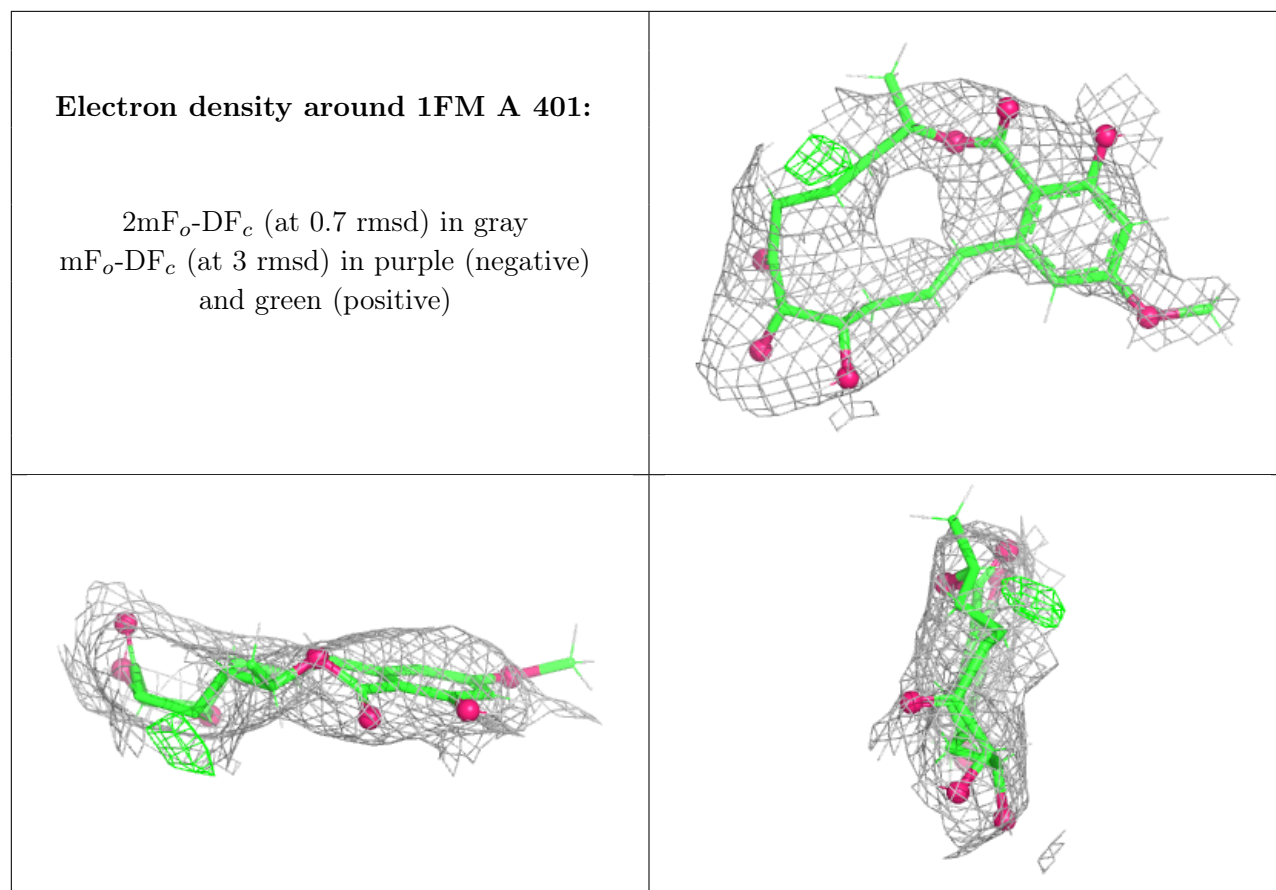




**Electron density around 1FM D 401:**

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





## 6.5 Other polymers ⓘ

There are no such residues in this entry.