WORLDWIDE wwPDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Oct 30, 2023 – 08:48 PM JST

PDB ID	:	4Z7F
Title	:	Crystal structure of FolT bound with folic acid
Authors	:	Zhao, Q.; Wang, C.C.; Wang, C.Y.; Zhang, P.
Deposited on	:	2015-04-07
Resolution	:	3.19 Å(reported)

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

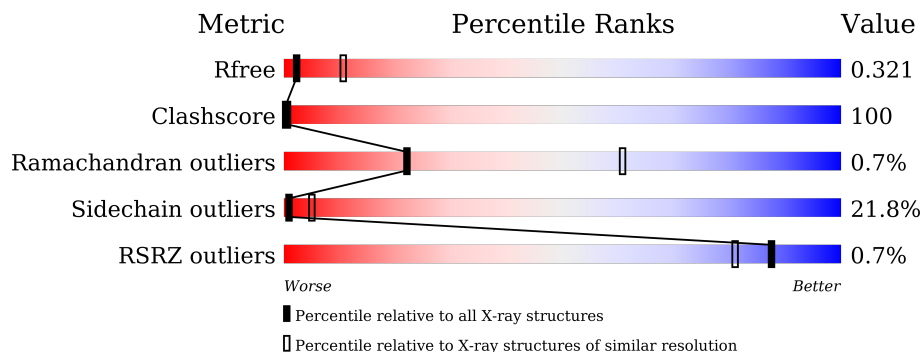|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.19 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	Percentile Ranks	Value
Rfree		0.321
Clashscore		100
Ramachandran outliers		0.7%
Sidechain outliers		21.8%
RSRZ outliers		0.7%

Worse ... *Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	199	% 25% 46% 10% · 18%
1	B	199	% 29% 47% 7% · 16%
1	C	199	% 19% 45% 19% · 17%
1	D	199	31% 41% 10% · 17%
1	E	199	% 11% 43% 17% · 26%
1	F	199	2% 15% 35% 25% · 25%

WORLDWIDE wwPDB PROTEIN DATA BANK

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	FOL	A	201	-	-	X	-
2	FOL	B	201	-	-	X	-
2	FOL	D	201	-	-	X	-
2	FOL	E	201	-	-	X	-
2	FOL	F	201	-	-	X	-

Full wwPDB X-ray Structure Validation Report

2 Entry composition ⓘ

There are 2 unique types of molecules in this entry. The entry contains 7862 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 Folate ECF transporter.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	163	Total	C	N	O	S	0	0	0
			1300	899	192	204	5			
1	B	168	Total	C	N	O	S	0	0	0
			1341	927	197	212	5			
1	C	166	Total	C	N	O	S	0	0	0
			1331	920	199	207	5			
1	D	166	Total	C	N	O	S	0	0	0
			1330	919	196	210	5			
1	E	147	Total	C	N	O	S	0	0	0
			1175	817	173	181	4			
1	F	150	Total	C	N	O	S	0	0	0
			1193	827	175	186	5			

There are 120 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP Q837A3
A	-18	GLY	-	expression tag	UNP Q837A3
A	-17	SER	-	expression tag	UNP Q837A3
A	-16	SER	-	expression tag	UNP Q837A3
A	-15	HIS	-	expression tag	UNP Q837A3
A	-14	HIS	-	expression tag	UNP Q837A3
A	-13	HIS	-	expression tag	UNP Q837A3
A	-12	HIS	-	expression tag	UNP Q837A3
A	-11	HIS	-	expression tag	UNP Q837A3
A	-10	HIS	-	expression tag	UNP Q837A3
A	-9	SER	-	expression tag	UNP Q837A3
A	-8	SER	-	expression tag	UNP Q837A3
A	-7	GLY	-	expression tag	UNP Q837A3
A	-6	LEU	-	expression tag	UNP Q837A3
A	-5	VAL	-	expression tag	UNP Q837A3
A	-4	PRO	-	expression tag	UNP Q837A3
A	-3	ARG	-	expression tag	UNP Q837A3

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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q837A3
A	-1	SER	-	expression tag	UNP Q837A3
A	0	HIS	-	expression tag	UNP Q837A3
B	-19	MET	-	expression tag	UNP Q837A3
B	-18	GLY	-	expression tag	UNP Q837A3
B	-17	SER	-	expression tag	UNP Q837A3
B	-16	SER	-	expression tag	UNP Q837A3
B	-15	HIS	-	expression tag	UNP Q837A3
B	-14	HIS	-	expression tag	UNP Q837A3
B	-13	HIS	-	expression tag	UNP Q837A3
B	-12	HIS	-	expression tag	UNP Q837A3
B	-11	HIS	-	expression tag	UNP Q837A3
B	-10	HIS	-	expression tag	UNP Q837A3
B	-9	SER	-	expression tag	UNP Q837A3
B	-8	SER	-	expression tag	UNP Q837A3
B	-7	GLY	-	expression tag	UNP Q837A3
B	-6	LEU	-	expression tag	UNP Q837A3
B	-5	VAL	-	expression tag	UNP Q837A3
B	-4	PRO	-	expression tag	UNP Q837A3
B	-3	ARG	-	expression tag	UNP Q837A3
B	-2	GLY	-	expression tag	UNP Q837A3
B	-1	SER	-	expression tag	UNP Q837A3
B	0	HIS	-	expression tag	UNP Q837A3
C	-19	MET	-	expression tag	UNP Q837A3
C	-18	GLY	-	expression tag	UNP Q837A3
C	-17	SER	-	expression tag	UNP Q837A3
C	-16	SER	-	expression tag	UNP Q837A3
C	-15	HIS	-	expression tag	UNP Q837A3
C	-14	HIS	-	expression tag	UNP Q837A3
C	-13	HIS	-	expression tag	UNP Q837A3
C	-12	HIS	-	expression tag	UNP Q837A3
C	-11	HIS	-	expression tag	UNP Q837A3
C	-10	HIS	-	expression tag	UNP Q837A3
C	-9	SER	-	expression tag	UNP Q837A3
C	-8	SER	-	expression tag	UNP Q837A3
C	-7	GLY	-	expression tag	UNP Q837A3
C	-6	LEU	-	expression tag	UNP Q837A3
C	-5	VAL	-	expression tag	UNP Q837A3
C	-4	PRO	-	expression tag	UNP Q837A3
C	-3	ARG	-	expression tag	UNP Q837A3
C	-2	GLY	-	expression tag	UNP Q837A3
C	-1	SER	-	expression tag	UNP Q837A3

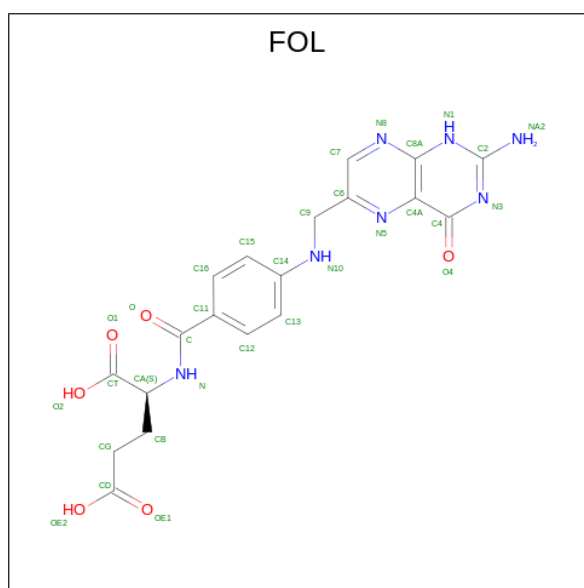*Continued on next page...*

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP Q837A3
D	-19	MET	-	expression tag	UNP Q837A3
D	-18	GLY	-	expression tag	UNP Q837A3
D	-17	SER	-	expression tag	UNP Q837A3
D	-16	SER	-	expression tag	UNP Q837A3
D	-15	HIS	-	expression tag	UNP Q837A3
D	-14	HIS	-	expression tag	UNP Q837A3
D	-13	HIS	-	expression tag	UNP Q837A3
D	-12	HIS	-	expression tag	UNP Q837A3
D	-11	HIS	-	expression tag	UNP Q837A3
D	-10	HIS	-	expression tag	UNP Q837A3
D	-9	SER	-	expression tag	UNP Q837A3
D	-8	SER	-	expression tag	UNP Q837A3
D	-7	GLY	-	expression tag	UNP Q837A3
D	-6	LEU	-	expression tag	UNP Q837A3
D	-5	VAL	-	expression tag	UNP Q837A3
D	-4	PRO	-	expression tag	UNP Q837A3
D	-3	ARG	-	expression tag	UNP Q837A3
D	-2	GLY	-	expression tag	UNP Q837A3
D	-1	SER	-	expression tag	UNP Q837A3
D	0	HIS	-	expression tag	UNP Q837A3
E	-19	MET	-	expression tag	UNP Q837A3
E	-18	GLY	-	expression tag	UNP Q837A3
E	-17	SER	-	expression tag	UNP Q837A3
E	-16	SER	-	expression tag	UNP Q837A3
E	-15	HIS	-	expression tag	UNP Q837A3
E	-14	HIS	-	expression tag	UNP Q837A3
E	-13	HIS	-	expression tag	UNP Q837A3
E	-12	HIS	-	expression tag	UNP Q837A3
E	-11	HIS	-	expression tag	UNP Q837A3
E	-10	HIS	-	expression tag	UNP Q837A3
E	-9	SER	-	expression tag	UNP Q837A3
E	-8	SER	-	expression tag	UNP Q837A3
E	-7	GLY	-	expression tag	UNP Q837A3
E	-6	LEU	-	expression tag	UNP Q837A3
E	-5	VAL	-	expression tag	UNP Q837A3
E	-4	PRO	-	expression tag	UNP Q837A3
E	-3	ARG	-	expression tag	UNP Q837A3
E	-2	GLY	-	expression tag	UNP Q837A3
E	-1	SER	-	expression tag	UNP Q837A3
E	0	HIS	-	expression tag	UNP Q837A3
F	-19	MET	-	expression tag	UNP Q837A3

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-18	GLY	-	expression tag	UNP Q837A3
F	-17	SER	-	expression tag	UNP Q837A3
F	-16	SER	-	expression tag	UNP Q837A3
F	-15	HIS	-	expression tag	UNP Q837A3
F	-14	HIS	-	expression tag	UNP Q837A3
F	-13	HIS	-	expression tag	UNP Q837A3
F	-12	HIS	-	expression tag	UNP Q837A3
F	-11	HIS	-	expression tag	UNP Q837A3
F	-10	HIS	-	expression tag	UNP Q837A3
F	-9	SER	-	expression tag	UNP Q837A3
F	-8	SER	-	expression tag	UNP Q837A3
F	-7	GLY	-	expression tag	UNP Q837A3
F	-6	LEU	-	expression tag	UNP Q837A3
F	-5	VAL	-	expression tag	UNP Q837A3
F	-4	PRO	-	expression tag	UNP Q837A3
F	-3	ARG	-	expression tag	UNP Q837A3
F	-2	GLY	-	expression tag	UNP Q837A3
F	-1	SER	-	expression tag	UNP Q837A3
F	0	HIS	-	expression tag	UNP Q837A3

- Molecule 2 is FOLIC ACID (three-letter code: FOL) (formula: $C_{19}H_{19}N_7O_6$).

FOL

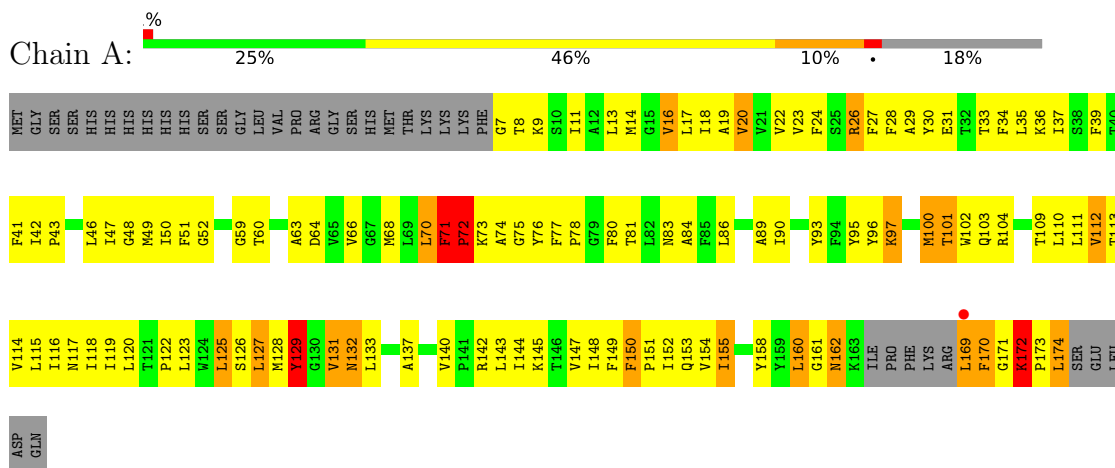| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			32	19	7	6		
2	B	1	Total	C	N	O	0	0
			32	19	7	6		

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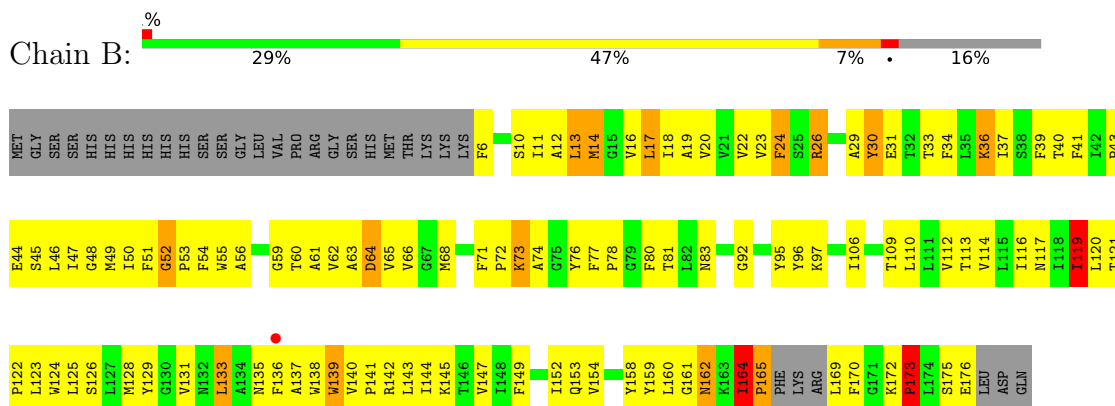| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			32	19	7	6		
2	D	1	Total	C	N	O	0	0
			32	19	7	6		
2	E	1	Total	C	N	O	0	0
			32	19	7	6		
2	F	1	Total	C	N	O	0	0
			32	19	7	6		

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.
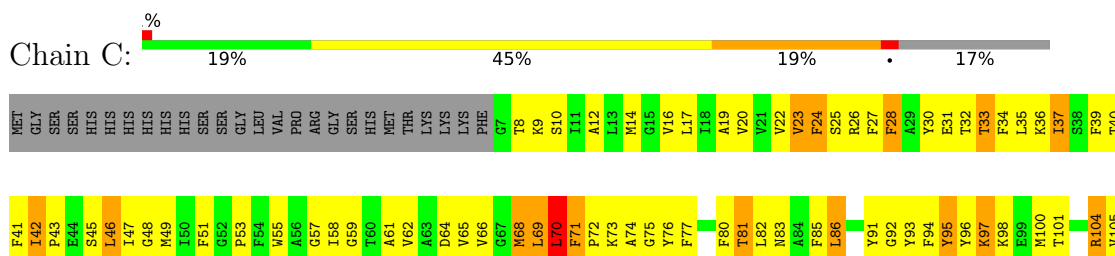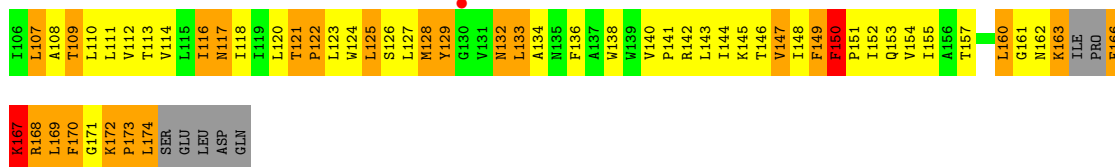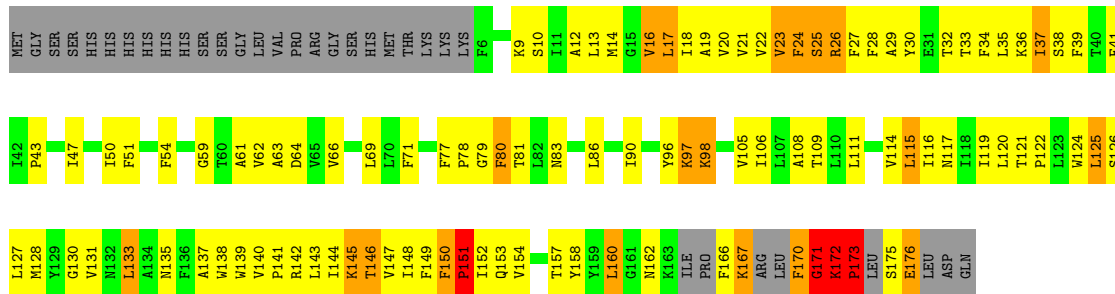
• Molecule 1: Folate ECF transporter

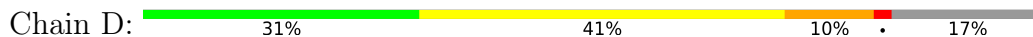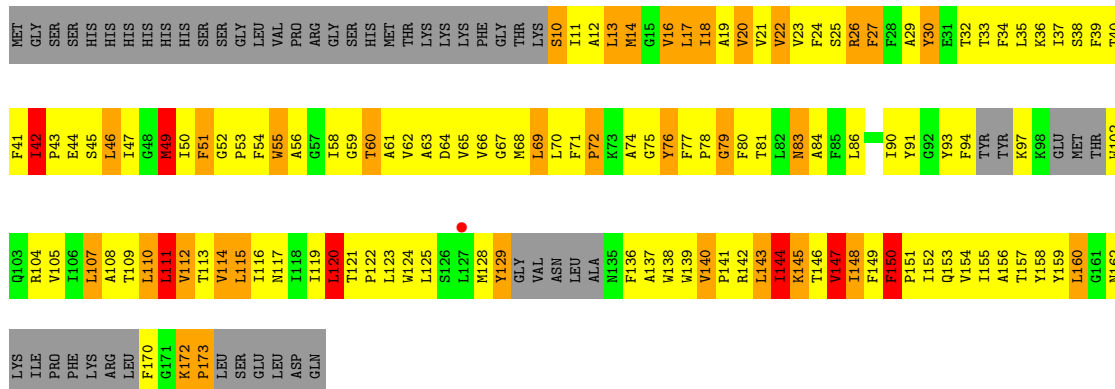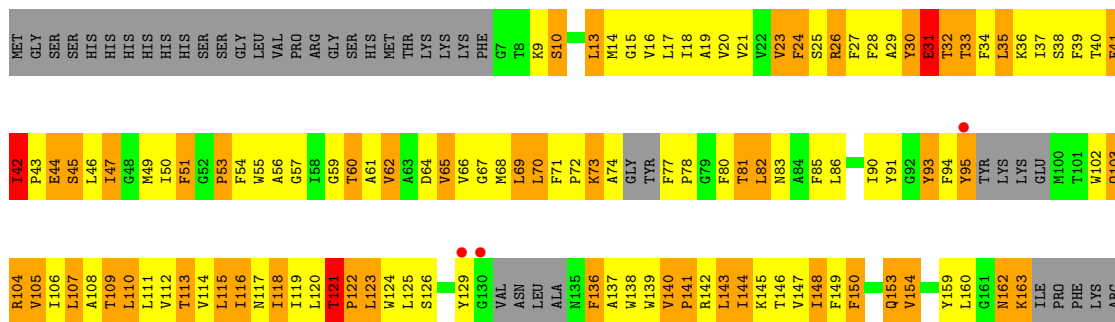• Molecule 1: Folate ECF transporter

• Molecule 1: Folate ECF transporter

I106 L107 A108 T109 L110 L111 V112 T113 V114 L115 I116 N117 I118 I119 L120 T121 P122 L123 W124 L125 S126 L127 M128 Y129 G130 V131 N132 L133 A134 N135 F136 A137 W138 W139 V140 P141 R142 L143 I144 K145 T146 V147 I148 F149 F150 P151 I152 Q153 V154 I155 A156 T157 L160 G161 N162 K163 ILE PRO F166

K167 R168 L169 F170 G171 K172 P173 L174 SER GLU LEU ASP GLN

• Molecule 1: Folate ECF transporter

Chain D: 31% 41% 10% • 17%

MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET THR LYS LYS LYS F6 K9 S10 I11 A12 L13 M14 G15 V16 L17 I18 A19 V20 V21 V22 V23 F24 S25 R26 F27 F28 A29 Y30 E31 T32 T33 F34 L35 K36 I37 S38 F39 T40 F41

I42 P43 I47 I50 F51 F54 G59 T60 A61 V62 A63 D64 V65 V66 L69 L70 F71 F77 P78 G79 F80 T81 L82 N83 L86 I90 Y96 K97 K98 V105 I106 L107 A108 T109 L110 L111 V114 L115 I116 N117 I118 I119 L120 T121 P122 L123 W124 L125 S126

L127 M128 Y129 G130 V131 N132 L133 A134 N135 F136 A137 W138 W139 V140 P141 R142 L143 I144 K145 T146 V147 I148 F149 F150 P151 I152 Q153 V154 T157 Y158 Y159 L160 G161 N162 K163 ILE PRO F166 K167 ARG LEU F170 G171 K172 P173 LEU S175 E176 LEU ASP GLN

• Molecule 1: Folate ECF transporter

Chain E: % 11% 43% 17% • 26%

MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET THR LYS LYS LYS PHE GLY THR LYS S10 I11 A12 L13 M14 G15 V16 L17 I18 A19 V20 V21 V22 V23 F24 S25 R26 F27 F28 A29 Y30 E31 T32 T33 F34 L35 K36 I37 S38 F39 T40

F41 I42 P43 E44 S45 L46 I47 G48 M49 I50 F51 G52 P53 F54 W55 A56 G57 I58 G59 T60 A61 V62 A63 D64 V65 V66 G67 M68 L69 L70 F71 P72 K73 A74 G75 Y76 F77 P78 G79 F80 T81 L82 N83 A84 F85 L86 I90 Y91 G92 Y93 F94 TYR TYR K97 K98 GLU MET THR W102

Q103 R104 V105 I106 L107 A108 T109 L110 L111 V112 T113 V114 L115 I116 N117 I118 I119 L120 T121 P122 L123 W124 L125 S126 L127 M128 Y129 GLY VAL ASN LEU ALA N135 F136 A137 W138 W139 V140 P141 R142 L143 I144 K145 T146 V147 I148 F149 F150 P151 I152 Q153 V154 I155 A156 T157 Y158 Y159 L160 G161 N162

LYS ILE PRO PHE LYS ARG LEU F170 G171 K172 P173 LEU SER GLU LEU ASP GLN

• Molecule 1: Folate ECF transporter

Chain F: 2% 15% 35% 25% • 25%

MET GLY SER SER HIS HIS HIS HIS HIS SER SER GLY LEU VAL PRO ARG GLY SER HIS MET THR LYS LYS LYS PHE G7 T8 K9 S10 L13 M14 G15 V16 L17 I18 A19 V20 V21 V22 V23 F24 S25 R26 F27 F28 A29 Y30 E31 T32 T33 F34 L35 K36 I37 S38 F39 T40 F41

I42 P43 E44 S45 L46 I47 G48 M49 I50 F51 G52 P53 F54 W55 A56 G57 I58 G59 T60 A61 V62 A63 D64 V65 V66 G67 M68 L69 L70 F71 P72 K73 A74 GLY TYR F77 P78 G79 F80 T81 L82 N83 A84 F85 L86 I90 Y91 G92 Y93 F94 Y95 TYR LYS LYS GLU M100 T101 W102 Q103

R104 V105 I106 L107 A108 T109 L110 L111 V112 T113 V114 L115 I116 N117 I118 I119 L120 T121 P122 L123 W124 L125 S126 Y129 G130 VAL ASN LEU ALA N135 F136 A137 W138 W139 V140 P141 R142 L143 I144 K145 T146 V147 I148 F149 F150 Q153 V154 Y159 L160 G161 N162 K163 ILE PRO PHE LYS ARG

L169 F170 G171 LYS PRO LEU SER GLU LEU ASP GLN

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α, β, γ	92.75Å 92.75Å 183.44Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	33.57 – 3.19 33.57 – 3.19	Depositor EDS
% Data completeness (in resolution range)	76.1 (33.57-3.19) 68.3 (33.57-3.19)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	5.79 (at 3.18Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1692)	Depositor
R, R_{free}	0.293 , 0.356 0.290 , 0.321	Depositor DCC
R_{free} test set	2011 reflections (8.97%)	wwPDB-VP
Wilson B-factor (Å^2)	68.8	Xtriage
Anisotropy	0.857	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.20 , 10.9	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.034 for -h,-k,l 0.380 for h,-h-k,-l 0.035 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.90	EDS
Total number of atoms	7862	wwPDB-VP
Average B, all atoms (Å^2)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: FOL

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	0.81	1/1342 (0.1%)	1.01	6/1830 (0.3%)
1	B	0.75	1/1385 (0.1%)	1.05	6/1889 (0.3%)
1	C	0.91	3/1374 (0.2%)	1.01	8/1871 (0.4%)
1	D	0.84	2/1372 (0.1%)	1.00	7/1865 (0.4%)
1	E	0.80	2/1212 (0.2%)	1.34	17/1650 (1.0%)
1	F	0.90	5/1229 (0.4%)	1.16	14/1673 (0.8%)
All	All	0.84	14/7914 (0.2%)	1.10	58/10778 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	C	0	1
1	D	0	2
1	E	0	6
1	F	0	5
All	All	0	15

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	62	VAL	CB-CG2	7.45	1.68	1.52
1	F	62	VAL	CB-CG1	6.92	1.67	1.52
1	F	122	PRO	N-CD	6.73	1.57	1.47
1	D	80	PHE	CE1-CZ	-6.49	1.25	1.37
1	C	122	PRO	N-CD	6.19	1.56	1.47
1	D	80	PHE	CB-CG	-5.92	1.41	1.51
1	C	95	TYR	CD1-CE1	5.49	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	173	PRO	N-CD	5.34	1.55	1.47
1	B	165	PRO	N-CD	5.24	1.55	1.47
1	A	72	PRO	N-CD	5.20	1.55	1.47
1	E	72	PRO	N-CD	5.17	1.55	1.47
1	F	121	THR	C-N	5.15	1.44	1.34
1	F	72	PRO	N-CD	5.13	1.55	1.47
1	E	173	PRO	N-CD	5.12	1.55	1.47

All (58) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	30	TYR	N-CA-C	11.70	142.58	111.00
1	C	71	PHE	C-N-CD	-9.64	99.39	120.60
1	E	111	LEU	CA-CB-CG	9.35	136.79	115.30
1	E	120	LEU	CA-CB-CG	9.21	136.50	115.30
1	C	122	PRO	CA-N-CD	-8.67	99.36	111.50
1	B	173	PRO	N-CA-CB	-8.47	93.14	103.30
1	E	115	LEU	N-CA-C	7.96	132.48	111.00
1	E	115	LEU	CB-CA-C	-7.92	95.14	110.20
1	E	143	LEU	CB-CA-C	-7.64	95.68	110.20
1	F	122	PRO	CA-N-CD	-7.63	100.82	111.50
1	A	172	LYS	N-CA-C	7.59	131.49	111.00
1	C	129	TYR	N-CA-C	-7.34	91.17	111.00
1	E	46	LEU	CA-CB-CG	7.29	132.07	115.30
1	F	31	GLU	N-CA-C	7.00	129.91	111.00
1	F	105	VAL	CB-CA-C	-6.87	98.35	111.40
1	E	30	TYR	CB-CA-C	-6.68	97.04	110.40
1	E	49	MET	CA-CB-CG	6.67	124.65	113.30
1	D	151	PRO	CA-N-CD	-6.55	102.33	111.50
1	F	62	VAL	CA-CB-CG2	6.51	120.67	110.90
1	E	144	ILE	N-CA-C	-6.49	93.48	111.00
1	B	68	MET	CA-CB-CG	-6.42	102.38	113.30
1	B	119	ILE	CG1-CB-CG2	-6.36	97.42	111.40
1	E	148	ILE	CG1-CB-CG2	-6.29	97.56	111.40
1	E	42	ILE	C-N-CD	6.21	141.44	128.40
1	B	52	GLY	C-N-CD	6.17	141.37	128.40
1	D	125	LEU	CA-CB-CG	-6.16	101.13	115.30
1	D	172	LYS	C-N-CD	6.14	141.29	128.40
1	D	171	GLY	N-CA-C	6.12	128.40	113.10
1	F	148	ILE	CB-CA-C	-6.07	99.47	111.60
1	F	42	ILE	C-N-CD	5.90	140.80	128.40
1	A	52	GLY	C-N-CD	5.88	140.75	128.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	68	MET	CG-SD-CE	-5.88	90.80	100.20
1	F	77	PHE	C-N-CD	5.87	140.72	128.40
1	A	150	PHE	C-N-CD	5.84	140.67	128.40
1	C	167	LYS	N-CA-C	5.84	126.76	111.00
1	C	150	PHE	C-N-CD	5.82	140.62	128.40
1	A	71	PHE	C-N-CD	5.80	140.59	128.40
1	E	140	VAL	C-N-CD	5.78	140.53	128.40
1	F	71	PHE	C-N-CD	5.74	140.46	128.40
1	A	129	TYR	N-CA-C	-5.68	95.65	111.00
1	C	172	LYS	C-N-CD	5.67	140.31	128.40
1	A	172	LYS	CB-CA-C	-5.67	99.07	110.40
1	F	149	PHE	C-N-CA	-5.63	107.63	121.70
1	C	46	LEU	CA-CB-CG	5.61	128.20	115.30
1	B	164	ILE	C-N-CD	5.56	140.07	128.40
1	D	150	PHE	C-N-CD	5.38	139.70	128.40
1	E	120	LEU	CB-CG-CD2	-5.38	101.85	111.00
1	D	120	LEU	CB-CG-CD2	-5.38	101.86	111.00
1	C	70	LEU	N-CA-C	-5.34	96.59	111.00
1	F	105	VAL	N-CA-C	-5.30	96.69	111.00
1	F	95	TYR	CA-CB-CG	-5.23	103.46	113.40
1	F	143	LEU	CA-CB-CG	5.22	127.31	115.30
1	F	150	PHE	C-N-CD	5.22	139.36	128.40
1	D	173	PRO	CA-N-CD	-5.15	104.29	111.50
1	E	172	LYS	C-N-CD	5.13	139.17	128.40
1	E	160	LEU	CB-CG-CD2	5.06	119.61	111.00
1	F	154	VAL	CG1-CB-CG2	-5.06	102.80	110.90
1	E	147	VAL	N-CA-C	5.06	124.66	111.00

There are no chirality outliers.

All (15) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	139	TRP	Peptide
1	C	117	ASN	Mainchain
1	D	171	GLY	Peptide
1	D	32	THR	Peptide
1	E	112	VAL	Peptide
1	E	144	ILE	Peptide
1	E	145	LYS	Peptide
1	E	150	PHE	Peptide
1	E	49	MET	Peptide
1	E	79	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	F	105	VAL	Peptide
1	F	141	PRO	Peptide
1	F	30	TYR	Peptide
1	F	31	GLU	Peptide
1	F	51	PHE	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	1300	0	1357	221	4
1	B	1341	0	1395	196	4
1	C	1331	0	1392	273	0
1	D	1330	0	1375	179	0
1	E	1175	0	1222	390	0
1	F	1193	0	1239	348	0
2	A	32	0	17	13	0
2	B	32	0	17	14	0
2	C	32	0	17	6	0
2	D	32	0	17	10	0
2	E	32	0	17	25	0
2	F	32	0	17	46	0
All	All	7862	0	8082	1597	4

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 100.

All (1597) 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:B:96:TYR:CZ	1:B:97:LYS:HE3	1.19	1.66
1:E:68:MET:HE3	2:E:201:FOL:C2	1.30	1.59
1:D:14:MET:CE	1:D:51:PHE:CE2	1.82	1.57
1:B:96:TYR:CE2	1:B:97:LYS:HE3	1.38	1.56
1:D:14:MET:HE2	1:D:51:PHE:CE2	1.07	1.54
1:D:33:THR:HG22	1:D:34:PHE:CE1	1.39	1.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:SER:HB3	1:C:170:PHE:CE1	1.43	1.53
1:E:40:THR:CG2	1:E:44:GLU:HG2	1.38	1.51
1:D:14:MET:HE1	1:D:51:PHE:CD2	1.44	1.50
1:E:39:PHE:CD1	1:E:41:PHE:CE1	2.00	1.50
1:C:49:MET:HE2	1:C:100:MET:CE	1.40	1.49
1:E:54:PHE:CE2	1:E:55:TRP:HZ3	1.32	1.48
1:D:14:MET:CE	1:D:51:PHE:CD2	1.91	1.47
1:E:40:THR:HG21	1:E:44:GLU:CD	1.33	1.46
1:E:40:THR:HG21	1:E:44:GLU:CG	1.44	1.46
1:C:49:MET:HE3	1:C:95:TYR:CD2	1.50	1.44
1:E:115:LEU:HD13	1:E:116:ILE:N	1.28	1.42
1:F:30:TYR:N	1:F:36:LYS:HZ1	0.92	1.42
1:C:49:MET:CE	1:C:100:MET:HE3	1.47	1.42
1:E:69:LEU:HD13	1:E:70:LEU:N	1.21	1.41
1:E:68:MET:CE	2:E:201:FOL:C2	2.01	1.39
1:A:50:ILE:O	1:A:173:PRO:CB	1.73	1.37
1:D:10:SER:OG	1:D:172:LYS:CB	1.72	1.36
1:F:30:TYR:O	1:F:36:LYS:HD3	1.23	1.35
1:E:68:MET:CE	2:E:201:FOL:N3	1.92	1.32
1:B:96:TYR:CE2	1:B:97:LYS:CE	2.10	1.32
1:F:30:TYR:N	1:F:36:LYS:NZ	1.78	1.31
1:C:112:VAL:O	1:C:116:ILE:HG22	1.22	1.31
1:B:96:TYR:CZ	1:B:97:LYS:CE	2.13	1.30
1:E:54:PHE:CE2	1:E:55:TRP:CZ3	2.20	1.29
1:A:100:MET:SD	1:A:161:GLY:HA3	1.70	1.29
1:E:39:PHE:HD1	1:E:41:PHE:CE1	1.43	1.28
1:E:54:PHE:CD2	1:E:55:TRP:CZ3	2.20	1.28
1:E:40:THR:HG21	1:E:44:GLU:OE2	1.27	1.28
1:F:73:LYS:HD2	2:F:201:FOL:C7	1.63	1.27
1:A:50:ILE:O	1:A:173:PRO:HB2	1.28	1.26
1:E:68:MET:HE1	2:E:201:FOL:C4	1.66	1.26
1:E:115:LEU:O	1:E:119:ILE:HG12	1.25	1.26
1:E:139:TRP:CZ3	1:E:142:ARG:HD2	1.67	1.26
1:C:49:MET:CE	1:C:95:TYR:CD2	2.17	1.25
1:F:39:PHE:HA	1:F:41:PHE:CE2	1.72	1.24
1:C:10:SER:CB	1:C:170:PHE:CE1	2.18	1.24
1:E:39:PHE:CD1	1:E:41:PHE:HE1	1.46	1.23
1:F:68:MET:SD	2:F:201:FOL:N1	2.10	1.23
1:C:49:MET:CE	1:C:100:MET:CE	2.05	1.22
1:E:18:ILE:HG23	1:E:63:ALA:CB	1.67	1.22
1:D:33:THR:CG2	1:D:34:PHE:CE1	2.22	1.21

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:THR:CG2	1:E:44:GLU:OE2	1.88	1.21
1:F:80:PHE:HE1	2:F:201:FOL:OE2	1.21	1.20
1:E:18:ILE:CG2	1:E:63:ALA:HB2	1.72	1.19
1:D:10:SER:OG	1:D:172:LYS:HB2	1.03	1.19
1:A:126:SER:HA	1:A:131:VAL:CG2	1.72	1.19
1:F:83:ASN:OD1	1:F:116:ILE:HD11	1.36	1.18
1:D:33:THR:HG22	1:D:34:PHE:CD1	1.79	1.18
1:B:96:TYR:OH	1:B:97:LYS:HE3	1.37	1.18
1:F:80:PHE:CD2	2:F:201:FOL:N3	2.12	1.17
1:E:40:THR:CG2	1:E:44:GLU:CG	2.09	1.17
1:F:13:LEU:HD21	1:F:51:PHE:CE2	1.80	1.16
1:C:70:LEU:C	1:C:72:PRO:HD3	1.64	1.16
1:C:49:MET:HE3	1:C:95:TYR:CG	1.80	1.14
1:C:71:PHE:N	1:C:72:PRO:CD	2.10	1.14
1:F:160:LEU:O	1:F:163:LYS:HG3	1.46	1.14
1:F:61:ALA:HB2	1:F:85:PHE:CD1	1.82	1.13
1:E:69:LEU:CD1	1:E:70:LEU:N	2.11	1.13
1:F:80:PHE:CE2	2:F:201:FOL:N3	2.16	1.13
1:E:68:MET:HE3	2:E:201:FOL:N1	1.63	1.13
1:B:36:LYS:HE2	1:B:37:ILE:H	1.02	1.13
1:E:35:LEU:CD2	1:E:142:ARG:HG2	1.78	1.12
1:F:61:ALA:O	1:F:65:VAL:HG23	1.47	1.12
1:E:35:LEU:HD21	1:E:142:ARG:CG	1.79	1.12
1:F:73:LYS:HD2	2:F:201:FOL:C6	1.79	1.12
1:B:30:TYR:N	1:B:36:LYS:NZ	1.98	1.11
1:F:95:TYR:OH	1:F:108:ALA:HB3	1.48	1.11
1:E:115:LEU:CD1	1:E:116:ILE:N	2.12	1.11
1:E:18:ILE:CG2	1:E:63:ALA:CB	2.28	1.10
1:B:30:TYR:N	1:B:36:LYS:HZ1	1.46	1.10
1:B:30:TYR:HB3	1:B:36:LYS:HE3	1.24	1.10
1:C:98:LYS:NZ	1:C:104:ARG:NH1	1.98	1.10
1:E:23:VAL:HA	1:E:26:ARG:HD2	1.16	1.09
1:A:126:SER:HA	1:A:131:VAL:HG21	1.25	1.09
1:B:96:TYR:OH	1:B:97:LYS:CE	1.96	1.09
1:D:12:ALA:O	1:D:16:VAL:HG22	1.53	1.09
1:F:64:ASP:HB2	1:F:80:PHE:CE2	1.87	1.08
1:F:122:PRO:HA	1:F:125:LEU:HD12	1.15	1.08
1:F:94:PHE:HD2	1:F:108:ALA:HB2	1.10	1.08
1:A:23:VAL:O	1:A:26:ARG:NE	1.87	1.08
1:F:39:PHE:HA	1:F:41:PHE:HE2	0.98	1.08
1:A:100:MET:SD	1:A:161:GLY:CA	2.42	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:54:PHE:HD2	1:E:55:TRP:CE3	1.70	1.07
1:F:16:VAL:HG23	1:F:17:LEU:HD22	1.37	1.07
1:A:26:ARG:HG2	1:A:27:PHE:CD1	1.90	1.06
1:E:77:PHE:CG	1:E:78:PRO:HD2	1.89	1.06
1:E:115:LEU:O	1:E:115:LEU:HD22	1.53	1.06
1:D:54:PHE:CZ	1:D:176:GLU:HB2	1.90	1.06
1:E:112:VAL:HB	1:E:115:LEU:HB3	1.38	1.06
1:F:94:PHE:CD2	1:F:108:ALA:HB2	1.88	1.06
1:C:25:SER:OG	1:C:26:ARG:NH1	1.88	1.06
1:E:141:PRO:O	1:E:144:ILE:HG22	1.53	1.06
1:D:10:SER:CB	1:D:172:LYS:HG3	1.85	1.06
1:C:105:VAL:O	1:C:109:THR:OG1	1.74	1.05
1:E:23:VAL:HA	1:E:26:ARG:CD	1.87	1.05
1:E:77:PHE:CD1	1:E:78:PRO:HD2	1.91	1.05
1:F:32:THR:O	1:F:35:LEU:CD2	2.04	1.04
1:E:30:TYR:HB2	1:E:37:ILE:HG22	1.38	1.04
1:A:68:MET:CE	1:A:75:GLY:O	2.05	1.04
1:F:94:PHE:HD2	1:F:108:ALA:CB	1.69	1.04
1:F:102:TRP:O	1:F:103:GLN:NE2	1.91	1.03
1:B:135:ASN:O	1:B:138:TRP:N	1.91	1.03
1:C:148:ILE:O	1:C:151:PRO:HD2	1.59	1.03
1:F:80:PHE:CE1	2:F:201:FOL:OE2	2.12	1.03
1:B:30:TYR:CB	1:B:36:LYS:HE3	1.85	1.02
1:C:34:PHE:CD2	1:C:138:TRP:NE1	2.25	1.02
1:F:10:SER:O	1:F:14:MET:HG2	1.59	1.02
1:E:14:MET:CE	1:E:18:ILE:HD11	1.89	1.01
1:E:23:VAL:O	1:E:26:ARG:HB2	1.60	1.01
1:C:30:TYR:HB2	1:C:37:ILE:HG13	1.38	1.01
1:C:71:PHE:N	1:C:72:PRO:HD2	1.71	1.01
1:A:125:LEU:HD12	1:A:125:LEU:H	1.19	1.01
1:F:30:TYR:O	1:F:36:LYS:CD	2.07	1.01
1:B:96:TYR:CE2	1:B:97:LYS:CD	2.44	1.01
1:F:32:THR:HG22	1:F:33:THR:H	1.25	1.01
1:C:122:PRO:HA	1:C:125:LEU:HD12	1.40	1.00
1:A:26:ARG:CZ	1:A:27:PHE:HB2	1.91	1.00
1:C:27:PHE:HE1	1:C:71:PHE:CZ	1.78	1.00
1:D:10:SER:HB3	1:D:172:LYS:CG	1.90	1.00
1:E:69:LEU:CD1	1:E:70:LEU:H	1.69	1.00
1:E:141:PRO:O	1:E:144:ILE:CG2	2.10	1.00
1:F:68:MET:SD	2:F:201:FOL:C2	2.50	1.00
1:C:70:LEU:HD23	1:C:70:LEU:H	1.26	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:95:TYR:OH	1:F:108:ALA:CB	2.08	0.99
1:A:103:GLN:OE1	1:A:104:ARG:HD3	1.59	0.99
1:F:122:PRO:CA	1:F:125:LEU:HD12	1.91	0.99
1:C:112:VAL:O	1:C:116:ILE:CG2	2.11	0.99
1:C:10:SER:HB3	1:C:170:PHE:CZ	1.98	0.99
1:E:18:ILE:HG23	1:E:63:ALA:HB2	1.02	0.99
1:E:40:THR:CB	1:E:44:GLU:OE2	2.11	0.99
1:F:94:PHE:CD2	1:F:108:ALA:CB	2.44	0.98
1:F:42:ILE:HG23	1:F:43:PRO:HD3	1.45	0.98
1:E:115:LEU:O	1:E:119:ILE:CG1	2.10	0.98
1:C:168:ARG:HH21	1:C:170:PHE:HD2	1.10	0.98
1:A:173:PRO:O	1:A:174:LEU:HB2	1.60	0.98
1:F:30:TYR:HB2	1:F:36:LYS:HE3	1.44	0.98
1:D:33:THR:C	1:D:34:PHE:HD1	1.66	0.98
1:E:19:ALA:O	1:E:23:VAL:HG12	1.64	0.98
1:F:118:ILE:HG22	1:F:119:ILE:HD12	1.44	0.98
1:A:97:LYS:CE	1:A:170:PHE:HD1	1.75	0.98
1:D:121:THR:O	1:D:125:LEU:HD12	1.63	0.98
1:F:116:ILE:HA	1:F:120:LEU:HD13	1.45	0.98
1:C:49:MET:HE3	1:C:95:TYR:HD2	1.19	0.97
1:D:54:PHE:CE2	1:D:176:GLU:HB2	1.98	0.97
1:E:40:THR:HG22	1:E:44:GLU:HG2	1.47	0.97
1:D:35:LEU:HD23	1:D:36:LYS:N	1.80	0.97
1:E:13:LEU:H	1:E:13:LEU:HD22	1.25	0.97
1:F:32:THR:O	1:F:35:LEU:HD23	1.65	0.97
1:B:36:LYS:HE2	1:B:37:ILE:N	1.79	0.97
1:C:98:LYS:HZ2	1:C:104:ARG:NH1	1.61	0.96
1:E:54:PHE:CD2	1:E:55:TRP:CE3	2.47	0.96
1:C:122:PRO:HA	1:C:125:LEU:CD1	1.94	0.96
1:E:35:LEU:HD21	1:E:142:ARG:HG2	0.97	0.96
1:D:10:SER:CB	1:D:172:LYS:CG	2.41	0.96
1:E:112:VAL:HB	1:E:115:LEU:CB	1.94	0.96
1:E:145:LYS:HB2	1:E:148:ILE:HG22	1.46	0.96
1:D:12:ALA:O	1:D:16:VAL:CG2	2.14	0.95
1:C:30:TYR:CB	1:C:37:ILE:HG13	1.95	0.95
1:E:139:TRP:CZ3	1:E:142:ARG:CD	2.48	0.95
1:E:143:LEU:CD2	1:E:146:THR:HG22	1.95	0.95
1:C:10:SER:CB	1:C:170:PHE:HE1	1.69	0.95
1:F:61:ALA:HB2	1:F:85:PHE:HD1	1.24	0.95
1:C:98:LYS:NZ	1:C:104:ARG:HH12	1.65	0.94
1:F:30:TYR:CA	1:F:36:LYS:HZ1	1.79	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:162:ASN:O	1:F:162:ASN:ND2	1.99	0.94
1:A:70:LEU:H	1:A:70:LEU:HD12	1.31	0.94
1:D:14:MET:CE	1:D:51:PHE:HE2	1.42	0.94
1:E:56:ALA:O	1:E:60:THR:OG1	1.85	0.94
1:C:32:THR:OG1	1:C:35:LEU:O	1.85	0.94
1:E:128:MET:O	1:E:129:TYR:HD2	1.50	0.94
1:E:145:LYS:HZ2	1:E:149:PHE:HD2	1.10	0.94
1:F:14:MET:HE3	1:F:14:MET:HA	1.50	0.94
1:D:14:MET:HE2	1:D:51:PHE:CD2	1.73	0.94
1:E:17:LEU:O	1:E:20:VAL:HG23	1.67	0.93
1:E:90:ILE:HG12	1:E:112:VAL:HG11	1.51	0.93
1:A:18:ILE:O	1:A:22:VAL:HG23	1.68	0.93
1:F:13:LEU:HD21	1:F:51:PHE:HE2	1.29	0.93
1:E:128:MET:C	1:E:129:TYR:HD2	1.72	0.92
1:E:115:LEU:HD13	1:E:115:LEU:C	1.88	0.92
1:F:118:ILE:CG2	1:F:119:ILE:HD12	1.99	0.92
1:E:14:MET:HA	1:E:17:LEU:CD2	1.99	0.92
1:A:70:LEU:HB2	1:A:71:PHE:CD1	2.05	0.92
1:F:160:LEU:O	1:F:163:LYS:CG	2.18	0.92
1:D:30:TYR:HE2	1:D:39:PHE:CE2	1.88	0.91
1:C:77:PHE:H	2:C:201:FOL:HN1	1.09	0.91
1:F:120:LEU:HD23	1:F:124:TRP:CZ3	2.04	0.91
1:D:30:TYR:HE2	1:D:39:PHE:HE2	1.18	0.91
1:E:115:LEU:HD13	1:E:116:ILE:CA	2.00	0.91
1:D:26:ARG:HH11	1:D:26:ARG:HG2	1.33	0.91
1:E:36:LYS:HE3	1:E:38:SER:OG	1.69	0.91
1:C:168:ARG:NH2	1:C:170:PHE:HD2	1.68	0.91
1:D:33:THR:HG22	1:D:34:PHE:HE1	1.08	0.91
1:E:23:VAL:CA	1:E:26:ARG:HD2	2.01	0.91
1:E:54:PHE:HE2	1:E:55:TRP:CZ3	1.73	0.91
1:C:114:VAL:HG21	1:D:144:ILE:HD11	1.53	0.90
1:E:36:LYS:O	2:E:201:FOL:HG1	1.71	0.90
1:E:145:LYS:HD3	1:E:149:PHE:H	1.33	0.90
1:F:116:ILE:HD12	1:F:120:LEU:HD13	1.54	0.90
1:B:30:TYR:H	1:B:36:LYS:HZ1	1.20	0.90
1:E:16:VAL:O	1:E:20:VAL:HG22	1.70	0.90
1:F:23:VAL:HA	1:F:27:PHE:CD2	2.06	0.90
1:D:14:MET:O	1:D:18:ILE:HG13	1.72	0.90
1:E:172:LYS:HB3	1:E:173:PRO:HA	1.52	0.90
1:E:128:MET:C	1:E:129:TYR:CD2	2.46	0.90
1:D:10:SER:HG	1:D:172:LYS:HB2	1.25	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:112:VAL:O	1:F:116:ILE:HG22	1.72	0.90
1:C:49:MET:HE1	1:C:100:MET:CE	2.00	0.89
1:F:35:LEU:HB2	1:F:145:LYS:NZ	1.87	0.89
1:A:26:ARG:HD2	1:A:27:PHE:CD2	2.07	0.89
1:A:50:ILE:O	1:A:173:PRO:HB3	1.70	0.89
1:F:61:ALA:HB1	1:F:85:PHE:HE1	1.38	0.89
1:E:112:VAL:CB	1:E:115:LEU:HB3	2.02	0.89
1:D:117:ASN:ND2	2:D:201:FOL:O1	2.06	0.89
1:C:96:TYR:OH	1:C:169:LEU:HD23	1.71	0.89
1:E:40:THR:HG23	1:E:44:GLU:HG2	1.51	0.89
1:E:47:ILE:HA	1:E:50:ILE:HG22	1.54	0.89
1:E:69:LEU:HD13	1:E:70:LEU:CA	2.01	0.89
1:F:61:ALA:CB	1:F:85:PHE:CE1	2.56	0.89
1:B:164:ILE:HG12	1:B:165:PRO:HD2	1.53	0.89
1:A:68:MET:HE1	1:A:75:GLY:O	1.72	0.88
1:A:158:TYR:O	1:A:162:ASN:ND2	2.06	0.88
1:E:68:MET:HE1	2:E:201:FOL:N3	1.69	0.88
1:A:96:TYR:OH	1:A:174:LEU:HD11	1.73	0.88
1:D:50:ILE:HG22	1:D:51:PHE:CD1	2.08	0.88
1:F:19:ALA:O	1:F:23:VAL:HG12	1.74	0.88
1:C:49:MET:HE3	1:C:95:TYR:CB	2.03	0.88
1:B:74:ALA:HB1	2:B:201:FOL:H92	1.55	0.88
1:B:96:TYR:HE2	1:B:97:LYS:CE	1.85	0.88
1:E:119:ILE:HG13	1:E:120:LEU:HB3	1.52	0.88
1:D:33:THR:O	1:D:34:PHE:HD1	1.57	0.88
1:F:14:MET:O	1:F:18:ILE:HG23	1.74	0.88
1:A:132:ASN:O	1:A:132:ASN:ND2	2.07	0.88
1:F:65:VAL:O	1:F:69:LEU:HD12	1.74	0.88
1:E:139:TRP:HZ3	1:E:142:ARG:CD	1.87	0.88
1:D:10:SER:HB3	1:D:172:LYS:CD	2.04	0.87
1:D:14:MET:HE1	1:D:51:PHE:HD2	0.81	0.87
1:F:103:GLN:HE21	1:F:103:GLN:HA	1.36	0.87
1:C:151:PRO:O	1:C:155:ILE:HG12	1.74	0.87
1:B:135:ASN:HB2	1:B:138:TRP:HB2	1.55	0.87
1:F:73:LYS:CD	2:F:201:FOL:C7	2.51	0.87
1:E:143:LEU:CD2	1:E:146:THR:CG2	2.53	0.87
1:A:97:LYS:HE3	1:A:170:PHE:CD1	2.08	0.87
1:C:49:MET:HE1	1:C:95:TYR:CD2	2.10	0.87
1:E:13:LEU:O	1:E:16:VAL:HG23	1.75	0.87
1:F:74:ALA:HB2	2:F:201:FOL:H7	1.57	0.87
1:E:54:PHE:HD2	1:E:55:TRP:CZ3	1.72	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:43:PRO:O	1:F:47:ILE:HD13	1.75	0.86
1:F:116:ILE:CD1	1:F:120:LEU:HD13	2.05	0.86
1:F:141:PRO:HB2	1:F:142:ARG:HG3	1.56	0.86
1:E:139:TRP:HZ3	1:E:142:ARG:HD2	1.32	0.86
1:E:14:MET:HA	1:E:17:LEU:HD23	1.54	0.86
1:F:74:ALA:CB	2:F:201:FOL:H7	2.05	0.86
1:C:162:ASN:O	1:C:163:LYS:C	2.14	0.86
1:E:36:LYS:HB2	2:E:201:FOL:C12	2.05	0.86
1:F:16:VAL:HG23	1:F:17:LEU:CD2	2.05	0.86
1:F:16:VAL:O	1:F:20:VAL:HG23	1.76	0.86
1:B:30:TYR:CA	1:B:36:LYS:NZ	2.36	0.86
1:F:160:LEU:HA	1:F:163:LYS:HG2	1.58	0.86
1:F:116:ILE:CD1	1:F:120:LEU:HD22	2.04	0.86
1:D:10:SER:HB3	1:D:172:LYS:HD2	1.58	0.86
1:E:26:ARG:N	1:E:27:PHE:HA	1.89	0.86
1:D:150:PHE:O	1:D:154:VAL:HG23	1.75	0.85
1:E:10:SER:OG	1:E:170:PHE:CD2	2.28	0.85
1:D:33:THR:CG2	1:D:34:PHE:HE1	1.76	0.85
1:E:17:LEU:O	1:E:21:VAL:HG23	1.76	0.85
1:F:80:PHE:CE1	2:F:201:FOL:O4	2.28	0.85
1:B:49:MET:HE1	1:B:160:LEU:HG	1.58	0.85
1:B:135:ASN:HB2	1:B:138:TRP:CB	2.07	0.85
1:C:109:THR:HG22	1:C:153:GLN:NE2	1.92	0.85
1:C:109:THR:O	1:C:113:THR:HG22	1.77	0.85
1:D:33:THR:C	1:D:34:PHE:CD1	2.50	0.85
1:F:13:LEU:HD22	1:F:14:MET:N	1.92	0.85
1:F:80:PHE:HE1	2:F:201:FOL:CD	1.89	0.85
1:E:23:VAL:C	1:E:26:ARG:HB2	1.97	0.85
1:B:137:ALA:HB1	1:B:140:VAL:CG2	2.06	0.85
1:C:27:PHE:CE1	1:C:71:PHE:CZ	2.64	0.85
1:E:62:VAL:O	1:E:66:VAL:HG23	1.75	0.84
1:E:147:VAL:HB	1:F:150:PHE:CZ	2.12	0.84
1:F:46:LEU:O	1:F:50:ILE:HG12	1.76	0.84
1:E:145:LYS:HD3	1:E:149:PHE:HB3	1.59	0.84
1:F:15:GLY:O	1:F:18:ILE:HG13	1.76	0.84
1:F:110:LEU:O	1:F:114:VAL:HG12	1.75	0.84
1:A:26:ARG:HG2	1:A:27:PHE:CG	2.12	0.84
1:B:121:THR:HG21	2:B:201:FOL:HA	1.58	0.84
1:E:40:THR:OG1	1:E:44:GLU:OE2	1.95	0.84
1:D:10:SER:CB	1:D:172:LYS:CB	2.55	0.84
1:D:140:VAL:HG13	1:D:141:PRO:HD3	1.56	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:10:SER:HA	1:E:170:PHE:HE2	1.43	0.84
1:E:143:LEU:HD23	1:E:146:THR:HG22	1.57	0.84
1:F:13:LEU:HD11	1:F:51:PHE:HZ	1.42	0.84
1:F:30:TYR:O	1:F:36:LYS:NZ	2.10	0.84
1:F:145:LYS:HA	1:F:148:ILE:HG13	1.59	0.84
1:A:24:PHE:CD2	1:A:39:PHE:O	2.31	0.84
1:B:30:TYR:CB	1:B:36:LYS:CE	2.55	0.84
1:A:171:GLY:C	1:A:173:PRO:HD3	1.97	0.84
1:D:19:ALA:O	1:D:23:VAL:HG22	1.77	0.84
1:E:40:THR:HG23	1:E:43:PRO:HG2	1.60	0.84
1:A:50:ILE:HG22	1:A:173:PRO:HB3	1.60	0.83
1:F:86:LEU:O	1:F:90:ILE:HG13	1.77	0.83
1:F:122:PRO:HA	1:F:125:LEU:CD1	2.05	0.83
1:F:42:ILE:HG23	1:F:43:PRO:CD	2.07	0.83
1:F:61:ALA:HB2	1:F:85:PHE:CE1	2.13	0.83
1:A:126:SER:CA	1:A:131:VAL:HG21	2.08	0.83
1:E:59:GLY:O	1:E:62:VAL:HG22	1.78	0.83
1:F:42:ILE:CG2	1:F:43:PRO:HD3	2.09	0.83
1:F:138:TRP:O	1:F:139:TRP:CE3	2.31	0.83
1:C:124:TRP:O	1:C:128:MET:HG2	1.79	0.83
1:F:68:MET:HE1	2:F:201:FOL:N8	1.93	0.83
1:C:71:PHE:N	1:C:72:PRO:HD3	1.85	0.83
1:C:114:VAL:HG21	1:D:144:ILE:CD1	2.08	0.83
1:C:150:PHE:O	1:C:153:GLN:HG2	1.78	0.83
1:C:83:ASN:ND2	1:C:124:TRP:HE1	1.77	0.82
1:C:70:LEU:C	1:C:72:PRO:CD	2.42	0.82
1:E:145:LYS:HE3	1:E:150:PHE:N	1.94	0.82
1:A:14:MET:CE	1:A:51:PHE:CE2	2.62	0.82
1:A:97:LYS:CE	1:A:170:PHE:CD1	2.63	0.82
1:F:81:THR:HG23	1:F:85:PHE:CZ	2.13	0.82
1:E:69:LEU:HD13	1:E:70:LEU:H	1.00	0.82
1:E:13:LEU:HA	1:E:16:VAL:CG2	2.10	0.82
1:E:54:PHE:HE2	1:E:55:TRP:HZ3	0.86	0.82
1:B:36:LYS:HG3	1:B:37:ILE:N	1.92	0.82
1:F:30:TYR:H	1:F:36:LYS:HZ1	0.83	0.82
1:F:26:ARG:HG3	1:F:26:ARG:HH11	1.45	0.82
1:E:142:ARG:O	1:E:143:LEU:HB2	1.78	0.81
1:A:97:LYS:HE2	1:A:170:PHE:HD1	1.42	0.81
1:D:97:LYS:O	1:D:98:LYS:HD3	1.81	0.81
1:E:115:LEU:HD22	1:E:115:LEU:C	1.99	0.81
1:F:108:ALA:O	1:F:112:VAL:HG23	1.79	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:MET:CE	1:C:95:TYR:HD2	1.75	0.81
1:F:119:ILE:HG22	1:F:123:LEU:CD1	2.10	0.81
1:F:120:LEU:HD23	1:F:124:TRP:HZ3	1.42	0.81
1:F:120:LEU:HB3	1:F:124:TRP:HZ3	1.45	0.81
1:A:18:ILE:CD1	1:A:59:GLY:O	2.28	0.81
1:C:55:TRP:HD1	1:C:172:LYS:HB2	1.46	0.81
1:E:39:PHE:CE1	1:E:41:PHE:HE1	1.98	0.81
1:A:123:LEU:O	1:A:126:SER:OG	1.99	0.80
1:C:111:LEU:HD23	1:C:111:LEU:O	1.81	0.80
1:D:148:ILE:HG13	1:D:149:PHE:N	1.94	0.80
1:A:170:PHE:HD2	1:A:171:GLY:H	1.29	0.80
1:E:39:PHE:CE1	1:E:41:PHE:CE1	2.68	0.80
1:F:120:LEU:HB3	1:F:124:TRP:CZ3	2.16	0.80
1:A:171:GLY:O	1:A:173:PRO:CD	2.29	0.80
1:A:171:GLY:O	1:A:173:PRO:HD2	1.82	0.80
1:F:73:LYS:HD2	2:F:201:FOL:H7	1.62	0.80
1:D:13:LEU:HA	1:D:16:VAL:HG23	1.64	0.80
1:E:14:MET:SD	1:E:18:ILE:HD11	2.21	0.80
1:F:64:ASP:HB2	1:F:80:PHE:CZ	2.16	0.80
1:C:48:GLY:O	1:C:92:GLY:HA2	1.82	0.79
1:F:68:MET:SD	2:F:201:FOL:C8A	2.71	0.79
1:A:97:LYS:HE3	1:A:170:PHE:HD1	1.44	0.79
1:B:164:ILE:HD13	1:B:165:PRO:N	1.96	0.79
1:A:103:GLN:OE1	1:A:104:ARG:CD	2.30	0.79
1:D:125:LEU:HD12	1:D:125:LEU:H	1.46	0.79
1:E:29:ALA:HB2	1:E:39:PHE:CE2	2.17	0.79
1:A:125:LEU:O	1:A:129:TYR:HB2	1.83	0.79
1:C:98:LYS:HZ1	1:C:104:ARG:NH1	1.76	0.79
1:E:112:VAL:CA	1:E:115:LEU:HB3	2.12	0.79
1:F:117:ASN:O	1:F:121:THR:OG1	1.99	0.78
1:D:10:SER:OG	1:D:172:LYS:CG	2.30	0.78
1:E:36:LYS:HB2	2:E:201:FOL:H12	1.65	0.78
1:A:126:SER:HA	1:A:131:VAL:HG22	1.64	0.78
1:D:50:ILE:HG22	1:D:51:PHE:HD1	1.46	0.78
1:C:30:TYR:CG	1:C:37:ILE:HG13	2.19	0.78
1:F:30:TYR:H	1:F:36:LYS:NZ	1.61	0.78
1:E:52:GLY:O	1:E:56:ALA:HB2	1.84	0.78
1:E:30:TYR:HB2	1:E:37:ILE:CG2	2.12	0.78
1:D:121:THR:O	1:D:125:LEU:CD1	2.32	0.78
1:C:168:ARG:NH2	1:C:170:PHE:CD2	2.52	0.78
1:A:173:PRO:O	1:A:174:LEU:CB	2.32	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:50:ILE:HG22	1:B:51:PHE:CD1	2.19	0.77
1:B:145:LYS:NZ	2:B:201:FOL:OE1	2.18	0.77
1:C:34:PHE:HE1	1:C:129:TYR:HD2	1.31	0.77
1:C:45:SER:O	1:C:49:MET:SD	2.43	0.77
1:C:68:MET:HE1	1:C:71:PHE:O	1.85	0.77
1:D:20:VAL:O	1:D:23:VAL:HG23	1.84	0.77
1:E:29:ALA:HB2	1:E:39:PHE:CD2	2.20	0.77
1:F:28:PHE:HB2	1:F:39:PHE:CE2	2.18	0.77
1:F:61:ALA:CB	1:F:85:PHE:CD1	2.67	0.77
1:F:64:ASP:OD1	1:F:65:VAL:N	2.17	0.77
1:F:73:LYS:HD2	2:F:201:FOL:C9	2.13	0.77
1:F:119:ILE:O	1:F:123:LEU:HD12	1.85	0.77
1:E:115:LEU:CD2	1:E:119:ILE:HD11	2.14	0.77
1:B:30:TYR:CA	1:B:36:LYS:HZ1	1.94	0.77
1:D:142:ARG:O	1:D:146:THR:OG1	2.03	0.77
1:E:14:MET:O	1:E:17:LEU:HD23	1.84	0.77
1:E:14:MET:HE3	1:E:18:ILE:HD11	1.63	0.77
1:E:153:GLN:OE1	1:E:153:GLN:N	2.18	0.77
1:F:18:ILE:HD12	1:F:19:ALA:N	1.99	0.77
1:C:96:TYR:CE1	1:C:169:LEU:HD21	2.20	0.77
1:B:36:LYS:CE	1:B:37:ILE:H	1.90	0.76
1:C:125:LEU:HA	1:C:128:MET:HG3	1.65	0.76
1:E:40:THR:HG22	1:E:43:PRO:HD2	1.68	0.76
1:B:37:ILE:H	1:B:37:ILE:HD12	1.48	0.76
1:E:14:MET:SD	1:E:17:LEU:HD21	2.24	0.76
1:F:30:TYR:CA	1:F:36:LYS:NZ	2.42	0.76
1:F:109:THR:HG22	1:F:153:GLN:HE21	1.48	0.76
1:E:109:THR:O	1:E:113:THR:OG1	2.01	0.76
1:F:104:ARG:HG2	1:F:104:ARG:HH21	1.51	0.76
1:C:26:ARG:HG2	1:C:26:ARG:HH11	1.49	0.76
1:B:31:GLU:HB3	1:B:36:LYS:HD3	1.66	0.76
1:C:168:ARG:HD3	1:C:168:ARG:C	2.06	0.76
1:E:68:MET:CE	2:E:201:FOL:C4	2.42	0.76
1:F:61:ALA:CB	1:F:85:PHE:HE1	1.97	0.76
1:A:14:MET:HE3	1:A:51:PHE:CE2	2.21	0.76
1:A:49:MET:SD	1:A:95:TYR:HB3	2.26	0.76
1:E:23:VAL:HA	1:E:26:ARG:HB2	1.67	0.75
1:B:30:TYR:N	1:B:36:LYS:HZ2	1.83	0.75
1:B:77:PHE:H	2:B:201:FOL:HN1	1.34	0.75
1:E:17:LEU:HA	1:E:20:VAL:CG2	2.17	0.75
1:E:61:ALA:HA	1:E:64:ASP:OD2	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:80:PHE:CZ	2:F:201:FOL:O4	2.40	0.75
1:F:94:PHE:CD2	1:F:108:ALA:HB1	2.22	0.75
1:F:25:SER:O	1:F:29:ALA:CB	2.34	0.75
1:C:55:TRP:CD1	1:C:172:LYS:HB2	2.21	0.75
1:D:26:ARG:HG2	1:D:26:ARG:NH1	1.97	0.75
1:F:17:LEU:O	1:F:21:VAL:HG23	1.86	0.75
1:F:39:PHE:CA	1:F:41:PHE:CE2	2.63	0.75
1:D:14:MET:CE	1:D:51:PHE:HD2	1.58	0.74
1:C:163:LYS:HE2	1:C:166:PHE:HB3	1.68	0.74
1:E:52:GLY:O	1:E:56:ALA:CB	2.35	0.74
1:E:115:LEU:HD22	1:E:119:ILE:CD1	2.17	0.74
1:E:128:MET:O	1:E:129:TYR:CD2	2.38	0.74
1:D:36:LYS:HE2	1:D:38:SER:HB3	1.68	0.74
1:E:23:VAL:O	1:E:26:ARG:CB	2.34	0.74
1:F:116:ILE:HA	1:F:120:LEU:CD1	2.17	0.74
1:C:10:SER:HB3	1:C:170:PHE:HE1	0.92	0.74
1:C:148:ILE:O	1:C:151:PRO:CD	2.34	0.74
1:A:49:MET:O	1:A:96:TYR:HD1	1.69	0.74
1:B:12:ALA:O	1:B:16:VAL:HG23	1.88	0.74
1:B:73:LYS:O	1:B:74:ALA:HB3	1.87	0.74
1:D:26:ARG:HG3	1:D:71:PHE:CD2	2.22	0.74
1:E:14:MET:CA	1:E:17:LEU:HD23	2.18	0.74
1:D:10:SER:HB3	1:D:172:LYS:HG3	1.55	0.74
1:C:30:TYR:HD2	1:C:32:THR:HG23	1.53	0.74
1:D:137:ALA:O	1:D:140:VAL:HG12	1.88	0.74
1:D:144:ILE:O	1:D:147:VAL:HG22	1.88	0.74
1:E:143:LEU:HD22	1:E:146:THR:HG22	1.69	0.74
1:F:160:LEU:C	1:F:163:LYS:HG3	2.06	0.74
1:A:30:TYR:HB3	1:A:37:ILE:HB	1.71	0.73
1:D:30:TYR:CE2	1:D:39:PHE:HE2	2.02	0.73
1:E:13:LEU:C	1:E:16:VAL:HG23	2.07	0.73
1:C:30:TYR:HB2	1:C:37:ILE:CG1	2.18	0.73
1:E:42:ILE:N	1:E:42:ILE:HD13	2.02	0.73
1:C:116:ILE:HG23	1:C:117:ASN:N	2.02	0.73
1:E:143:LEU:HD23	1:E:146:THR:CG2	2.15	0.73
1:A:148:ILE:O	1:A:151:PRO:HD2	1.88	0.73
1:C:80:PHE:O	1:C:83:ASN:HB2	1.87	0.73
1:D:147:VAL:O	1:D:151:PRO:HD2	1.87	0.73
1:B:96:TYR:CE2	1:B:97:LYS:HD2	2.24	0.73
1:F:61:ALA:HB1	1:F:85:PHE:CE1	2.18	0.73
1:C:98:LYS:NZ	1:C:104:ARG:HH11	1.85	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:168:ARG:O	1:C:169:LEU:HD12	1.88	0.73
1:E:55:TRP:CE3	1:E:55:TRP:HA	2.23	0.73
1:F:80:PHE:CD2	2:F:201:FOL:C2	2.71	0.73
1:F:109:THR:CG2	1:F:153:GLN:HE21	2.00	0.73
1:A:17:LEU:HB3	1:A:47:ILE:HD11	1.70	0.73
1:A:169:LEU:HD12	1:A:169:LEU:O	1.88	0.73
1:C:61:ALA:HB2	1:C:85:PHE:HB2	1.71	0.73
1:E:68:MET:HE2	2:E:201:FOL:N3	2.01	0.73
1:E:110:LEU:HD21	1:F:144:ILE:HD12	1.71	0.72
1:A:24:PHE:HD2	1:A:39:PHE:O	1.71	0.72
1:A:126:SER:CA	1:A:131:VAL:CG2	2.62	0.72
1:C:122:PRO:O	1:C:126:SER:OG	2.03	0.72
1:E:22:VAL:CG2	1:E:67:GLY:CA	2.67	0.72
1:F:116:ILE:HD13	1:F:120:LEU:HD22	1.69	0.72
1:A:42:ILE:HD12	1:A:160:LEU:HD13	1.71	0.72
1:D:125:LEU:HD12	1:D:125:LEU:N	2.03	0.72
1:E:115:LEU:HD13	1:E:116:ILE:H	1.50	0.72
1:F:14:MET:HA	1:F:14:MET:CE	2.19	0.72
1:B:11:ILE:HG13	1:B:12:ALA:N	2.04	0.72
1:C:42:ILE:HG22	1:C:160:LEU:HD13	1.72	0.72
1:E:153:GLN:NE2	1:E:154:VAL:HG13	2.05	0.72
1:B:30:TYR:HB2	1:B:36:LYS:HZ1	1.54	0.72
1:C:66:VAL:O	1:C:70:LEU:HD23	1.90	0.72
1:C:96:TYR:CE1	1:C:169:LEU:CD2	2.72	0.72
1:C:171:GLY:O	1:C:172:LYS:HD3	1.90	0.72
1:F:10:SER:O	1:F:13:LEU:CD1	2.38	0.72
1:F:51:PHE:O	1:F:55:TRP:HB2	1.90	0.72
1:C:30:TYR:CD2	1:C:32:THR:HG23	2.25	0.72
1:F:82:LEU:HA	1:F:85:PHE:CD2	2.25	0.72
1:A:70:LEU:HB2	1:A:71:PHE:CE1	2.25	0.72
1:B:20:VAL:O	1:B:23:VAL:HG22	1.90	0.72
1:D:18:ILE:HG23	1:D:63:ALA:HB2	1.71	0.72
1:E:13:LEU:N	1:E:13:LEU:HD13	2.04	0.72
1:A:170:PHE:HD2	1:A:171:GLY:N	1.87	0.71
1:B:133:LEU:N	1:B:133:LEU:HD12	2.04	0.71
1:D:122:PRO:HA	1:D:125:LEU:HD13	1.70	0.71
1:B:138:TRP:CE3	1:B:139:TRP:HA	2.25	0.71
1:E:39:PHE:HD1	1:E:41:PHE:CD1	2.06	0.71
1:E:105:VAL:O	1:E:109:THR:HG23	1.90	0.71
1:B:37:ILE:N	1:B:37:ILE:HD12	2.05	0.71
1:C:33:THR:HG22	1:C:129:TYR:HE2	1.56	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:46:LEU:HA	1:C:49:MET:SD	2.30	0.71
1:A:122:PRO:HA	1:A:125:LEU:HD13	1.72	0.71
1:E:139:TRP:C	1:E:141:PRO:HD2	2.10	0.71
1:B:131:VAL:HG12	1:B:133:LEU:CD1	2.21	0.71
1:E:25:SER:C	1:E:27:PHE:HA	2.11	0.71
1:E:42:ILE:O	1:E:46:LEU:N	2.22	0.71
1:D:80:PHE:CE1	2:D:201:FOL:NA2	2.58	0.71
1:E:36:LYS:CE	1:E:38:SER:OG	2.38	0.71
1:F:119:ILE:HG22	1:F:123:LEU:HD11	1.72	0.71
1:B:30:TYR:CB	1:B:36:LYS:HZ1	2.04	0.71
1:D:80:PHE:CE1	1:D:81:THR:HG23	2.25	0.71
1:E:64:ASP:OD1	1:E:65:VAL:N	2.23	0.71
1:E:115:LEU:CD2	1:E:119:ILE:CD1	2.68	0.71
1:E:13:LEU:HA	1:E:16:VAL:HG23	1.73	0.70
1:E:74:ALA:HB1	1:E:75:GLY:C	2.11	0.70
1:B:13:LEU:HD23	1:B:14:MET:N	2.05	0.70
1:F:32:THR:HG22	1:F:33:THR:N	2.04	0.70
1:E:159:TYR:HA	1:E:162:ASN:OD1	1.91	0.70
1:F:38:SER:HB2	1:F:40:THR:HG22	1.73	0.70
1:F:104:ARG:HG2	1:F:104:ARG:NH2	2.05	0.70
1:A:160:LEU:HD23	1:A:161:GLY:N	2.05	0.70
1:C:49:MET:O	1:C:96:TYR:CD1	2.44	0.70
1:F:13:LEU:HD21	1:F:14:MET:SD	2.31	0.70
1:E:42:ILE:HD11	1:E:156:ALA:HB1	1.73	0.70
1:E:115:LEU:CD1	1:E:116:ILE:H	2.04	0.70
1:F:116:ILE:HD12	1:F:120:LEU:HB2	1.74	0.70
1:A:70:LEU:HB2	1:A:71:PHE:HD1	1.51	0.70
1:C:112:VAL:C	1:C:116:ILE:HG22	2.11	0.70
1:A:23:VAL:HA	1:A:26:ARG:HD3	1.73	0.69
1:B:13:LEU:HD23	1:B:13:LEU:C	2.12	0.69
1:E:10:SER:HA	1:E:170:PHE:CE2	2.26	0.69
1:F:35:LEU:HD23	1:F:35:LEU:O	1.92	0.69
1:C:65:VAL:O	1:C:69:LEU:HB2	1.92	0.69
1:E:18:ILE:HG23	1:E:63:ALA:HB1	1.72	0.69
1:E:22:VAL:CG2	1:E:67:GLY:HA2	2.22	0.69
1:E:29:ALA:HB1	1:E:30:TYR:HD2	1.56	0.69
1:A:125:LEU:H	1:A:125:LEU:CD1	1.97	0.69
1:C:70:LEU:H	1:C:70:LEU:CD2	2.04	0.69
1:F:120:LEU:CB	1:F:124:TRP:HZ3	2.06	0.69
1:F:64:ASP:HB2	1:F:80:PHE:HE2	1.52	0.69
1:B:30:TYR:HB3	1:B:37:ILE:HD13	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:ASN:O	1:D:142:ARG:NH1	2.25	0.69
1:A:68:MET:HE2	1:A:75:GLY:O	1.90	0.68
1:D:140:VAL:CG1	1:D:141:PRO:HD3	2.22	0.68
1:E:23:VAL:CA	1:E:26:ARG:HB2	2.23	0.68
1:E:36:LYS:HE3	1:E:38:SER:HG	1.58	0.68
1:C:49:MET:HE3	1:C:95:TYR:HB3	1.75	0.68
1:D:36:LYS:N	2:D:201:FOL:O	2.26	0.68
1:D:80:PHE:CZ	2:D:201:FOL:NA2	2.60	0.68
1:E:112:VAL:CB	1:E:115:LEU:CB	2.66	0.68
1:A:96:TYR:OH	1:A:174:LEU:CD1	2.41	0.68
1:A:101:THR:O	1:A:104:ARG:N	2.25	0.68
1:B:131:VAL:HG12	1:B:133:LEU:HD11	1.75	0.68
1:D:147:VAL:HG23	1:D:148:ILE:N	2.08	0.68
1:F:13:LEU:HD21	1:F:51:PHE:CZ	2.29	0.68
1:F:13:LEU:HD22	1:F:13:LEU:C	2.13	0.68
1:A:50:ILE:O	1:A:173:PRO:CG	2.42	0.68
1:A:50:ILE:HB	1:A:51:PHE:CD1	2.28	0.68
1:B:26:ARG:HG3	1:B:71:PHE:CG	2.29	0.68
1:C:10:SER:HB2	1:C:170:PHE:CE1	2.23	0.68
1:E:112:VAL:HA	1:E:115:LEU:H	1.58	0.68
1:E:145:LYS:CD	1:E:149:PHE:H	2.07	0.68
1:B:159:TYR:OH	1:B:164:ILE:HB	1.93	0.68
1:E:43:PRO:HG2	1:E:44:GLU:H	1.59	0.68
1:F:109:THR:O	1:F:113:THR:OG1	2.11	0.68
1:F:120:LEU:CD2	1:F:124:TRP:HZ3	2.06	0.68
1:A:117:ASN:O	1:A:142:ARG:NH1	2.26	0.68
1:E:115:LEU:HD22	1:E:119:ILE:HD11	1.75	0.68
1:F:73:LYS:CD	2:F:201:FOL:H92	2.24	0.68
1:E:70:LEU:HD23	1:E:70:LEU:C	2.15	0.68
1:F:64:ASP:OD1	1:F:65:VAL:HG22	1.94	0.68
1:E:66:VAL:O	1:E:69:LEU:HD12	1.94	0.67
1:E:79:GLY:O	1:E:81:THR:N	2.26	0.67
1:E:172:LYS:CB	1:E:173:PRO:HA	2.21	0.67
1:F:73:LYS:HD2	2:F:201:FOL:H92	1.74	0.67
1:F:13:LEU:HD13	1:F:14:MET:H	1.59	0.67
1:F:160:LEU:HA	1:F:163:LYS:CG	2.24	0.67
1:B:109:THR:O	1:B:113:THR:OG1	2.10	0.67
1:D:18:ILE:HG23	1:D:63:ALA:CB	2.24	0.67
1:A:100:MET:CE	1:A:161:GLY:HA2	2.24	0.67
1:C:66:VAL:O	1:C:70:LEU:CD2	2.42	0.67
1:B:149:PHE:HD1	1:B:152:ILE:HD12	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:MET:CE	1:C:100:MET:HE2	2.18	0.67
1:E:153:GLN:O	1:E:157:THR:HG23	1.95	0.67
1:E:115:LEU:CD1	1:E:115:LEU:C	2.52	0.67
1:C:34:PHE:CE2	1:C:138:TRP:NE1	2.62	0.67
1:A:160:LEU:HD23	1:A:160:LEU:C	2.15	0.67
1:C:97:LYS:HG3	1:C:169:LEU:CD2	2.25	0.67
1:E:20:VAL:HA	1:E:23:VAL:CG1	2.25	0.67
1:E:70:LEU:CD2	1:E:71:PHE:CD2	2.78	0.67
1:F:103:GLN:HE21	1:F:103:GLN:CA	2.00	0.67
1:B:173:PRO:HD2	1:B:173:PRO:O	1.94	0.66
1:C:30:TYR:CD1	1:C:37:ILE:HD12	2.30	0.66
1:F:26:ARG:HG3	1:F:26:ARG:NH1	2.11	0.66
1:A:151:PRO:O	1:A:155:ILE:HD13	1.94	0.66
1:D:21:VAL:HG22	1:D:43:PRO:HG2	1.78	0.66
1:C:174:LEU:C	1:C:174:LEU:HD22	2.15	0.66
1:E:13:LEU:CA	1:E:16:VAL:HG23	2.26	0.66
1:F:18:ILE:HD12	1:F:18:ILE:C	2.16	0.66
1:A:36:LYS:HG2	2:A:201:FOL:C11	2.26	0.66
1:F:111:LEU:C	1:F:111:LEU:HD23	2.15	0.66
1:F:116:ILE:HG23	1:F:117:ASN:N	2.11	0.66
1:D:140:VAL:HG13	1:D:141:PRO:CD	2.26	0.66
1:E:145:LYS:HE3	1:E:150:PHE:H	1.59	0.66
1:F:28:PHE:HB2	1:F:39:PHE:HE2	1.61	0.66
1:C:27:PHE:C	1:C:28:PHE:HD1	1.99	0.66
1:E:12:ALA:O	1:E:16:VAL:HG22	1.96	0.66
1:F:39:PHE:CA	1:F:41:PHE:HE2	1.91	0.66
1:C:117:ASN:OD1	1:C:142:ARG:NH2	2.30	0.65
1:F:110:LEU:C	1:F:110:LEU:HD23	2.15	0.65
1:E:147:VAL:HB	1:F:150:PHE:HZ	1.58	0.65
1:A:41:PHE:CE1	1:A:42:ILE:HG12	2.32	0.65
1:A:101:THR:O	1:A:102:TRP:C	2.33	0.65
1:D:54:PHE:CZ	1:D:176:GLU:CB	2.73	0.65
1:E:32:THR:HB	1:E:35:LEU:O	1.96	0.65
1:C:98:LYS:CE	1:C:104:ARG:HH11	2.10	0.65
1:E:79:GLY:C	1:E:81:THR:H	1.99	0.65
1:D:14:MET:SD	1:D:51:PHE:HE2	2.20	0.65
1:D:33:THR:CG2	1:D:34:PHE:CD1	2.68	0.65
1:E:77:PHE:CG	1:E:78:PRO:CD	2.77	0.65
1:F:35:LEU:HB2	1:F:145:LYS:HZ3	1.58	0.65
1:F:95:TYR:HH	1:F:108:ALA:HB3	1.60	0.65
1:A:14:MET:HE2	1:A:51:PHE:CZ	2.33	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:83:ASN:ND2	1:C:124:TRP:NE1	2.45	0.64
1:F:36:LYS:HG3	1:F:37:ILE:N	2.11	0.64
1:D:10:SER:OG	1:D:172:LYS:HB3	1.92	0.64
1:A:114:VAL:O	1:A:119:ILE:HG13	1.98	0.64
1:B:164:ILE:HD13	1:B:165:PRO:O	1.97	0.64
1:C:170:PHE:O	1:C:172:LYS:HD3	1.97	0.64
1:F:64:ASP:OD1	1:F:65:VAL:CG2	2.45	0.64
1:B:64:ASP:CG	1:B:81:THR:HG22	2.18	0.64
1:B:164:ILE:HD13	1:B:165:PRO:C	2.18	0.64
1:C:64:ASP:OD2	1:C:81:THR:HG23	1.98	0.64
1:D:143:LEU:O	1:D:147:VAL:HG13	1.96	0.64
1:E:58:ILE:O	1:E:62:VAL:HG13	1.97	0.64
1:F:30:TYR:O	1:F:36:LYS:CE	2.46	0.64
1:B:30:TYR:CB	1:B:36:LYS:NZ	2.61	0.64
1:B:77:PHE:O	2:B:201:FOL:NA2	2.30	0.64
1:C:153:GLN:O	1:C:157:THR:HG23	1.96	0.64
1:E:55:TRP:HA	1:E:58:ILE:CG1	2.27	0.64
1:F:80:PHE:CG	2:F:201:FOL:N3	2.66	0.64
1:A:7:GLY:O	1:A:11:ILE:HG13	1.97	0.64
1:B:164:ILE:HD13	1:B:164:ILE:C	2.17	0.64
1:A:18:ILE:HD11	1:A:59:GLY:O	1.96	0.64
1:A:19:ALA:O	1:A:23:VAL:HG23	1.98	0.64
1:E:39:PHE:CD1	1:E:41:PHE:CZ	2.80	0.64
1:F:150:PHE:CA	1:F:153:GLN:HB3	2.28	0.64
1:F:150:PHE:HA	1:F:153:GLN:HB3	1.79	0.64
1:A:64:ASP:OD2	1:A:81:THR:HG22	1.98	0.64
1:A:95:TYR:O	1:A:97:LYS:HA	1.98	0.64
1:C:34:PHE:CD2	1:C:138:TRP:CD1	2.85	0.64
1:C:97:LYS:HG3	1:C:169:LEU:HD21	1.80	0.64
1:F:45:SER:HA	1:F:91:TYR:CD2	2.33	0.64
1:B:50:ILE:HG22	1:B:51:PHE:HD1	1.62	0.63
1:C:71:PHE:H	1:C:72:PRO:HD2	1.62	0.63
1:D:171:GLY:O	1:D:173:PRO:HD3	1.98	0.63
1:E:149:PHE:CD1	1:E:152:ILE:HD11	2.32	0.63
1:B:36:LYS:HE2	1:B:37:ILE:CD1	2.28	0.63
1:C:94:PHE:CD1	1:C:108:ALA:CB	2.80	0.63
1:C:94:PHE:CE1	1:C:108:ALA:HA	2.33	0.63
1:D:133:LEU:HG	1:D:138:TRP:HZ3	1.62	0.63
1:D:30:TYR:CE2	1:D:39:PHE:CE2	2.79	0.63
1:D:77:PHE:O	1:D:80:PHE:CE2	2.51	0.63
1:C:58:ILE:O	1:C:62:VAL:HG13	1.97	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:39:PHE:HA	1:A:41:PHE:CE2	2.34	0.63
1:D:160:LEU:C	1:D:160:LEU:HD23	2.19	0.63
1:F:104:ARG:HH21	1:F:104:ARG:CG	2.11	0.63
1:F:120:LEU:HD23	1:F:124:TRP:CH2	2.34	0.63
1:B:137:ALA:HB1	1:B:140:VAL:CB	2.28	0.63
1:A:172:LYS:HA	1:A:172:LYS:CE	2.29	0.63
1:D:13:LEU:CA	1:D:16:VAL:HG23	2.28	0.63
1:E:42:ILE:HD11	1:E:156:ALA:CB	2.28	0.63
1:A:171:GLY:O	1:A:173:PRO:HD3	1.95	0.63
1:E:91:TYR:OH	1:E:109:THR:HG22	1.99	0.63
1:F:142:ARG:HG2	1:F:145:LYS:NZ	2.14	0.63
1:B:30:TYR:CB	1:B:37:ILE:HD13	2.29	0.62
1:C:33:THR:CG2	1:C:129:TYR:HE2	2.12	0.62
1:E:53:PRO:HG3	1:E:93:TYR:CD2	2.33	0.62
1:F:36:LYS:HE2	1:F:37:ILE:O	1.98	0.62
1:F:150:PHE:HB2	1:F:153:GLN:OE1	1.99	0.62
1:B:26:ARG:HG3	1:B:71:PHE:CD2	2.34	0.62
1:B:175:SER:O	1:B:176:GLU:HB2	1.99	0.62
1:E:55:TRP:O	1:E:58:ILE:HG13	1.99	0.62
1:E:66:VAL:O	1:E:69:LEU:HB3	1.99	0.62
1:A:170:PHE:CE2	1:A:173:PRO:CG	2.82	0.62
1:A:66:VAL:CG1	1:A:70:LEU:HD11	2.30	0.62
1:B:96:TYR:OH	1:B:97:LYS:HE2	1.95	0.62
1:E:17:LEU:HD11	1:E:47:ILE:CD1	2.29	0.62
1:C:33:THR:CG2	1:C:129:TYR:CE2	2.83	0.62
1:C:174:LEU:HD13	1:C:174:LEU:O	2.00	0.62
1:F:30:TYR:C	1:F:36:LYS:HZ2	2.02	0.62
1:E:36:LYS:HB3	2:E:201:FOL:C	2.30	0.62
1:A:172:LYS:HA	1:A:172:LYS:HE2	1.82	0.62
1:C:174:LEU:HD22	1:C:174:LEU:O	2.00	0.62
1:D:50:ILE:HG22	1:D:51:PHE:CE1	2.35	0.62
1:A:14:MET:HE2	1:A:14:MET:HA	1.82	0.62
1:B:135:ASN:HB2	1:B:138:TRP:HB3	1.82	0.62
1:B:139:TRP:O	1:B:142:ARG:HB3	2.00	0.62
1:E:64:ASP:OD1	1:E:65:VAL:HG23	1.99	0.62
1:E:32:THR:HG22	1:E:33:THR:N	2.15	0.62
1:F:142:ARG:HA	1:F:145:LYS:HE2	1.82	0.62
1:B:137:ALA:HB1	1:B:140:VAL:HB	1.81	0.61
1:C:49:MET:HE1	1:C:100:MET:HE2	1.79	0.61
1:C:68:MET:O	1:C:70:LEU:O	2.18	0.61
1:E:145:LYS:HD3	1:E:149:PHE:N	2.11	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:80:PHE:CE1	2:F:201:FOL:CD	2.74	0.61
1:B:36:LYS:HE2	1:B:37:ILE:HD12	1.81	0.61
1:D:78:PRO:O	1:D:81:THR:OG1	2.14	0.61
1:F:81:THR:HG23	1:F:85:PHE:CE2	2.34	0.61
1:A:26:ARG:HG2	1:A:27:PHE:CE1	2.35	0.61
1:A:100:MET:SD	1:A:161:GLY:HA2	2.39	0.61
1:E:145:LYS:NZ	1:E:149:PHE:CD2	2.67	0.61
1:A:26:ARG:NE	1:A:27:PHE:HB2	2.14	0.61
1:E:46:LEU:O	1:E:49:MET:HB2	1.98	0.61
1:F:30:TYR:C	1:F:36:LYS:NZ	2.52	0.61
1:A:112:VAL:HG23	1:A:116:ILE:HD11	1.83	0.61
1:E:145:LYS:NZ	1:E:149:PHE:HD2	1.92	0.61
1:D:109:THR:HG21	1:D:154:VAL:HG22	1.83	0.61
1:E:141:PRO:O	1:E:144:ILE:HG23	1.98	0.61
1:F:25:SER:O	1:F:29:ALA:HB2	2.00	0.61
1:C:132:ASN:N	1:C:132:ASN:OD1	2.32	0.61
1:A:33:THR:HG22	1:A:34:PHE:CD1	2.35	0.61
1:D:131:VAL:HG13	1:D:133:LEU:CD1	2.29	0.61
1:C:27:PHE:CE1	1:C:71:PHE:HZ	2.17	0.61
1:C:49:MET:CE	1:C:95:TYR:CG	2.65	0.61
1:E:42:ILE:HG23	1:E:45:SER:HB2	1.83	0.61
1:E:68:MET:HE3	2:E:201:FOL:C8A	2.30	0.61
1:A:23:VAL:HG13	1:A:26:ARG:HD3	1.83	0.60
1:A:80:PHE:CE1	2:A:201:FOL:H16	2.36	0.60
1:E:14:MET:C	1:E:17:LEU:HD23	2.22	0.60
1:E:53:PRO:HG3	1:E:93:TYR:HD2	1.67	0.60
1:E:141:PRO:C	1:E:144:ILE:HG22	2.20	0.60
1:E:149:PHE:O	1:E:152:ILE:HG13	2.01	0.60
1:F:20:VAL:O	1:F:23:VAL:HG13	2.01	0.60
1:A:144:ILE:O	1:A:148:ILE:HG12	2.01	0.60
1:C:116:ILE:HG23	1:C:117:ASN:H	1.65	0.60
1:F:45:SER:HA	1:F:91:TYR:HD2	1.65	0.60
1:E:10:SER:HA	1:E:13:LEU:HD23	1.82	0.60
1:E:18:ILE:CG2	1:E:63:ALA:HB1	2.25	0.60
1:F:119:ILE:CG2	1:F:123:LEU:HD11	2.31	0.60
1:B:46:LEU:HD12	1:B:49:MET:HE3	1.83	0.60
1:F:73:LYS:CD	2:F:201:FOL:C6	2.69	0.60
1:A:31:GLU:N	1:A:31:GLU:OE1	2.34	0.60
1:C:122:PRO:HA	1:C:125:LEU:HD11	1.83	0.60
1:F:160:LEU:O	1:F:163:LYS:CD	2.48	0.60
1:F:10:SER:O	1:F:13:LEU:HD11	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:38:SER:OG	2:F:201:FOL:O1	2.19	0.60
1:A:125:LEU:HD12	1:A:125:LEU:N	2.04	0.60
1:D:79:GLY:O	1:D:124:TRP:CZ3	2.55	0.60
1:F:140:VAL:N	1:F:141:PRO:HD3	2.17	0.60
1:A:42:ILE:HD12	1:A:160:LEU:CD1	2.31	0.60
1:B:96:TYR:O	1:B:97:LYS:HB2	2.01	0.60
1:C:64:ASP:OD2	1:C:81:THR:HA	2.02	0.60
1:F:44:GLU:OE2	1:F:60:THR:HG21	2.00	0.60
2:F:201:FOL:H15	2:F:201:FOL:N5	2.16	0.60
1:C:70:LEU:HD23	1:C:70:LEU:N	2.08	0.60
1:C:140:VAL:O	1:C:144:ILE:HG13	2.02	0.60
1:E:42:ILE:CG2	1:E:45:SER:HB2	2.31	0.60
1:A:171:GLY:C	1:A:173:PRO:CD	2.70	0.60
1:C:42:ILE:HB	1:C:43:PRO:HD3	1.83	0.59
1:C:121:THR:O	1:C:125:LEU:HG	2.02	0.59
1:C:168:ARG:HD3	1:C:169:LEU:N	2.17	0.59
1:D:26:ARG:HH11	1:D:26:ARG:CG	2.12	0.59
1:E:68:MET:HE1	2:E:201:FOL:C4A	2.30	0.59
1:F:141:PRO:O	1:F:144:ILE:HG23	2.01	0.59
1:B:61:ALA:O	1:B:65:VAL:HG23	2.02	0.59
1:B:73:LYS:O	1:B:74:ALA:CB	2.49	0.59
1:C:98:LYS:HZ1	1:C:104:ARG:HH12	1.38	0.59
1:D:133:LEU:CD1	1:D:138:TRP:CZ3	2.85	0.59
1:F:81:THR:CG2	1:F:85:PHE:CZ	2.85	0.59
1:F:83:ASN:OD1	1:F:116:ILE:CD1	2.30	0.59
1:A:26:ARG:CD	1:A:27:PHE:CD2	2.85	0.59
1:C:150:PHE:HA	1:C:153:GLN:HG2	1.84	0.59
1:D:35:LEU:HD23	1:D:35:LEU:C	2.22	0.59
1:D:166:PHE:CD1	1:D:167:LYS:N	2.71	0.59
1:A:14:MET:CE	1:A:51:PHE:CZ	2.85	0.59
1:C:30:TYR:HD2	1:C:32:THR:CG2	2.16	0.59
1:C:49:MET:CE	1:C:95:TYR:HB3	2.31	0.59
1:E:109:THR:HG21	1:E:154:VAL:HG12	1.84	0.59
1:F:160:LEU:O	1:F:163:LYS:HD2	2.02	0.59
1:A:101:THR:O	1:A:103:GLN:N	2.36	0.59
1:A:148:ILE:HD11	1:B:110:LEU:HD22	1.85	0.59
1:C:166:PHE:CE2	1:C:167:LYS:CE	2.85	0.59
1:C:30:TYR:CD2	1:C:32:THR:CG2	2.86	0.59
1:C:33:THR:O	1:C:34:PHE:HB2	2.00	0.59
1:C:49:MET:CE	1:C:100:MET:HE1	2.25	0.59
1:C:59:GLY:O	1:C:62:VAL:HG22	2.03	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:PHE:CE2	1:C:167:LYS:CD	2.85	0.59
1:D:13:LEU:HA	1:D:16:VAL:CG2	2.31	0.59
1:E:113:THR:HG21	1:E:150:PHE:CD2	2.37	0.59
1:A:27:PHE:O	1:A:28:PHE:HD1	1.84	0.59
1:C:68:MET:HE1	1:C:72:PRO:HA	1.85	0.59
1:B:77:PHE:N	2:B:201:FOL:HN1	2.00	0.59
1:E:39:PHE:CD1	1:E:41:PHE:CD1	2.83	0.59
1:F:95:TYR:OH	1:F:108:ALA:HB2	2.01	0.59
1:B:24:PHE:CD2	1:B:39:PHE:O	2.55	0.59
1:D:133:LEU:HG	1:D:138:TRP:CZ3	2.38	0.59
1:B:16:VAL:O	1:B:20:VAL:HG23	2.03	0.58
1:B:122:PRO:HA	1:B:125:LEU:HD12	1.85	0.58
1:F:74:ALA:HB3	2:F:201:FOL:C7	2.33	0.58
1:C:30:TYR:CD1	1:C:37:ILE:CD1	2.86	0.58
1:A:172:LYS:HA	1:A:172:LYS:NZ	2.18	0.58
1:E:20:VAL:O	1:E:23:VAL:HG13	2.03	0.58
1:E:17:LEU:O	1:E:20:VAL:CG2	2.46	0.58
1:E:143:LEU:CD2	1:E:146:THR:HG21	2.33	0.58
1:F:13:LEU:HD11	1:F:51:PHE:CZ	2.31	0.58
1:C:28:PHE:HD1	1:C:28:PHE:N	2.01	0.58
1:E:76:TYR:CD1	1:E:77:PHE:N	2.72	0.58
1:D:64:ASP:OD2	1:D:81:THR:HG22	2.03	0.58
1:E:66:VAL:HA	1:E:69:LEU:HB3	1.84	0.58
1:F:32:THR:CG2	1:F:33:THR:H	2.06	0.58
1:D:33:THR:O	1:D:34:PHE:CD1	2.49	0.58
1:B:36:LYS:CE	1:B:37:ILE:CD1	2.82	0.58
1:E:77:PHE:CD2	1:E:78:PRO:HD2	2.37	0.58
1:F:74:ALA:CB	2:F:201:FOL:C7	2.82	0.58
1:C:57:GLY:C	1:C:85:PHE:HD1	2.06	0.58
1:C:109:THR:CG2	1:C:153:GLN:NE2	2.66	0.57
1:A:77:PHE:H	2:A:201:FOL:HN1	1.51	0.57
1:C:148:ILE:C	1:C:151:PRO:HD2	2.24	0.57
1:D:37:ILE:CG1	1:D:145:LYS:HG3	2.34	0.57
1:E:94:PHE:HD2	1:E:108:ALA:HB2	1.69	0.57
1:E:142:ARG:O	1:E:143:LEU:CB	2.51	0.57
1:F:41:PHE:O	1:F:45:SER:OG	2.21	0.57
1:F:116:ILE:HD12	1:F:120:LEU:CD1	2.30	0.57
1:F:120:LEU:CB	1:F:124:TRP:CZ3	2.85	0.57
1:C:28:PHE:N	1:C:28:PHE:CD1	2.72	0.57
1:D:83:ASN:CG	1:D:116:ILE:HG23	2.24	0.57
1:E:68:MET:HE2	2:E:201:FOL:C2	2.21	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:13:LEU:HD13	1:F:13:LEU:N	2.19	0.57
1:A:36:LYS:O	2:A:201:FOL:HG1	2.04	0.57
1:A:70:LEU:CB	1:A:71:PHE:CD1	2.85	0.57
1:B:96:TYR:CE2	1:B:97:LYS:CG	2.88	0.57
1:C:166:PHE:CE2	1:C:167:LYS:NZ	2.73	0.57
1:D:117:ASN:HD21	2:D:201:FOL:HG2	1.68	0.57
1:E:40:THR:HG23	1:E:43:PRO:CG	2.33	0.57
1:F:24:PHE:O	1:F:39:PHE:CD2	2.57	0.57
1:F:142:ARG:O	1:F:146:THR:HG23	2.04	0.57
1:B:19:ALA:HA	1:B:22:VAL:CG2	2.34	0.57
1:B:124:TRP:O	1:B:128:MET:HG2	2.03	0.57
1:C:98:LYS:HZ2	1:C:104:ARG:HH12	1.32	0.57
1:B:96:TYR:CE2	1:B:97:LYS:HG3	2.40	0.57
1:B:140:VAL:O	1:B:141:PRO:C	2.41	0.57
1:B:158:TYR:O	1:B:162:ASN:ND2	2.34	0.57
1:C:19:ALA:O	1:C:22:VAL:HG12	2.04	0.57
1:C:166:PHE:CZ	1:C:167:LYS:CD	2.88	0.57
1:E:55:TRP:CE3	1:E:55:TRP:CA	2.87	0.57
1:A:90:ILE:HD12	1:A:111:LEU:HD22	1.87	0.57
1:B:36:LYS:CG	1:B:37:ILE:N	2.65	0.57
1:C:118:ILE:O	1:C:122:PRO:HG2	2.04	0.57
1:E:10:SER:CA	1:E:13:LEU:HD23	2.33	0.57
1:A:149:PHE:HD1	1:A:152:ILE:HD12	1.69	0.57
1:E:125:LEU:O	1:E:128:MET:O	2.23	0.57
1:D:160:LEU:HD23	1:D:160:LEU:O	2.05	0.57
1:E:43:PRO:HG2	1:E:44:GLU:N	2.18	0.57
1:E:129:TYR:CD2	1:E:129:TYR:N	2.73	0.57
1:F:150:PHE:O	1:F:153:GLN:HB3	2.04	0.57
1:B:34:PHE:O	1:B:142:ARG:NH2	2.37	0.57
1:E:119:ILE:O	1:E:123:LEU:HD13	2.05	0.56
1:F:10:SER:O	1:F:13:LEU:HD13	2.05	0.56
1:F:16:VAL:HG23	1:F:17:LEU:N	2.20	0.56
1:C:96:TYR:CZ	1:C:169:LEU:HD23	2.40	0.56
1:E:13:LEU:H	1:E:13:LEU:CD2	2.00	0.56
1:F:116:ILE:HD13	1:F:120:LEU:HD13	1.86	0.56
1:B:23:VAL:HG23	1:B:24:PHE:N	2.20	0.56
1:B:143:LEU:O	1:B:147:VAL:HG22	2.06	0.56
1:C:150:PHE:HA	1:C:153:GLN:OE1	2.05	0.56
1:C:166:PHE:CE2	1:C:167:LYS:HD3	2.40	0.56
1:E:14:MET:SD	1:E:18:ILE:CG1	2.94	0.56
1:E:27:PHE:HD2	1:E:27:PHE:O	1.86	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:166:PHE:N	1:C:166:PHE:CD2	2.73	0.56
1:E:55:TRP:HA	1:E:55:TRP:HE3	1.68	0.56
1:A:33:THR:HG22	1:A:34:PHE:CE1	2.40	0.56
1:A:149:PHE:CD1	1:A:152:ILE:HD12	2.41	0.56
1:B:36:LYS:HE3	1:B:37:ILE:HD13	1.88	0.56
1:E:14:MET:SD	1:E:17:LEU:CD2	2.94	0.56
1:F:29:ALA:C	1:F:36:LYS:NZ	2.54	0.56
1:F:35:LEU:O	1:F:36:LYS:HB2	2.05	0.56
1:F:74:ALA:HB3	2:F:201:FOL:H7	1.82	0.56
1:F:93:TYR:HD1	1:F:93:TYR:O	1.89	0.56
1:D:27:PHE:O	1:D:28:PHE:HD2	1.89	0.56
1:B:30:TYR:HB2	1:B:36:LYS:NZ	2.21	0.56
2:B:201:FOL:C6	2:B:201:FOL:H15	2.36	0.56
1:F:138:TRP:CD1	1:F:138:TRP:N	2.73	0.56
1:B:106:ILE:HG13	1:B:154:VAL:HG11	1.88	0.56
1:C:114:VAL:CG2	1:D:144:ILE:CD1	2.83	0.56
1:A:26:ARG:HE	1:A:27:PHE:H	1.54	0.56
1:B:74:ALA:O	2:B:201:FOL:H7	2.06	0.56
1:D:80:PHE:O	1:D:83:ASN:HB2	2.06	0.56
1:A:26:ARG:CG	1:A:27:PHE:CG	2.85	0.55
1:A:36:LYS:HG3	2:A:201:FOL:HB2	1.87	0.55
1:A:49:MET:CE	1:A:100:MET:CE	2.84	0.55
1:B:96:TYR:CD2	1:B:97:LYS:HG3	2.40	0.55
1:D:35:LEU:HD21	1:D:145:LYS:HD2	1.88	0.55
1:D:131:VAL:HG13	1:D:131:VAL:O	2.05	0.55
1:E:102:TRP:HB2	1:E:158:TYR:OH	2.06	0.55
1:E:110:LEU:O	1:E:114:VAL:HG12	2.06	0.55
1:F:13:LEU:CD2	1:F:14:MET:SD	2.94	0.55
1:F:160:LEU:CA	1:F:163:LYS:HG2	2.35	0.55
1:A:36:LYS:HG2	2:A:201:FOL:C12	2.36	0.55
1:A:60:THR:HG22	1:A:84:ALA:HB1	1.88	0.55
1:B:131:VAL:CG1	1:B:133:LEU:HD11	2.36	0.55
1:C:26:ARG:NH1	1:C:26:ARG:HG2	2.15	0.55
1:C:14:MET:HB2	1:C:51:PHE:CZ	2.41	0.55
1:C:34:PHE:CE1	1:C:129:TYR:HD2	2.18	0.55
1:D:133:LEU:HD11	1:D:138:TRP:CZ3	2.42	0.55
1:A:70:LEU:H	1:A:70:LEU:CD1	2.09	0.55
1:C:96:TYR:HE1	1:C:169:LEU:CD2	2.20	0.55
1:C:128:MET:HE2	1:C:129:TYR:CE1	2.41	0.55
1:F:31:GLU:HB2	1:F:32:THR:OG1	2.06	0.55
1:A:46:LEU:O	1:A:50:ILE:HG13	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:14:MET:HE1	1:E:59:GLY:HA3	1.89	0.55
1:E:18:ILE:CG2	1:E:63:ALA:CA	2.85	0.55
1:E:55:TRP:HA	1:E:58:ILE:HD11	1.89	0.55
1:E:83:ASN:OD1	1:E:83:ASN:N	2.39	0.55
1:F:94:PHE:HB3	1:F:95:TYR:CZ	2.41	0.55
1:B:19:ALA:HA	1:B:22:VAL:HG22	1.87	0.55
1:A:70:LEU:HD12	1:A:70:LEU:N	2.13	0.55
1:D:143:LEU:HA	1:D:146:THR:OG1	2.07	0.55
1:D:36:LYS:HB3	2:D:201:FOL:C	2.36	0.55
1:F:115:LEU:O	1:F:119:ILE:HD13	2.07	0.55
1:A:22:VAL:O	1:A:26:ARG:HB3	2.07	0.55
1:B:164:ILE:HG12	1:B:165:PRO:CD	2.30	0.55
1:D:77:PHE:H	1:D:80:PHE:HE2	1.55	0.55
1:B:30:TYR:HB2	1:B:36:LYS:CE	2.37	0.55
1:B:71:PHE:N	1:B:72:PRO:CD	2.69	0.55
1:E:120:LEU:O	1:E:124:TRP:HB2	2.07	0.55
1:A:132:ASN:HD22	1:A:132:ASN:C	2.02	0.54
1:B:33:THR:HG22	1:B:34:PHE:CD2	2.42	0.54
1:D:61:ALA:O	1:D:64:ASP:HB3	2.06	0.54
1:E:107:LEU:HD12	1:E:107:LEU:O	2.07	0.54
1:F:80:PHE:CZ	2:F:201:FOL:N3	2.72	0.54
1:F:160:LEU:C	1:F:163:LYS:CG	2.72	0.54
1:A:30:TYR:CD2	1:A:37:ILE:HD12	2.43	0.54
1:A:49:MET:HE3	1:A:100:MET:HE1	1.88	0.54
1:A:71:PHE:CD1	1:A:71:PHE:N	2.75	0.54
1:A:170:PHE:CD2	1:A:171:GLY:N	2.73	0.54
1:C:107:LEU:HD13	1:C:107:LEU:O	2.07	0.54
1:E:41:PHE:O	1:E:42:ILE:HG12	2.06	0.54
1:E:149:PHE:HD1	1:E:152:ILE:HD11	1.70	0.54
1:F:36:LYS:HG3	1:F:37:ILE:C	2.27	0.54
1:A:140:VAL:O	1:A:144:ILE:HG13	2.07	0.54
1:C:143:LEU:O	1:C:147:VAL:HG22	2.08	0.54
1:C:30:TYR:HB2	1:C:37:ILE:H	1.73	0.54
1:C:94:PHE:CG	1:C:108:ALA:HB2	2.42	0.54
1:D:20:VAL:HA	1:D:23:VAL:CG2	2.37	0.54
1:D:30:TYR:HD2	1:D:37:ILE:HG22	1.72	0.54
1:D:51:PHE:CD1	1:D:51:PHE:N	2.73	0.54
1:D:96:TYR:CE2	1:D:97:LYS:HG3	2.43	0.54
1:E:69:LEU:HD13	1:E:70:LEU:CB	2.37	0.54
1:E:145:LYS:HE2	1:E:146:THR:C	2.28	0.54
1:A:17:LEU:HD13	1:A:47:ILE:CG1	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:PHE:CE2	1:B:43:PRO:HD3	2.42	0.54
1:E:172:LYS:HB3	1:E:173:PRO:CA	2.31	0.54
1:B:31:GLU:CB	1:B:36:LYS:HD3	2.35	0.54
1:C:10:SER:CB	1:C:170:PHE:CZ	2.75	0.54
1:E:139:TRP:CZ3	1:E:142:ARG:NE	2.76	0.54
1:A:97:LYS:HE2	1:A:170:PHE:CD1	2.33	0.54
1:A:120:LEU:O	1:A:123:LEU:HB3	2.07	0.54
1:D:34:PHE:CD1	1:D:34:PHE:N	2.72	0.54
1:E:29:ALA:HB1	1:E:30:TYR:CD2	2.39	0.54
1:A:26:ARG:CD	1:A:27:PHE:CG	2.91	0.54
1:B:73:LYS:HE2	1:B:74:ALA:H	1.71	0.54
1:B:138:TRP:HE3	1:B:139:TRP:N	2.06	0.54
1:C:35:LEU:HD11	1:C:145:LYS:HD2	1.90	0.54
1:F:110:LEU:HD23	1:F:111:LEU:N	2.22	0.54
1:F:120:LEU:HA	1:F:123:LEU:HD13	1.88	0.54
1:A:18:ILE:HD13	1:A:63:ALA:HB2	1.90	0.54
1:F:23:VAL:HA	1:F:27:PHE:CE2	2.43	0.54
1:B:137:ALA:HB1	1:B:140:VAL:HG21	1.88	0.54
1:E:14:MET:SD	1:E:18:ILE:CD1	2.94	0.54
1:E:47:ILE:HA	1:E:50:ILE:CG2	2.32	0.54
1:E:70:LEU:HD23	1:E:71:PHE:CG	2.43	0.54
1:E:77:PHE:CD1	1:E:78:PRO:CD	2.79	0.54
1:F:94:PHE:CE2	1:F:108:ALA:HB2	2.40	0.54
1:E:76:TYR:HE1	1:E:78:PRO:HA	1.73	0.53
1:F:129:TYR:CG	1:F:129:TYR:O	2.60	0.53
1:A:170:PHE:CD2	1:A:173:PRO:HG3	2.42	0.53
1:D:64:ASP:CG	1:D:81:THR:HG22	2.28	0.53
1:E:34:PHE:O	1:E:35:LEU:HG	2.08	0.53
1:E:115:LEU:C	1:E:119:ILE:HG12	2.20	0.53
1:F:13:LEU:HD22	1:F:14:MET:CA	2.38	0.53
1:A:70:LEU:CB	1:A:71:PHE:CE1	2.91	0.53
1:A:116:ILE:HD12	1:A:117:ASN:N	2.24	0.53
1:A:172:LYS:CE	1:A:172:LYS:CA	2.86	0.53
1:C:57:GLY:HA3	1:C:85:PHE:CE1	2.43	0.53
1:E:112:VAL:HA	1:E:115:LEU:CB	2.39	0.53
1:B:49:MET:HG2	1:B:95:TYR:HB3	1.91	0.53
1:B:138:TRP:CE3	1:B:139:TRP:CA	2.91	0.53
1:E:10:SER:CA	1:E:13:LEU:CD2	2.86	0.53
1:A:100:MET:CE	1:A:161:GLY:CA	2.84	0.53
1:B:37:ILE:H	1:B:37:ILE:CD1	2.20	0.53
1:E:139:TRP:HZ3	1:E:142:ARG:NE	2.07	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:26:ARG:HE	1:A:27:PHE:N	2.07	0.53
1:A:39:PHE:CD2	1:A:41:PHE:HZ	2.26	0.53
1:A:49:MET:HE1	1:A:100:MET:CE	2.38	0.53
1:B:128:MET:CE	1:B:129:TYR:CE2	2.91	0.53
1:E:116:ILE:HD12	1:E:117:ASN:H	1.74	0.53
1:F:140:VAL:O	1:F:144:ILE:HG22	2.09	0.53
1:A:150:PHE:O	1:A:154:VAL:HG23	2.08	0.53
1:C:55:TRP:CD1	1:C:172:LYS:CB	2.89	0.53
1:E:22:VAL:HG22	1:E:67:GLY:HA2	1.89	0.53
1:E:150:PHE:CD1	1:E:153:GLN:HB3	2.44	0.53
1:F:83:ASN:OD1	1:F:120:LEU:HD22	2.09	0.53
1:F:95:TYR:CZ	1:F:108:ALA:HB3	2.41	0.53
1:C:100:MET:SD	1:C:161:GLY:HA3	2.48	0.53
1:E:86:LEU:HD13	1:E:115:LEU:HD21	1.91	0.53
1:F:80:PHE:CD2	2:F:201:FOL:NA2	2.77	0.53
1:F:80:PHE:CZ	2:F:201:FOL:C4	2.92	0.53
1:B:173:PRO:O	1:B:173:PRO:CD	2.56	0.53
1:E:145:LYS:HD2	1:E:147:VAL:N	2.24	0.53
1:B:14:MET:O	1:B:18:ILE:HG12	2.09	0.53
1:D:37:ILE:HD11	1:D:145:LYS:HG3	1.90	0.53
1:E:139:TRP:O	1:E:141:PRO:HD2	2.09	0.53
1:F:54:PHE:HD2	1:F:55:TRP:CD1	2.27	0.53
1:E:77:PHE:CE1	1:E:78:PRO:HD2	2.41	0.52
1:E:112:VAL:CA	1:E:115:LEU:CB	2.84	0.52
1:F:35:LEU:HD23	1:F:35:LEU:H	1.72	0.52
1:F:59:GLY:O	1:F:62:VAL:HG22	2.09	0.52
1:F:120:LEU:CG	1:F:124:TRP:HZ3	2.22	0.52
1:A:50:ILE:C	1:A:173:PRO:HB3	2.30	0.52
1:B:145:LYS:O	1:B:149:PHE:HD2	1.92	0.52
1:C:43:PRO:O	1:C:46:LEU:N	2.43	0.52
1:F:122:PRO:N	1:F:125:LEU:HD12	2.24	0.52
1:B:138:TRP:HE3	1:B:139:TRP:CA	2.22	0.52
1:E:17:LEU:HG	1:E:18:ILE:N	2.24	0.52
1:E:112:VAL:HB	1:E:115:LEU:CG	2.39	0.52
1:E:112:VAL:HA	1:E:115:LEU:HB3	1.91	0.52
1:F:29:ALA:HB1	1:F:36:LYS:HZ3	1.73	0.52
1:F:30:TYR:CB	1:F:36:LYS:HE3	2.28	0.52
1:F:35:LEU:CD2	1:F:35:LEU:N	2.73	0.52
1:B:137:ALA:CB	1:B:140:VAL:CG2	2.85	0.52
1:D:14:MET:HE2	1:D:51:PHE:HE2	0.73	0.52
1:D:147:VAL:CG2	1:D:148:ILE:N	2.73	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:18:ILE:HG21	1:E:63:ALA:HB2	1.82	0.52
1:B:19:ALA:O	1:B:22:VAL:HG23	2.10	0.52
1:C:116:ILE:O	1:C:120:LEU:HB2	2.10	0.52
1:F:116:ILE:HD11	1:F:120:LEU:HD22	1.89	0.52
1:E:42:ILE:N	1:E:43:PRO:CD	2.73	0.52
1:E:110:LEU:HD11	1:F:144:ILE:CD1	2.39	0.52
1:E:140:VAL:HG12	1:E:140:VAL:O	2.10	0.52
1:C:65:VAL:O	1:C:69:LEU:HD12	2.10	0.52
1:C:148:ILE:O	1:C:151:PRO:CG	2.57	0.52
1:D:59:GLY:O	1:D:62:VAL:HG22	2.10	0.52
1:E:40:THR:CG2	1:E:43:PRO:HG2	2.35	0.52
1:C:150:PHE:HE2	1:D:151:PRO:HG2	1.75	0.52
1:D:12:ALA:O	1:D:16:VAL:HG23	2.03	0.52
1:E:145:LYS:CD	1:E:149:PHE:HB3	2.36	0.52
1:E:150:PHE:HA	1:E:153:GLN:OE1	2.10	0.52
1:A:17:LEU:HD13	1:A:47:ILE:HG13	1.92	0.51
1:B:74:ALA:CB	2:B:201:FOL:H92	2.35	0.51
1:D:111:LEU:HD11	1:D:115:LEU:HD22	1.92	0.51
1:F:68:MET:HE1	2:F:201:FOL:C8A	2.39	0.51
1:B:55:TRP:O	1:B:59:GLY:N	2.40	0.51
1:C:24:PHE:CD2	1:C:39:PHE:O	2.62	0.51
1:E:22:VAL:HG21	1:E:67:GLY:CA	2.40	0.51
1:F:160:LEU:CA	1:F:163:LYS:CG	2.88	0.51
1:F:170:PHE:HD2	1:F:170:PHE:O	1.93	0.51
1:D:138:TRP:O	1:D:141:PRO:HD2	2.10	0.51
1:F:73:LYS:CD	2:F:201:FOL:C9	2.84	0.51
1:B:50:ILE:HG22	1:B:51:PHE:CE1	2.45	0.51
1:E:70:LEU:HD23	1:E:70:LEU:O	2.10	0.51
1:F:32:THR:O	1:F:35:LEU:HD22	2.03	0.51
1:F:119:ILE:C	1:F:123:LEU:HD12	2.30	0.51
1:B:128:MET:HE2	1:B:129:TYR:HE2	1.75	0.51
1:F:116:ILE:CA	1:F:120:LEU:HD13	2.28	0.51
1:C:36:LYS:HB2	2:C:201:FOL:HN	1.76	0.51
1:C:123:LEU:O	1:C:127:LEU:HG	2.10	0.51
1:F:13:LEU:CD1	1:F:13:LEU:H	2.22	0.51
1:A:109:THR:HA	1:A:112:VAL:CG1	2.40	0.51
1:D:66:VAL:HA	1:D:69:LEU:HD12	1.92	0.51
1:D:114:VAL:O	1:D:119:ILE:HG12	2.11	0.51
1:E:36:LYS:CB	2:E:201:FOL:H12	2.38	0.51
1:E:151:PRO:O	1:E:154:VAL:HG22	2.11	0.51
1:F:118:ILE:O	1:F:122:PRO:HG2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:17:LEU:HA	1:A:20:VAL:CG2	2.41	0.51
1:B:41:PHE:CD2	1:B:153:GLN:HG3	2.46	0.51
1:E:36:LYS:HB3	2:E:201:FOL:N	2.26	0.51
1:F:68:MET:CE	2:F:201:FOL:N1	2.74	0.51
1:C:33:THR:HG22	1:C:129:TYR:CE2	2.38	0.51
1:C:138:TRP:O	1:C:141:PRO:HD2	2.10	0.51
1:F:121:THR:O	1:F:125:LEU:HG	2.10	0.51
1:B:53:PRO:HG2	1:B:54:PHE:N	2.26	0.51
1:B:113:THR:HA	1:B:117:ASN:OD1	2.11	0.51
1:C:111:LEU:HD23	1:C:111:LEU:C	2.28	0.51
1:F:68:MET:SD	2:F:201:FOL:NA2	2.83	0.51
1:A:35:LEU:HD11	1:A:145:LYS:HD3	1.92	0.50
1:A:114:VAL:HG21	1:B:144:ILE:HG12	1.93	0.50
1:B:164:ILE:CD1	1:B:165:PRO:N	2.73	0.50
1:C:34:PHE:CE2	1:C:138:TRP:CD1	2.99	0.50
1:E:40:THR:CG2	1:E:43:PRO:HD2	2.39	0.50
1:F:13:LEU:CD1	1:F:13:LEU:N	2.73	0.50
1:F:14:MET:HE3	1:F:14:MET:CA	2.30	0.50
1:F:106:ILE:HD13	1:F:154:VAL:HG11	1.94	0.50
1:A:66:VAL:HG13	1:A:70:LEU:HD11	1.92	0.50
1:A:112:VAL:CG2	1:A:116:ILE:HD11	2.40	0.50
1:A:118:ILE:HD12	1:B:143:LEU:HD13	1.93	0.50
1:C:49:MET:O	1:C:96:TYR:HD1	1.91	0.50
1:A:36:LYS:HZ2	2:A:201:FOL:HN	1.58	0.50
1:A:160:LEU:HD23	1:A:161:GLY:CA	2.42	0.50
1:B:36:LYS:HE2	1:B:37:ILE:CA	2.42	0.50
1:C:166:PHE:CZ	1:C:167:LYS:HD3	2.47	0.50
1:D:97:LYS:HE2	1:D:170:PHE:CZ	2.46	0.50
1:D:148:ILE:HG13	1:D:149:PHE:H	1.73	0.50
1:F:13:LEU:HD13	1:F:14:MET:N	2.26	0.50
1:A:49:MET:CE	1:A:100:MET:HE1	2.42	0.50
1:E:145:LYS:HD2	1:E:148:ILE:N	2.27	0.50
1:F:33:THR:C	1:F:34:PHE:CG	2.85	0.50
1:C:70:LEU:CA	1:C:72:PRO:HD3	2.41	0.50
1:D:106:ILE:O	1:D:109:THR:HG22	2.12	0.50
1:A:26:ARG:NE	1:A:27:PHE:N	2.60	0.50
1:C:93:TYR:C	1:C:93:TYR:CD2	2.85	0.50
1:C:116:ILE:CG2	1:C:117:ASN:N	2.73	0.50
1:C:125:LEU:HA	1:C:128:MET:CG	2.38	0.50
1:D:50:ILE:CG2	1:D:51:PHE:CE1	2.94	0.50
1:D:126:SER:O	1:D:130:GLY:HA2	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:90:ILE:HG21	1:E:112:VAL:HG21	1.93	0.50
1:F:33:THR:C	1:F:34:PHE:CD2	2.85	0.50
1:F:103:GLN:NE2	1:F:103:GLN:CA	2.73	0.50
1:B:138:TRP:CE3	1:B:138:TRP:C	2.85	0.50
1:D:27:PHE:C	1:D:28:PHE:CD2	2.85	0.50
1:E:23:VAL:HA	1:E:26:ARG:CB	2.39	0.50
1:E:45:SER:HB2	1:E:160:LEU:CD1	2.42	0.50
1:F:16:VAL:CG2	1:F:17:LEU:CD2	2.85	0.50
1:F:61:ALA:O	1:F:65:VAL:CG2	2.40	0.50
1:A:26:ARG:O	1:A:27:PHE:HD1	1.94	0.50
1:B:54:PHE:CD1	1:B:54:PHE:C	2.85	0.50
1:B:64:ASP:OD2	1:B:81:THR:HG22	2.12	0.50
1:C:83:ASN:OD1	1:C:116:ILE:HG13	2.12	0.50
1:F:67:GLY:HA2	1:F:70:LEU:HB2	1.93	0.50
1:F:103:GLN:O	1:F:104:ARG:HG2	2.12	0.50
1:F:54:PHE:CD2	1:F:55:TRP:HD1	2.29	0.49
1:B:36:LYS:CE	1:B:37:ILE:HD12	2.41	0.49
1:C:57:GLY:C	1:C:85:PHE:CD1	2.84	0.49
1:C:96:TYR:CZ	1:C:169:LEU:CD2	2.95	0.49
1:E:112:VAL:O	1:E:115:LEU:HB3	2.12	0.49
1:F:116:ILE:HG23	1:F:117:ASN:H	1.75	0.49
1:C:70:LEU:CD2	1:C:70:LEU:N	2.73	0.49
1:C:96:TYR:O	1:C:98:LYS:HG3	2.11	0.49
1:E:22:VAL:HG21	1:E:67:GLY:HA2	1.91	0.49
1:E:76:TYR:HD1	1:E:77:PHE:N	2.10	0.49
1:A:24:PHE:CE2	1:A:43:PRO:HD3	2.47	0.49
1:B:133:LEU:HD12	1:B:133:LEU:H	1.74	0.49
1:E:18:ILE:HG21	1:E:63:ALA:CB	2.37	0.49
1:E:46:LEU:HD12	1:E:49:MET:SD	2.52	0.49
1:F:93:TYR:CD1	1:F:93:TYR:C	2.85	0.49
1:F:118:ILE:HG23	1:F:119:ILE:HD12	1.87	0.49
1:A:23:VAL:HG13	1:A:26:ARG:CD	2.42	0.49
1:B:45:SER:O	1:B:49:MET:HG3	2.12	0.49
1:D:79:GLY:O	1:D:124:TRP:CH2	2.66	0.49
1:E:32:THR:CG2	1:E:33:THR:N	2.75	0.49
1:C:150:PHE:C	1:C:150:PHE:CD2	2.85	0.49
1:A:126:SER:HG	1:A:127:LEU:N	2.11	0.49
1:B:138:TRP:CE3	1:B:139:TRP:N	2.81	0.49
1:E:137:ALA:C	1:E:138:TRP:CD1	2.86	0.49
1:A:150:PHE:CD1	1:A:150:PHE:C	2.86	0.49
1:A:162:ASN:ND2	1:A:162:ASN:N	2.60	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:172:LYS:N	1:A:173:PRO:HD3	2.25	0.49
1:B:162:ASN:ND2	1:B:162:ASN:N	2.60	0.49
1:E:13:LEU:CA	1:E:16:VAL:CG2	2.86	0.49
1:E:115:LEU:HD13	1:E:116:ILE:HA	1.93	0.49
1:B:135:ASN:CB	1:B:138:TRP:HB2	2.35	0.49
1:C:97:LYS:HG3	1:C:169:LEU:HD22	1.95	0.49
1:C:133:LEU:HG	1:C:134:ALA:N	2.27	0.49
1:C:125:LEU:CD2	2:C:201:FOL:H16	2.43	0.49
1:D:36:LYS:HB2	2:D:201:FOL:H12	1.94	0.49
1:E:37:ILE:HG23	1:E:37:ILE:O	2.13	0.49
1:E:76:TYR:HA	2:E:201:FOL:N8	2.28	0.49
1:E:76:TYR:CE1	1:E:78:PRO:HA	2.48	0.49
1:F:36:LYS:CG	1:F:37:ILE:N	2.76	0.49
1:A:36:LYS:HG2	2:A:201:FOL:C	2.43	0.48
1:A:126:SER:HG	1:A:127:LEU:H	1.61	0.48
1:A:35:LEU:C	2:A:201:FOL:H12	2.33	0.48
1:A:137:ALA:HA	1:A:140:VAL:HG23	1.94	0.48
1:E:13:LEU:N	1:E:13:LEU:CD1	2.73	0.48
1:F:78:PRO:O	1:F:81:THR:HG22	2.14	0.48
1:F:116:ILE:O	1:F:120:LEU:HB2	2.13	0.48
1:C:64:ASP:OD2	1:C:81:THR:CA	2.61	0.48
2:F:201:FOL:H16	2:F:201:FOL:HG1	1.94	0.48
1:C:173:PRO:HG2	1:C:174:LEU:N	2.28	0.48
1:A:49:MET:CE	1:A:100:MET:HE2	2.44	0.48
1:C:30:TYR:CB	1:C:37:ILE:H	2.25	0.48
1:C:68:MET:HE1	1:C:72:PRO:CA	2.43	0.48
1:C:166:PHE:N	1:C:166:PHE:HD2	2.11	0.48
1:E:90:ILE:HG21	1:E:112:VAL:CG2	2.44	0.48
1:F:150:PHE:CD1	1:F:153:GLN:OE1	2.67	0.48
1:B:128:MET:HE2	1:B:129:TYR:CE2	2.49	0.48
1:C:125:LEU:HD13	1:C:138:TRP:CZ2	2.49	0.48
1:E:119:ILE:HG13	1:E:120:LEU:CB	2.36	0.48
1:A:170:PHE:CE2	1:A:173:PRO:HG2	2.48	0.48
1:C:30:TYR:HB2	1:C:37:ILE:N	2.28	0.48
1:D:117:ASN:ND2	2:D:201:FOL:OE1	2.46	0.48
1:E:68:MET:CE	2:E:201:FOL:C4A	2.92	0.48
1:B:36:LYS:CE	1:B:37:ILE:HD13	2.44	0.48
1:B:53:PRO:HG2	1:B:54:PHE:H	1.78	0.48
1:C:10:SER:CA	1:C:170:PHE:CZ	2.96	0.48
1:E:40:THR:HG22	1:E:43:PRO:CD	2.42	0.48
1:E:76:TYR:CD1	1:E:76:TYR:C	2.86	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:79:GLY:C	1:E:81:THR:N	2.66	0.48
1:B:48:GLY:O	1:B:96:TYR:HB2	2.14	0.48
1:B:149:PHE:CD1	1:B:152:ILE:HD12	2.44	0.48
1:D:26:ARG:HA	1:D:26:ARG:HD3	1.53	0.48
1:E:11:ILE:HG13	1:E:12:ALA:N	2.29	0.48
1:E:107:LEU:O	1:E:111:LEU:HB2	2.13	0.48
1:C:41:PHE:CZ	1:C:42:ILE:HG12	2.48	0.48
1:D:105:VAL:HG21	1:D:158:TYR:HB2	1.95	0.48
1:C:51:PHE:HB3	1:C:55:TRP:HB2	1.96	0.47
1:E:34:PHE:O	1:E:35:LEU:HD23	2.13	0.47
1:F:150:PHE:O	1:F:153:GLN:OE1	2.32	0.47
1:A:155:ILE:N	1:A:155:ILE:CD1	2.77	0.47
1:B:128:MET:HE3	1:B:129:TYR:CE2	2.48	0.47
1:D:148:ILE:O	1:D:152:ILE:HG13	2.14	0.47
1:E:140:VAL:N	1:E:141:PRO:HD2	2.28	0.47
1:F:16:VAL:CG2	1:F:17:LEU:N	2.77	0.47
1:F:107:LEU:HD13	1:F:107:LEU:HA	1.76	0.47
1:C:96:TYR:HH	1:C:169:LEU:HD23	1.74	0.47
1:C:166:PHE:HE2	1:C:167:LYS:HZ3	1.61	0.47
1:E:51:PHE:CD1	1:E:170:PHE:HB3	2.49	0.47
1:F:18:ILE:CD1	1:F:19:ALA:N	2.73	0.47
1:A:8:THR:O	1:A:11:ILE:N	2.47	0.47
1:D:41:PHE:CD1	1:D:157:THR:OG1	2.67	0.47
1:F:35:LEU:HD23	1:F:35:LEU:N	2.28	0.47
1:A:39:PHE:CD2	1:A:41:PHE:CZ	3.01	0.47
1:A:51:PHE:CD1	1:A:51:PHE:N	2.82	0.47
1:B:62:VAL:O	1:B:66:VAL:HG13	2.15	0.47
1:C:8:THR:C	1:C:9:LYS:HD3	2.35	0.47
1:C:118:ILE:O	1:C:122:PRO:HD2	2.15	0.47
1:E:145:LYS:HD3	1:E:149:PHE:CB	2.39	0.47
1:B:145:LYS:HG2	1:B:149:PHE:CD2	2.50	0.47
1:C:112:VAL:CG1	1:C:116:ILE:HG21	2.44	0.47
1:D:124:TRP:HD1	1:D:127:LEU:HD12	1.79	0.47
1:F:54:PHE:CD2	1:F:55:TRP:CD1	3.02	0.47
1:F:114:VAL:HG13	1:F:115:LEU:N	2.30	0.47
1:A:17:LEU:O	1:A:20:VAL:HG23	2.14	0.47
1:A:172:LYS:NZ	1:A:172:LYS:CA	2.78	0.47
1:C:17:LEU:HB3	1:C:47:ILE:HD11	1.97	0.47
1:C:70:LEU:O	1:C:71:PHE:HB2	2.15	0.47
1:D:24:PHE:CE2	1:D:43:PRO:HD3	2.50	0.47
1:D:33:THR:HG21	1:D:34:PHE:CE1	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:86:LEU:O	1:E:90:ILE:HD13	2.14	0.47
1:E:115:LEU:C	1:E:115:LEU:CD2	2.60	0.47
1:E:17:LEU:CA	1:E:20:VAL:CG2	2.92	0.47
1:E:145:LYS:NZ	1:E:150:PHE:CD2	2.82	0.47
1:F:119:ILE:HD12	1:F:119:ILE:N	2.30	0.47
1:A:114:VAL:O	1:A:118:ILE:HG12	2.15	0.47
1:B:142:ARG:HH12	2:B:201:FOL:HG2	1.80	0.47
1:F:119:ILE:CG2	1:F:123:LEU:CD1	2.86	0.47
1:A:16:VAL:O	1:A:20:VAL:HG22	2.14	0.47
1:C:86:LEU:HD23	1:C:86:LEU:HA	1.75	0.47
1:C:157:THR:O	1:C:160:LEU:HB3	2.16	0.47
1:E:23:VAL:CA	1:E:26:ARG:CD	2.74	0.47
1:E:52:GLY:O	1:E:56:ALA:HB3	2.13	0.47
1:F:80:PHE:HD2	2:F:201:FOL:HN22	1.63	0.47
1:F:116:ILE:CD1	1:F:120:LEU:CD1	2.86	0.47
1:F:170:PHE:N	1:F:170:PHE:CD2	2.82	0.47
1:A:77:PHE:CD1	1:A:78:PRO:HD2	2.50	0.46
1:B:80:PHE:HD2	2:B:201:FOL:C8A	2.27	0.46
1:B:114:VAL:O	1:B:119:ILE:HD13	2.15	0.46
1:C:149:PHE:O	1:C:152:ILE:N	2.48	0.46
1:D:105:VAL:HG21	1:D:158:TYR:HD1	1.81	0.46
1:D:135:ASN:ND2	1:D:137:ALA:HB3	2.30	0.46
1:E:27:PHE:CD2	1:E:27:PHE:N	2.73	0.46
1:F:17:LEU:HD13	1:F:17:LEU:HA	1.69	0.46
1:D:9:LYS:HG3	1:D:10:SER:N	2.30	0.46
1:D:150:PHE:C	1:D:150:PHE:CD2	2.88	0.46
1:E:117:ASN:HA	1:E:121:THR:OG1	2.15	0.46
1:E:128:MET:HB3	1:E:129:TYR:CE2	2.49	0.46
1:F:117:ASN:HA	1:F:121:THR:OG1	2.15	0.46
1:C:27:PHE:N	1:C:27:PHE:HD1	2.14	0.46
1:C:110:LEU:HA	1:C:113:THR:CG2	2.45	0.46
1:D:10:SER:HB2	1:D:172:LYS:HG3	1.90	0.46
1:E:137:ALA:C	1:E:138:TRP:HD1	2.17	0.46
1:B:164:ILE:CG1	1:B:165:PRO:HD2	2.37	0.46
1:E:55:TRP:HA	1:E:58:ILE:CD1	2.45	0.46
1:A:76:TYR:C	1:A:76:TYR:CD2	2.89	0.46
1:C:112:VAL:HG13	1:C:116:ILE:HG21	1.97	0.46
1:F:30:TYR:HB2	1:F:36:LYS:CE	2.32	0.46
1:A:23:VAL:CA	1:A:26:ARG:HD3	2.44	0.46
1:C:19:ALA:O	1:C:23:VAL:HG12	2.15	0.46
1:C:45:SER:HB3	1:C:95:TYR:HE2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:18:ILE:HG23	1:B:63:ALA:HA	1.97	0.46
1:E:18:ILE:HG21	1:E:63:ALA:HA	1.96	0.46
1:F:17:LEU:O	1:F:20:VAL:HB	2.15	0.46
1:F:111:LEU:O	1:F:114:VAL:HG13	2.16	0.46
1:A:80:PHE:O	1:A:83:ASN:HB2	2.16	0.46
1:B:18:ILE:O	1:B:22:VAL:HG22	2.15	0.46
1:B:48:GLY:HA2	1:B:92:GLY:HA2	1.98	0.46
1:C:150:PHE:C	1:C:153:GLN:HG2	2.35	0.46
1:F:32:THR:C	1:F:33:THR:OG1	2.53	0.46
1:F:73:LYS:CG	2:F:201:FOL:C7	2.94	0.46
1:B:14:MET:HG2	1:B:51:PHE:HZ	1.15	0.46
1:C:40:THR:O	1:C:43:PRO:HD2	2.15	0.46
1:D:17:LEU:N	1:D:17:LEU:HD23	2.31	0.46
1:D:108:ALA:O	1:D:111:LEU:N	2.49	0.46
1:F:24:PHE:O	1:F:39:PHE:HD2	1.98	0.46
1:A:23:VAL:O	1:A:26:ARG:HB3	2.16	0.46
1:A:26:ARG:NH1	1:A:28:PHE:HB2	2.31	0.46
1:C:150:PHE:N	1:C:151:PRO:HD2	2.31	0.46
1:D:18:ILE:O	1:D:22:VAL:HG23	2.16	0.46
1:D:80:PHE:CD1	1:D:80:PHE:C	2.89	0.46
1:E:40:THR:CG2	1:E:43:PRO:CG	2.93	0.46
1:E:152:ILE:HA	1:E:155:ILE:HD13	1.98	0.46
1:A:26:ARG:NH2	1:A:27:PHE:HB2	2.29	0.45
1:C:94:PHE:CD1	1:C:108:ALA:HA	2.51	0.45
1:D:64:ASP:OD1	1:D:80:PHE:HE1	1.99	0.45
1:F:116:ILE:CD1	1:F:120:LEU:CD2	2.85	0.45
1:F:122:PRO:HD3	1:F:142:ARG:HH12	1.80	0.45
1:B:74:ALA:O	2:B:201:FOL:C7	2.65	0.45
1:F:116:ILE:HD13	1:F:120:LEU:CD2	2.44	0.45
1:C:48:GLY:O	1:C:92:GLY:CA	2.57	0.45
1:C:149:PHE:O	1:C:152:ILE:HB	2.17	0.45
1:E:29:ALA:CB	1:E:39:PHE:CD2	2.94	0.45
1:E:69:LEU:CD1	1:E:70:LEU:HB2	2.47	0.45
1:E:80:PHE:HD2	2:E:201:FOL:N1	2.15	0.45
1:E:148:ILE:C	1:E:151:PRO:HD2	2.36	0.45
2:F:201:FOL:C6	2:F:201:FOL:H15	2.46	0.45
1:A:101:THR:C	1:A:103:GLN:N	2.66	0.45
1:B:29:ALA:C	1:B:36:LYS:HZ2	2.19	0.45
1:C:170:PHE:HD1	1:C:172:LYS:CE	2.29	0.45
1:E:18:ILE:CG2	1:E:63:ALA:HA	2.46	0.45
1:F:14:MET:CE	1:F:14:MET:CA	2.86	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:111:LEU:HA	1:F:114:VAL:CG1	2.46	0.45
1:F:150:PHE:HA	1:F:153:GLN:H	1.81	0.45
1:A:50:ILE:HB	1:A:51:PHE:HD1	1.77	0.45
1:A:111:LEU:O	1:A:115:LEU:HB3	2.17	0.45
1:D:139:TRP:O	1:D:142:ARG:HB3	2.17	0.45
1:E:18:ILE:HG21	1:E:63:ALA:CA	2.46	0.45
1:E:41:PHE:C	1:E:43:PRO:CD	2.85	0.45
1:E:113:THR:HA	1:E:116:ILE:HD11	1.98	0.45
1:B:26:ARG:CD	1:B:71:PHE:CD1	3.00	0.45
1:B:76:TYR:C	1:B:76:TYR:CD2	2.90	0.45
1:B:81:THR:HG23	2:B:201:FOL:HN22	1.82	0.45
1:B:120:LEU:HD22	1:B:124:TRP:CZ2	2.51	0.45
1:C:22:VAL:O	1:C:26:ARG:HB2	2.17	0.45
1:C:107:LEU:CD1	1:C:107:LEU:C	2.85	0.45
1:F:25:SER:O	1:F:29:ALA:HB3	2.14	0.45
1:F:116:ILE:HD12	1:F:120:LEU:CB	2.43	0.45
1:F:120:LEU:HB3	1:F:124:TRP:CE3	2.51	0.45
1:C:27:PHE:N	1:C:27:PHE:CD1	2.84	0.45
1:C:98:LYS:HE3	1:C:104:ARG:HH11	1.79	0.45
1:E:55:TRP:C	1:E:58:ILE:HG13	2.36	0.45
1:F:53:PRO:O	1:F:56:ALA:HB3	2.17	0.45
1:A:30:TYR:O	1:A:36:LYS:HA	2.16	0.45
1:A:49:MET:O	1:A:96:TYR:CD1	2.60	0.45
1:C:68:MET:HE3	1:C:74:ALA:N	2.32	0.45
1:C:114:VAL:CG2	1:D:144:ILE:HD13	2.47	0.45
1:E:54:PHE:O	1:E:58:ILE:HG13	2.17	0.45
1:E:66:VAL:C	1:E:69:LEU:HB3	2.36	0.45
1:C:122:PRO:CA	1:C:125:LEU:HD12	2.28	0.45
1:C:124:TRP:HE3	1:C:124:TRP:HA	1.81	0.45
1:E:80:PHE:HA	1:E:124:TRP:CE3	2.51	0.45
1:A:143:LEU:O	1:A:147:VAL:HG12	2.17	0.45
1:C:110:LEU:O	1:C:113:THR:HG23	2.17	0.45
1:D:86:LEU:O	1:D:90:ILE:HG13	2.17	0.45
1:E:10:SER:OG	1:E:170:PHE:HD2	1.92	0.45
1:F:81:THR:O	1:F:85:PHE:CD1	2.70	0.45
1:F:150:PHE:HB2	1:F:153:GLN:HB3	1.99	0.45
1:A:89:ALA:O	1:A:93:TYR:N	2.44	0.44
1:D:126:SER:O	1:D:130:GLY:N	2.50	0.44
1:E:43:PRO:CG	1:E:44:GLU:N	2.80	0.44
1:E:58:ILE:HD12	1:E:59:GLY:N	2.31	0.44
1:E:137:ALA:O	1:E:138:TRP:CD1	2.70	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:LEU:HD12	1:B:46:LEU:HA	1.73	0.44
1:D:35:LEU:C	1:D:35:LEU:CD2	2.86	0.44
1:E:69:LEU:HD13	1:E:69:LEU:C	2.18	0.44
1:E:76:TYR:CD1	1:E:77:PHE:O	2.70	0.44
1:E:151:PRO:O	1:E:155:ILE:HD12	2.17	0.44
1:F:120:LEU:O	1:F:124:TRP:CE3	2.70	0.44
1:F:153:GLN:OE1	1:F:154:VAL:HG23	2.17	0.44
1:B:13:LEU:C	1:B:13:LEU:CD2	2.85	0.44
1:B:47:ILE:O	1:B:47:ILE:HG22	2.16	0.44
1:C:12:ALA:O	1:C:16:VAL:HG13	2.17	0.44
1:E:66:VAL:CA	1:E:69:LEU:HB3	2.48	0.44
1:F:40:THR:O	1:F:43:PRO:HD2	2.17	0.44
1:F:111:LEU:C	1:F:111:LEU:CD2	2.85	0.44
1:B:23:VAL:CG2	1:B:24:PHE:N	2.80	0.44
1:B:137:ALA:CB	1:B:140:VAL:HG21	2.48	0.44
1:C:68:MET:C	1:C:70:LEU:O	2.56	0.44
1:D:157:THR:HG22	1:D:157:THR:O	2.17	0.44
1:F:114:VAL:HG13	1:F:115:LEU:H	1.82	0.44
1:F:116:ILE:HD12	1:F:116:ILE:O	2.17	0.44
1:F:118:ILE:CG2	1:F:119:ILE:N	2.80	0.44
1:F:142:ARG:HG2	1:F:145:LYS:HZ1	1.82	0.44
1:A:49:MET:HE1	1:A:100:MET:HE2	1.99	0.44
1:C:91:TYR:HE1	1:C:112:VAL:HG21	1.81	0.44
1:E:111:LEU:O	1:E:114:VAL:HG13	2.18	0.44
1:F:170:PHE:O	1:F:170:PHE:CD2	2.70	0.44
1:A:100:MET:HE1	1:A:161:GLY:HA2	1.95	0.44
1:B:10:SER:O	1:B:14:MET:HB2	2.17	0.44
1:A:36:LYS:HZ3	2:A:201:FOL:HB2	1.83	0.44
1:B:36:LYS:HE2	1:B:37:ILE:CB	2.47	0.44
1:C:65:VAL:HG12	1:C:69:LEU:HD12	1.99	0.44
1:D:26:ARG:C	1:D:27:PHE:HD1	2.21	0.44
1:E:34:PHE:O	1:E:35:LEU:CG	2.66	0.44
1:E:76:TYR:CE1	1:E:77:PHE:O	2.70	0.44
1:E:115:LEU:HD22	1:E:119:ILE:HG12	2.00	0.44
1:B:112:VAL:O	1:B:116:ILE:HB	2.18	0.44
1:C:26:ARG:HA	1:C:26:ARG:HD3	1.72	0.44
1:C:110:LEU:O	1:C:113:THR:CG2	2.66	0.44
1:D:27:PHE:N	1:D:27:PHE:CD1	2.85	0.44
1:E:10:SER:OG	1:E:170:PHE:CE2	2.51	0.44
1:E:68:MET:CE	2:E:201:FOL:C8A	2.94	0.44
1:F:121:THR:C	1:F:125:LEU:HD12	2.38	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:24:PHE:HB3	1:B:40:THR:HG22	1.98	0.43
1:B:137:ALA:HB1	1:B:140:VAL:HG23	1.93	0.43
1:D:30:TYR:HE2	1:D:39:PHE:CD2	2.34	0.43
1:E:55:TRP:HA	1:E:58:ILE:HG12	2.00	0.43
1:F:68:MET:CE	2:F:201:FOL:C8A	2.96	0.43
1:F:150:PHE:HB2	1:F:153:GLN:CD	2.38	0.43
1:F:33:THR:O	1:F:34:PHE:CG	2.70	0.43
1:F:94:PHE:CE2	1:F:108:ALA:CB	2.99	0.43
1:F:121:THR:H	1:F:121:THR:HG1	1.57	0.43
1:B:164:ILE:HD13	1:B:165:PRO:CA	2.49	0.43
1:C:76:TYR:CE2	2:C:201:FOL:NA2	2.87	0.43
1:C:144:ILE:O	1:C:147:VAL:HG23	2.18	0.43
1:D:37:ILE:CD1	1:D:145:LYS:HG3	2.49	0.43
1:F:66:VAL:O	1:F:70:LEU:N	2.43	0.43
1:F:159:TYR:O	1:F:163:LYS:HG2	2.17	0.43
1:A:160:LEU:HD23	1:A:161:GLY:HA2	2.00	0.43
1:B:96:TYR:HE2	1:B:97:LYS:NZ	2.16	0.43
1:D:117:ASN:ND2	2:D:201:FOL:HG2	2.31	0.43
1:E:13:LEU:HA	1:E:16:VAL:HG21	1.97	0.43
1:E:150:PHE:HD1	1:E:153:GLN:HB3	1.82	0.43
1:A:26:ARG:NE	1:A:27:PHE:CB	2.81	0.43
1:A:41:PHE:HE1	1:A:42:ILE:HG12	1.82	0.43
1:C:118:ILE:O	1:C:122:PRO:CD	2.67	0.43
1:C:166:PHE:CZ	1:C:167:LYS:HD2	2.53	0.43
1:E:36:LYS:CB	2:E:201:FOL:C12	2.89	0.43
1:E:74:ALA:HB1	2:E:201:FOL:H7	2.00	0.43
1:A:36:LYS:NZ	2:A:201:FOL:HB2	2.33	0.43
1:D:35:LEU:HD22	1:D:37:ILE:HD12	1.99	0.43
1:F:170:PHE:CD2	1:F:170:PHE:C	2.92	0.43
1:A:18:ILE:HD12	1:A:59:GLY:O	2.17	0.43
1:A:26:ARG:O	1:A:27:PHE:CD1	2.70	0.43
1:A:86:LEU:HA	1:A:86:LEU:HD23	1.73	0.43
1:C:94:PHE:CD1	1:C:108:ALA:HB1	2.51	0.43
1:D:36:LYS:HB2	2:D:201:FOL:C12	2.49	0.43
1:E:115:LEU:HD22	1:E:119:ILE:CG1	2.49	0.43
1:A:122:PRO:HA	1:A:125:LEU:CD1	2.47	0.43
1:B:123:LEU:O	1:B:126:SER:OG	2.29	0.43
1:C:39:PHE:HB3	1:C:42:ILE:HD11	2.01	0.43
1:E:42:ILE:N	1:E:42:ILE:CD1	2.73	0.43
1:E:104:ARG:NH1	1:E:107:LEU:HD23	2.34	0.43
1:E:115:LEU:CD1	1:E:116:ILE:HG23	2.49	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:8:THR:O	1:A:9:LYS:C	2.58	0.43
1:C:49:MET:HE2	1:C:100:MET:HE3	0.55	0.43
1:D:27:PHE:O	1:D:28:PHE:CD2	2.70	0.43
1:E:17:LEU:HD11	1:E:47:ILE:HD13	1.97	0.43
1:E:41:PHE:C	1:E:42:ILE:CG1	2.86	0.43
1:F:18:ILE:C	1:F:18:ILE:CD1	2.86	0.43
1:F:26:ARG:HD2	1:F:26:ARG:HA	1.76	0.43
1:A:172:LYS:HA	1:A:172:LYS:HZ3	1.84	0.43
1:B:37:ILE:N	1:B:37:ILE:CD1	2.73	0.43
1:E:104:ARG:HH11	1:E:107:LEU:HD23	1.84	0.43
1:F:74:ALA:HB3	2:F:201:FOL:N8	2.34	0.43
1:B:44:GLU:HG2	1:B:60:THR:HG21	2.01	0.42
1:C:68:MET:HE3	1:C:75:GLY:H	1.83	0.42
1:E:115:LEU:CD2	1:E:119:ILE:HD13	2.49	0.42
1:F:73:LYS:HG3	2:F:201:FOL:C7	2.49	0.42
1:A:18:ILE:CD1	1:A:63:ALA:HB2	2.49	0.42
1:A:48:GLY:O	1:A:96:TYR:HB2	2.18	0.42
1:A:149:PHE:O	1:A:153:GLN:N	2.40	0.42
1:C:97:LYS:O	1:C:97:LYS:HE3	2.19	0.42
1:D:17:LEU:HB3	1:D:47:ILE:HD11	2.01	0.42
1:E:81:THR:O	1:E:84:ALA:N	2.51	0.42
1:F:80:PHE:CE1	2:F:201:FOL:C4	3.01	0.42
1:F:138:TRP:H	1:F:138:TRP:HD1	1.67	0.42
1:F:138:TRP:C	1:F:139:TRP:CE3	2.92	0.42
1:F:150:PHE:HD1	1:F:153:GLN:OE1	2.02	0.42
1:C:163:LYS:CB	1:C:163:LYS:NZ	2.83	0.42
1:E:83:ASN:HB3	1:E:116:ILE:HG22	2.01	0.42
1:F:13:LEU:C	1:F:13:LEU:CD2	2.86	0.42
1:F:20:VAL:HA	1:F:23:VAL:CG1	2.50	0.42
1:B:47:ILE:HG22	1:B:56:ALA:CB	2.48	0.42
1:B:59:GLY:O	1:B:62:VAL:HG22	2.20	0.42
1:C:125:LEU:HD21	2:C:201:FOL:H16	2.02	0.42
1:C:150:PHE:O	1:C:154:VAL:HG23	2.20	0.42
1:D:51:PHE:HD1	1:D:51:PHE:N	2.16	0.42
1:E:43:PRO:CG	1:E:44:GLU:H	2.29	0.42
1:F:68:MET:CE	2:F:201:FOL:HN1	2.33	0.42
1:A:110:LEU:HD21	1:B:144:ILE:HG23	2.02	0.42
1:E:113:THR:HG21	1:E:150:PHE:HD2	1.82	0.42
1:F:116:ILE:CG2	1:F:117:ASN:N	2.81	0.42
1:F:118:ILE:O	1:F:122:PRO:CD	2.67	0.42
1:F:140:VAL:N	1:F:141:PRO:CD	2.82	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:77:PHE:HA	1:B:78:PRO:HD3	1.87	0.42
1:C:145:LYS:O	1:C:145:LYS:HG2	2.18	0.42
1:C:174:LEU:C	1:C:174:LEU:CD2	2.85	0.42
1:E:70:LEU:HD23	1:E:71:PHE:CD2	2.54	0.42
1:F:35:LEU:O	1:F:36:LYS:CB	2.68	0.42
1:F:120:LEU:O	1:F:124:TRP:HE3	2.02	0.42
1:B:52:GLY:HA2	1:B:96:TYR:CG	2.54	0.42
1:C:20:VAL:O	1:C:23:VAL:HG13	2.19	0.42
1:D:131:VAL:HG13	1:D:133:LEU:HD13	1.99	0.42
1:D:173:PRO:O	1:D:173:PRO:HG2	2.19	0.42
1:F:17:LEU:HD22	1:F:17:LEU:N	2.34	0.42
1:F:136:PHE:HA	1:F:137:ALA:HA	1.65	0.42
1:A:109:THR:O	1:A:112:VAL:HG13	2.19	0.42
1:B:138:TRP:CZ3	1:B:139:TRP:HA	2.55	0.42
1:C:30:TYR:HB2	1:C:37:ILE:CB	2.49	0.42
1:C:124:TRP:HA	1:C:124:TRP:CE3	2.54	0.42
1:D:10:SER:OG	1:D:172:LYS:HG3	2.04	0.42
1:E:55:TRP:CA	1:E:55:TRP:HE3	2.30	0.42
1:E:58:ILE:HG13	1:E:58:ILE:H	1.61	0.42
1:C:35:LEU:HD12	1:C:35:LEU:HA	1.81	0.42
1:C:83:ASN:OD1	1:C:116:ILE:CG1	2.67	0.42
1:D:150:PHE:CE2	1:D:154:VAL:HG21	2.55	0.42
1:F:18:ILE:HD12	1:F:19:ALA:CA	2.49	0.42
1:F:81:THR:CG2	1:F:85:PHE:HZ	2.32	0.42
1:A:23:VAL:HA	1:A:26:ARG:HB3	2.02	0.42
1:C:94:PHE:CD1	1:C:108:ALA:HB2	2.53	0.42
1:E:20:VAL:HA	1:E:23:VAL:HG12	2.00	0.42
1:E:27:PHE:O	1:E:27:PHE:CD2	2.70	0.42
1:B:161:GLY:C	1:B:162:ASN:ND2	2.73	0.41
1:C:150:PHE:CA	1:C:153:GLN:HG2	2.48	0.41
1:E:42:ILE:N	1:E:43:PRO:HD2	2.34	0.41
1:E:83:ASN:CG	1:E:120:LEU:HD21	2.40	0.41
1:E:153:GLN:CD	1:E:154:VAL:N	2.73	0.41
1:F:118:ILE:CG2	1:F:119:ILE:CD1	2.85	0.41
1:A:16:VAL:O	1:A:19:ALA:HB3	2.19	0.41
1:A:66:VAL:HG12	1:A:70:LEU:HD11	2.01	0.41
1:A:170:PHE:CD2	1:A:173:PRO:CG	3.02	0.41
1:B:36:LYS:H	2:B:201:FOL:HB2	1.84	0.41
1:B:46:LEU:CD1	1:B:49:MET:HE3	2.50	0.41
1:C:91:TYR:CE1	1:C:112:VAL:HG21	2.56	0.41
1:F:35:LEU:N	2:F:201:FOL:H12	2.34	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:133:LEU:CG	1:D:138:TRP:CZ3	3.03	0.41
1:E:13:LEU:HD22	1:E:13:LEU:N	2.09	0.41
1:E:66:VAL:O	1:E:66:VAL:HG12	2.19	0.41
1:E:94:PHE:CD2	1:E:108:ALA:HB2	2.51	0.41
1:C:80:PHE:O	1:C:83:ASN:CB	2.63	0.41
1:E:74:ALA:HB1	1:E:75:GLY:CA	2.51	0.41
1:E:75:GLY:O	2:E:201:FOL:H7	2.20	0.41
1:F:93:TYR:O	1:F:93:TYR:CD1	2.70	0.41
1:F:145:LYS:HA	1:F:148:ILE:CG1	2.41	0.41
1:C:25:SER:CB	1:C:26:ARG:NH1	2.82	0.41
1:E:145:LYS:HD2	1:E:148:ILE:H	1.83	0.41
1:A:14:MET:CE	1:A:14:MET:HA	2.44	0.41
1:B:164:ILE:C	1:B:164:ILE:CD1	2.86	0.41
1:F:42:ILE:HG23	1:F:43:PRO:N	2.36	0.41
1:F:121:THR:O	1:F:125:LEU:HD12	2.20	0.41
1:A:144:ILE:O	1:A:147:VAL:HG12	2.20	0.41
1:B:17:LEU:HD13	1:B:20:VAL:HG21	2.02	0.41
1:B:26:ARG:HD3	1:B:71:PHE:CD1	2.56	0.41
1:C:124:TRP:CE3	1:C:124:TRP:CA	3.03	0.41
1:D:24:PHE:CD2	1:D:39:PHE:O	2.73	0.41
1:E:39:PHE:CE1	1:E:41:PHE:CZ	3.07	0.41
1:F:118:ILE:HG22	1:F:119:ILE:CD1	2.33	0.41
1:F:138:TRP:N	1:F:138:TRP:HD1	2.17	0.41
1:A:17:LEU:HD13	1:A:47:ILE:HG12	2.02	0.41
1:A:74:ALA:HB1	2:A:201:FOL:H92	2.03	0.41
1:A:113:THR:HA	1:A:117:ASN:ND2	2.36	0.41
1:C:117:ASN:O	1:C:121:THR:OG1	2.16	0.41
1:E:47:ILE:HD11	1:E:60:THR:HG23	2.03	0.41
1:E:117:ASN:HA	1:E:121:THR:HG1	1.86	0.41
1:A:23:VAL:HA	1:A:26:ARG:CD	2.47	0.41
1:C:10:SER:HA	1:C:170:PHE:CZ	2.56	0.41
1:C:76:TYR:CD2	2:C:201:FOL:NA2	2.89	0.41
1:C:123:LEU:HD12	1:C:123:LEU:HA	1.80	0.41
1:E:113:THR:CG2	1:E:150:PHE:CD2	3.03	0.41
1:F:143:LEU:O	1:F:147:VAL:HG23	2.20	0.41
1:A:29:ALA:C	1:A:31:GLU:OE1	2.59	0.41
1:C:166:PHE:CD2	1:C:167:LYS:HD3	2.55	0.41
1:F:13:LEU:HD22	1:F:14:MET:HA	2.02	0.41
1:B:36:LYS:HA	1:B:37:ILE:HD12	2.02	0.40
1:C:45:SER:HB3	1:C:95:TYR:CE2	2.56	0.40
1:C:109:THR:HG22	1:C:153:GLN:HE21	1.82	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:121:THR:HG22	1:D:125:LEU:HD11	2.03	0.40
1:E:14:MET:SD	1:E:14:MET:O	2.78	0.40
1:E:23:VAL:HG23	1:E:26:ARG:HD3	2.03	0.40
1:E:34:PHE:O	1:E:35:LEU:CD2	2.68	0.40
1:F:23:VAL:HG23	1:F:27:PHE:CG	2.56	0.40
1:F:81:THR:O	1:F:85:PHE:CE1	2.74	0.40
1:A:122:PRO:CA	1:A:125:LEU:HD13	2.49	0.40
1:B:29:ALA:C	1:B:36:LYS:NZ	2.70	0.40
1:B:145:LYS:HG2	1:B:149:PHE:HD2	1.85	0.40
1:C:98:LYS:CE	1:C:104:ARG:NH1	2.71	0.40
1:D:124:TRP:HD1	1:D:127:LEU:CD1	2.35	0.40
1:A:14:MET:CE	1:A:51:PHE:CD2	3.03	0.40
1:A:50:ILE:HB	1:A:51:PHE:CE1	2.55	0.40
1:C:150:PHE:CE2	1:D:151:PRO:HG2	2.54	0.40
1:D:172:LYS:CG	1:D:172:LYS:O	2.69	0.40
1:E:42:ILE:O	1:E:42:ILE:HG22	2.22	0.40
1:E:76:TYR:CE1	1:E:77:PHE:C	2.95	0.40
1:E:115:LEU:HD23	1:E:119:ILE:HD13	2.03	0.40
1:F:9:LYS:O	1:F:13:LEU:HD12	2.21	0.40
1:A:36:LYS:N	2:A:201:FOL:H12	2.36	0.40
1:B:80:PHE:O	1:B:83:ASN:HB2	2.20	0.40
1:B:96:TYR:CG	1:B:97:LYS:HG3	2.57	0.40
1:B:138:TRP:C	1:B:138:TRP:CD2	2.95	0.40
1:D:25:SER:O	1:D:29:ALA:CB	2.70	0.40
1:E:35:LEU:O	2:E:201:FOL:H12	2.21	0.40
1:E:41:PHE:O	1:E:42:ILE:CB	2.70	0.40
1:F:57:GLY:O	1:F:85:PHE:HA	2.22	0.40
1:B:36:LYS:NZ	1:B:37:ILE:O	2.40	0.40
1:B:46:LEU:HD12	1:B:49:MET:CE	2.51	0.40
1:B:136:PHE:HA	1:B:137:ALA:HA	1.81	0.40
1:E:117:ASN:O	1:E:122:PRO:HD3	2.22	0.40
1:F:34:PHE:HB2	1:F:125:LEU:CD2	2.51	0.40
1:F:118:ILE:O	1:F:122:PRO:HD2	2.20	0.40

All (4) 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:72:PRO:CB	1:B:11:ILE:CD1[2_555]	1.00	1.20
1:A:128:MET:CE	1:B:6:PHE:CZ[2_555]	1.92	0.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:MET:CE	1:B:6:PHE:CG[2_555]	1.98	0.22
1:A:72:PRO:CG	1:B:11:ILE:CD1[2_555]	2.19	0.01

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	159/199 (80%)	151 (95%)	7 (4%)	1 (1%)	25	64
1	B	164/199 (82%)	157 (96%)	7 (4%)	0	100	100
1	C	162/199 (81%)	152 (94%)	9 (6%)	1 (1%)	25	64
1	D	158/199 (79%)	151 (96%)	7 (4%)	0	100	100
1	E	137/199 (69%)	121 (88%)	13 (10%)	3 (2%)	6	35
1	F	140/199 (70%)	131 (94%)	8 (6%)	1 (1%)	22	61
All	All	920/1194 (77%)	863 (94%)	51 (6%)	6 (1%)	22	61

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	172	LYS
1	E	42	ILE
1	F	53	PRO
1	C	53	PRO
1	E	72	PRO
1	E	150	PHE

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	135/168 (80%)	110 (82%)	25 (18%)	1	8
1	B	140/168 (83%)	123 (88%)	17 (12%)	5	22
1	C	138/168 (82%)	100 (72%)	38 (28%)	0	1
1	D	138/168 (82%)	114 (83%)	24 (17%)	2	10
1	E	122/168 (73%)	94 (77%)	28 (23%)	1	3
1	F	124/168 (74%)	82 (66%)	42 (34%)	0	0
All	All	797/1008 (79%)	623 (78%)	174 (22%)	1	5

All (174) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	LEU
1	A	16	VAL
1	A	20	VAL
1	A	26	ARG
1	A	70	LEU
1	A	71	PHE
1	A	72	PRO
1	A	73	LYS
1	A	97	LYS
1	A	100	MET
1	A	101	THR
1	A	112	VAL
1	A	125	LEU
1	A	127	LEU
1	A	129	TYR
1	A	131	VAL
1	A	132	ASN
1	A	133	LEU
1	A	155	ILE
1	A	160	LEU
1	A	162	ASN
1	A	169	LEU
1	A	170	PHE
1	A	172	LYS
1	A	174	LEU
1	B	13	LEU
1	B	14	MET

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Mol	Chain	Res	Type
1	B	17	LEU
1	B	24	PHE
1	B	26	ARG
1	B	30	TYR
1	B	36	LYS
1	B	64	ASP
1	B	73	LYS
1	B	119	ILE
1	B	133	LEU
1	B	162	ASN
1	B	164	ILE
1	B	169	LEU
1	B	170	PHE
1	B	172	LYS
1	B	173	PRO
1	C	23	VAL
1	C	24	PHE
1	C	28	PHE
1	C	31	GLU
1	C	33	THR
1	C	37	ILE
1	C	42	ILE
1	C	68	MET
1	C	69	LEU
1	C	70	LEU
1	C	73	LYS
1	C	81	THR
1	C	82	LEU
1	C	86	LEU
1	C	97	LYS
1	C	101	THR
1	C	104	ARG
1	C	107	LEU
1	C	109	THR
1	C	116	ILE
1	C	121	THR
1	C	125	LEU
1	C	128	MET
1	C	132	ASN
1	C	133	LEU
1	C	136	PHE
1	C	146	THR

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Mol	Chain	Res	Type
1	C	147	VAL
1	C	149	PHE
1	C	150	PHE
1	C	160	LEU
1	C	163	LYS
1	C	166	PHE
1	C	167	LYS
1	C	168	ARG
1	C	169	LEU
1	C	170	PHE
1	C	174	LEU
1	D	16	VAL
1	D	17	LEU
1	D	23	VAL
1	D	24	PHE
1	D	25	SER
1	D	26	ARG
1	D	37	ILE
1	D	97	LYS
1	D	98	LYS
1	D	115	LEU
1	D	128	MET
1	D	133	LEU
1	D	145	LYS
1	D	146	THR
1	D	151	PRO
1	D	153	GLN
1	D	160	LEU
1	D	162	ASN
1	D	167	LYS
1	D	170	PHE
1	D	172	LYS
1	D	173	PRO
1	D	175	SER
1	D	176	GLU
1	E	10	SER
1	E	13	LEU
1	E	14	MET
1	E	16	VAL
1	E	17	LEU
1	E	18	ILE
1	E	20	VAL

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Mol	Chain	Res	Type
1	E	22	VAL
1	E	24	PHE
1	E	26	ARG
1	E	27	PHE
1	E	42	ILE
1	E	51	PHE
1	E	55	TRP
1	E	60	THR
1	E	69	LEU
1	E	76	TYR
1	E	83	ASN
1	E	97	LYS
1	E	107	LEU
1	E	110	LEU
1	E	111	LEU
1	E	114	VAL
1	E	120	LEU
1	E	129	TYR
1	E	136	PHE
1	E	144	ILE
1	E	147	VAL
1	F	10	SER
1	F	13	LEU
1	F	23	VAL
1	F	24	PHE
1	F	26	ARG
1	F	32	THR
1	F	33	THR
1	F	35	LEU
1	F	41	PHE
1	F	42	ILE
1	F	44	GLU
1	F	45	SER
1	F	47	ILE
1	F	49	MET
1	F	60	THR
1	F	65	VAL
1	F	69	LEU
1	F	70	LEU
1	F	73	LYS
1	F	81	THR
1	F	82	LEU

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Mol	Chain	Res	Type
1	F	93	TYR
1	F	103	GLN
1	F	104	ARG
1	F	107	LEU
1	F	109	THR
1	F	110	LEU
1	F	113	THR
1	F	115	LEU
1	F	116	ILE
1	F	118	ILE
1	F	121	THR
1	F	123	LEU
1	F	126	SER
1	F	136	PHE
1	F	140	VAL
1	F	144	ILE
1	F	153	GLN
1	F	162	ASN
1	F	163	LYS
1	F	169	LEU
1	F	170	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	83	ASN
1	F	103	GLN
1	F	153	GLN

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 monosaccharides in this entry.

5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	FOL	D	201	-	34,34,34	1.30	2 (5%)	44,47,47	2.03	9 (20%)
2	FOL	B	201	-	34,34,34	1.36	3 (8%)	44,47,47	2.27	11 (25%)
2	FOL	F	201	-	34,34,34	1.32	3 (8%)	44,47,47	2.18	12 (27%)
2	FOL	A	201	-	34,34,34	1.36	4 (11%)	44,47,47	2.20	14 (31%)
2	FOL	E	201	-	34,34,34	1.47	4 (11%)	44,47,47	2.21	11 (25%)
2	FOL	C	201	-	34,34,34	1.26	3 (8%)	44,47,47	2.42	14 (31%)

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	FOL	D	201	-	-	11/22/22/22	0/3/3/3
2	FOL	B	201	-	-	13/22/22/22	0/3/3/3
2	FOL	F	201	-	-	12/22/22/22	0/3/3/3
2	FOL	A	201	-	-	10/22/22/22	0/3/3/3
2	FOL	E	201	-	-	12/22/22/22	0/3/3/3
2	FOL	C	201	-	-	7/22/22/22	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	201	FOL	C4A-C4	4.49	1.49	1.41
2	F	201	FOL	C4A-C4	4.34	1.48	1.41
2	E	201	FOL	C4A-C4	4.33	1.48	1.41
2	E	201	FOL	C4A-C8A	4.26	1.48	1.40
2	D	201	FOL	C4A-C4	4.22	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	201	FOL	C4A-C8A	3.96	1.48	1.40
2	A	201	FOL	C4A-C4	3.91	1.48	1.41
2	D	201	FOL	C4A-C8A	3.87	1.48	1.40
2	B	201	FOL	C4A-C8A	3.85	1.48	1.40
2	C	201	FOL	C4A-C8A	3.81	1.48	1.40
2	F	201	FOL	C4A-C8A	3.67	1.47	1.40
2	C	201	FOL	C4A-C4	3.20	1.46	1.41
2	A	201	FOL	C7-N8	2.43	1.35	1.31
2	B	201	FOL	C6-N5	2.39	1.36	1.32
2	F	201	FOL	C6-N5	2.39	1.36	1.32
2	E	201	FOL	C6-N5	2.31	1.36	1.32
2	A	201	FOL	C6-N5	2.16	1.36	1.32
2	E	201	FOL	C4A-N5	2.07	1.36	1.33
2	C	201	FOL	C6-N5	2.00	1.36	1.32

All (71) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	201	FOL	N8-C8A-N1	7.38	124.25	115.82
2	C	201	FOL	C6-C9-N10	-6.91	97.79	113.07
2	F	201	FOL	C2-N1-C8A	6.25	122.50	115.36
2	B	201	FOL	C2-N1-C8A	6.24	122.48	115.36
2	B	201	FOL	N8-C8A-N1	5.87	122.53	115.82
2	D	201	FOL	C2-N1-C8A	5.59	121.74	115.36
2	F	201	FOL	N8-C8A-N1	5.58	122.19	115.82
2	D	201	FOL	N8-C8A-N1	5.54	122.15	115.82
2	E	201	FOL	N8-C8A-N1	5.34	121.92	115.82
2	E	201	FOL	C8A-C4A-C4	-5.31	116.44	119.95
2	C	201	FOL	C8A-C4A-C4	-5.14	116.55	119.95
2	C	201	FOL	C2-N1-C8A	5.03	121.10	115.36
2	B	201	FOL	C4-C4A-N5	5.03	124.35	118.60
2	E	201	FOL	C2-N1-C8A	4.92	120.97	115.36
2	F	201	FOL	C4-C4A-N5	4.70	123.97	118.60
2	A	201	FOL	C2-N1-C8A	4.65	120.67	115.36
2	D	201	FOL	C8A-C4A-C4	-4.44	117.01	119.95
2	C	201	FOL	C4A-C4-N3	-4.43	117.38	123.43
2	E	201	FOL	C4A-C4-N3	-4.43	117.38	123.43
2	F	201	FOL	C4A-C4-N3	-4.38	117.44	123.43
2	C	201	FOL	C4-C4A-N5	4.35	123.57	118.60
2	C	201	FOL	C2-N3-C4	4.33	122.81	115.93
2	B	201	FOL	C8A-C4A-C4	-4.31	117.10	119.95
2	E	201	FOL	C2-N3-C4	4.13	122.49	115.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	E	201	FOL	C4-C4A-N5	4.12	123.30	118.60
2	D	201	FOL	C4A-C4-N3	-4.11	117.81	123.43
2	D	201	FOL	C4-C4A-N5	4.00	123.17	118.60
2	F	201	FOL	C8A-C4A-C4	-4.00	117.30	119.95
2	A	201	FOL	C7-N8-C8A	3.91	120.62	116.69
2	B	201	FOL	C4A-C4-N3	-3.83	118.19	123.43
2	C	201	FOL	N1-C2-N3	-3.77	122.19	127.22
2	A	201	FOL	C4A-C4-N3	-3.74	118.32	123.43
2	D	201	FOL	C2-N3-C4	3.70	121.80	115.93
2	C	201	FOL	N8-C8A-N1	3.69	120.03	115.82
2	B	201	FOL	C7-N8-C8A	3.52	120.23	116.69
2	B	201	FOL	C2-N3-C4	3.49	121.47	115.93
2	B	201	FOL	N1-C2-N3	-3.49	122.57	127.22
2	A	201	FOL	C8A-C4A-C4	-3.44	117.67	119.95
2	B	201	FOL	C8A-C4A-N5	-3.39	118.48	122.33
2	D	201	FOL	N1-C2-N3	-3.33	122.78	127.22
2	E	201	FOL	N1-C2-N3	-3.30	122.82	127.22
2	F	201	FOL	NA2-C2-N3	3.26	122.33	117.25
2	F	201	FOL	C2-N3-C4	3.25	121.09	115.93
2	F	201	FOL	C8A-C4A-N5	-3.19	118.71	122.33
2	C	201	FOL	C9-C6-C7	-3.18	116.01	121.55
2	F	201	FOL	C7-N8-C8A	3.08	119.79	116.69
2	A	201	FOL	C2-N3-C4	3.05	120.77	115.93
2	A	201	FOL	CT-CA-N	-2.89	103.70	110.55
2	C	201	FOL	C7-C6-N5	2.86	122.71	120.85
2	A	201	FOL	C4-C4A-N5	2.84	121.84	118.60
2	E	201	FOL	C7-N8-C8A	2.75	119.46	116.69
2	D	201	FOL	C7-N8-C8A	2.74	119.45	116.69
2	F	201	FOL	N1-C2-N3	-2.62	123.73	127.22
2	A	201	FOL	C9-N10-C14	2.60	128.82	122.15
2	E	201	FOL	C9-C6-N5	2.57	121.23	116.66
2	C	201	FOL	C9-C6-N5	2.53	121.16	116.66
2	A	201	FOL	CB-CA-CT	-2.42	104.51	110.35
2	F	201	FOL	NA2-C2-N1	-2.41	113.87	117.79
2	F	201	FOL	C4A-C8A-N1	-2.33	117.88	121.80
2	E	201	FOL	C7-C6-N5	-2.27	119.36	120.85
2	D	201	FOL	C8A-C4A-N5	-2.22	119.81	122.33
2	A	201	FOL	N1-C2-N3	-2.20	124.29	127.22
2	A	201	FOL	CA-N-C	2.18	126.93	121.60
2	B	201	FOL	C6-C7-N8	-2.17	121.00	123.13
2	B	201	FOL	C4A-C8A-N1	-2.16	118.17	121.80
2	C	201	FOL	C8A-C4A-N5	-2.16	119.88	122.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	201	FOL	CB-CA-N	-2.12	106.58	110.88
2	A	201	FOL	C11-C-N	2.12	121.12	117.06
2	E	201	FOL	CG-CB-CA	-2.11	109.21	113.16
2	A	201	FOL	C4A-C8A-N1	-2.10	118.28	121.80
2	C	201	FOL	C7-N8-C8A	2.09	118.79	116.69

There are no chirality outliers.

All (65) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	201	FOL	N-CA-CB-CG
2	D	201	FOL	CT-CA-CB-CG
2	E	201	FOL	N-CA-CB-CG
2	F	201	FOL	C11-C-N-CA
2	F	201	FOL	O-C-N-CA
2	A	201	FOL	N-CA-CB-CG
2	D	201	FOL	N-CA-CB-CG
2	A	201	FOL	C13-C14-N10-C9
2	B	201	FOL	C13-C14-N10-C9
2	D	201	FOL	C15-C14-N10-C9
2	E	201	FOL	C13-C14-N10-C9
2	E	201	FOL	N-C-C11-C12
2	A	201	FOL	C15-C14-N10-C9
2	D	201	FOL	C13-C14-N10-C9
2	E	201	FOL	C15-C14-N10-C9
2	E	201	FOL	O-C-C11-C12
2	E	201	FOL	N-C-C11-C16
2	C	201	FOL	O-C-N-CA
2	A	201	FOL	CT-CA-CB-CG
2	B	201	FOL	CT-CA-CB-CG
2	E	201	FOL	CT-CA-CB-CG
2	E	201	FOL	O-C-C11-C16
2	B	201	FOL	CT-CA-N-C
2	B	201	FOL	C15-C14-N10-C9
2	C	201	FOL	C11-C-N-CA
2	F	201	FOL	C13-C14-N10-C9
2	F	201	FOL	C15-C14-N10-C9
2	E	201	FOL	N-CA-CT-O1
2	E	201	FOL	N-CA-CT-O2
2	D	201	FOL	CA-CB-CG-CD
2	A	201	FOL	N-C-C11-C12
2	F	201	FOL	N-CA-CT-O1

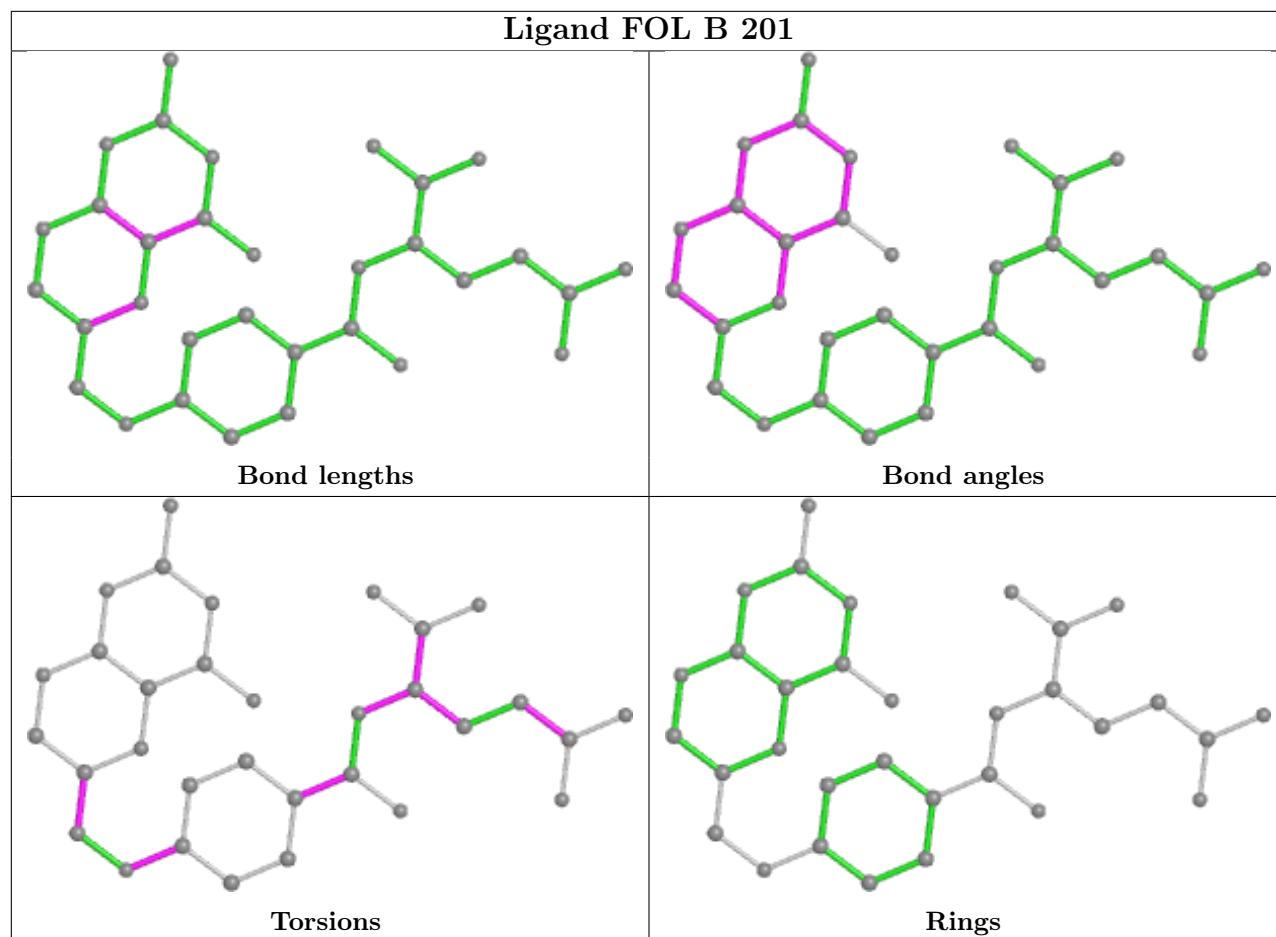*Continued on next page...*

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Mol	Chain	Res	Type	Atoms
2	F	201	FOL	N-CA-CT-O2
2	B	201	FOL	CB-CA-CT-O2
2	D	201	FOL	C11-C-N-CA
2	B	201	FOL	CB-CA-N-C
2	A	201	FOL	O-C-C11-C12
2	B	201	FOL	CB-CA-CT-O1
2	C	201	FOL	C7-C6-C9-N10
2	D	201	FOL	O-C-N-CA
2	A	201	FOL	N-C-C11-C16
2	C	201	FOL	OE1-CD-CG-CB
2	B	201	FOL	C7-C6-C9-N10
2	B	201	FOL	OE2-CD-CG-CB
2	C	201	FOL	N5-C6-C9-N10
2	B	201	FOL	OE1-CD-CG-CB
2	F	201	FOL	OE2-CD-CG-CB
2	F	201	FOL	OE1-CD-CG-CB
2	F	201	FOL	CB-CA-CT-O1
2	C	201	FOL	OE2-CD-CG-CB
2	B	201	FOL	N5-C6-C9-N10
2	D	201	FOL	OE2-CD-CG-CB
2	F	201	FOL	CB-CA-CT-O2
2	D	201	FOL	OE1-CD-CG-CB
2	E	201	FOL	N5-C6-C9-N10
2	F	201	FOL	N5-C6-C9-N10
2	C	201	FOL	N-CA-CT-O2
2	E	201	FOL	C7-C6-C9-N10
2	A	201	FOL	N5-C6-C9-N10
2	D	201	FOL	N5-C6-C9-N10
2	A	201	FOL	C7-C6-C9-N10
2	D	201	FOL	C7-C6-C9-N10
2	F	201	FOL	C7-C6-C9-N10
2	A	201	FOL	O-C-C11-C16
2	B	201	FOL	O-C-C11-C12

There are no ring outliers.

6 monomers are involved in 114 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	201	FOL	10	0
2	B	201	FOL	14	0
2	F	201	FOL	46	0
2	A	201	FOL	13	0

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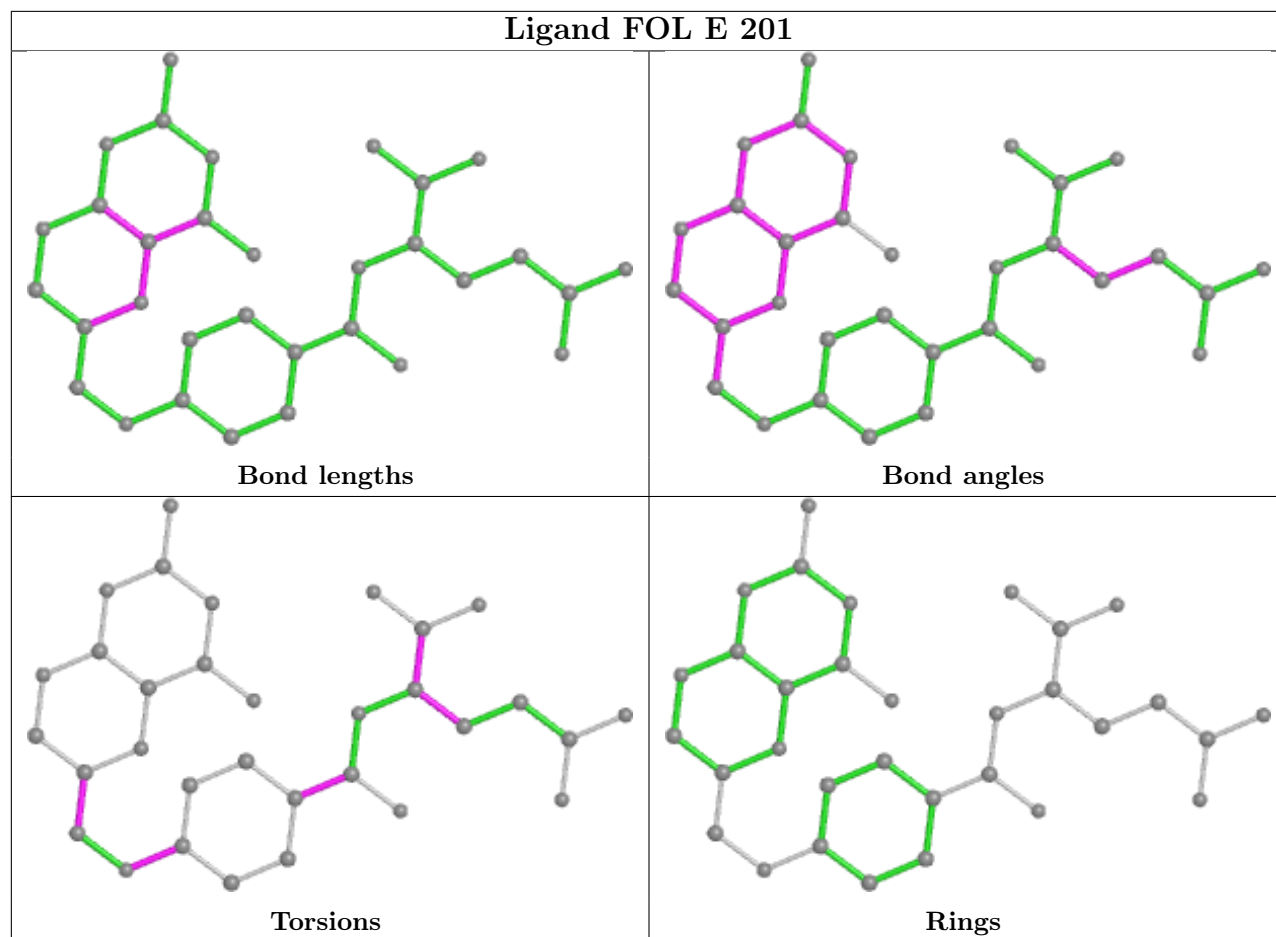| Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	201	FOL	25	0
2	C	201	FOL	6	0

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 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 FOL D 201

Bond lengths

Bond angles

Torsions

Rings

Ligand FOL B 201

Bond lengths

Bond angles

Torsions

Rings

Ligand FOL F 201

Bond lengths

Bond angles

Torsions

Rings

Ligand FOL A 201

Bond lengths

Bond angles

Torsions

Rings

Ligand FOL E 201

Bond lengths

Bond angles

Torsions

Rings

Ligand FOL C 201

Bond lengths

Bond angles

Torsions

Rings
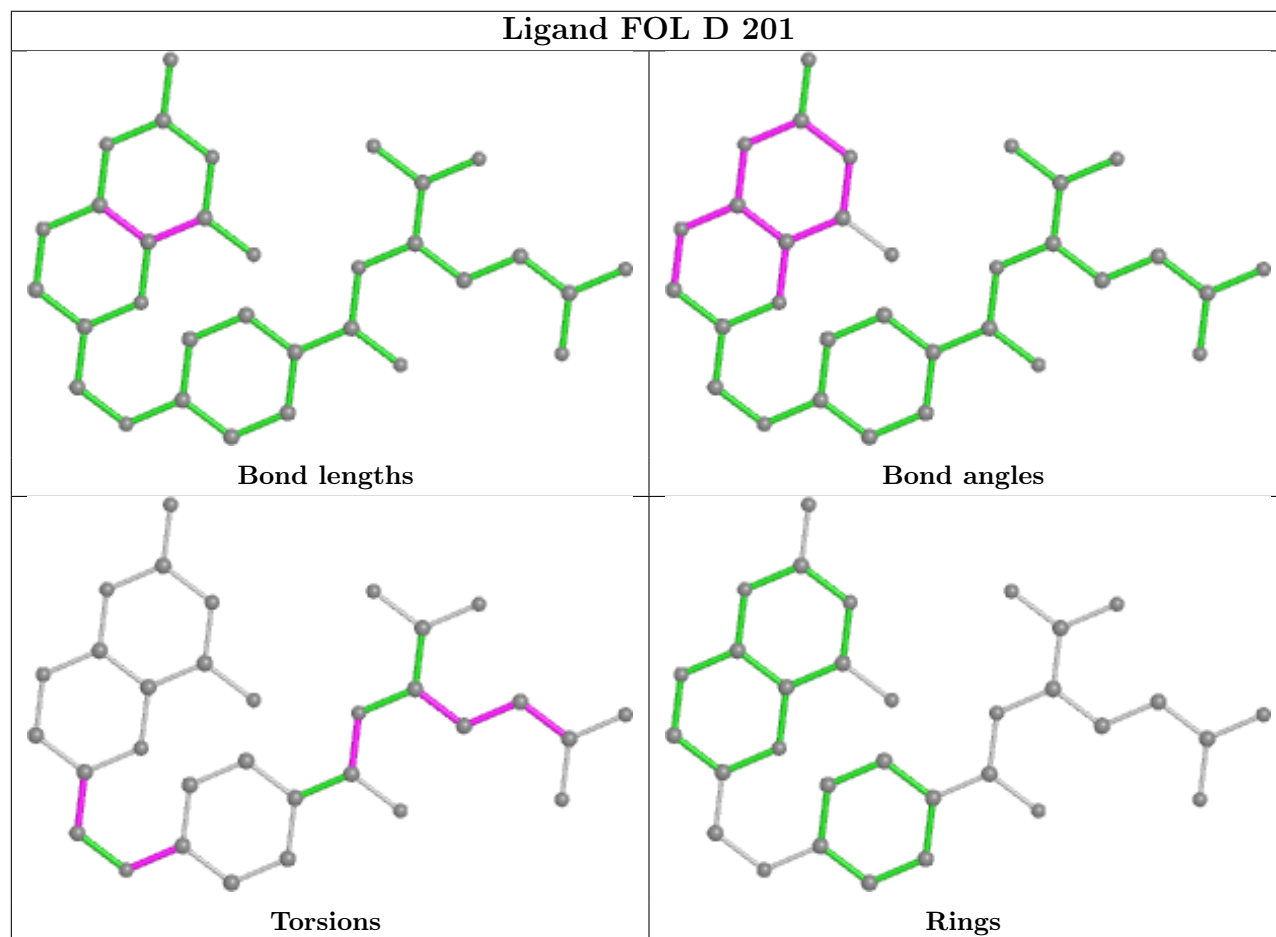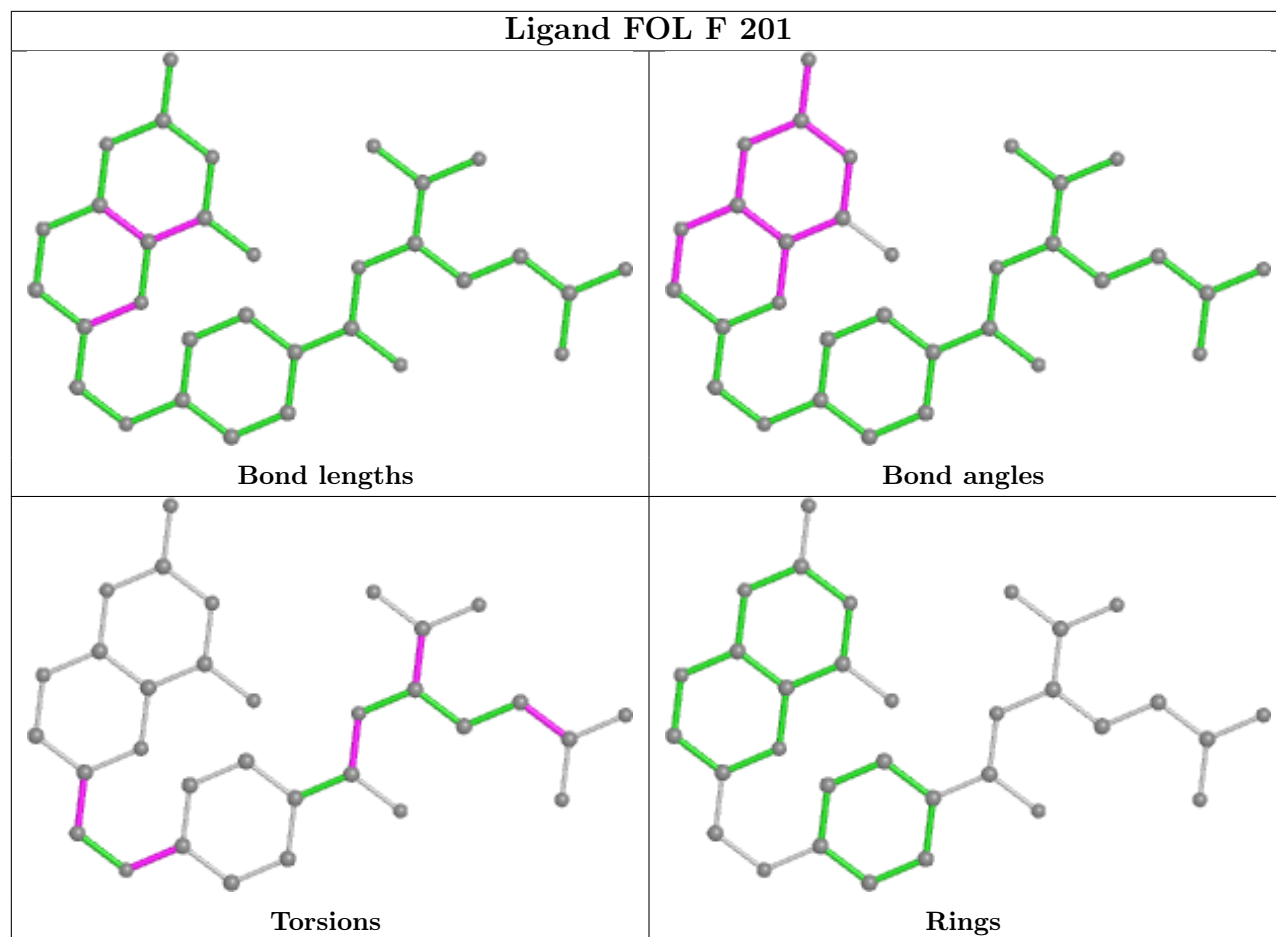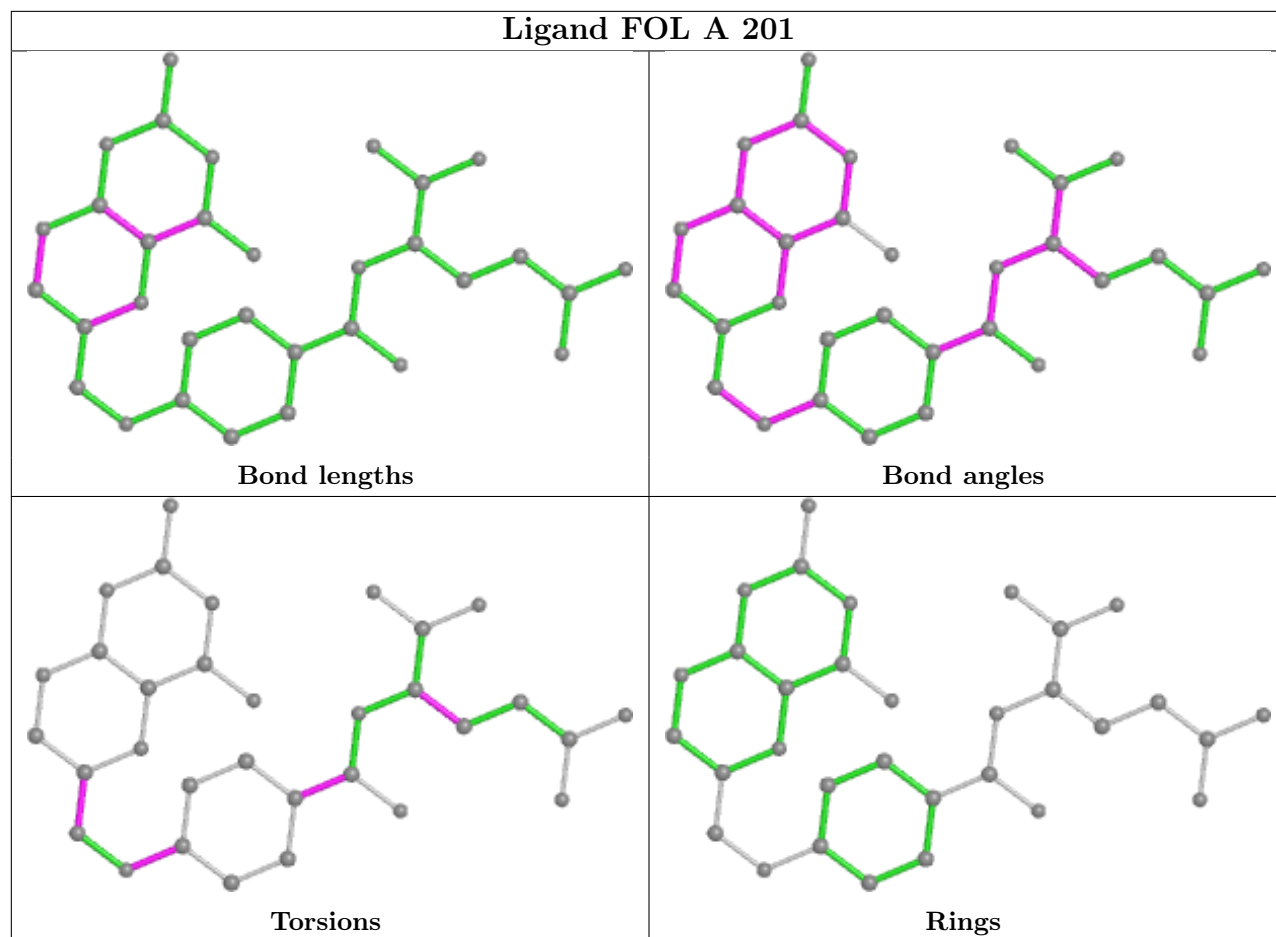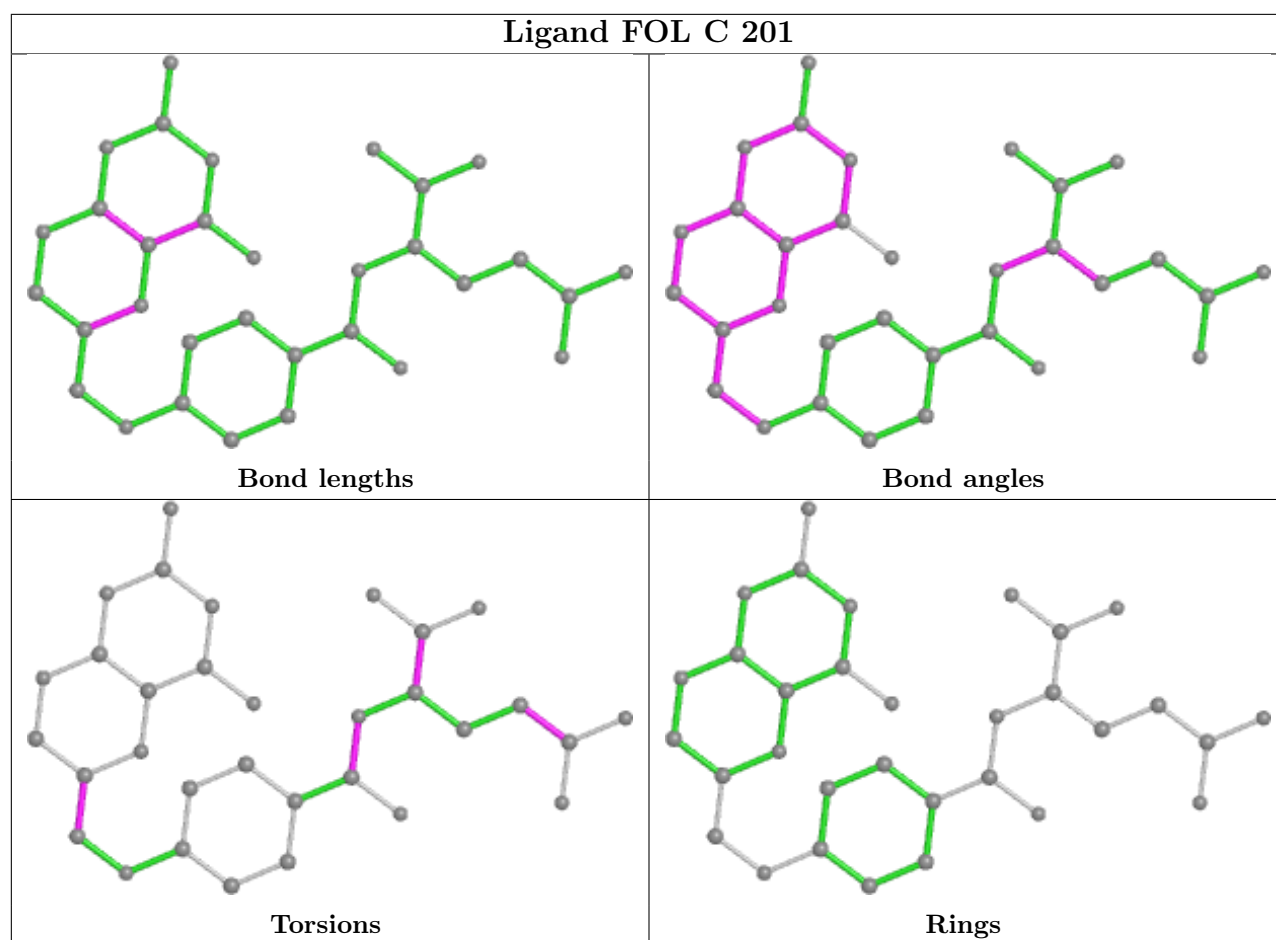
5.7 Other polymers ⓘ

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	163/199 (81%)	-0.61	1 (0%)	89	83	51, 83, 134, 151	0
1	B	168/199 (84%)	-0.56	1 (0%)	89	83	52, 81, 126, 169	0
1	C	166/199 (83%)	-0.61	1 (0%)	89	83	24, 82, 128, 163	0
1	D	166/199 (83%)	-0.62	0	100	100	56, 84, 122, 138	0
1	E	147/199 (73%)	-0.46	1 (0%)	87	81	25, 160, 191, 215	0
1	F	150/199 (75%)	-0.41	3 (2%)	65	51	62, 146, 187, 233	0
All	All	960/1194 (80%)	-0.55	7 (0%)	87	81	24, 94, 176, 233	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	95	TYR	8.0
1	C	130	GLY	4.2
1	F	129	TYR	4.1
1	F	130	GLY	2.8
1	B	136	PHE	2.4
1	A	169	LEU	2.2
1	E	127	LEU	2.1

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands (i)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	FOL	F	201	32/32	0.64	0.28	130,174,186,189	0
2	FOL	E	201	32/32	0.77	0.28	127,158,201,207	0
2	FOL	D	201	32/32	0.77	0.36	88,116,160,163	0
2	FOL	C	201	32/32	0.85	0.20	71,104,159,185	0
2	FOL	B	201	32/32	0.85	0.26	75,99,164,170	0
2	FOL	A	201	32/32	0.87	0.18	69,98,137,146	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.
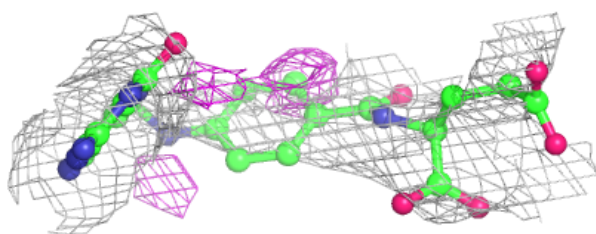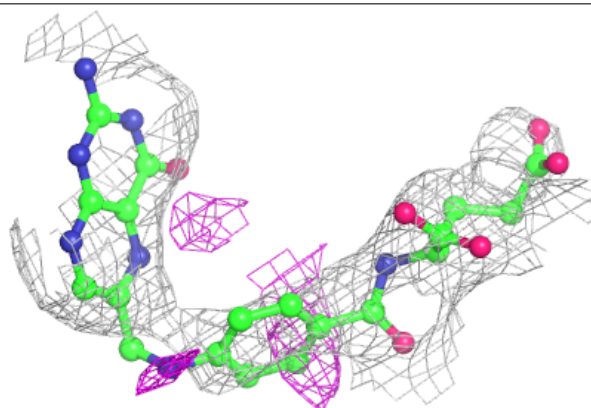
Electron density around FOL F 201:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative) and green (positive)
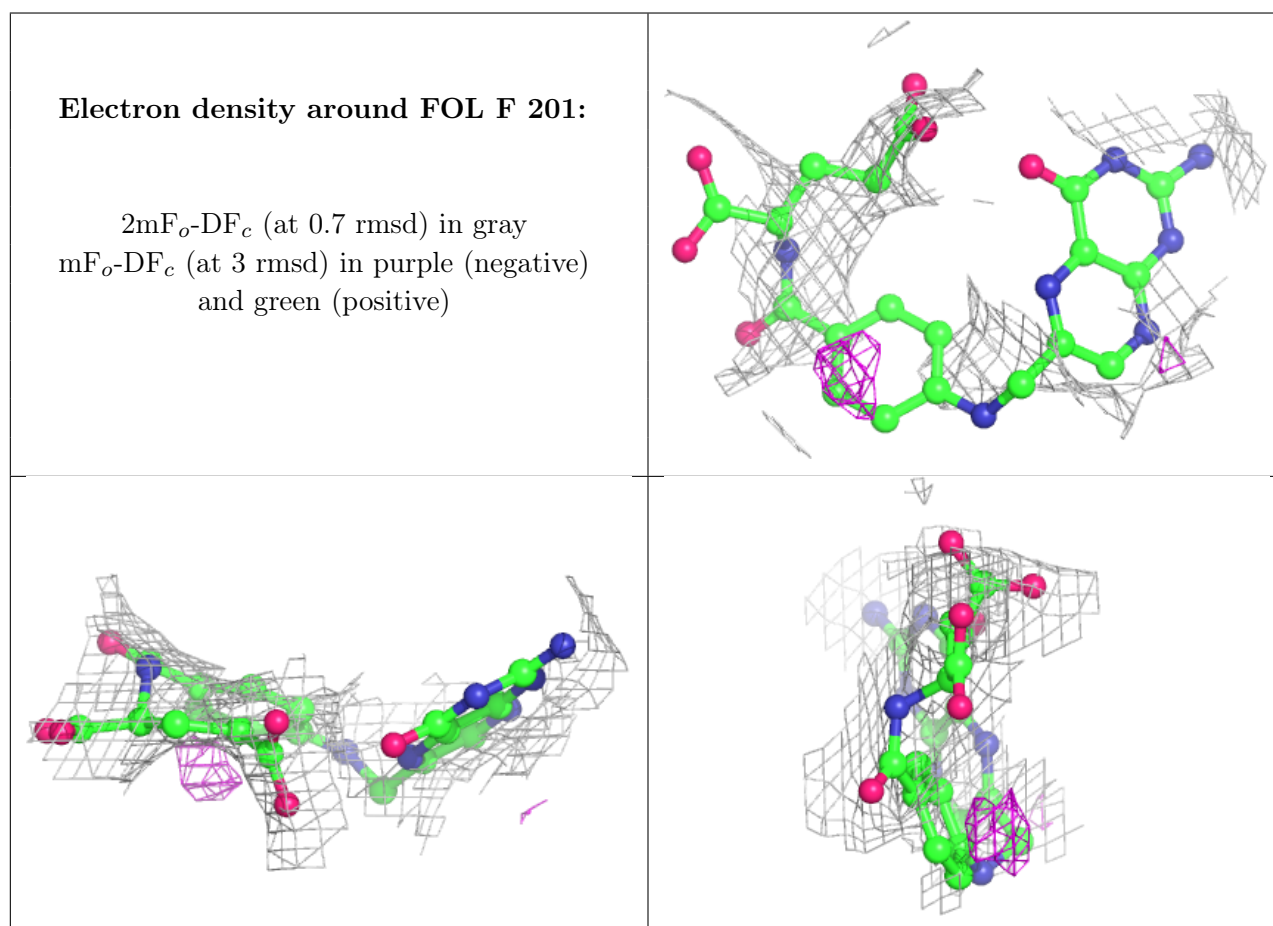
Electron density around FOL E 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
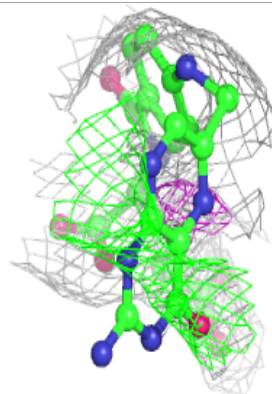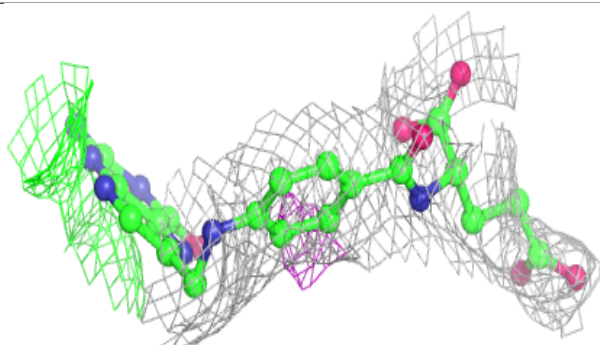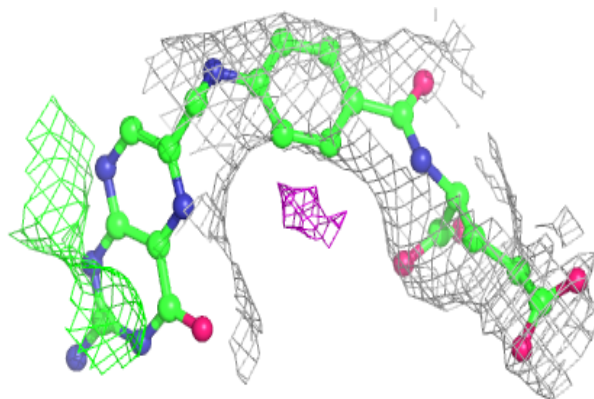and green (positive)
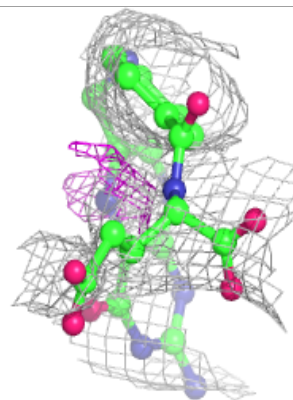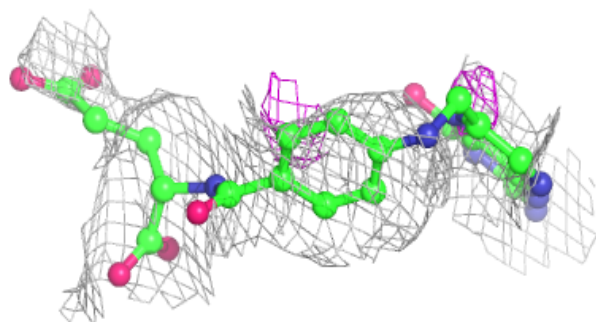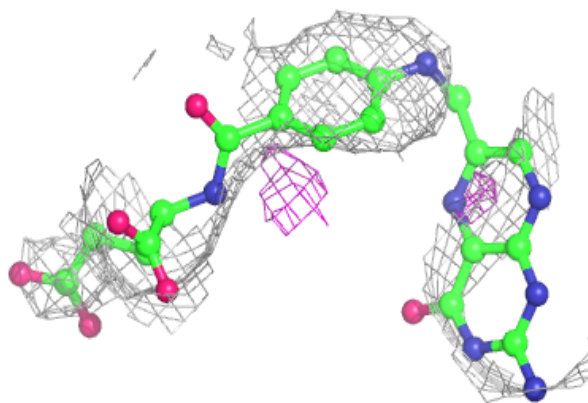
Electron density around FOL D 201:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
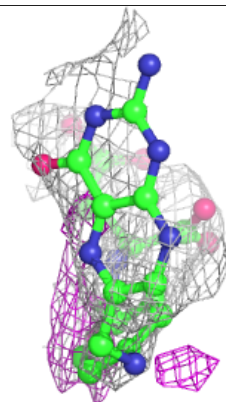
Electron density around FOL C 201:

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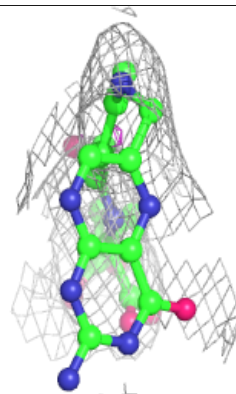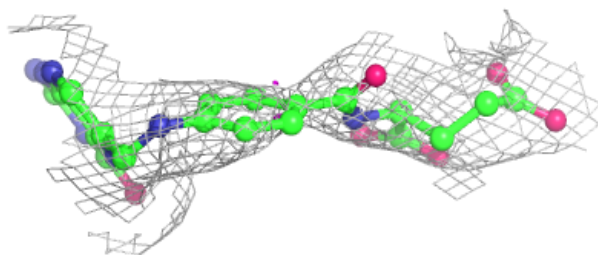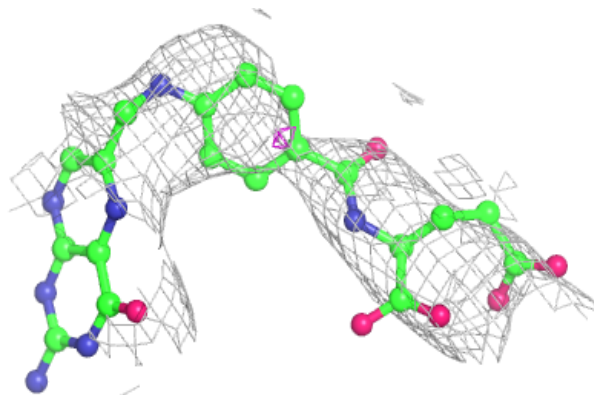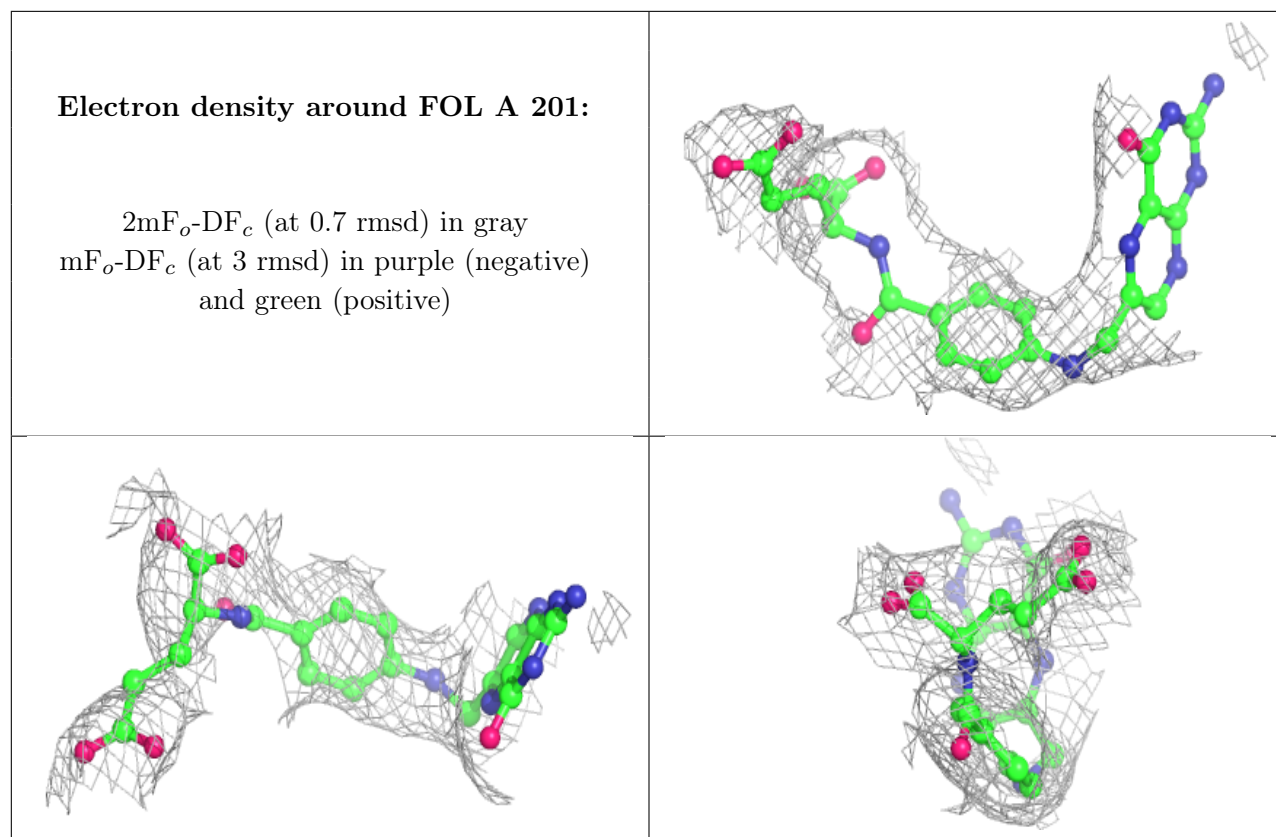mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around FOL B 201:

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

Electron density around FOL A 201:

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

6.5   Other polymers ⓘ

There are no such residues in this entry.