



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 12:59 PM BST

PDB ID : 4LRM  
Title : EGFR D770\_N771insNPG in complex with PD168393  
Authors : Yun, C.H.; Eck, M.J.  
Deposited on : 2013-07-20  
Resolution : 3.53 Å(reported)

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

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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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 : 2.13.1  
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) : 2.13.1

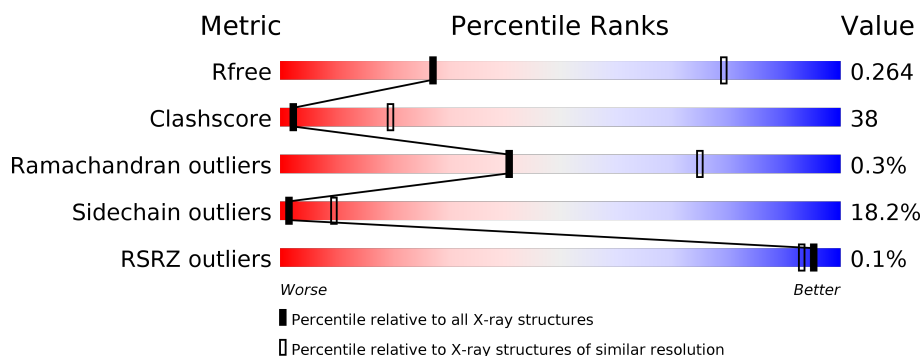
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.53 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1161 (3.60-3.44)
Clashscore	141614	1244 (3.60-3.44)
Ramachandran outliers	138981	1206 (3.60-3.44)
Sidechain outliers	138945	1207 (3.60-3.44)
RSRZ outliers	127900	1080 (3.60-3.44)

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

Mol	Chain	Length	Quality of chain
1	A	334	<div> <div></div> <div>47%</div> <div>33%</div> <div>13%</div> <div>8%</div> </div>
1	B	334	<div> <div></div> <div>52%</div> <div>27%</div> <div>9%</div> <div>12%</div> </div>
1	C	334	<div> <div></div> <div>49%</div> <div>30%</div> <div>8%</div> <div>12%</div> </div>
1	D	334	<div> <div></div> <div>56%</div> <div>25%</div> <div>5%</div> <div>13%</div> </div>
1	E	334	<div> <div></div> <div>52%</div> <div>27%</div> <div>7%</div> <div>13%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11696 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 Epidermal growth factor receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	307	Total	C	N	O	S	0	0	0
			2391	1538	407	430	16			
1	B	293	Total	C	N	O	S	0	0	0
			2313	1492	391	415	15			
1	C	293	Total	C	N	O	S	0	0	0
			2293	1479	387	412	15			
1	D	289	Total	C	N	O	S	0	0	0
			2279	1473	383	408	15			
1	E	290	Total	C	N	O	S	0	0	0
			2289	1477	391	406	15			

There are 25 discrepancies between the modelled and reference sequences:

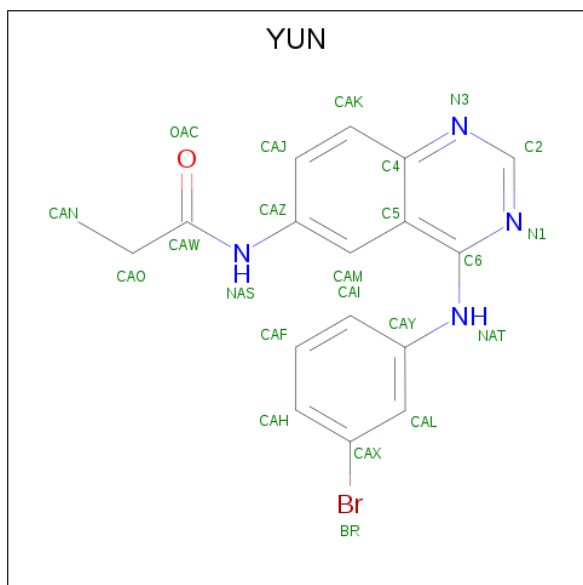
Chain	Residue	Modelled	Actual	Comment	Reference
A	692	GLY	-	EXPRESSION TAG	UNP P00533
A	693	SER	-	EXPRESSION TAG	UNP P00533
A	771	ASN	-	INSERTION	UNP P00533
A	772	PRO	-	INSERTION	UNP P00533
A	773	GLY	-	INSERTION	UNP P00533
B	692	GLY	-	EXPRESSION TAG	UNP P00533
B	693	SER	-	EXPRESSION TAG	UNP P00533
B	771	ASN	-	INSERTION	UNP P00533
B	772	PRO	-	INSERTION	UNP P00533
B	773	GLY	-	INSERTION	UNP P00533
C	692	GLY	-	EXPRESSION TAG	UNP P00533
C	693	SER	-	EXPRESSION TAG	UNP P00533
C	771	ASN	-	INSERTION	UNP P00533
C	772	PRO	-	INSERTION	UNP P00533
C	773	GLY	-	INSERTION	UNP P00533
D	692	GLY	-	EXPRESSION TAG	UNP P00533
D	693	SER	-	EXPRESSION TAG	UNP P00533
D	771	ASN	-	INSERTION	UNP P00533
D	772	PRO	-	INSERTION	UNP P00533

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Chain	Residue	Modelled	Actual	Comment	Reference
D	773	GLY	-	INSERTION	UNP P00533
E	692	GLY	-	EXPRESSION TAG	UNP P00533
E	693	SER	-	EXPRESSION TAG	UNP P00533
E	771	ASN	-	INSERTION	UNP P00533
E	772	PRO	-	INSERTION	UNP P00533
E	773	GLY	-	INSERTION	UNP P00533

- Molecule 2 is N-{4-[(3-bromophenyl)amino]quinazolin-6-yl}propanamide (three-letter code: YUN) (formula: C<sub>17</sub>H<sub>15</sub>BrN<sub>4</sub>O).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	Br	C	N	O	0	0
			23	1	17	4	1		
2	B	1	Total	Br	C	N	O	0	0
			23	1	17	4	1		
2	C	1	Total	Br	C	N	O	0	0
			23	1	17	4	1		
2	D	1	Total	Br	C	N	O	0	0
			23	1	17	4	1		
2	E	1	Total	Br	C	N	O	0	0
			23	1	17	4	1		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	5	Total	O	0	0
			5	5		

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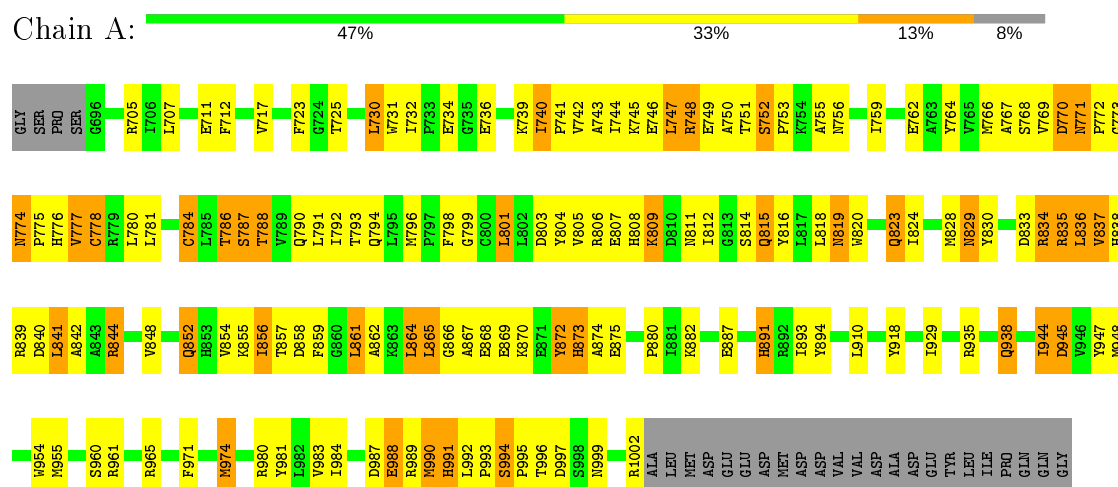
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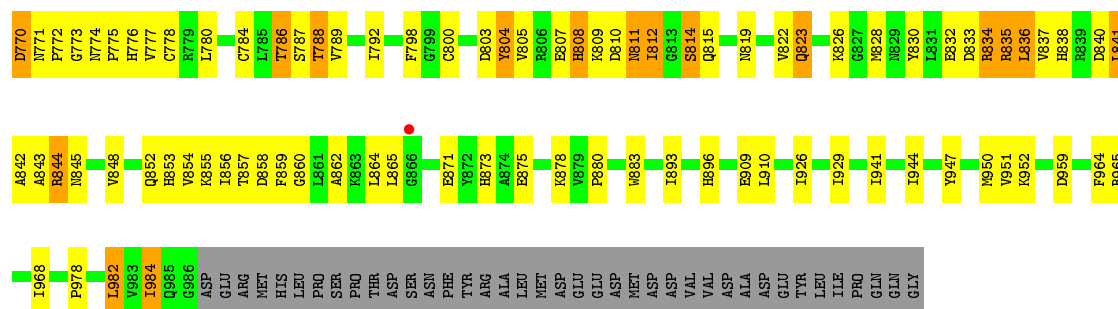
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	2	Total 2	O 2	0	0
3	C	3	Total 3	O 3	0	0
3	D	2	Total 2	O 2	0	0
3	E	4	Total 4	O 4	0	0

### 3 Residue-property plots

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

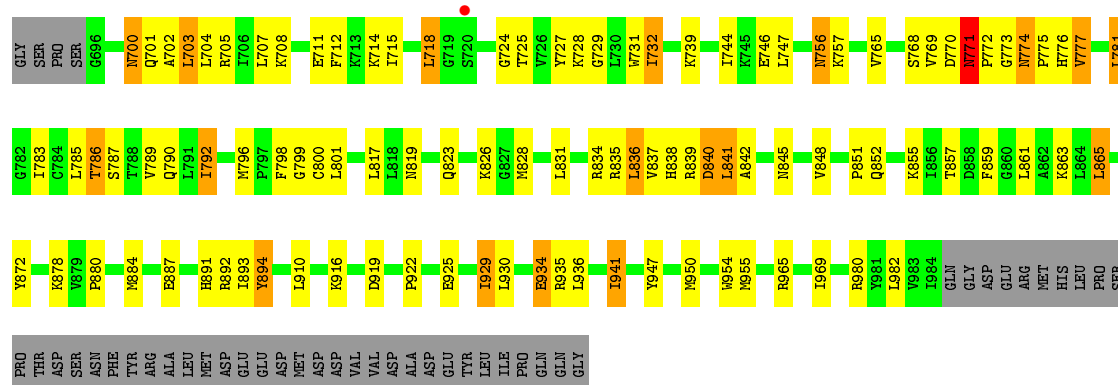
#### • Molecule 1: Epidermal growth factor receptor





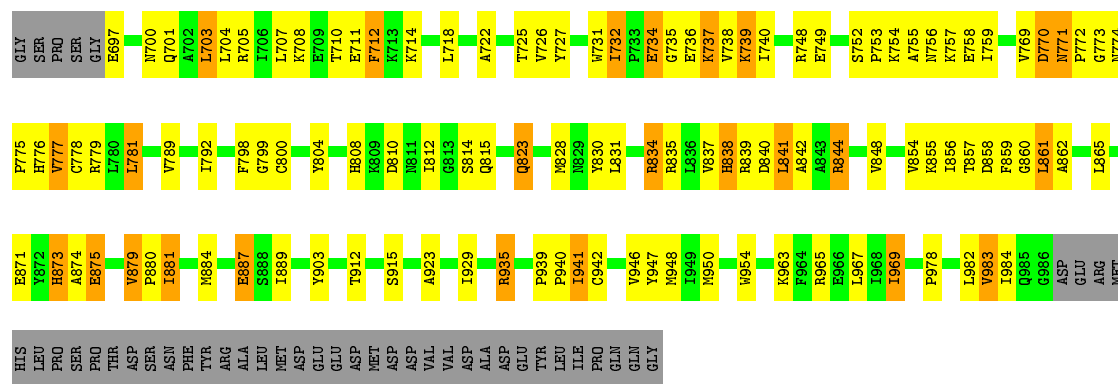
• Molecule 1: Epidermal growth factor receptor

Chain D: 56% 25% 5% 13%



• Molecule 1: Epidermal growth factor receptor

Chain E: 52% 27% 7% 13%



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	114.92Å 425.85Å 95.10Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.18 – 3.53 49.18 – 3.53	Depositor EDS
% Data completeness (in resolution range)	84.5 (49.18-3.53) 84.6 (49.18-3.53)	Depositor EDS
$R_{merge}$	0.15	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.74 (at 3.48Å)	Xtrriage
Refinement program	PHENIX (phenix.refine: 1.8_1069)	Depositor
R, $R_{free}$	0.225 , 0.264 0.227 , 0.264	Depositor DCC
$R_{free}$ test set	1264 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	94.0	Xtrriage
Anisotropy	0.603	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 48.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.43$ , $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	11696	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	76.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.74% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.43	0/2446	0.55	0/3318
1	B	0.33	0/2365	0.51	0/3202
1	C	0.40	0/2346	0.51	0/3181
1	D	0.30	0/2331	0.48	0/3159
1	E	0.36	0/2341	0.53	0/3172
All	All	0.37	0/11829	0.51	0/16032

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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	2391	0	2393	232	0
1	B	2313	0	2358	141	0
1	C	2293	0	2318	242	0
1	D	2279	0	2320	122	0
1	E	2289	0	2336	169	0
2	A	23	0	14	3	0
2	B	23	0	14	3	0
2	C	23	0	13	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	23	0	14	1	0
2	E	23	0	13	1	0
3	A	5	0	0	0	0
3	B	2	0	0	0	0
3	C	3	0	0	1	0
3	D	2	0	0	0	0
3	E	4	0	0	0	0
All	All	11696	0	11793	898	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 38.

All (898) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:740:ILE:HD13	1:C:741:PRO:CD	1.42	1.47
1:C:740:ILE:CD1	1:C:741:PRO:HD2	1.46	1.46
1:E:776:HIS:CE1	1:E:823:GLN:HG3	1.48	1.46
1:A:740:ILE:HD12	1:A:741:PRO:CD	1.51	1.38
1:C:755:ALA:HB1	1:C:759:ILE:CD1	1.53	1.38
1:A:740:ILE:HD12	1:A:741:PRO:N	1.35	1.37
1:B:747:LEU:HD12	1:B:748:ARG:N	1.38	1.36
1:A:771:ASN:CB	1:A:772:PRO:HD2	1.56	1.33
1:C:836:LEU:HD12	1:C:836:LEU:C	1.51	1.29
1:A:836:LEU:C	1:A:836:LEU:HD12	1.51	1.28
1:B:771:ASN:CB	1:B:772:PRO:HD2	1.61	1.28
1:D:839:ARG:CG	1:D:894:TYR:HD2	1.48	1.27
1:C:732:ILE:HD12	1:C:732:ILE:C	1.55	1.27
1:C:769:VAL:O	1:C:772:PRO:HD2	1.35	1.24
1:E:881:ILE:H	1:E:881:ILE:CD1	1.50	1.23
1:E:774:ASN:CG	1:E:775:PRO:HD2	1.58	1.23
1:C:736:GLU:CG	1:C:738:VAL:HG23	1.69	1.22
1:D:703:LEU:C	1:D:703:LEU:HD12	1.59	1.22
1:A:872:TYR:CE2	1:A:874:ALA:HB2	1.74	1.21
1:A:836:LEU:HD12	1:A:837:VAL:N	1.53	1.21
1:C:755:ALA:CA	1:C:759:ILE:HD12	1.70	1.20
1:C:747:LEU:HD23	1:C:748:ARG:N	1.56	1.19
1:D:703:LEU:HD12	1:D:704:LEU:N	1.58	1.18
1:D:836:LEU:HD23	1:D:837:VAL:N	1.57	1.18
1:B:836:LEU:HD12	1:B:836:LEU:C	1.59	1.18
1:B:771:ASN:ND2	1:B:772:PRO:HD3	1.60	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:772:PRO:HG3	1:C:834:ARG:CZ	1.74	1.16
1:C:836:LEU:HD12	1:C:837:VAL:N	1.56	1.16
1:D:771:ASN:HB3	1:D:772:PRO:HD2	1.26	1.15
1:D:704:LEU:HD23	1:D:705:ARG:N	1.61	1.12
1:B:771:ASN:HB3	1:B:772:PRO:CD	1.78	1.11
1:C:755:ALA:HB1	1:C:759:ILE:HD11	1.27	1.11
1:C:775:PRO:O	1:C:855:LYS:HE2	1.50	1.10
1:A:774:ASN:ND2	1:A:776:HIS:H	1.46	1.10
1:E:879:VAL:HG23	1:E:880:PRO:HD2	1.29	1.10
1:C:755:ALA:CB	1:C:759:ILE:CD1	2.30	1.10
1:D:836:LEU:HD23	1:D:836:LEU:C	1.71	1.10
1:C:772:PRO:CG	1:C:834:ARG:CZ	2.30	1.09
1:D:771:ASN:CB	1:D:772:PRO:HD2	1.83	1.09
1:E:881:ILE:N	1:E:881:ILE:HD13	1.58	1.09
1:D:839:ARG:CG	1:D:894:TYR:CD2	2.35	1.09
1:C:828:MET:HE2	1:C:856:ILE:CD1	1.83	1.08
1:C:747:LEU:HD12	1:C:759:ILE:HD11	1.28	1.08
1:A:740:ILE:CD1	1:A:741:PRO:CD	2.30	1.08
1:A:771:ASN:CB	1:A:772:PRO:CD	2.30	1.07
1:E:776:HIS:CE1	1:E:823:GLN:CG	2.36	1.07
1:C:755:ALA:C	1:C:759:ILE:HD12	1.74	1.07
1:C:776:HIS:O	1:C:856:ILE:HG22	1.54	1.07
1:D:839:ARG:HD3	1:D:894:TYR:CD2	1.90	1.07
1:C:828:MET:HE3	1:C:841:LEU:HD21	1.37	1.05
1:A:839:ARG:HD2	1:A:894:TYR:CD2	1.90	1.05
1:C:772:PRO:HG3	1:C:834:ARG:NH2	1.69	1.05
1:E:776:HIS:HE1	1:E:823:GLN:CG	1.67	1.05
1:A:747:LEU:HD12	1:A:748:ARG:H	1.16	1.05
1:D:839:ARG:HD3	1:D:894:TYR:CE2	1.92	1.05
1:A:872:TYR:C	1:A:872:TYR:HD2	1.59	1.04
1:E:774:ASN:OD1	1:E:775:PRO:HD2	1.56	1.04
1:A:864:LEU:HD12	1:A:865:LEU:N	1.70	1.04
1:A:740:ILE:CD1	1:A:741:PRO:HD2	1.87	1.04
1:A:872:TYR:CZ	1:A:874:ALA:HB2	1.91	1.04
1:D:771:ASN:CB	1:D:772:PRO:CD	2.30	1.03
1:A:712:PHE:HB3	1:A:731:TRP:HD1	1.23	1.03
1:C:736:GLU:HG3	1:C:738:VAL:HG23	1.40	1.03
1:B:771:ASN:CB	1:B:772:PRO:CD	2.29	1.02
1:C:828:MET:HE2	1:C:856:ILE:HD13	1.39	1.02
1:B:776:HIS:ND1	1:B:823:GLN:HG3	1.75	1.01
1:A:835:ARG:NH2	1:A:867:ALA:CB	2.23	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:703:LEU:C	1:E:703:LEU:CD2	2.30	1.01
1:B:836:LEU:HD12	1:B:837:VAL:N	1.74	1.00
1:D:771:ASN:CG	1:D:772:PRO:CD	2.30	1.00
1:A:774:ASN:HD22	1:A:775:PRO:N	1.59	0.99
1:C:838:HIS:CE1	1:C:840:ASP:C	2.35	0.99
1:D:839:ARG:CD	1:D:894:TYR:CD2	2.45	0.99
1:B:776:HIS:CE1	1:B:823:GLN:HG3	1.95	0.99
1:E:703:LEU:C	1:E:703:LEU:HD23	1.82	0.99
1:D:836:LEU:CD2	1:D:836:LEU:C	2.30	0.99
1:C:836:LEU:CD1	1:C:836:LEU:C	2.30	0.99
1:E:857:THR:HG22	1:E:858:ASP:N	1.78	0.99
1:E:703:LEU:HD21	1:E:705:ARG:HG3	1.38	0.98
1:B:836:LEU:C	1:B:836:LEU:CD1	2.30	0.98
1:D:775:PRO:O	1:D:855:LYS:HE2	1.63	0.98
1:A:864:LEU:CD1	1:A:865:LEU:H	1.77	0.98
1:C:838:HIS:HE1	1:C:840:ASP:C	1.66	0.98
1:A:776:HIS:CE1	1:A:823:GLN:HG3	1.99	0.98
1:E:771:ASN:HD22	1:E:772:PRO:CD	1.77	0.97
1:A:857:THR:HG22	1:A:858:ASP:N	1.79	0.97
1:C:838:HIS:HE1	1:C:840:ASP:O	1.46	0.97
1:C:755:ALA:O	1:C:759:ILE:HB	1.64	0.96
1:C:857:THR:CG2	1:C:858:ASP:H	1.78	0.96
1:D:828:MET:HE1	1:D:841:LEU:HD22	1.46	0.96
1:C:828:MET:CE	1:C:856:ILE:CD1	2.44	0.96
1:A:872:TYR:CE2	1:A:874:ALA:CB	2.48	0.95
1:B:750:ALA:HB2	1:B:756:ASN:OD1	1.66	0.95
1:C:857:THR:HG22	1:C:858:ASP:N	1.81	0.95
1:B:747:LEU:CD1	1:B:748:ARG:N	2.30	0.95
1:E:771:ASN:HD22	1:E:772:PRO:HD3	1.31	0.95
1:A:836:LEU:CD1	1:A:836:LEU:C	2.30	0.95
1:E:881:ILE:H	1:E:881:ILE:HD13	0.79	0.95
1:A:864:LEU:CD1	1:A:865:LEU:N	2.30	0.95
1:B:736:GLU:O	1:B:737:LYS:HG2	1.67	0.95
1:D:771:ASN:HB3	1:D:772:PRO:CD	1.87	0.95
1:A:872:TYR:C	1:A:872:TYR:CD2	2.35	0.94
1:A:836:LEU:CD1	1:A:837:VAL:N	2.30	0.94
1:B:747:LEU:HD12	1:B:748:ARG:H	1.19	0.94
1:A:740:ILE:CD1	1:A:741:PRO:N	2.30	0.94
1:A:872:TYR:HE2	1:A:874:ALA:HB2	1.29	0.94
1:C:747:LEU:CD2	1:C:748:ARG:N	2.30	0.94
1:A:872:TYR:HE2	1:A:874:ALA:CB	1.79	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:836:LEU:CD1	1:B:837:VAL:N	2.30	0.94
1:E:857:THR:CG2	1:E:858:ASP:N	2.30	0.94
1:A:740:ILE:HD12	1:A:741:PRO:HD2	1.45	0.93
1:C:732:ILE:CD1	1:C:732:ILE:C	2.30	0.93
1:A:857:THR:CG2	1:A:858:ASP:N	2.30	0.93
1:B:771:ASN:ND2	1:B:772:PRO:CD	2.30	0.93
1:A:841:LEU:HD12	1:A:842:ALA:N	1.84	0.93
1:B:771:ASN:CG	1:B:772:PRO:CD	2.37	0.93
1:A:857:THR:CG2	1:A:858:ASP:H	1.81	0.93
1:B:765:VAL:HG11	1:B:859:PHE:HB3	1.49	0.93
1:C:740:ILE:HD13	1:C:741:PRO:N	1.82	0.93
1:C:747:LEU:CD1	1:C:755:ALA:CB	2.47	0.93
1:D:839:ARG:HG2	1:D:894:TYR:HD2	1.29	0.93
1:D:771:ASN:CG	1:D:772:PRO:HD3	1.88	0.92
1:A:711:GLU:HG2	1:A:734:GLU:H	1.35	0.92
1:C:731:TRP:O	1:C:740:ILE:HG22	1.68	0.92
1:C:755:ALA:O	1:C:759:ILE:HD12	1.69	0.92
1:E:879:VAL:HG23	1:E:880:PRO:CD	1.98	0.91
1:A:740:ILE:HD11	1:A:741:PRO:O	1.70	0.91
1:A:747:LEU:HD12	1:A:748:ARG:N	1.85	0.91
1:B:771:ASN:HB3	1:B:772:PRO:HD2	0.92	0.91
1:C:732:ILE:HD12	1:C:733:PRO:N	1.84	0.91
1:E:732:ILE:HG22	1:E:738:VAL:O	1.70	0.91
1:D:839:ARG:HG2	1:D:894:TYR:CD2	2.04	0.91
1:C:828:MET:CE	1:C:841:LEU:CD2	2.49	0.90
1:D:839:ARG:CD	1:D:894:TYR:CE2	2.53	0.90
1:A:839:ARG:HD2	1:A:894:TYR:HD2	1.29	0.90
1:A:872:TYR:OH	1:A:874:ALA:HB2	1.72	0.90
1:C:732:ILE:HD12	1:C:732:ILE:O	1.70	0.89
1:E:737:LYS:HD3	1:E:737:LYS:C	1.91	0.89
1:E:703:LEU:O	1:E:703:LEU:HD22	1.72	0.89
1:A:784:CYS:SG	1:A:790:GLN:OE1	2.30	0.89
1:C:756:ASN:O	1:C:760:LEU:HD13	1.74	0.88
1:C:736:GLU:CG	1:C:738:VAL:CG2	2.51	0.88
1:C:776:HIS:ND1	1:C:823:GLN:HG3	1.88	0.87
1:C:828:MET:CE	1:C:841:LEU:HD21	2.04	0.87
1:D:771:ASN:CG	1:D:772:PRO:HD2	1.94	0.87
1:A:839:ARG:CZ	1:A:894:TYR:HE2	1.86	0.87
1:B:983:VAL:O	1:B:984:ILE:HG12	1.74	0.87
1:E:776:HIS:ND1	1:E:823:GLN:HG3	1.89	0.87
1:E:731:TRP:O	1:E:740:ILE:HG22	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:712:PHE:HB3	1:A:731:TRP:CD1	2.09	0.86
1:E:860:GLY:O	1:E:861:LEU:HD23	1.75	0.86
1:C:755:ALA:CA	1:C:759:ILE:CD1	2.52	0.86
1:A:814:SER:HB3	1:A:984:ILE:HD12	1.57	0.86
1:C:828:MET:HE1	1:C:841:LEU:HD22	1.56	0.86
1:C:747:LEU:HD13	1:C:755:ALA:CB	2.06	0.85
1:D:703:LEU:C	1:D:703:LEU:CD1	2.37	0.85
1:C:740:ILE:HD13	1:C:741:PRO:HD2	0.86	0.85
1:E:776:HIS:HE1	1:E:823:GLN:HG3	1.06	0.85
1:C:736:GLU:HG2	1:C:738:VAL:HG23	1.59	0.85
1:C:736:GLU:HG3	1:C:738:VAL:CG2	2.07	0.85
1:D:828:MET:CE	1:D:841:LEU:CD2	2.54	0.85
1:D:838:HIS:CE1	1:D:840:ASP:O	2.30	0.85
1:C:747:LEU:CD1	1:C:755:ALA:HB2	2.05	0.84
1:A:861:LEU:HD23	1:A:861:LEU:N	1.93	0.84
1:C:838:HIS:CE1	1:C:840:ASP:O	2.30	0.84
1:A:873:HIS:N	1:A:873:HIS:CD2	2.45	0.84
1:E:703:LEU:HD23	1:E:704:LEU:N	1.91	0.84
1:E:879:VAL:HG21	1:E:884:MET:SD	2.18	0.84
1:C:747:LEU:HD23	1:C:748:ARG:H	1.39	0.84
1:B:775:PRO:O	1:B:855:LYS:HE2	1.78	0.83
1:E:774:ASN:CG	1:E:775:PRO:CD	2.44	0.83
1:B:736:GLU:C	1:B:737:LYS:HG2	1.97	0.83
1:A:872:TYR:HD2	1:A:873:HIS:N	1.75	0.83
1:A:740:ILE:HD12	1:A:740:ILE:C	1.97	0.82
1:B:771:ASN:CG	1:B:772:PRO:HD3	1.99	0.82
1:C:747:LEU:CD1	1:C:755:ALA:HB1	2.09	0.82
1:A:835:ARG:NH2	1:A:867:ALA:HB2	1.94	0.82
1:C:755:ALA:HA	1:C:759:ILE:HD12	1.61	0.82
1:C:755:ALA:CB	1:C:759:ILE:HD12	2.02	0.82
1:A:747:LEU:O	1:A:788:THR:CG2	2.28	0.82
1:B:747:LEU:HD11	1:B:748:ARG:O	1.80	0.81
1:A:740:ILE:HD13	1:A:741:PRO:HD2	1.61	0.81
1:C:809:LYS:HG3	1:C:810:ASP:N	1.94	0.81
1:C:755:ALA:C	1:C:759:ILE:CD1	2.49	0.81
1:C:775:PRO:HB2	1:C:776:HIS:CD2	2.14	0.81
1:C:812:ILE:O	1:C:812:ILE:HG23	1.78	0.81
1:C:828:MET:HE1	1:C:856:ILE:HD11	1.62	0.81
1:D:839:ARG:HG3	1:D:894:TYR:HD2	1.42	0.81
1:A:774:ASN:HD22	1:A:776:HIS:H	1.29	0.81
1:C:828:MET:CE	1:C:856:ILE:HD11	2.11	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:864:LEU:HD13	1:A:865:LEU:H	1.44	0.81
1:A:747:LEU:O	1:A:788:THR:HG22	1.81	0.81
1:D:828:MET:CE	1:D:841:LEU:HD22	2.10	0.81
1:A:749:GLU:HA	1:A:788:THR:HG23	1.61	0.81
1:B:771:ASN:CG	1:B:772:PRO:HD2	2.01	0.81
1:D:776:HIS:CE1	1:D:823:GLN:HE21	1.98	0.80
1:E:769:VAL:O	1:E:772:PRO:HD2	1.81	0.80
1:C:828:MET:HE3	1:C:841:LEU:CD2	2.12	0.80
1:E:838:HIS:CE1	1:E:840:ASP:H	1.99	0.80
1:E:860:GLY:O	1:E:861:LEU:CD2	2.30	0.80
1:A:837:VAL:O	1:A:837:VAL:CG2	2.30	0.80
1:A:872:TYR:OH	1:A:874:ALA:CB	2.30	0.80
1:B:747:LEU:CD1	1:B:748:ARG:O	2.30	0.80
1:C:755:ALA:HB1	1:C:759:ILE:HD13	1.62	0.80
1:B:836:LEU:HB2	1:B:864:LEU:HD23	1.64	0.80
1:C:755:ALA:O	1:C:759:ILE:CB	2.30	0.80
1:C:836:LEU:CD1	1:C:837:VAL:N	2.40	0.80
1:E:838:HIS:HE1	1:E:840:ASP:HB3	1.45	0.80
1:A:741:PRO:O	1:A:742:VAL:HG22	1.82	0.80
1:A:766:MET:HG2	1:A:780:LEU:HB2	1.64	0.79
1:A:740:ILE:CD1	1:A:741:PRO:O	2.30	0.79
1:E:860:GLY:O	1:E:861:LEU:CG	2.30	0.79
1:A:774:ASN:ND2	1:A:775:PRO:N	2.30	0.79
1:C:740:ILE:CD1	1:C:741:PRO:O	2.30	0.79
1:E:771:ASN:ND2	1:E:772:PRO:N	2.30	0.79
1:E:828:MET:SD	1:E:841:LEU:CD2	2.70	0.79
1:C:740:ILE:CG1	1:C:741:PRO:HD2	2.13	0.79
1:A:776:HIS:CE1	1:A:823:GLN:CG	2.66	0.79
1:A:835:ARG:NH2	1:A:867:ALA:HB1	1.96	0.79
1:B:736:GLU:O	1:B:737:LYS:CG	2.30	0.79
1:A:771:ASN:CB	1:A:834:ARG:CZ	2.61	0.79
1:C:732:ILE:HD12	1:C:733:PRO:C	2.04	0.79
1:D:828:MET:HE1	1:D:841:LEU:CD2	2.13	0.78
1:D:771:ASN:OD1	1:D:772:PRO:CD	2.30	0.78
1:C:755:ALA:O	1:C:759:ILE:CD1	2.30	0.78
1:C:747:LEU:CD1	1:C:759:ILE:HD11	2.10	0.78
1:E:703:LEU:O	1:E:703:LEU:CD2	2.30	0.78
1:E:774:ASN:OD1	1:E:775:PRO:CD	2.30	0.78
1:C:732:ILE:CD1	1:C:733:PRO:O	2.31	0.78
1:A:857:THR:HG23	1:A:858:ASP:H	1.47	0.78
1:D:771:ASN:OD1	1:D:772:PRO:HD2	1.83	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:985:GLN:HG2	1:B:986:GLY:N	1.95	0.78
1:C:772:PRO:HG2	1:C:834:ARG:CZ	2.12	0.78
1:E:857:THR:CG2	1:E:858:ASP:H	1.95	0.77
1:B:764:TYR:HD1	1:B:764:TYR:O	1.68	0.77
1:C:857:THR:HG22	1:C:858:ASP:H	1.41	0.77
1:E:771:ASN:ND2	1:E:772:PRO:CD	2.47	0.77
1:D:703:LEU:CD1	1:D:704:LEU:N	2.45	0.77
1:A:841:LEU:HD12	1:A:842:ALA:H	1.46	0.77
1:E:838:HIS:HE1	1:E:840:ASP:CA	1.99	0.76
1:E:838:HIS:CE1	1:E:840:ASP:C	2.59	0.76
1:D:704:LEU:HD23	1:D:705:ARG:H	1.50	0.76
1:A:740:ILE:HD12	1:A:741:PRO:CG	2.16	0.76
1:C:732:ILE:CD1	1:C:732:ILE:O	2.30	0.76
1:A:774:ASN:ND2	1:A:776:HIS:N	2.29	0.76
1:E:838:HIS:ND1	1:E:840:ASP:N	2.30	0.76
1:C:772:PRO:CG	1:C:834:ARG:NH1	2.49	0.75
1:A:873:HIS:H	1:A:873:HIS:CD2	2.04	0.75
1:E:740:ILE:O	1:E:740:ILE:CG2	2.35	0.75
1:C:742:VAL:HG12	1:C:743:ALA:N	2.00	0.75
1:D:770:ASP:O	1:D:773:GLY:CA	2.35	0.75
1:A:836:LEU:HD12	1:A:837:VAL:CA	2.16	0.75
1:E:838:HIS:CE1	1:E:840:ASP:CA	2.69	0.75
1:C:776:HIS:CE1	1:C:823:GLN:HG3	2.21	0.75
1:A:741:PRO:O	1:A:742:VAL:CG2	2.35	0.74
1:C:828:MET:HE1	1:C:841:LEU:CD2	2.15	0.74
1:B:764:TYR:HD1	1:B:764:TYR:C	1.91	0.74
1:A:938:GLN:NE2	1:A:947:TYR:CD2	2.55	0.74
1:E:776:HIS:HE1	1:E:823:GLN:CD	1.91	0.74
1:B:732:ILE:CD1	1:B:736:GLU:CB	2.66	0.74
1:D:841:LEU:HD12	1:D:842:ALA:N	2.02	0.74
1:A:814:SER:OG	1:A:987:ASP:CG	2.27	0.73
1:A:774:ASN:HD22	1:A:774:ASN:C	1.91	0.73
1:B:764:TYR:C	1:B:764:TYR:CD1	2.60	0.73
1:A:872:TYR:CD2	1:A:873:HIS:N	2.55	0.73
1:A:839:ARG:CZ	1:A:894:TYR:CE2	2.70	0.73
1:E:838:HIS:HE1	1:E:840:ASP:CB	2.01	0.73
1:A:835:ARG:O	1:A:865:LEU:HB2	1.89	0.72
1:B:747:LEU:HD12	1:B:748:ARG:CA	2.19	0.72
1:C:772:PRO:HB2	1:C:830:TYR:OH	1.88	0.72
1:C:857:THR:HG23	1:C:858:ASP:H	1.54	0.72
1:D:934:GLU:HB2	1:E:708:LYS:HG2	1.71	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:873:HIS:HD2	1:A:873:HIS:H	1.37	0.72
1:B:765:VAL:CG1	1:B:859:PHE:HB3	2.20	0.72
1:E:774:ASN:ND2	1:E:775:PRO:HD2	2.03	0.72
1:A:801:LEU:HD21	1:A:910:LEU:HD21	1.71	0.71
1:A:865:LEU:CD1	1:A:869:GLU:O	2.38	0.71
1:C:836:LEU:HD12	1:C:837:VAL:CA	2.19	0.71
1:C:778:CYS:SG	1:C:857:THR:OG1	2.48	0.71
1:C:761:ASP:O	1:C:764:TYR:HB3	1.89	0.71
1:D:704:LEU:HD23	1:D:704:LEU:C	2.11	0.71
1:B:776:HIS:CE1	1:B:823:GLN:CG	2.74	0.71
1:C:732:ILE:CD1	1:C:733:PRO:C	2.58	0.71
1:B:836:LEU:HD12	1:B:836:LEU:O	1.90	0.71
1:A:838:HIS:O	1:A:862:ALA:HB2	1.90	0.71
1:E:734:GLU:HG2	1:E:736:GLU:H	1.56	0.70
1:C:742:VAL:HG11	1:C:792:ILE:HG13	1.73	0.70
1:E:860:GLY:O	1:E:861:LEU:HG	1.90	0.70
1:C:747:LEU:HD12	1:C:755:ALA:HB1	1.72	0.70
1:D:786:THR:OG1	1:D:787:SER:N	2.24	0.70
1:E:703:LEU:HD11	1:E:705:ARG:CZ	2.22	0.70
1:C:756:ASN:O	1:C:760:LEU:CD1	2.39	0.70
1:A:829:ASN:C	1:A:829:ASN:OD1	2.30	0.70
1:C:770:ASP:OD2	1:C:770:ASP:C	2.29	0.70
1:E:838:HIS:CE1	1:E:840:ASP:HB3	2.25	0.70
1:C:811:ASN:O	1:C:811:ASN:CG	2.30	0.70
1:E:838:HIS:CE1	1:E:840:ASP:N	2.59	0.70
1:A:804:TYR:OH	1:A:992:LEU:HD21	1.90	0.70
1:D:980:ARG:HD2	1:E:697:GLU:CB	2.22	0.70
1:E:700:ASN:OD1	1:E:700:ASN:C	2.30	0.70
1:A:774:ASN:ND2	1:A:775:PRO:HD2	2.07	0.69
1:A:745:LYS:NZ	1:A:762:GLU:OE1	2.25	0.69
1:B:770:ASP:OD1	1:B:770:ASP:C	2.30	0.69
1:B:732:ILE:HD12	1:B:736:GLU:CB	2.22	0.69
1:C:812:ILE:O	1:C:812:ILE:CG2	2.40	0.69
1:E:857:THR:HG23	1:E:858:ASP:H	1.56	0.69
1:C:739:LYS:H	1:C:739:LYS:HD3	1.57	0.69
1:E:781:LEU:HB3	1:E:792:ILE:HG22	1.75	0.69
1:A:815:GLN:NE2	1:A:819:ASN:OD1	2.23	0.69
1:A:711:GLU:HB3	1:A:732:ILE:O	1.92	0.69
1:C:747:LEU:CD2	1:C:748:ARG:C	2.61	0.69
1:C:766:MET:HG2	1:C:780:LEU:HB2	1.75	0.69
1:A:814:SER:CB	1:A:984:ILE:HD12	2.24	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:828:MET:HE2	1:D:841:LEU:HD23	1.75	0.68
1:A:837:VAL:HG23	1:A:837:VAL:O	1.91	0.68
1:C:747:LEU:CD2	1:C:747:LEU:C	2.59	0.68
1:C:732:ILE:CG1	1:C:732:ILE:O	2.39	0.68
1:A:983:VAL:HG12	1:A:983:VAL:O	1.94	0.68
1:E:838:HIS:O	1:E:839:ARG:HB2	1.94	0.68
1:B:836:LEU:HD12	1:B:837:VAL:CA	2.24	0.68
1:D:774:ASN:OD1	1:D:776:HIS:N	2.26	0.68
1:C:838:HIS:O	1:C:862:ALA:HB2	1.94	0.68
1:A:774:ASN:ND2	1:A:775:PRO:CD	2.57	0.67
1:A:747:LEU:HD12	1:A:748:ARG:HG3	1.77	0.67
1:B:765:VAL:HG11	1:B:859:PHE:CB	2.21	0.67
1:E:837:VAL:HG12	1:E:839:ARG:HG3	1.74	0.67
1:D:704:LEU:CD2	1:D:705:ARG:N	2.52	0.67
1:B:772:PRO:HG2	1:B:773:GLY:N	2.09	0.67
1:B:748:ARG:NE	1:B:751:THR:HG22	2.10	0.67
1:E:823:GLN:HG2	1:E:854:VAL:HG22	1.77	0.67
1:D:724:GLY:HA2	1:D:747:LEU:HA	1.77	0.67
1:C:828:MET:CE	1:C:841:LEU:HD22	2.19	0.66
1:E:770:ASP:C	1:E:770:ASP:OD1	2.32	0.66
1:C:736:GLU:CD	1:C:738:VAL:CG2	2.63	0.66
1:B:762:GLU:HB2	1:B:860:GLY:HA2	1.78	0.66
1:C:742:VAL:HG11	1:C:792:ILE:CG1	2.26	0.66
1:D:828:MET:CE	1:D:841:LEU:HD23	2.26	0.66
1:A:866:GLY:O	1:A:869:GLU:HB3	1.95	0.66
1:B:748:ARG:NE	1:B:751:THR:CG2	2.59	0.66
1:E:838:HIS:C	1:E:838:HIS:ND1	2.49	0.66
1:A:992:LEU:HD22	1:A:993:PRO:HD2	1.78	0.66
1:A:740:ILE:CD1	1:A:741:PRO:CG	2.74	0.66
1:C:810:ASP:O	1:C:811:ASN:HB3	1.96	0.66
1:A:774:ASN:HD22	1:A:776:HIS:N	1.93	0.65
1:E:771:ASN:N	1:E:772:PRO:CD	2.59	0.65
1:A:747:LEU:O	1:A:788:THR:HG21	1.97	0.65
1:B:770:ASP:O	1:B:773:GLY:CA	2.44	0.65
1:A:812:ILE:O	1:A:990:MET:SD	2.54	0.65
1:A:996:THR:O	1:A:996:THR:HG22	1.96	0.65
1:E:774:ASN:OD1	1:E:776:HIS:N	2.30	0.65
1:E:875:GLU:OE1	1:E:875:GLU:N	2.30	0.65
1:A:980:ARG:HG2	1:A:981:TYR:CD1	2.31	0.65
1:B:836:LEU:HD13	1:B:837:VAL:N	2.09	0.65
1:C:777:VAL:HA	1:C:856:ILE:CG2	2.27	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:843:ALA:HB2	1:C:909:GLU:CD	2.17	0.65
1:D:770:ASP:O	1:D:773:GLY:N	2.30	0.65
1:D:770:ASP:O	1:D:773:GLY:HA2	1.96	0.65
1:B:745:LYS:NZ	1:B:762:GLU:OE1	2.30	0.65
1:B:774:ASN:OD1	1:B:775:PRO:N	2.30	0.65
1:A:873:HIS:HD2	1:A:873:HIS:N	1.90	0.65
1:C:751:THR:O	1:C:756:ASN:ND2	2.30	0.65
1:C:774:ASN:OD1	1:C:775:PRO:N	2.29	0.65
1:C:838:HIS:ND1	1:C:840:ASP:N	2.41	0.65
1:A:835:ARG:HH21	1:A:867:ALA:CB	2.10	0.65
1:D:838:HIS:ND1	1:D:840:ASP:O	2.30	0.65
1:B:841:LEU:HD12	1:B:842:ALA:N	2.12	0.64
1:C:811:ASN:O	1:C:811:ASN:ND2	2.30	0.64
1:D:836:LEU:HD23	1:D:837:VAL:CA	2.25	0.64
1:B:772:PRO:CD	1:B:773:GLY:H	2.10	0.64
1:C:755:ALA:O	1:C:759:ILE:N	2.30	0.64
1:C:747:LEU:HD13	1:C:755:ALA:HB1	1.76	0.64
1:E:722:ALA:HA	1:E:748:ARG:NH1	2.12	0.64
1:A:859:PHE:O	1:A:862:ALA:N	2.29	0.64
1:A:980:ARG:HG2	1:A:981:TYR:CE1	2.33	0.64
1:A:770:ASP:O	1:A:773:GLY:N	2.30	0.64
1:A:866:GLY:N	1:A:869:GLU:OE2	2.30	0.64
1:C:732:ILE:HD12	1:C:733:PRO:CA	2.27	0.64
1:C:739:LYS:HD3	1:C:739:LYS:N	2.11	0.64
1:A:741:PRO:C	1:A:742:VAL:CG2	2.66	0.64
1:B:774:ASN:OD1	1:B:776:HIS:N	2.30	0.64
1:E:770:ASP:O	1:E:773:GLY:N	2.30	0.64
1:A:811:ASN:HB3	1:A:991:HIS:HB2	1.79	0.64
1:B:753:PRO:O	1:B:757:LYS:N	2.31	0.64
1:E:775:PRO:O	1:E:855:LYS:HE2	1.97	0.64
1:A:865:LEU:HD13	1:A:869:GLU:O	1.97	0.64
1:C:740:ILE:HD12	1:C:741:PRO:O	1.97	0.64
1:E:770:ASP:O	1:E:773:GLY:CA	2.47	0.63
1:E:838:HIS:HE1	1:E:840:ASP:C	2.00	0.63
1:E:881:ILE:N	1:E:881:ILE:CD1	2.30	0.63
1:A:774:ASN:HD21	1:A:776:HIS:H	1.41	0.63
1:D:840:ASP:C	1:D:840:ASP:OD2	2.37	0.63
1:B:772:PRO:CG	1:B:773:GLY:N	2.61	0.63
1:D:746:GLU:OE1	1:D:790:GLN:NE2	2.30	0.63
1:E:731:TRP:HB3	1:E:740:ILE:CG2	2.29	0.63
1:A:828:MET:SD	1:A:841:LEU:HD22	2.39	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:836:LEU:CD1	1:B:837:VAL:C	2.67	0.63
1:C:814:SER:HB3	1:C:982:LEU:HD13	1.81	0.63
1:A:741:PRO:C	1:A:742:VAL:HG23	2.18	0.62
1:C:770:ASP:O	1:C:773:GLY:N	2.32	0.62
1:E:879:VAL:CG2	1:E:884:MET:SD	2.87	0.62
1:C:836:LEU:O	1:C:836:LEU:HD12	1.97	0.62
1:C:838:HIS:HA	1:C:862:ALA:CB	2.29	0.62
1:E:753:PRO:HG2	1:E:754:LYS:HG2	1.82	0.62
1:B:765:VAL:HG12	1:B:766:MET:N	2.15	0.62
1:C:750:ALA:O	1:C:753:PRO:CD	2.47	0.62
1:C:804:TYR:O	1:C:808:HIS:HB2	1.99	0.62
1:D:834:ARG:O	1:D:835:ARG:HG2	1.99	0.62
1:B:983:VAL:HG12	1:B:983:VAL:O	1.98	0.62
1:D:841:LEU:HD12	1:D:842:ALA:H	1.64	0.62
1:B:736:GLU:O	1:B:737:LYS:CB	2.48	0.61
1:C:944:ILE:HG22	1:D:700:ASN:OD1	2.00	0.61
1:C:774:ASN:OD1	1:C:776:HIS:N	2.30	0.61
1:D:839:ARG:NH2	1:D:861:LEU:O	2.33	0.61
1:E:737:LYS:HD3	1:E:737:LYS:O	2.01	0.61
1:E:772:PRO:HG2	1:E:830:TYR:OH	2.00	0.61
1:B:759:ILE:CG2	1:B:760:LEU:N	2.63	0.61
1:B:765:VAL:CG1	1:B:859:PHE:CB	2.79	0.61
1:C:752:SER:N	1:C:753:PRO:HD3	2.15	0.61
1:B:756:ASN:HD21	1:B:789:VAL:HG12	1.66	0.60
1:C:809:LYS:O	1:C:812:ILE:HB	2.00	0.60
1:D:834:ARG:O	1:D:835:ARG:CG	2.49	0.60
1:A:837:VAL:HG23	1:A:839:ARG:HB2	1.83	0.60
1:C:736:GLU:CD	1:C:738:VAL:HG23	2.21	0.60
1:B:771:ASN:HD22	1:B:772:PRO:CD	2.11	0.60
1:C:736:GLU:CD	1:C:738:VAL:HG21	2.22	0.60
1:A:774:ASN:HB3	1:A:777:VAL:HG23	1.83	0.60
1:C:809:LYS:HG3	1:C:810:ASP:H	1.66	0.60
1:A:971:PHE:HA	1:A:974:MET:HG3	1.83	0.60
1:C:742:VAL:CG1	1:C:743:ALA:N	2.65	0.60
1:A:999:ASN:ND2	1:A:999:ASN:O	2.34	0.60
1:A:747:LEU:CD1	1:A:748:ARG:H	2.01	0.60
1:A:814:SER:HA	1:A:984:ILE:CD1	2.32	0.60
1:B:833:ASP:OD1	1:B:965:ARG:NH1	2.34	0.60
1:C:729:GLY:N	1:C:742:VAL:O	2.32	0.60
1:B:772:PRO:CG	1:B:773:GLY:H	2.15	0.59
1:D:837:VAL:CG2	1:D:865:LEU:HD11	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:776:HIS:O	1:B:855:LYS:HA	2.02	0.59
1:C:775:PRO:O	1:C:855:LYS:CE	2.38	0.59
1:C:741:PRO:O	1:C:742:VAL:CG2	2.50	0.59
1:C:838:HIS:CE1	1:C:840:ASP:CA	2.85	0.59
1:B:747:LEU:C	1:B:747:LEU:HD12	2.19	0.59
1:E:740:ILE:HG23	1:E:740:ILE:O	2.02	0.59
1:C:844:ARG:NH1	1:C:845:ASN:OD1	2.36	0.59
1:A:988:GLU:O	1:A:989:ARG:CB	2.51	0.59
1:B:983:VAL:C	1:B:984:ILE:HG12	2.22	0.59
1:A:836:LEU:CD1	1:A:837:VAL:C	2.70	0.59
1:C:857:THR:CG2	1:C:858:ASP:N	2.35	0.59
1:C:838:HIS:HA	1:C:862:ALA:HB2	1.85	0.59
1:D:704:LEU:CD2	1:D:704:LEU:C	2.70	0.59
1:E:722:ALA:HA	1:E:748:ARG:HH11	1.68	0.59
1:C:732:ILE:HD13	1:C:733:PRO:O	2.03	0.58
1:C:732:ILE:HG13	1:C:732:ILE:O	2.01	0.58
1:C:752:SER:N	1:C:753:PRO:CD	2.66	0.58
1:C:777:VAL:HG23	1:C:777:VAL:O	2.01	0.58
1:E:770:ASP:OD2	1:E:779:ARG:HD3	2.02	0.58
1:E:814:SER:HB3	1:E:984:ILE:HD13	1.84	0.58
1:E:776:HIS:O	1:E:855:LYS:HA	2.03	0.58
1:E:839:ARG:HD3	1:E:861:LEU:O	2.03	0.58
1:E:881:ILE:HG22	1:E:889:ILE:HD13	1.85	0.58
1:E:859:PHE:O	1:E:862:ALA:CB	2.52	0.58
1:A:740:ILE:HD12	1:A:741:PRO:CA	2.30	0.58
1:D:774:ASN:OD1	1:D:777:VAL:HG23	2.04	0.58
1:D:819:ASN:ND2	1:D:852:GLN:OE1	2.36	0.58
1:D:801:LEU:HD21	1:D:910:LEU:HD21	1.86	0.58
1:A:778:CYS:SG	1:A:857:THR:OG1	2.62	0.58
1:B:774:ASN:C	1:B:774:ASN:OD1	2.41	0.58
1:C:769:VAL:O	1:C:772:PRO:CD	2.30	0.58
1:B:807:GLU:HG3	1:B:808:HIS:ND1	2.18	0.57
1:B:984:ILE:HG22	1:B:985:GLN:H	1.68	0.57
1:C:740:ILE:HD13	1:C:740:ILE:C	2.25	0.57
1:C:947:TYR:HD1	1:C:950:MET:HE3	1.69	0.57
1:E:815:GLN:HG2	1:E:978:PRO:HG3	1.87	0.57
1:B:772:PRO:HG2	1:B:773:GLY:H	1.69	0.57
1:E:714:LYS:HB3	1:E:727:TYR:HD2	1.69	0.57
1:D:935:ARG:NH1	1:D:954:TRP:O	2.37	0.57
1:A:740:ILE:CD1	1:A:741:PRO:HG2	2.34	0.57
1:A:786:THR:O	1:A:787:SER:C	2.43	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:992:LEU:CD2	1:A:993:PRO:HD2	2.35	0.57
1:A:872:TYR:HE2	1:A:874:ALA:N	2.01	0.57
1:C:836:LEU:CD1	1:C:837:VAL:C	2.73	0.57
1:C:944:ILE:HG21	1:D:700:ASN:HD21	1.70	0.57
1:D:703:LEU:HD12	1:D:704:LEU:CA	2.34	0.57
1:A:804:TYR:OH	1:A:992:LEU:CD2	2.53	0.57
1:B:895:THR:OG1	1:B:896:HIS:N	2.37	0.56
1:A:836:LEU:O	1:A:836:LEU:HD12	1.99	0.56
1:D:715:ILE:HG13	1:D:729:GLY:HA2	1.86	0.56
1:D:776:HIS:NE2	1:D:823:GLN:NE2	2.53	0.56
1:A:778:CYS:HB2	1:A:856:ILE:O	2.05	0.56
1:A:864:LEU:HD12	1:A:864:LEU:C	2.25	0.56
1:A:938:GLN:NE2	1:A:947:TYR:HD2	2.04	0.56
1:E:939:PRO:HG2	1:E:942:CYS:HB2	1.86	0.56
1:A:824:ILE:HG23	1:A:856:ILE:HD11	1.87	0.56
1:B:765:VAL:CG1	1:B:766:MET:N	2.65	0.56
1:B:984:ILE:HG22	1:B:985:GLN:N	2.21	0.56
1:E:828:MET:SD	1:E:841:LEU:HD22	2.45	0.56
1:B:828:MET:HE1	1:B:841:LEU:HD22	1.88	0.56
1:C:814:SER:HB3	1:C:982:LEU:CD1	2.37	0.56
1:E:881:ILE:HG13	1:E:923:ALA:HB1	1.88	0.56
1:C:712:PHE:HB3	1:C:731:TRP:HA	1.88	0.55
1:B:756:ASN:ND2	1:B:789:VAL:HG12	2.21	0.55
1:B:841:LEU:HD12	1:B:842:ALA:H	1.70	0.55
1:A:811:ASN:HA	1:A:990:MET:SD	2.46	0.55
1:E:731:TRP:CE3	1:E:740:ILE:HG21	2.41	0.55
1:E:707:LEU:HD11	1:E:731:TRP:CZ2	2.42	0.55
1:C:840:ASP:OD2	1:C:880:PRO:HG3	2.06	0.55
1:D:704:LEU:HD21	1:D:783:ILE:HG22	1.89	0.55
1:E:731:TRP:HE3	1:E:740:ILE:HG21	1.72	0.55
1:C:740:ILE:HD13	1:C:741:PRO:O	2.07	0.55
1:C:798:PHE:HB2	1:C:848:VAL:HB	1.89	0.55
1:C:747:LEU:HD21	1:C:749:GLU:CB	2.37	0.54
1:D:836:LEU:HD23	1:D:837:VAL:C	2.28	0.54
1:E:808:HIS:O	1:E:812:ILE:HG12	2.07	0.54
1:B:777:VAL:O	1:B:777:VAL:CG2	2.51	0.54
1:D:941:ILE:HG13	1:D:982:LEU:HD22	1.88	0.54
1:A:742:VAL:CG1	1:A:793:THR:O	2.55	0.54
1:D:774:ASN:C	1:D:774:ASN:OD1	2.45	0.54
1:A:835:ARG:HH22	1:A:867:ALA:CB	2.15	0.54
1:C:777:VAL:HA	1:C:856:ILE:HG22	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:770:ASP:O	1:B:773:GLY:N	2.40	0.54
1:E:738:VAL:HG12	1:E:738:VAL:O	2.06	0.54
1:A:711:GLU:CB	1:A:732:ILE:O	2.56	0.54
1:B:745:LYS:NZ	1:B:762:GLU:OE2	2.39	0.54
1:B:745:LYS:NZ	1:B:762:GLU:CD	2.61	0.54
1:C:741:PRO:O	1:C:742:VAL:HG23	2.08	0.54
1:C:838:HIS:CE1	1:C:840:ASP:H	2.26	0.54
1:E:771:ASN:ND2	1:E:772:PRO:HD3	2.12	0.54
1:B:777:VAL:O	1:B:777:VAL:HG22	2.07	0.54
1:B:980:ARG:HA	1:C:699:PRO:HD3	1.90	0.54
1:E:834:ARG:HH11	1:E:834:ARG:HA	1.73	0.54
1:E:859:PHE:O	1:E:862:ALA:N	2.38	0.54
1:A:811:ASN:CA	1:A:990:MET:SD	2.96	0.53
1:A:742:VAL:HG12	1:A:743:ALA:N	2.23	0.53
1:A:712:PHE:HZ	1:A:790:GLN:OE1	1.90	0.53
1:B:771:ASN:HD22	1:B:772:PRO:HD3	1.61	0.53
1:C:747:LEU:HD12	1:C:755:ALA:CB	2.31	0.53
1:C:803:ASP:O	1:C:807:GLU:HG2	2.08	0.53
1:C:772:PRO:CD	1:C:834:ARG:NH1	2.71	0.53
1:D:711:GLU:HB2	1:D:732:ILE:O	2.08	0.53
1:B:786:THR:HG22	1:B:788:THR:H	1.74	0.53
1:C:747:LEU:HD13	1:C:755:ALA:HB2	1.80	0.53
1:E:772:PRO:CG	1:E:830:TYR:OH	2.56	0.53
1:E:776:HIS:O	1:E:855:LYS:HG2	2.09	0.53
1:D:840:ASP:OD2	1:D:845:ASN:ND2	2.42	0.53
1:C:747:LEU:HD22	1:C:748:ARG:C	2.28	0.53
1:C:761:ASP:O	1:C:764:TYR:N	2.42	0.53
1:B:808:HIS:O	1:B:812:ILE:HG12	2.09	0.53
1:B:835:ARG:O	1:B:865:LEU:HB2	2.09	0.53
1:E:754:LYS:O	1:E:757:LYS:N	2.41	0.53
1:B:857:THR:HG22	1:B:858:ASP:H	1.73	0.53
1:A:764:TYR:O	1:A:767:ALA:HB3	2.09	0.52
1:E:712:PHE:HD2	1:E:731:TRP:CD1	2.26	0.52
1:B:756:ASN:ND2	1:B:789:VAL:CG1	2.72	0.52
1:E:740:ILE:HG22	1:E:740:ILE:O	2.08	0.52
1:D:839:ARG:CD	1:D:894:TYR:HE2	2.18	0.52
1:C:777:VAL:HA	1:C:856:ILE:HG23	1.91	0.52
1:A:814:SER:CA	1:A:984:ILE:HD12	2.40	0.52
1:A:974:MET:HB3	1:A:981:TYR:HD2	1.75	0.52
1:B:769:VAL:O	1:B:769:VAL:HG23	2.09	0.52
1:C:740:ILE:CD1	1:C:741:PRO:CD	2.30	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:815:GLN:HG2	1:C:978:PRO:HG3	1.91	0.52
1:C:777:VAL:HG12	1:C:856:ILE:HG21	1.91	0.52
1:C:853:HIS:CE1	1:C:855:LYS:HE3	2.44	0.52
1:D:916:LYS:HB2	1:D:919:ASP:HB3	1.91	0.52
1:A:770:ASP:O	1:A:773:GLY:CA	2.57	0.52
1:C:740:ILE:HD11	1:C:741:PRO:HD2	1.74	0.52
1:C:836:LEU:HD12	1:C:837:VAL:C	2.29	0.52
1:D:799:GLY:HA2	2:D:1101:YUN:H9	1.92	0.52
1:A:759:ILE:HD11	1:A:791:LEU:HG	1.92	0.52
1:A:770:ASP:O	1:A:771:ASN:C	2.46	0.52
1:C:740:ILE:HG23	1:C:740:ILE:O	2.09	0.52
1:A:820:TRP:O	1:A:823:GLN:N	2.43	0.51
1:E:947:TYR:HD1	1:E:950:MET:HE3	1.75	0.51
1:B:838:HIS:O	1:B:862:ALA:HB2	2.11	0.51
1:D:771:ASN:OD1	1:D:772:PRO:HD3	2.01	0.51
1:E:777:VAL:HG11	1:E:831:LEU:HD11	1.92	0.51
1:B:801:LEU:HA	1:B:804:TYR:HB3	1.93	0.51
1:B:926:ILE:HA	1:B:929:ILE:HG22	1.93	0.51
1:C:755:ALA:CB	1:C:759:ILE:HD11	2.15	0.51
1:A:944:ILE:O	1:A:948:MET:HG2	2.11	0.51
1:C:771:ASN:N	1:C:772:PRO:CD	2.73	0.51
1:C:777:VAL:HG12	1:C:856:ILE:CG2	2.40	0.51
1:E:859:PHE:O	1:E:862:ALA:HB2	2.09	0.51
1:A:837:VAL:HG22	1:A:837:VAL:O	2.10	0.51
1:C:944:ILE:HB	1:D:702:ALA:O	2.10	0.51
1:E:703:LEU:HD11	1:E:705:ARG:NH1	2.26	0.51
1:E:737:LYS:HE3	1:E:739:LYS:NZ	2.26	0.51
1:A:858:ASP:O	1:A:858:ASP:OD1	2.29	0.51
1:C:786:THR:OG1	1:C:787:SER:N	2.43	0.51
1:E:753:PRO:HG2	1:E:754:LYS:N	2.26	0.51
1:B:748:ARG:HE	1:B:751:THR:CG2	2.22	0.50
1:A:742:VAL:HG12	1:A:793:THR:O	2.10	0.50
1:B:741:PRO:HB2	1:B:795:LEU:HD23	1.94	0.50
1:C:750:ALA:HB3	1:C:753:PRO:HG3	1.92	0.50
1:E:775:PRO:HG2	1:E:776:HIS:HD2	1.76	0.50
1:A:712:PHE:CB	1:A:731:TRP:HD1	2.09	0.50
1:B:983:VAL:C	1:B:984:ILE:CG1	2.80	0.50
1:C:742:VAL:HG12	1:C:743:ALA:H	1.74	0.50
1:D:774:ASN:OD1	1:D:777:VAL:N	2.43	0.50
1:C:770:ASP:O	1:C:773:GLY:CA	2.60	0.50
1:C:843:ALA:CB	1:C:909:GLU:CD	2.80	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:840:ASP:O	1:C:840:ASP:OD1	2.30	0.50
1:D:936:LEU:HB2	1:D:954:TRP:CH2	2.47	0.50
1:E:731:TRP:HB3	1:E:740:ILE:HG22	1.92	0.50
1:A:711:GLU:HG2	1:A:734:GLU:N	2.17	0.50
1:E:748:ARG:O	1:E:749:GLU:C	2.49	0.50
1:B:770:ASP:OD1	1:B:770:ASP:O	2.30	0.50
1:B:840:ASP:OD2	1:B:840:ASP:O	2.30	0.50
1:B:985:GLN:O	1:B:987:ASP:OD1	2.30	0.50
1:C:762:GLU:HB2	1:C:860:GLY:HA2	1.93	0.50
1:A:752:SER:O	1:A:755:ALA:HB3	2.12	0.50
1:E:753:PRO:CG	1:E:754:LYS:N	2.75	0.50
1:E:873:HIS:N	1:E:873:HIS:ND1	2.58	0.50
1:A:838:HIS:O	1:A:839:ARG:HB3	2.11	0.50
1:A:868:GLU:O	1:A:869:GLU:C	2.50	0.50
1:D:863:LYS:CG	1:D:872:TYR:CE1	2.95	0.50
1:E:753:PRO:HG2	1:E:754:LYS:H	1.77	0.50
1:A:866:GLY:CA	1:A:869:GLU:OE2	2.59	0.49
1:A:811:ASN:CB	1:A:991:HIS:HB2	2.41	0.49
1:B:948:MET:CE	3:C:1203:HOH:O	2.60	0.49
1:D:776:HIS:O	1:D:855:LYS:HA	2.11	0.49
1:A:807:GLU:HG3	1:A:808:HIS:ND1	2.27	0.49
1:C:770:ASP:OD2	1:C:770:ASP:O	2.30	0.49
1:C:775:PRO:HB2	1:C:776:HIS:HD2	1.70	0.49
1:C:843:ALA:HB2	1:C:909:GLU:OE1	2.12	0.49
1:D:700:ASN:OD1	1:D:700:ASN:O	2.30	0.49
1:E:879:VAL:CG2	1:E:880:PRO:N	2.73	0.49
1:B:836:LEU:CD1	1:B:837:VAL:CA	2.88	0.49
1:B:828:MET:CE	1:B:841:LEU:HD22	2.41	0.49
1:C:740:ILE:CG2	1:C:740:ILE:O	2.60	0.49
1:D:711:GLU:CD	1:D:731:TRP:HE1	2.15	0.49
1:E:770:ASP:O	1:E:770:ASP:OD1	2.30	0.49
1:C:858:ASP:O	1:C:858:ASP:OD1	2.30	0.49
1:A:814:SER:HA	1:A:984:ILE:HD12	1.93	0.49
1:B:840:ASP:CG	1:B:840:ASP:O	2.49	0.49
1:D:840:ASP:O	1:D:840:ASP:OD2	2.30	0.49
1:E:737:LYS:CD	1:E:737:LYS:O	2.60	0.49
1:C:729:GLY:O	1:C:742:VAL:O	2.31	0.49
1:C:772:PRO:HD3	1:C:834:ARG:NH1	2.26	0.49
1:A:840:ASP:OD1	1:A:840:ASP:O	2.30	0.49
1:C:747:LEU:HD22	1:C:749:GLU:N	2.26	0.49
1:C:751:THR:HG22	1:C:788:THR:HG23	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:725:THR:HB	1:D:727:TYR:HE1	1.77	0.49
1:D:831:LEU:HG	1:D:836:LEU:HD13	1.94	0.49
1:E:799:GLY:HA2	2:E:1101:YUN:H9	1.95	0.49
1:E:772:PRO:HD2	1:E:773:GLY:H	1.77	0.49
1:A:772:PRO:HG2	1:A:773:GLY:H	1.76	0.49
1:A:711:GLU:HG2	1:A:732:ILE:O	2.13	0.48
1:A:730:LEU:HD23	1:A:740:ILE:O	2.13	0.48
1:B:751:THR:OG1	1:B:752:SER:N	2.46	0.48
1:C:707:LEU:HD12	1:C:792:ILE:HG21	1.93	0.48
1:C:822:VAL:O	1:C:826:LYS:HB2	2.13	0.48
1:D:746:GLU:HG2	1:D:790:GLN:HG2	1.95	0.48
1:A:786:THR:O	1:A:788:THR:O	2.30	0.48
1:E:880:PRO:O	1:E:880:PRO:CG	2.60	0.48
1:A:747:LEU:CD1	1:A:748:ARG:HG3	2.43	0.48
1:B:796:MET:HE3	1:B:849:LYS:HB2	1.95	0.48
1:A:935:ARG:NH1	1:A:954:TRP:O	2.34	0.48
1:A:835:ARG:HH21	1:A:867:ALA:HB1	1.74	0.48
1:B:849:LYS:HG3	1:B:850:THR:HG23	1.96	0.48
1:E:708:LYS:HB2	1:E:711:GLU:OE1	2.14	0.48
1:D:836:LEU:HD22	1:D:836:LEU:C	2.30	0.48
1:E:838:HIS:CE1	1:E:840:ASP:CB	2.88	0.48
1:C:726:VAL:HA	1:C:744:ILE:O	2.14	0.48
1:C:764:TYR:O	1:C:768:SER:OG	2.30	0.48
1:D:703:LEU:O	1:D:703:LEU:HD12	2.09	0.48
1:D:718:LEU:HD21	1:D:728:LYS:HB2	1.94	0.48
1:E:879:VAL:CG2	1:E:880:PRO:CD	2.83	0.48
1:A:749:GLU:CA	1:A:788:THR:HG23	2.40	0.48
1:C:838:HIS:O	1:C:862:ALA:CB	2.61	0.48
1:D:769:VAL:O	1:D:771:ASN:HB2	2.13	0.48
1:A:864:LEU:HD13	1:A:865:LEU:N	2.13	0.48
1:E:753:PRO:CG	1:E:754:LYS:H	2.27	0.48
1:A:872:TYR:HE2	1:A:874:ALA:CA	2.26	0.47
1:A:945:ASP:N	1:A:945:ASP:OD1	2.46	0.47
1:B:750:ALA:CB	1:B:756:ASN:OD1	2.52	0.47
1:C:765:VAL:HG22	1:C:766:MET:N	2.28	0.47
1:A:712:PHE:CZ	1:A:790:GLN:OE1	2.66	0.47
1:A:828:MET:SD	1:A:841:LEU:CD2	3.02	0.47
1:B:759:ILE:HG22	1:B:760:LEU:N	2.29	0.47
1:C:832:GLU:HA	1:C:896:HIS:CE1	2.49	0.47
1:A:882:LYS:HD3	1:A:918:TYR:HD2	1.78	0.47
1:C:838:HIS:HA	1:C:862:ALA:HB1	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:805:VAL:HG21	1:C:910:LEU:HD23	1.96	0.47
1:D:777:VAL:HG11	1:D:831:LEU:HD11	1.96	0.47
1:E:703:LEU:HD23	1:E:704:LEU:CA	2.42	0.47
1:A:753:PRO:O	1:A:756:ASN:N	2.47	0.47
1:C:741:PRO:C	1:C:742:VAL:HG23	2.35	0.47
1:A:955:MET:HG2	1:A:960:SER:HB2	1.96	0.47
1:C:736:GLU:OE1	1:C:738:VAL:HG21	2.14	0.47
1:D:836:LEU:CD2	1:D:837:VAL:C	2.83	0.47
1:A:840:ASP:CG	1:A:840:ASP:O	2.51	0.47
1:A:864:LEU:CD1	1:A:864:LEU:C	2.75	0.47
1:A:858:ASP:C	1:A:858:ASP:OD1	2.52	0.47
1:A:818:LEU:HD13	1:A:974:MET:HB2	1.97	0.47
1:D:836:LEU:O	1:D:836:LEU:HD22	2.15	0.47
1:A:835:ARG:HH21	1:A:867:ALA:HA	1.79	0.47
1:B:745:LYS:HB2	2:B:1101:YUN:BR	2.69	0.47
1:C:742:VAL:CG1	1:C:743:ALA:H	2.27	0.47
1:C:772:PRO:HD3	1:C:834:ARG:HH12	1.80	0.47
1:D:834:ARG:C	1:D:835:ARG:HG2	2.36	0.47
1:D:756:ASN:OD1	1:D:756:ASN:N	2.41	0.47
1:E:912:THR:HG23	1:E:915:SER:H	1.80	0.47
1:B:771:ASN:HD22	1:B:772:PRO:N	2.13	0.46
1:D:837:VAL:HG23	1:D:865:LEU:HD11	1.96	0.46
1:D:947:TYR:HA	1:D:950:MET:HE3	1.98	0.46
1:A:742:VAL:HG12	1:A:743:ALA:H	1.80	0.46
1:C:747:LEU:HD11	1:C:755:ALA:HB2	1.92	0.46
1:A:745:LYS:HD3	2:A:1101:YUN:CAH	2.45	0.46
1:A:725:THR:OG1	1:A:746:GLU:O	2.32	0.46
1:A:811:ASN:CG	1:A:991:HIS:HB2	2.35	0.46
1:B:712:PHE:HB3	1:B:731:TRP:CD1	2.50	0.46
1:C:731:TRP:HE3	1:C:740:ILE:HG21	1.80	0.46
1:A:835:ARG:NH2	1:A:867:ALA:CA	2.76	0.46
1:A:994:SER:N	1:A:995:PRO:HD2	2.31	0.46
1:C:840:ASP:OD1	1:C:845:ASN:OD1	2.33	0.46
1:E:879:VAL:HG23	1:E:880:PRO:N	2.25	0.46
1:E:700:ASN:OD1	1:E:701:GLN:N	2.49	0.46
1:E:732:ILE:HG12	1:E:732:ILE:O	2.16	0.46
1:E:798:PHE:HB2	1:E:848:VAL:HB	1.98	0.46
1:B:764:TYR:HE1	1:B:768:SER:HG	1.62	0.46
1:C:778:CYS:HB2	1:C:857:THR:OG1	2.16	0.46
1:E:734:GLU:CG	1:E:735:GLY:N	2.79	0.46
1:A:746:GLU:HG3	1:A:747:LEU:N	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:835:ARG:HH21	1:A:867:ALA:CA	2.29	0.45
1:E:754:LYS:O	1:E:755:ALA:C	2.53	0.45
1:A:872:TYR:HD2	1:A:872:TYR:O	1.94	0.45
1:B:707:LEU:HD12	1:B:792:ILE:HG13	1.97	0.45
1:C:747:LEU:CD2	1:C:749:GLU:CB	2.94	0.45
1:C:762:GLU:HA	1:C:765:VAL:HG13	1.97	0.45
1:A:799:GLY:HA2	2:A:1101:YUN:CAJ	2.47	0.45
1:E:734:GLU:CG	1:E:736:GLU:H	2.27	0.45
1:A:745:LYS:NZ	1:A:762:GLU:CD	2.69	0.45
1:B:799:GLY:HA2	2:B:1101:YUN:CAJ	2.47	0.45
1:C:740:ILE:CD1	1:C:740:ILE:C	2.85	0.45
1:C:878:LYS:HA	1:C:878:LYS:HD3	1.72	0.45
1:D:836:LEU:O	1:D:836:LEU:CD2	2.62	0.45
1:D:892:ARG:HA	1:D:892:ARG:HD3	1.82	0.45
1:E:823:GLN:HB2	1:E:823:GLN:HE21	1.49	0.45
1:A:799:GLY:HA2	2:A:1101:YUN:H9	1.98	0.45
1:A:844:ARG:HH22	1:A:880:PRO:HB3	1.81	0.45
1:D:798:PHE:HB2	1:D:848:VAL:HB	1.98	0.45
1:E:770:ASP:O	1:E:773:GLY:HA2	2.15	0.45
1:E:874:ALA:C	1:E:875:GLU:OE1	2.55	0.45
1:E:880:PRO:HG2	1:E:880:PRO:O	2.16	0.45
1:B:803:ASP:O	1:B:807:GLU:HG2	2.17	0.45
1:C:769:VAL:HG23	1:C:770:ASP:N	2.32	0.45
1:C:772:PRO:HG2	1:C:834:ARG:NH1	2.27	0.45
1:A:872:TYR:CE2	1:A:873:HIS:C	2.91	0.45
1:B:754:LYS:HA	1:B:757:LYS:HB3	1.99	0.45
1:C:727:TYR:N	1:C:744:ILE:O	2.44	0.45
1:C:774:ASN:CG	1:C:775:PRO:HD2	2.37	0.45
1:C:776:HIS:HA	1:C:855:LYS:HG2	1.99	0.45
1:A:835:ARG:NH2	1:A:867:ALA:HA	2.32	0.45
1:E:731:TRP:N	1:E:740:ILE:O	2.41	0.45
1:B:823:GLN:HE21	1:B:823:GLN:HB2	1.50	0.45
1:E:860:GLY:C	1:E:861:LEU:HD23	2.35	0.45
1:A:750:ALA:CB	1:A:756:ASN:HD21	2.30	0.44
1:B:838:HIS:C	1:B:838:HIS:HD1	2.21	0.44
1:E:775:PRO:HG2	1:E:776:HIS:H	1.81	0.44
1:A:742:VAL:HG13	1:A:794:GLN:HA	1.99	0.44
1:A:999:ASN:ND2	1:A:999:ASN:C	2.70	0.44
1:D:701:GLN:O	1:D:702:ALA:C	2.55	0.44
1:D:769:VAL:O	1:D:770:ASP:C	2.53	0.44
1:B:802:LEU:HD23	1:B:844:ARG:HG3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:834:ARG:C	1:C:835:ARG:CG	2.84	0.44
1:D:839:ARG:HG3	1:D:894:TYR:CD2	2.30	0.44
1:E:774:ASN:HB3	1:E:777:VAL:HG23	1.99	0.44
1:E:774:ASN:OD1	1:E:774:ASN:C	2.56	0.44
1:E:804:TYR:O	1:E:808:HIS:HB2	2.18	0.44
1:E:857:THR:HG22	1:E:858:ASP:HB2	1.99	0.44
1:B:957:ASP:OD2	1:C:751:THR:HB	2.17	0.44
1:B:799:GLY:HA2	2:B:1101:YUN:H9	2.00	0.44
1:C:750:ALA:O	1:C:753:PRO:HD2	2.16	0.44
1:C:814:SER:OG	1:C:984:ILE:HG21	2.18	0.44
1:D:714:LYS:NZ	1:D:746:GLU:OE1	2.51	0.44
1:D:776:HIS:CE1	1:D:823:GLN:HB3	2.52	0.44
1:E:774:ASN:HB2	1:E:830:TYR:CD2	2.52	0.44
1:C:838:HIS:CE1	1:C:840:ASP:N	2.85	0.44
1:C:858:ASP:C	1:C:858:ASP:OD1	2.55	0.44
1:C:952:LYS:HD3	1:D:757:LYS:HE2	2.00	0.44
1:E:771:ASN:HD22	1:E:772:PRO:CG	2.26	0.44
1:E:963:LYS:HD3	1:E:965:ARG:NH1	2.33	0.44
1:A:872:TYR:HD2	1:A:873:HIS:CA	2.30	0.44
1:C:823:GLN:HB2	1:C:823:GLN:HE21	1.52	0.44
1:C:838:HIS:HE1	1:C:840:ASP:CA	2.26	0.43
1:A:811:ASN:OD1	1:A:991:HIS:HB2	2.18	0.43
1:B:734:GLU:HG2	1:B:735:GLY:H	1.83	0.43
1:C:883:TRP:NE1	1:C:909:GLU:OE1	2.44	0.43
1:A:974:MET:HB3	1:A:981:TYR:CD2	2.53	0.43
1:B:831:LEU:HD21	1:B:859:PHE:HE1	1.83	0.43
1:C:755:ALA:O	1:C:759:ILE:CG1	2.65	0.43
1:C:926:ILE:HA	1:C:929:ILE:HG22	2.00	0.43
1:E:753:PRO:CD	1:E:754:LYS:H	2.31	0.43
1:E:756:ASN:HA	1:E:759:ILE:HG22	2.01	0.43
1:C:842:ALA:CB	1:C:844:ARG:CZ	2.96	0.43
1:C:814:SER:OG	1:C:984:ILE:CB	2.67	0.43
1:D:929:ILE:HG13	1:D:930:LEU:N	2.32	0.43
1:A:772:PRO:HG2	1:A:773:GLY:N	2.33	0.43
1:B:834:ARG:O	1:B:835:ARG:CB	2.64	0.43
1:B:776:HIS:HE1	1:B:823:GLN:CG	2.30	0.43
1:D:714:LYS:H	1:D:714:LYS:HG2	1.58	0.43
1:E:874:ALA:CA	1:E:875:GLU:OE1	2.66	0.43
1:A:740:ILE:CD1	1:A:740:ILE:C	2.63	0.43
1:A:938:GLN:HB2	1:A:947:TYR:CE2	2.52	0.43
1:A:814:SER:CA	1:A:984:ILE:CD1	2.97	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:785:LEU:HD23	1:D:785:LEU:HA	1.87	0.43
1:B:828:MET:CE	1:B:841:LEU:CD2	2.96	0.42
1:B:979:GLN:HB2	1:C:694:PRO:HG3	2.00	0.42
1:D:839:ARG:HD2	1:D:894:TYR:HE2	1.84	0.42
1:E:775:PRO:CG	1:E:776:HIS:N	2.82	0.42
1:A:786:THR:C	1:A:788:THR:O	2.58	0.42
1:A:796:MET:SD	1:A:855:LYS:HD2	2.58	0.42
1:E:769:VAL:HG23	1:E:770:ASP:N	2.34	0.42
1:E:775:PRO:CG	1:E:776:HIS:H	2.32	0.42
1:E:828:MET:SD	1:E:841:LEU:HD23	2.58	0.42
1:E:903:TYR:CE2	1:E:967:LEU:HD13	2.54	0.42
1:A:707:LEU:HD13	1:A:731:TRP:CZ2	2.53	0.42
1:A:744:ILE:HD12	1:A:792:ILE:HG13	2.00	0.42
1:A:811:ASN:C	1:A:990:MET:SD	2.98	0.42
1:A:852:GLN:H	1:A:852:GLN:HG2	1.60	0.42
1:A:992:LEU:HA	1:A:993:PRO:HD3	1.86	0.42
1:B:938:GLN:HA	1:B:947:TYR:CE1	2.55	0.42
1:C:772:PRO:HG2	1:C:834:ARG:NE	2.35	0.42
1:A:707:LEU:HD13	1:A:731:TRP:CH2	2.54	0.42
1:E:941:ILE:HA	1:E:983:VAL:HG12	2.01	0.42
1:B:964:PHE:O	1:B:968:ILE:HG13	2.19	0.42
1:D:712:PHE:HB3	1:D:731:TRP:CD1	2.54	0.42
1:E:841:LEU:HD12	1:E:842:ALA:N	2.34	0.42
1:C:774:ASN:OD1	1:C:774:ASN:C	2.57	0.42
1:D:708:LYS:O	1:D:711:GLU:HG2	2.19	0.42
1:D:781:LEU:HD13	1:D:792:ILE:HD11	2.02	0.42
1:D:922:PRO:HG2	1:D:925:GLU:HB2	2.00	0.42
1:A:730:LEU:HD23	1:A:740:ILE:C	2.40	0.42
1:D:707:LEU:HD12	1:D:792:ILE:HG21	2.00	0.42
1:E:969:ILE:HG12	1:E:969:ILE:H	1.48	0.42
1:A:836:LEU:HD12	1:A:837:VAL:C	2.36	0.42
1:A:891:HIS:HB2	1:A:893:ILE:HG12	2.01	0.42
1:E:939:PRO:HA	1:E:940:PRO:HD2	1.81	0.42
1:E:941:ILE:HG13	1:E:982:LEU:HD22	2.02	0.42
1:A:747:LEU:HD11	1:A:748:ARG:HD2	2.01	0.42
1:A:865:LEU:HD22	1:A:865:LEU:HA	1.87	0.42
1:B:770:ASP:O	1:B:773:GLY:HA2	2.18	0.42
1:C:739:LYS:CD	1:C:739:LYS:N	2.78	0.42
1:B:798:PHE:CE1	1:B:851:PRO:HD3	2.54	0.42
1:C:834:ARG:O	1:C:835:ARG:CB	2.66	0.42
1:A:772:PRO:CG	1:A:773:GLY:H	2.33	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:816:TYR:HE2	1:A:992:LEU:HB3	1.84	0.41
1:B:718:LEU:HD11	1:B:728:LYS:HB2	2.01	0.41
1:C:751:THR:C	1:C:753:PRO:CD	2.88	0.41
1:A:994:SER:N	1:A:995:PRO:CD	2.83	0.41
1:B:980:ARG:C	1:B:981:TYR:HD1	2.22	0.41
1:C:753:PRO:CD	1:C:754:LYS:H	2.34	0.41
1:D:880:PRO:O	1:D:884:MET:HG3	2.20	0.41
1:E:844:ARG:H	1:E:844:ARG:HG3	1.62	0.41
1:A:806:ARG:O	1:A:809:LYS:NZ	2.52	0.41
1:C:732:ILE:HD12	1:C:733:PRO:O	2.11	0.41
1:C:774:ASN:CG	1:C:775:PRO:N	2.73	0.41
1:C:947:TYR:O	1:C:951:VAL:HG23	2.20	0.41
1:D:700:ASN:ND2	1:D:768:SER:OG	2.54	0.41
1:A:711:GLU:O	1:A:732:ILE:N	2.37	0.41
1:A:829:ASN:OD1	1:A:830:TYR:N	2.53	0.41
1:C:766:MET:CE	1:C:859:PHE:HD2	2.34	0.41
1:C:838:HIS:O	1:C:862:ALA:CA	2.69	0.41
1:D:891:HIS:HB2	1:D:893:ILE:HG12	2.02	0.41
1:A:745:LYS:HZ1	1:A:762:GLU:CD	2.24	0.41
1:A:809:LYS:HB3	1:A:809:LYS:HZ2	1.84	0.41
1:E:887:GLU:H	1:E:887:GLU:HG3	1.39	0.41
1:A:798:PHE:HB2	1:A:848:VAL:HB	2.02	0.41
1:E:772:PRO:HB2	1:E:830:TYR:OH	2.20	0.41
1:E:775:PRO:HG2	1:E:776:HIS:CD2	2.54	0.41
1:E:935:ARG:NH1	1:E:954:TRP:O	2.54	0.41
1:B:776:HIS:CE1	1:B:823:GLN:CD	2.94	0.41
1:C:742:VAL:CG1	1:C:792:ILE:HG13	2.48	0.41
1:E:776:HIS:O	1:E:855:LYS:CB	2.69	0.41
1:E:859:PHE:O	1:E:860:GLY:C	2.58	0.41
1:E:942:CYS:SG	1:E:946:VAL:HB	2.61	0.41
1:B:759:ILE:HG23	1:B:760:LEU:N	2.36	0.41
1:B:798:PHE:HB2	1:B:848:VAL:HG13	2.03	0.41
1:D:727:TYR:N	1:D:744:ILE:O	2.37	0.41
1:D:774:ASN:CG	1:D:777:VAL:HG23	2.42	0.41
1:E:963:LYS:HD3	1:E:965:ARG:HH12	1.86	0.41
1:A:872:TYR:CD2	1:A:872:TYR:O	2.69	0.41
1:B:921:ILE:HA	1:B:922:PRO:HD2	1.95	0.40
1:A:769:VAL:O	1:A:770:ASP:C	2.59	0.40
1:B:885:ALA:O	1:B:889:ILE:HG13	2.22	0.40
1:E:772:PRO:CD	1:E:773:GLY:H	2.34	0.40
1:A:801:LEU:O	1:A:805:VAL:HG23	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:809:LYS:HB3	1:A:809:LYS:NZ	2.37	0.40
1:B:708:LYS:HB3	1:B:710:THR:HG22	2.03	0.40
1:B:834:ARG:C	1:B:835:ARG:HG2	2.41	0.40
1:A:803:ASP:O	1:A:807:GLU:HG2	2.21	0.40
1:D:955:MET:HE3	1:D:955:MET:HB3	1.96	0.40
1:A:872:TYR:CZ	1:A:874:ALA:CB	2.75	0.40
1:B:885:ALA:HA	1:B:901:TRP:CD2	2.57	0.40
2:C:1101:YUN:OAC	2:C:1101:YUN:H6	2.22	0.40
1:C:747:LEU:CD2	1:C:748:ARG:CA	2.98	0.40
1:C:842:ALA:HB2	1:C:844:ARG:NH2	2.36	0.40
1:C:964:PHE:O	1:C:968:ILE:HG13	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	305/334 (91%)	288 (94%)	16 (5%)	1 (0%)	41	75
1	B	291/334 (87%)	272 (94%)	17 (6%)	2 (1%)	22	62
1	C	291/334 (87%)	278 (96%)	13 (4%)	0	100	100
1	D	287/334 (86%)	273 (95%)	12 (4%)	2 (1%)	22	62
1	E	288/334 (86%)	277 (96%)	11 (4%)	0	100	100
All	All	1462/1670 (88%)	1388 (95%)	69 (5%)	5 (0%)	41	75

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	771	ASN
1	B	771	ASN
1	D	771	ASN

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Mol	Chain	Res	Type
1	B	733	PRO
1	D	851	PRO

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	255/292 (87%)	196 (77%)	59 (23%)	1	5
1	B	251/292 (86%)	205 (82%)	46 (18%)	1	9
1	C	246/292 (84%)	198 (80%)	48 (20%)	1	8
1	D	246/292 (84%)	214 (87%)	32 (13%)	4	22
1	E	247/292 (85%)	206 (83%)	41 (17%)	2	13
All	All	1245/1460 (85%)	1019 (82%)	226 (18%)	1	9

All (226) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	705	ARG
1	A	717	VAL
1	A	723	PHE
1	A	730	LEU
1	A	736	GLU
1	A	739	LYS
1	A	740	ILE
1	A	747	LEU
1	A	748	ARG
1	A	751	THR
1	A	752	SER
1	A	768	SER
1	A	770	ASP
1	A	774	ASN
1	A	777	VAL
1	A	778	CYS
1	A	781	LEU

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Mol	Chain	Res	Type
1	A	784	CYS
1	A	786	THR
1	A	787	SER
1	A	788	THR
1	A	801	LEU
1	A	809	LYS
1	A	815	GLN
1	A	819	ASN
1	A	823	GLN
1	A	829	ASN
1	A	833	ASP
1	A	834	ARG
1	A	835	ARG
1	A	836	LEU
1	A	837	VAL
1	A	841	LEU
1	A	844	ARG
1	A	852	GLN
1	A	854	VAL
1	A	856	ILE
1	A	861	LEU
1	A	864	LEU
1	A	865	LEU
1	A	870	LYS
1	A	872	TYR
1	A	873	HIS
1	A	875	GLU
1	A	887	GLU
1	A	891	HIS
1	A	929	ILE
1	A	938	GLN
1	A	944	ILE
1	A	945	ASP
1	A	961	ARG
1	A	965	ARG
1	A	974	MET
1	A	988	GLU
1	A	990	MET
1	A	991	HIS
1	A	994	SER
1	A	997	ASP
1	A	1002	ARG

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Mol	Chain	Res	Type
1	B	704	LEU
1	B	714	LYS
1	B	718	LEU
1	B	726	VAL
1	B	732	ILE
1	B	737	LYS
1	B	738	VAL
1	B	740	ILE
1	B	746	GLU
1	B	747	LEU
1	B	748	ARG
1	B	751	THR
1	B	756	ASN
1	B	759	ILE
1	B	764	TYR
1	B	765	VAL
1	B	766	MET
1	B	769	VAL
1	B	771	ASN
1	B	774	ASN
1	B	781	LEU
1	B	783	ILE
1	B	786	THR
1	B	789	VAL
1	B	794	GLN
1	B	801	LEU
1	B	810	ASP
1	B	823	GLN
1	B	833	ASP
1	B	835	ARG
1	B	836	LEU
1	B	839	ARG
1	B	841	LEU
1	B	844	ARG
1	B	848	VAL
1	B	852	GLN
1	B	857	THR
1	B	868	GLU
1	B	875	GLU
1	B	895	THR
1	B	956	ILE
1	B	980	ARG

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Mol	Chain	Res	Type
1	B	982	LEU
1	B	983	VAL
1	B	985	GLN
1	B	987	ASP
1	C	701	GLN
1	C	704	LEU
1	C	708	LYS
1	C	718	LEU
1	C	723	PHE
1	C	726	VAL
1	C	732	ILE
1	C	736	GLU
1	C	739	LYS
1	C	740	ILE
1	C	744	ILE
1	C	747	LEU
1	C	751	THR
1	C	761	ASP
1	C	765	VAL
1	C	768	SER
1	C	770	ASP
1	C	784	CYS
1	C	786	THR
1	C	788	THR
1	C	789	VAL
1	C	800	CYS
1	C	804	TYR
1	C	808	HIS
1	C	811	ASN
1	C	812	ILE
1	C	814	SER
1	C	819	ASN
1	C	823	GLN
1	C	833	ASP
1	C	834	ARG
1	C	835	ARG
1	C	836	LEU
1	C	841	LEU
1	C	844	ARG
1	C	852	GLN
1	C	854	VAL
1	C	864	LEU

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Mol	Chain	Res	Type
1	C	865	LEU
1	C	871	GLU
1	C	873	HIS
1	C	875	GLU
1	C	893	ILE
1	C	941	ILE
1	C	959	ASP
1	C	965	ARG
1	C	982	LEU
1	C	984	ILE
1	D	700	ASN
1	D	703	LEU
1	D	718	LEU
1	D	732	ILE
1	D	739	LYS
1	D	756	ASN
1	D	765	VAL
1	D	771	ASN
1	D	774	ASN
1	D	777	VAL
1	D	781	LEU
1	D	786	THR
1	D	789	VAL
1	D	792	ILE
1	D	796	MET
1	D	800	CYS
1	D	817	LEU
1	D	826	LYS
1	D	836	LEU
1	D	840	ASP
1	D	841	LEU
1	D	857	THR
1	D	859	PHE
1	D	865	LEU
1	D	878	LYS
1	D	887	GLU
1	D	894	TYR
1	D	929	ILE
1	D	934	GLU
1	D	941	ILE
1	D	965	ARG
1	D	969	ILE

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Mol	Chain	Res	Type
1	E	703	LEU
1	E	710	THR
1	E	712	PHE
1	E	718	LEU
1	E	725	THR
1	E	726	VAL
1	E	732	ILE
1	E	734	GLU
1	E	737	LYS
1	E	739	LYS
1	E	752	SER
1	E	758	GLU
1	E	770	ASP
1	E	771	ASN
1	E	777	VAL
1	E	778	CYS
1	E	781	LEU
1	E	789	VAL
1	E	800	CYS
1	E	810	ASP
1	E	823	GLN
1	E	834	ARG
1	E	835	ARG
1	E	838	HIS
1	E	841	LEU
1	E	844	ARG
1	E	856	ILE
1	E	861	LEU
1	E	865	LEU
1	E	871	GLU
1	E	873	HIS
1	E	875	GLU
1	E	879	VAL
1	E	881	ILE
1	E	887	GLU
1	E	929	ILE
1	E	935	ARG
1	E	941	ILE
1	E	948	MET
1	E	969	ILE
1	E	983	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such

sidechains are listed below:

Mol	Chain	Res	Type
1	A	774	ASN
1	A	776	HIS
1	A	873	HIS
1	A	938	GLN
1	B	756	ASN
1	B	771	ASN
1	B	776	HIS
1	B	815	GLN
1	C	776	HIS
1	C	811	ASN
1	C	823	GLN
1	C	896	HIS
1	D	819	ASN
1	D	823	GLN
1	D	852	GLN
1	E	756	ASN
1	E	771	ASN
1	E	776	HIS
1	E	823	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

5 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	YUN	E	1101	1	25,25,25	2.32	8 (32%)	34,34,34	2.22	11 (32%)
2	YUN	D	1101	1	25,25,25	2.31	8 (32%)	34,34,34	2.24	10 (29%)
2	YUN	C	1101	1	25,25,25	2.30	8 (32%)	34,34,34	2.27	8 (23%)
2	YUN	B	1101	1	25,25,25	2.26	7 (28%)	34,34,34	2.37	10 (29%)
2	YUN	A	1101	1	25,25,25	2.28	8 (32%)	34,34,34	2.31	11 (32%)

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	YUN	E	1101	1	-	2/10/10/10	0/3/3/3
2	YUN	D	1101	1	-	0/10/10/10	0/3/3/3
2	YUN	C	1101	1	-	2/10/10/10	0/3/3/3
2	YUN	B	1101	1	-	2/10/10/10	0/3/3/3
2	YUN	A	1101	1	-	2/10/10/10	0/3/3/3

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1101	YUN	C6-NAT	7.07	1.46	1.36
2	E	1101	YUN	C6-NAT	7.03	1.46	1.36
2	D	1101	YUN	C6-NAT	7.00	1.46	1.36
2	A	1101	YUN	C6-NAT	6.93	1.46	1.36
2	B	1101	YUN	C6-NAT	6.92	1.46	1.36
2	C	1101	YUN	CAW-NAS	5.29	1.47	1.35
2	E	1101	YUN	CAW-NAS	5.28	1.47	1.35
2	D	1101	YUN	CAW-NAS	5.27	1.47	1.35
2	A	1101	YUN	CAW-NAS	5.21	1.47	1.35
2	B	1101	YUN	CAW-NAS	5.19	1.47	1.35
2	D	1101	YUN	CAZ-NAS	3.19	1.48	1.41
2	A	1101	YUN	CAZ-NAS	3.11	1.47	1.41
2	C	1101	YUN	CAZ-NAS	3.10	1.47	1.41
2	A	1101	YUN	C2-N1	3.09	1.39	1.33
2	E	1101	YUN	CAZ-NAS	3.06	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1101	YUN	C2-N1	3.03	1.39	1.33
2	D	1101	YUN	C2-N1	2.98	1.39	1.33
2	B	1101	YUN	C2-N1	2.90	1.39	1.33
2	B	1101	YUN	CAZ-NAS	2.82	1.47	1.41
2	E	1101	YUN	C2-N1	2.78	1.39	1.33
2	C	1101	YUN	CAJ-CAZ	2.56	1.43	1.39
2	E	1101	YUN	CAY-NAT	2.53	1.46	1.40
2	D	1101	YUN	CAJ-CAZ	2.41	1.43	1.39
2	B	1101	YUN	CAY-NAT	2.38	1.46	1.40
2	D	1101	YUN	CAY-NAT	2.33	1.45	1.40
2	C	1101	YUN	CAY-NAT	2.33	1.45	1.40
2	E	1101	YUN	CAM-CAZ	2.33	1.42	1.37
2	A	1101	YUN	CAJ-CAZ	2.32	1.43	1.39
2	A	1101	YUN	CAY-NAT	2.29	1.45	1.40
2	D	1101	YUN	CAM-CAZ	2.19	1.42	1.37
2	E	1101	YUN	CAJ-CAZ	2.16	1.42	1.39
2	B	1101	YUN	CAJ-CAZ	2.16	1.42	1.39
2	B	1101	YUN	CAM-CAZ	2.13	1.42	1.37
2	D	1101	YUN	C5-C4	-2.12	1.39	1.42
2	C	1101	YUN	CAM-CAZ	2.10	1.42	1.37
2	A	1101	YUN	CAM-CAZ	2.06	1.42	1.37
2	A	1101	YUN	C5-C4	-2.05	1.39	1.42
2	C	1101	YUN	C5-C4	-2.02	1.39	1.42
2	E	1101	YUN	CAK-C4	2.02	1.45	1.41

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	1101	YUN	C2-N1-C6	6.27	121.96	116.59
2	B	1101	YUN	C2-N1-C6	5.92	121.66	116.59
2	E	1101	YUN	N3-C2-N1	-5.73	119.72	128.68
2	D	1101	YUN	C2-N1-C6	5.70	121.48	116.59
2	A	1101	YUN	C2-N1-C6	5.56	121.36	116.59
2	C	1101	YUN	C2-N1-C6	5.53	121.33	116.59
2	B	1101	YUN	N3-C2-N1	-5.49	120.10	128.68
2	D	1101	YUN	N3-C2-N1	-5.44	120.18	128.68
2	C	1101	YUN	C6-C5-C4	5.24	119.18	115.88
2	A	1101	YUN	N3-C2-N1	-5.22	120.51	128.68
2	C	1101	YUN	N3-C2-N1	-5.14	120.64	128.68
2	A	1101	YUN	CAM-C5-C6	-5.06	120.31	124.88
2	A	1101	YUN	C6-C5-C4	5.05	119.06	115.88
2	C	1101	YUN	CAM-C5-C6	-4.92	120.44	124.88

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1101	YUN	C6-C5-C4	4.86	118.94	115.88
2	B	1101	YUN	C6-C5-C4	4.84	118.93	115.88
2	E	1101	YUN	C2-N3-C4	4.46	121.55	115.40
2	B	1101	YUN	C2-N3-C4	4.34	121.38	115.40
2	D	1101	YUN	C2-N3-C4	4.26	121.27	115.40
2	B	1101	YUN	CAM-C5-C6	-4.26	121.04	124.88
2	D	1101	YUN	CAM-C5-C6	-4.12	121.16	124.88
2	C	1101	YUN	C2-N3-C4	4.01	120.93	115.40
2	B	1101	YUN	CAZ-NAS-CAW	-3.95	120.58	127.50
2	A	1101	YUN	C2-N3-C4	3.88	120.75	115.40
2	C	1101	YUN	C5-C6-N1	-3.59	118.39	121.35
2	E	1101	YUN	C6-C5-C4	3.51	118.09	115.88
2	A	1101	YUN	C5-C6-N1	-3.35	118.59	121.35
2	B	1101	YUN	C5-C6-N1	-3.32	118.61	121.35
2	B	1101	YUN	C5-C4-N3	-3.30	119.32	122.83
2	D	1101	YUN	C5-C6-N1	-3.24	118.68	121.35
2	D	1101	YUN	C5-C4-N3	-3.17	119.45	122.83
2	C	1101	YUN	C5-C4-N3	-3.10	119.53	122.83
2	E	1101	YUN	CAM-C5-C6	-2.99	122.18	124.88
2	E	1101	YUN	C5-C6-N1	-2.97	118.90	121.35
2	A	1101	YUN	C5-C4-N3	-2.91	119.73	122.83
2	E	1101	YUN	C5-C4-N3	-2.87	119.77	122.83
2	C	1101	YUN	NAT-C6-N1	2.79	122.46	118.72
2	E	1101	YUN	CAZ-NAS-CAW	-2.73	122.71	127.50
2	E	1101	YUN	C5-C6-NAT	2.38	122.35	119.73
2	E	1101	YUN	CAY-NAT-C6	-2.33	122.19	128.26
2	B	1101	YUN	CAO-CAW-NAS	2.31	120.92	114.75
2	A	1101	YUN	CAO-CAW-NAS	2.25	120.76	114.75
2	A	1101	YUN	NAT-C6-N1	2.24	121.72	118.72
2	D	1101	YUN	CAY-NAT-C6	-2.18	122.58	128.26
2	B	1101	YUN	CAY-NAT-C6	-2.16	122.63	128.26
2	A	1101	YUN	CAZ-NAS-CAW	-2.15	123.72	127.50
2	E	1101	YUN	CAO-CAW-NAS	2.15	120.49	114.75
2	A	1101	YUN	CAY-NAT-C6	-2.14	122.69	128.26
2	D	1101	YUN	CAZ-NAS-CAW	-2.08	123.86	127.50
2	D	1101	YUN	CAO-CAW-NAS	2.01	120.12	114.75

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1101	YUN	C5-C6-NAT-CAY

*Continued on next page...*

*Continued from previous page...*

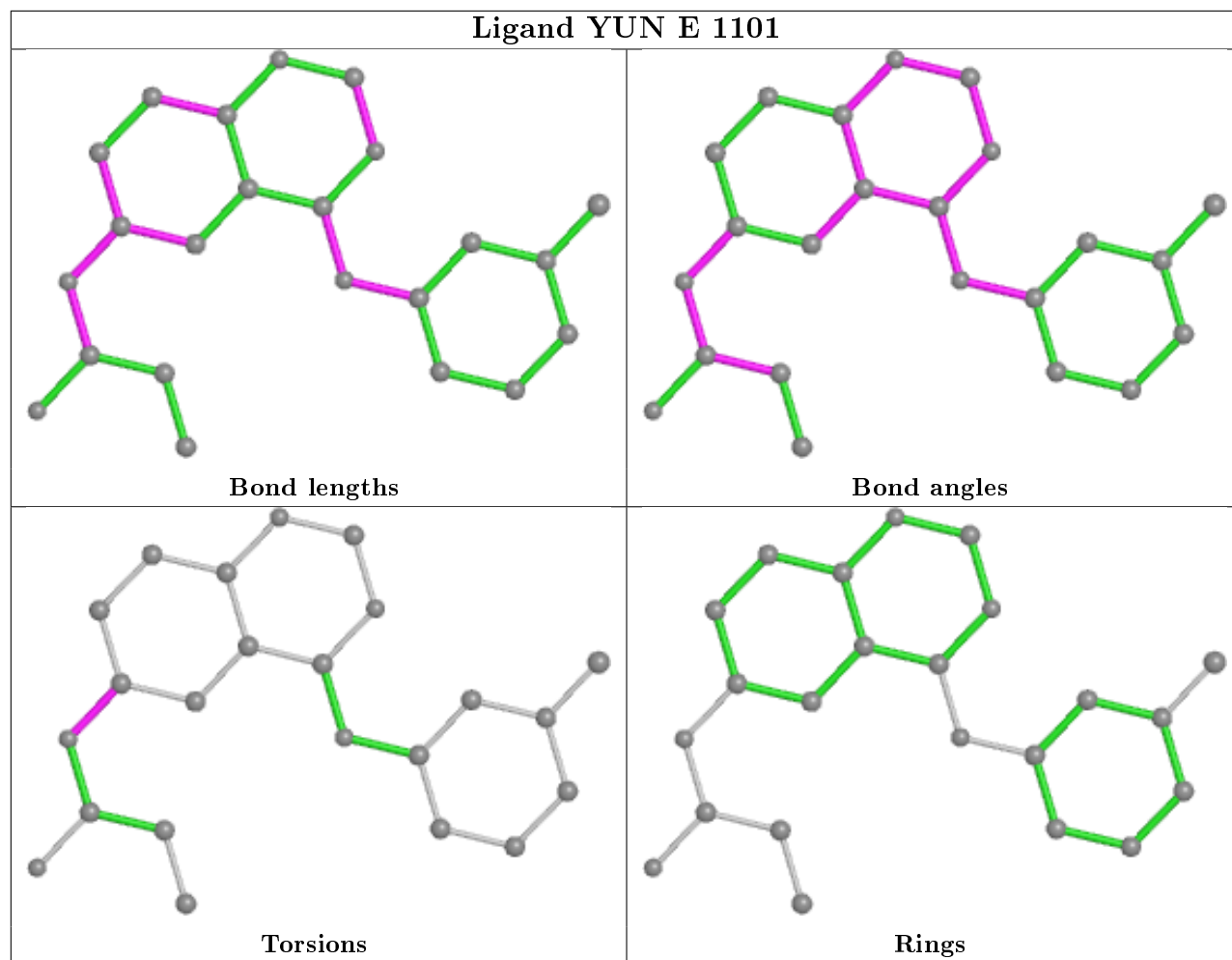
Mol	Chain	Res	Type	Atoms
2	A	1101	YUN	N1-C6-NAT-CAY
2	E	1101	YUN	CAJ-CAZ-NAS-CAW
2	E	1101	YUN	CAM-CAZ-NAS-CAW
2	B	1101	YUN	CAJ-CAZ-NAS-CAW
2	C	1101	YUN	CAN-CAO-CAW-NAS
2	C	1101	YUN	CAN-CAO-CAW-OAC
2	B	1101	YUN	CAM-CAZ-NAS-CAW

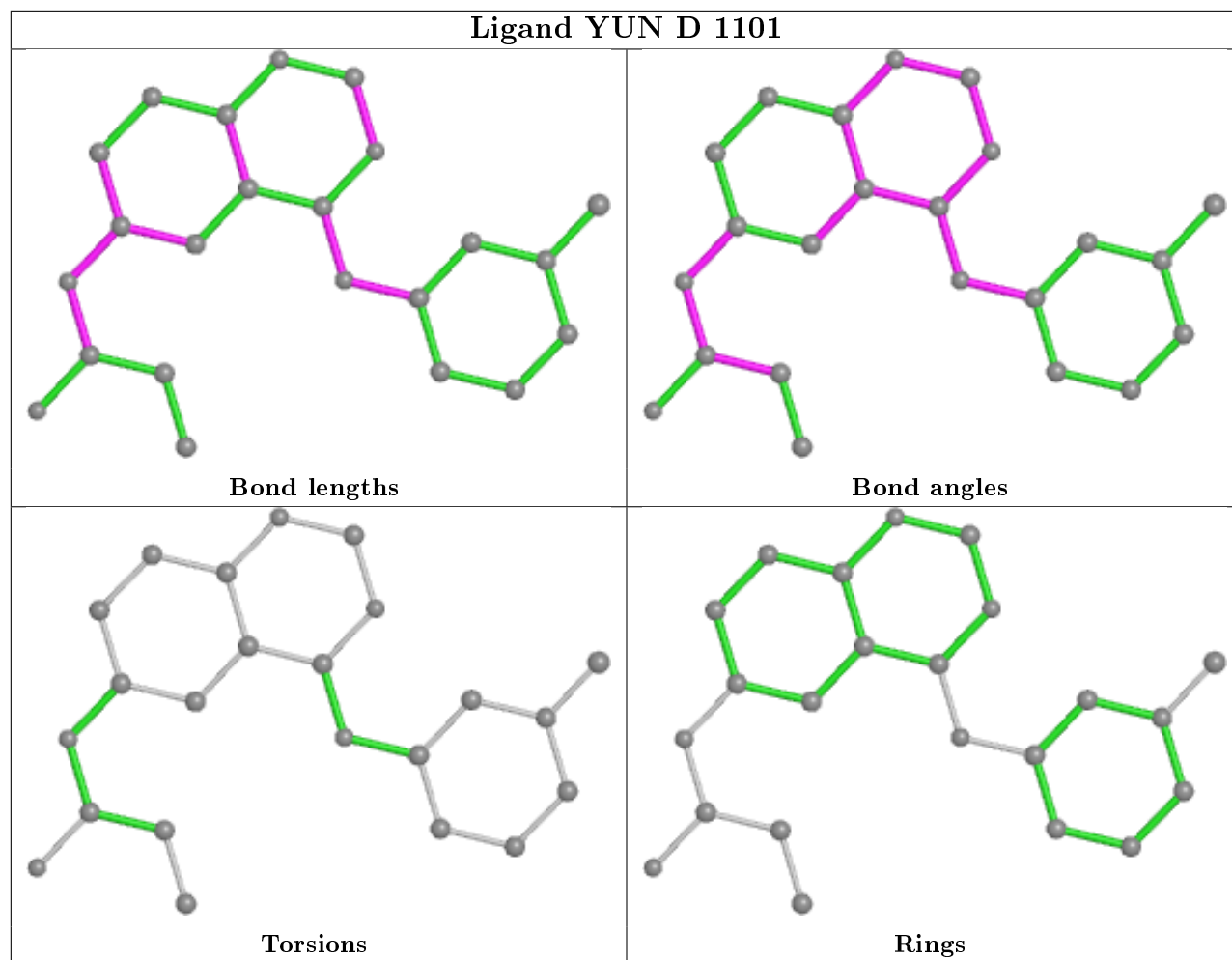
There are no ring outliers.

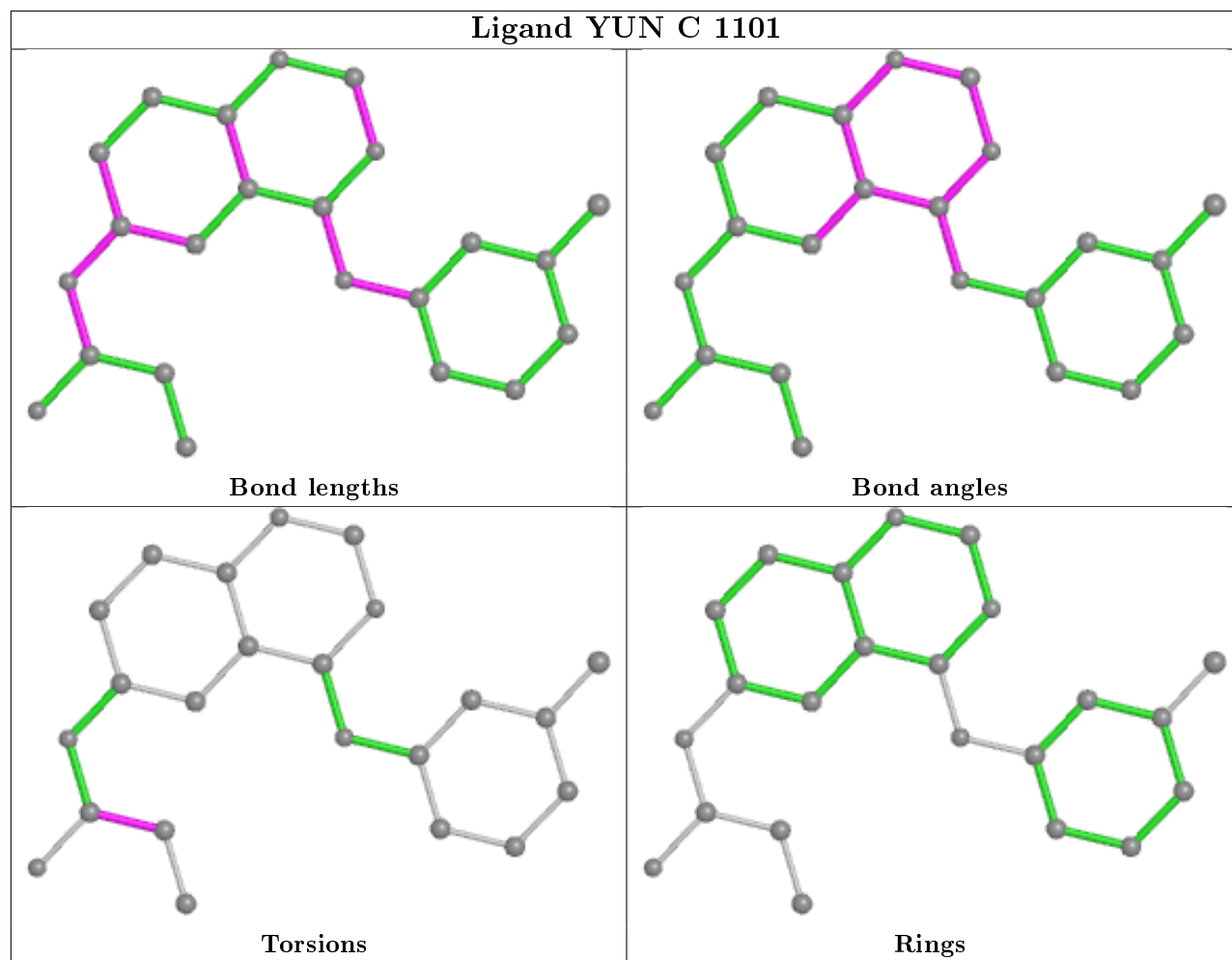
5 monomers are involved in 9 short contacts:

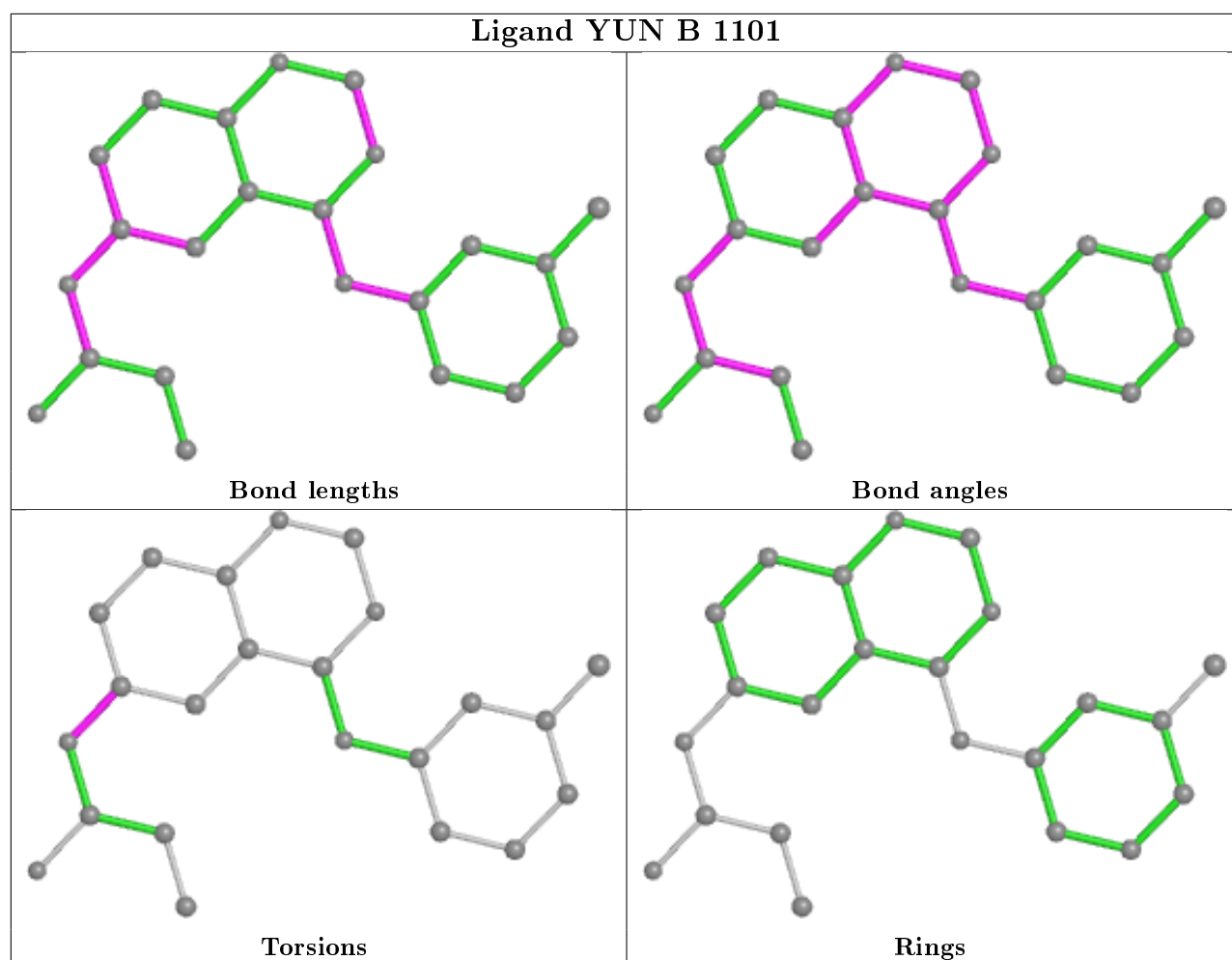
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1101	YUN	1	0
2	D	1101	YUN	1	0
2	C	1101	YUN	1	0
2	B	1101	YUN	3	0
2	A	1101	YUN	3	0

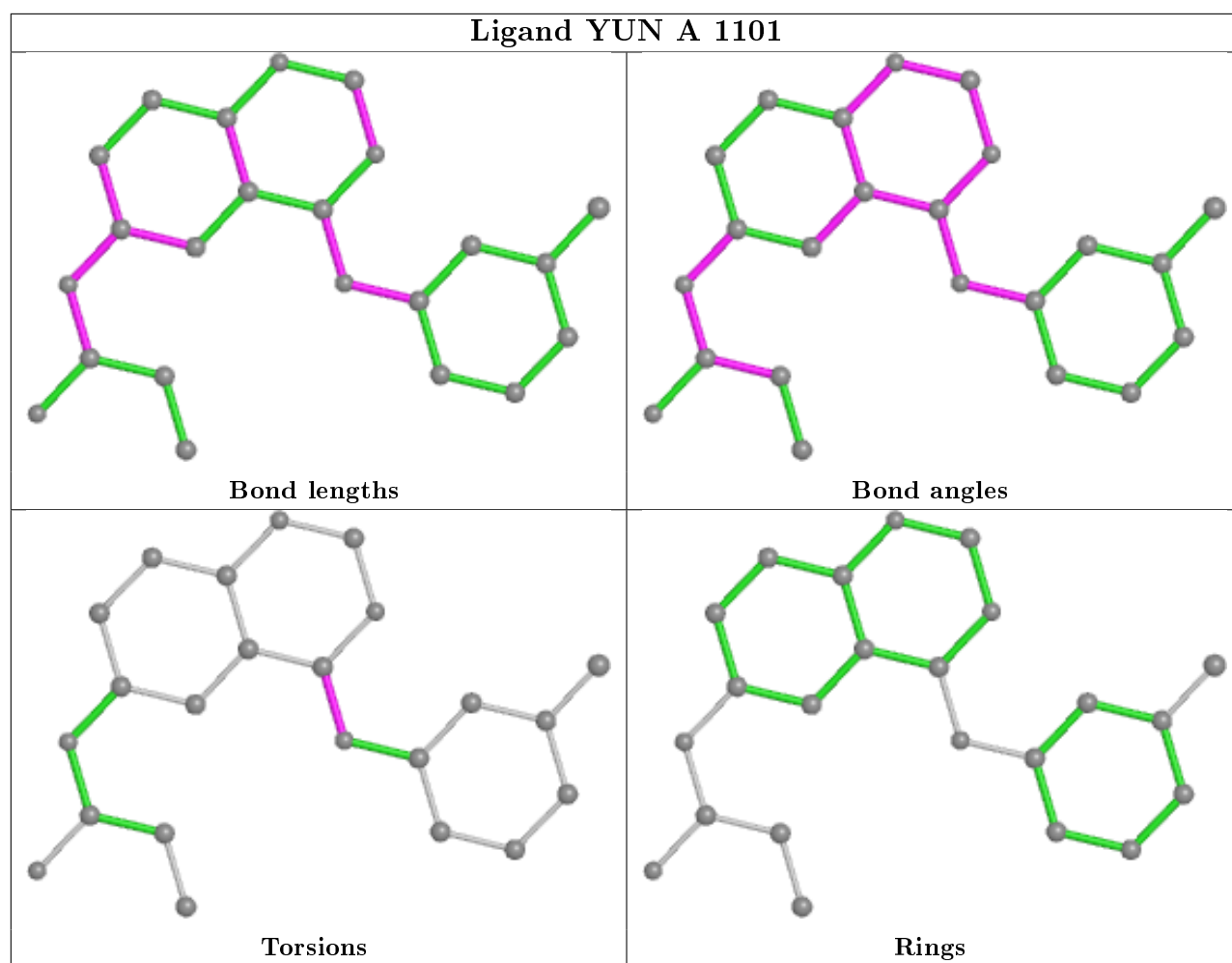
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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











## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



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

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	A	307/334 (91%)	-0.45	0	100	100	26, 60, 112, 138	0
1	B	293/334 (87%)	-0.42	0	100	100	34, 62, 117, 149	0
1	C	293/334 (87%)	-0.16	1 (0%)	94	89	41, 83, 130, 148	0
1	D	289/334 (86%)	-0.27	1 (0%)	94	89	40, 88, 130, 151	0
1	E	290/334 (86%)	-0.32	0	100	100	38, 72, 117, 137	0
All	All	1472/1670 (88%)	-0.33	2 (0%)	95	93	26, 74, 124, 151	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	720	SER	2.7
1	C	866	GLY	2.7

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

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

### 6.3 Carbohydrates [i](#)

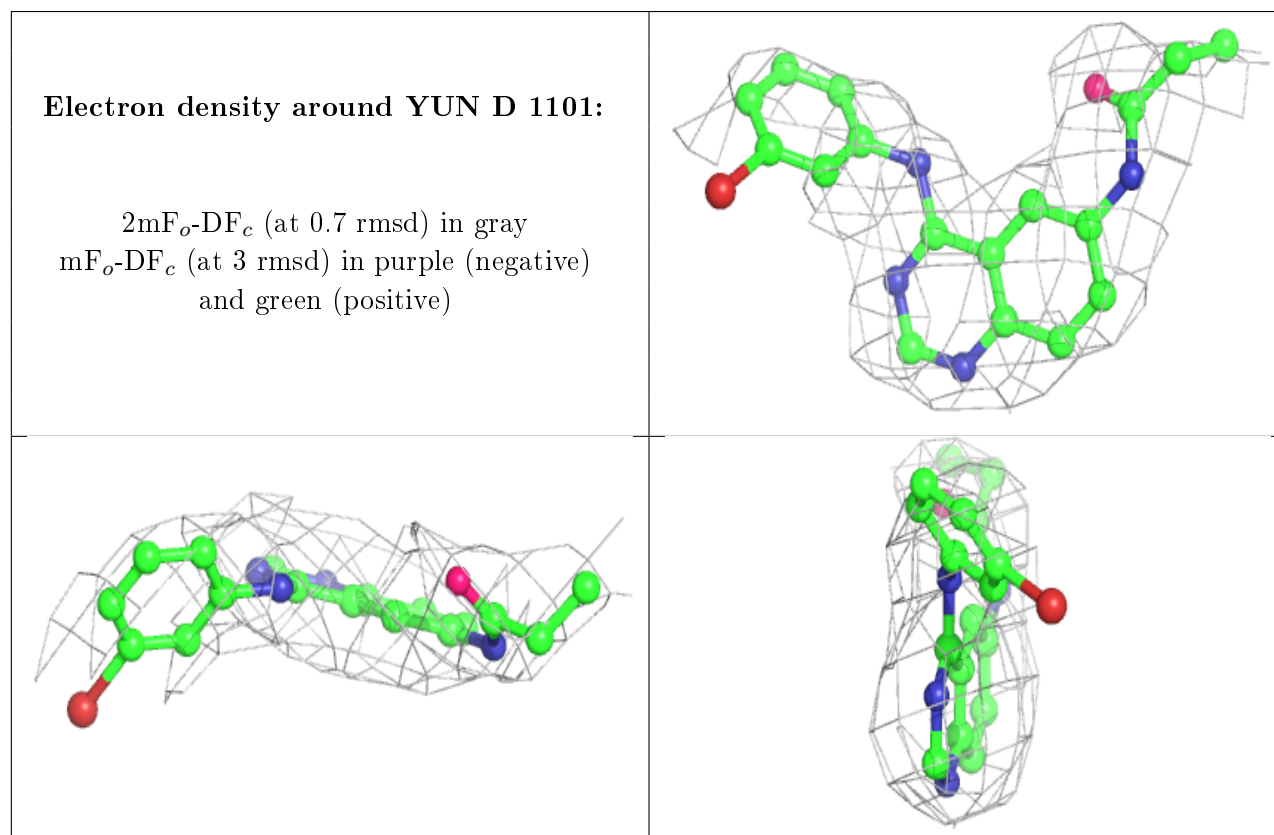
There are no monosaccharides in this entry.

### 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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

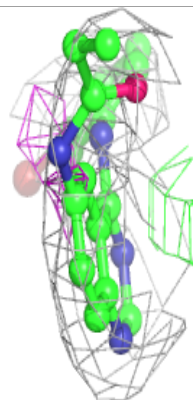
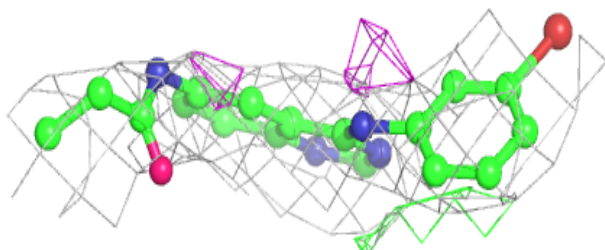
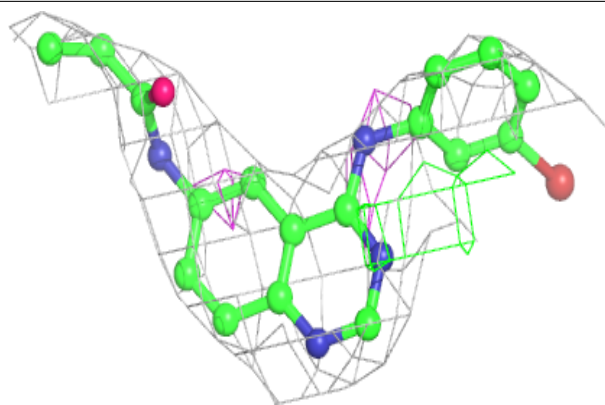
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	YUN	D	1101	23/23	0.92	0.26	65,78,100,172	0
2	YUN	E	1101	23/23	0.93	0.28	38,59,73,105	0
2	YUN	C	1101	23/23	0.94	0.25	61,72,107,117	0
2	YUN	B	1101	23/23	0.96	0.26	49,65,102,104	0
2	YUN	A	1101	23/23	0.96	0.22	28,43,76,90	0

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.

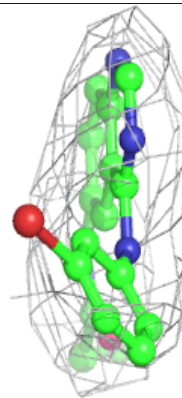
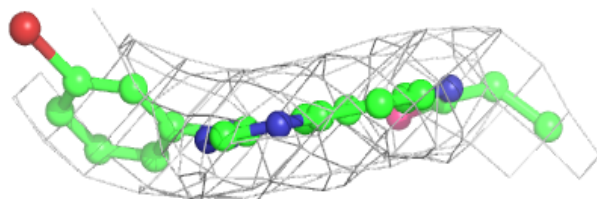
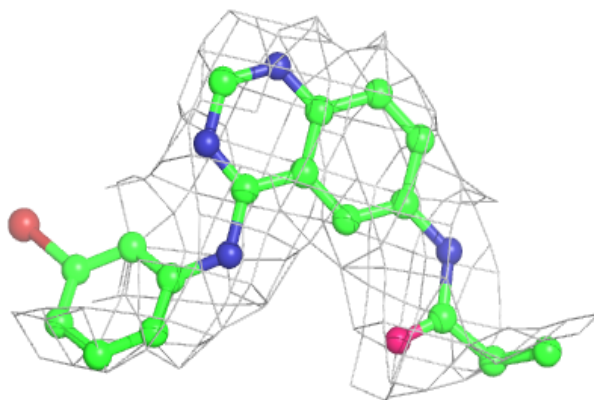


**Electron density around YUN E 1101:**

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

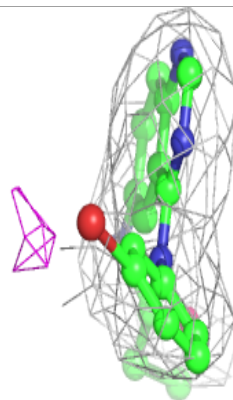
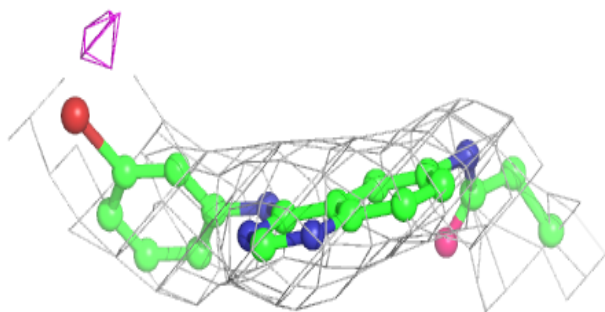
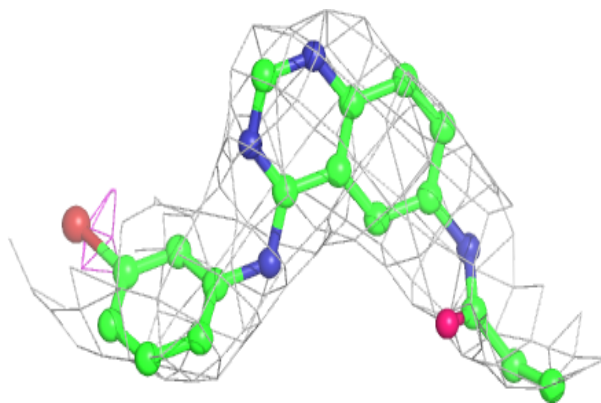
**Electron density around YUN C 1101:**

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

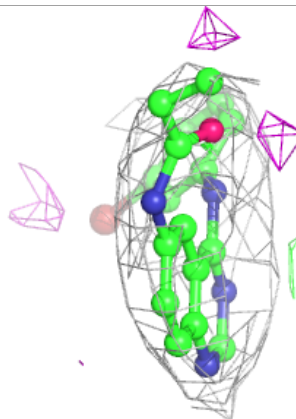
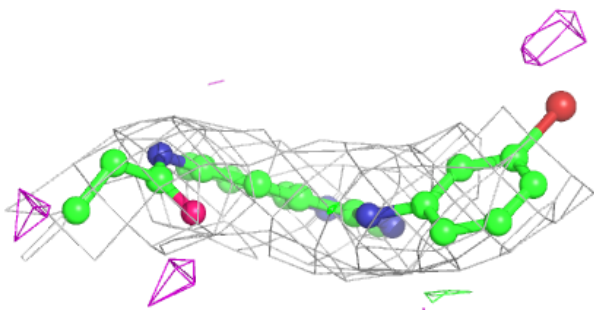
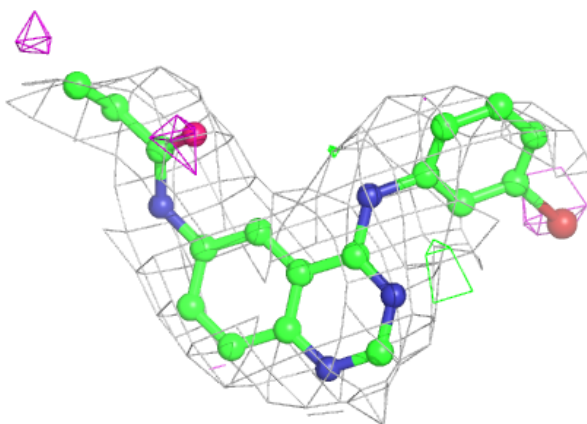


**Electron density around YUN B 1101:**

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

**Electron density around YUN A 1101:**

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



## 6.5 Other polymers ⓘ

There are no such residues in this entry.