



# Full wwPDB X-ray Structure Validation Report ⓘ

Jul 25, 2023 – 02:06 PM EDT

PDB ID : 8GJH  
Title : Salmonella ArnA  
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Deposited on : 2023-03-15  
Resolution : 3.60 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.34  
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) : 2.34

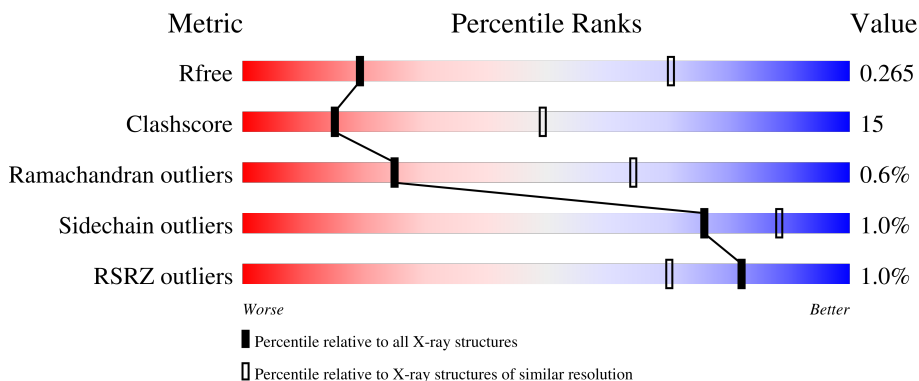
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.60 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.



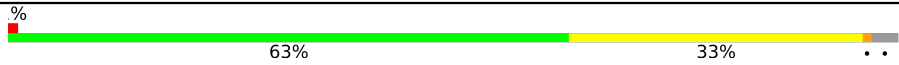
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1257 (3.70-3.50)
Clashscore	141614	1353 (3.70-3.50)
Ramachandran outliers	138981	1307 (3.70-3.50)
Sidechain outliers	138945	1307 (3.70-3.50)
RSRZ outliers	127900	1161 (3.70-3.50)

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

Mol	Chain	Length	Quality of chain
1	A	660	
1	B	660	
1	C	660	
1	D	660	
1	E	660	

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Mol	Chain	Length	Quality of chain
1	F	660	 <p>A horizontal bar chart representing the quality of chain. The bar is divided into two segments: a green segment on the left labeled '63%' and a yellow segment on the right labeled '33%'. The bar starts with a small red square at the beginning and ends with a small grey square at the end. There are two small black dots at the far right end of the bar.</p>

## 2 Entry composition [i](#)

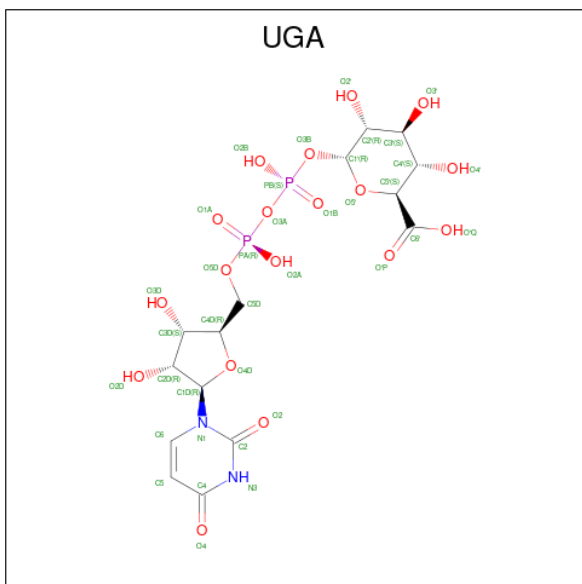
There are 2 unique types of molecules in this entry. The entry contains 30375 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Bifunctional polymyxin resistance protein ArnA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	639	Total 5028	C 3196	N 893	O 918	S 21	0	0	0
1	B	638	Total 5023	C 3193	N 892	O 917	S 21	0	0	0
1	C	639	Total 5028	C 3196	N 893	O 918	S 21	0	0	0
1	D	638	Total 5023	C 3193	N 892	O 917	S 21	0	0	0
1	E	638	Total 5023	C 3193	N 892	O 917	S 21	0	0	0
1	F	639	Total 5028	C 3196	N 893	O 918	S 21	0	0	0

- Molecule 2 is URIDINE-5'-DIPHOSPHATE-GLUCURONIC ACID (three-letter code: UGA) (formula:  $C_{15}H_{22}N_2O_{18}P_2$ ) (labeled as "Ligand of Interest" by depositor).

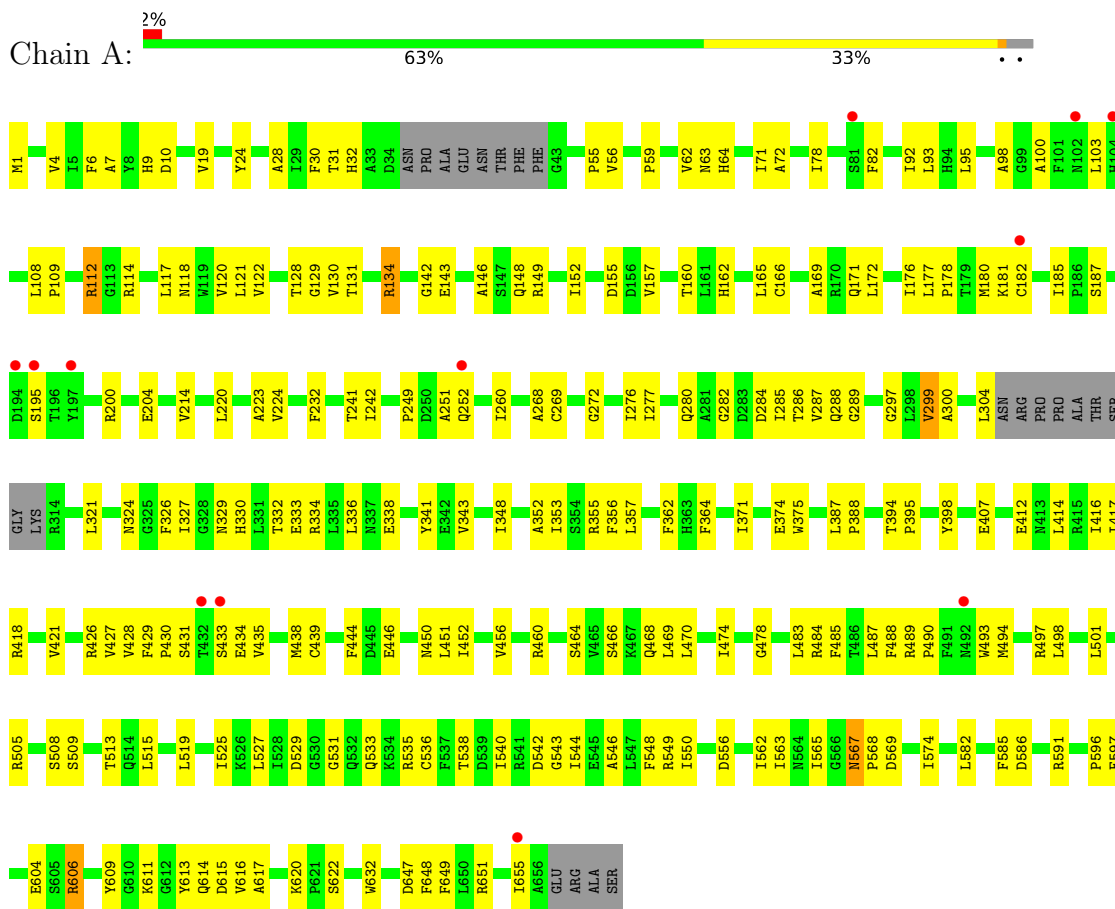


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 37	C 15	N 2	O 18	P 2	0	0
2	B	1	Total 37	C 15	N 2	O 18	P 2	0	0
2	C	1	Total 37	C 15	N 2	O 18	P 2	0	0
2	D	1	Total 37	C 15	N 2	O 18	P 2	0	0
2	E	1	Total 37	C 15	N 2	O 18	P 2	0	0
2	F	1	Total 37	C 15	N 2	O 18	P 2	0	0

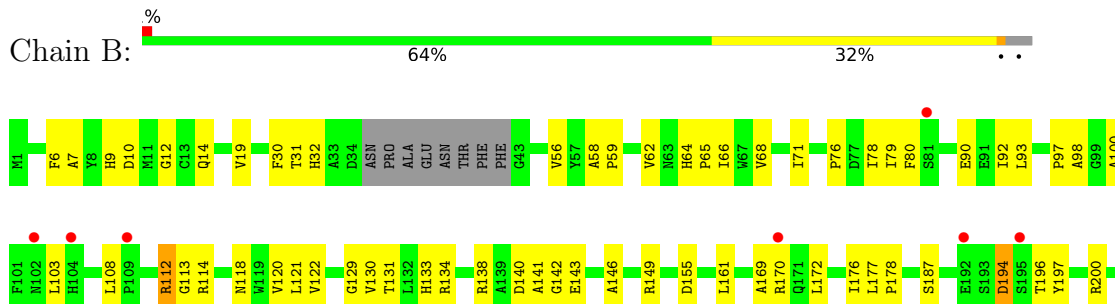
### 3 Residue-property plots

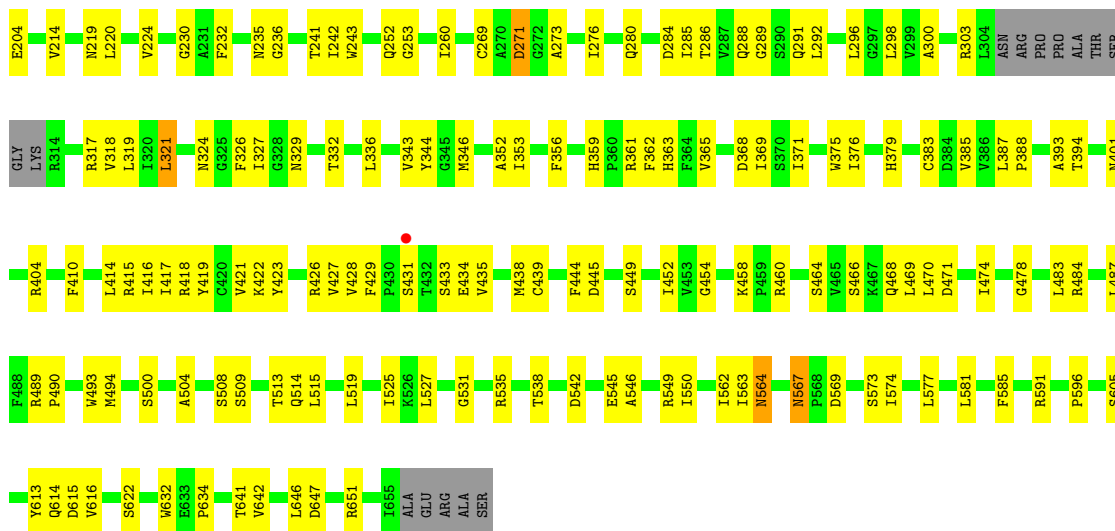
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Bifunctional polymyxin resistance protein ArnA

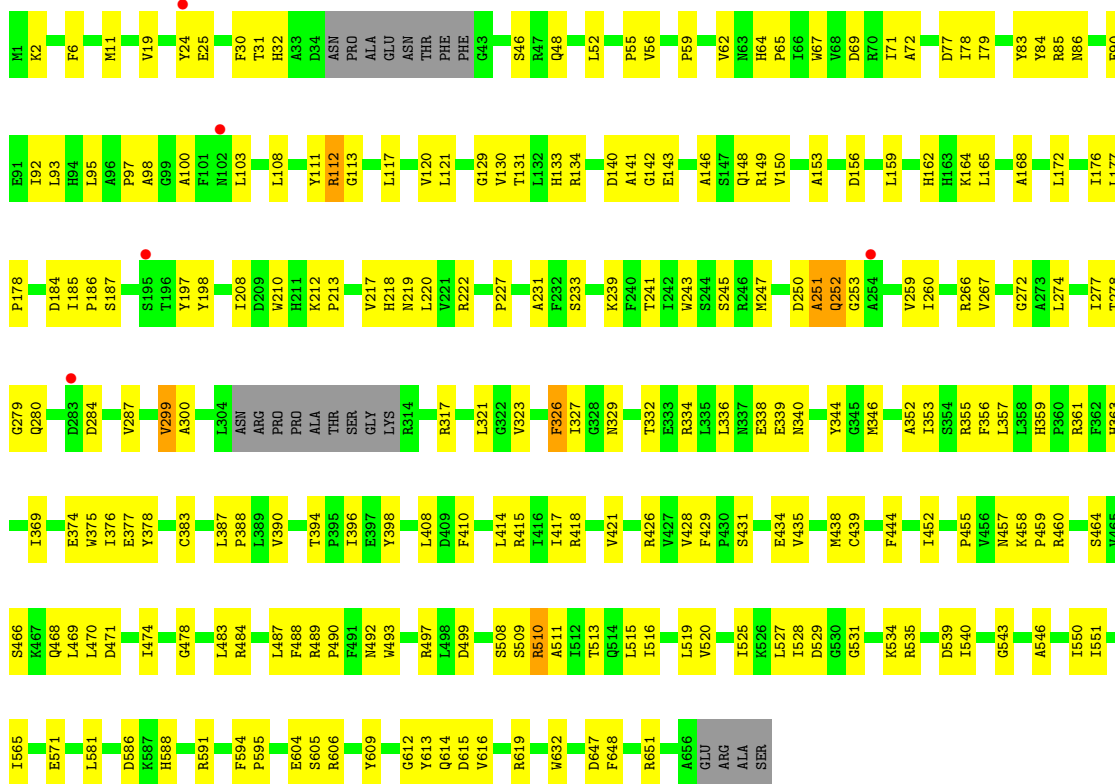


- Molecule 1: Bifunctional polymyxin resistance protein ArnA

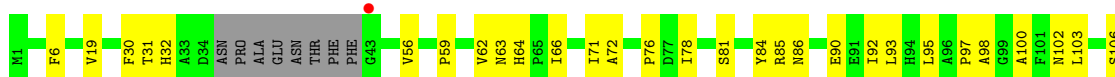


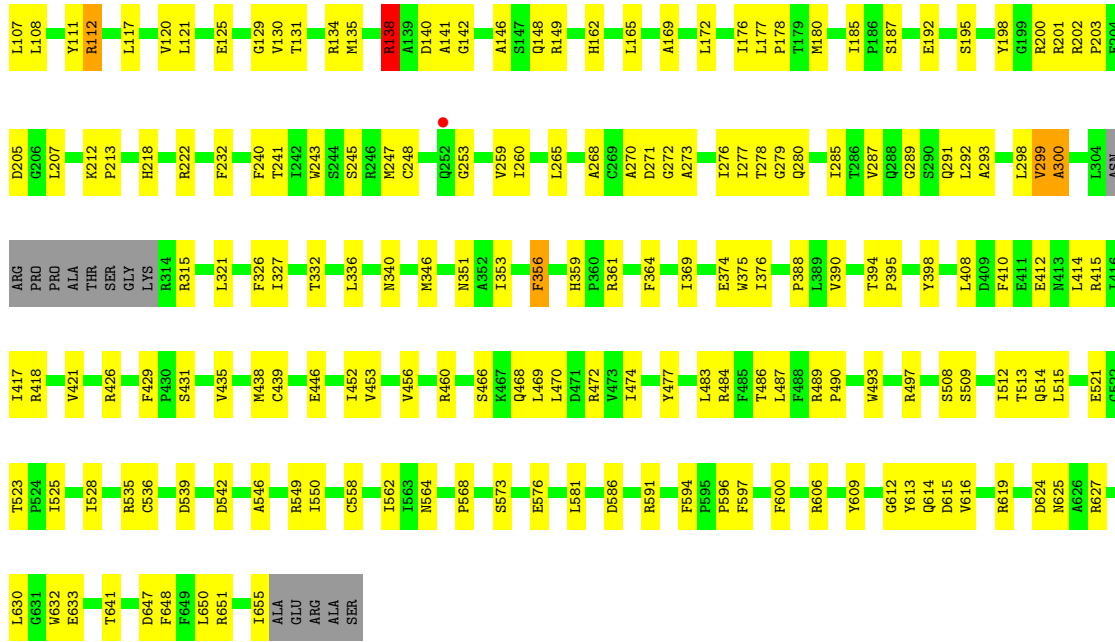


● Molecule 1: Bifunctional polymyxin resistance protein ArnA



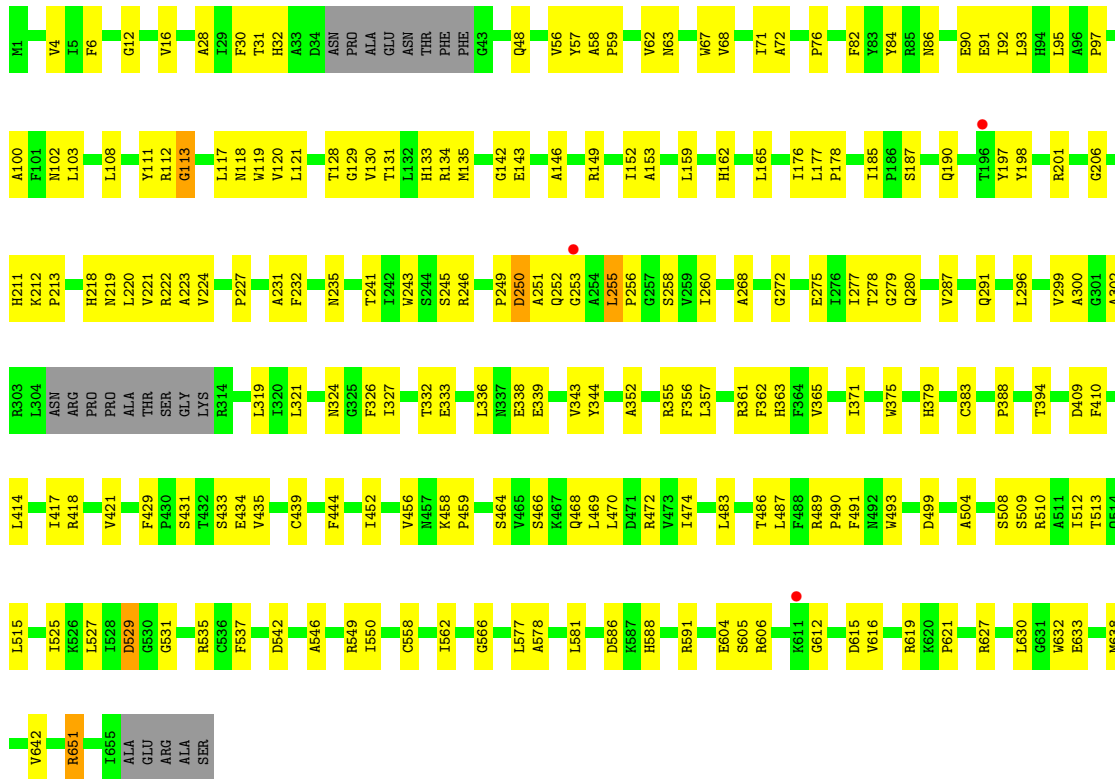
● Molecule 1: Bifunctional polymyxin resistance protein ArnA





• Molecule 1: Bifunctional polymyxin resistance protein ArnA

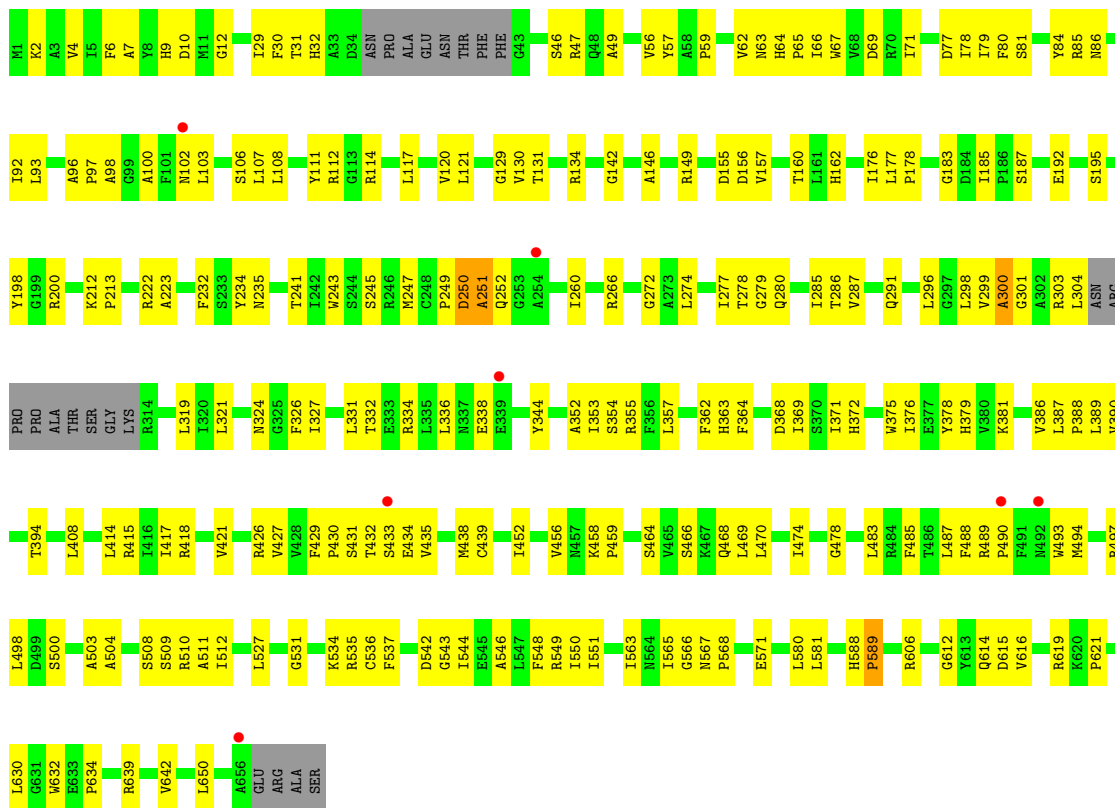
Chain E: 65% 30%



• Molecule 1: Bifunctional polymyxin resistance protein ArnA

Chain F: 63% 33%





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	90.83Å 129.44Å 140.19Å 62.99° 71.66° 77.76°	Depositor
Resolution (Å)	29.83 – 3.60 29.83 – 3.60	Depositor EDS
% Data completeness (in resolution range)	95.0 (29.83-3.60) 95.1 (29.83-3.60)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.29 (at 3.56Å)	Xtrriage
Refinement program	PHENIX 1.20.1_4487	Depositor
R, $R_{free}$	0.218 , 0.267 0.220 , 0.265	Depositor DCC
$R_{free}$ test set	2000 reflections (3.37%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	108.4	Xtrriage
Anisotropy	0.214	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 65.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	30375	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	111.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.78% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.27	0/5143	0.54	0/6984
1	B	0.26	0/5138	0.54	1/6977 (0.0%)
1	C	0.28	0/5143	0.55	0/6984
1	D	0.27	0/5138	0.56	0/6977
1	E	0.28	0/5138	0.54	1/6977 (0.0%)
1	F	0.26	0/5143	0.54	0/6984
All	All	0.27	0/30843	0.54	2/41883 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	D	0	1
1	E	0	1
All	All	0	2

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	B	321	LEU	CB-CG-CD2	-5.20	102.16	111.00
1	E	255	LEU	CA-CB-CG	5.04	126.90	115.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	138	ARG	Sidechain
1	E	651	ARG	Sidechain

## 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	5028	0	4994	159	0
1	B	5023	0	4989	156	0
1	C	5028	0	4994	169	0
1	D	5023	0	4989	151	0
1	E	5023	0	4989	156	0
1	F	5028	0	4994	158	0
2	A	37	0	19	2	0
2	B	37	0	19	4	0
2	C	37	0	19	5	0
2	D	37	0	19	3	0
2	E	37	0	19	2	0
2	F	37	0	19	3	0
All	All	30375	0	30063	908	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 15.

All (908) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1:MET:SD	1:A:181:LYS:NZ	2.16	1.17
1:A:129:GLY:HA3	1:A:149:ARG:HA	1.52	0.91
1:E:299:VAL:HG23	1:E:300:ALA:H	1.37	0.88
1:C:129:GLY:HA3	1:C:149:ARG:HA	1.55	0.86
1:A:582:LEU:HD11	1:A:597:PHE:CE2	2.10	0.85
1:D:394:THR:HG21	1:D:508:SER:HA	1.61	0.81
1:E:627:ARG:HD3	1:E:633:GLU:HG3	1.62	0.80
1:A:299:VAL:HG22	1:A:300:ALA:H	1.43	0.80
1:E:434:GLU:HG2	1:E:464:SER:HB2	1.66	0.78
1:D:326:PHE:HD2	1:D:327:ILE:HG13	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:245:SER:HB2	1:C:274:LEU:HD11	1.64	0.77
1:F:251:ALA:HA	1:F:272:GLY:HA2	1.67	0.77
1:E:326:PHE:HD1	1:E:327:ILE:HG13	1.49	0.76
1:E:251:ALA:HA	1:E:272:GLY:HA2	1.66	0.76
1:A:326:PHE:HD1	1:A:327:ILE:HG13	1.49	0.76
1:C:134:ARG:HH21	1:C:187:SER:HB3	1.51	0.75
1:E:255:LEU:HD12	1:E:256:PRO:HD2	1.67	0.75
1:A:435:VAL:HG23	1:A:468:GLN:HB2	1.68	0.75
1:B:103:LEU:HD11	1:B:130:VAL:HB	1.69	0.74
1:E:102:ASN:HD22	1:E:133:HIS:HE1	1.36	0.74
1:E:112:ARG:NH2	1:E:190:GLN:OE1	2.19	0.73
1:B:515:LEU:HD22	1:B:525:ILE:HG23	1.70	0.73
1:F:234:TYR:HD2	1:F:304:LEU:HD21	1.51	0.72
1:F:59:PRO:HG2	1:F:62:VAL:HG22	1.71	0.72
1:F:129:GLY:HA3	1:F:149:ARG:HA	1.73	0.71
1:B:434:GLU:HG2	1:B:464:SER:HB2	1.70	0.71
1:A:59:PRO:HG2	1:A:62:VAL:HG22	1.72	0.71
1:F:434:GLU:HG2	1:F:464:SER:HB2	1.73	0.71
1:F:619:ARG:HH12	2:F:1100:UGA:H5'1	1.57	0.70
1:B:108:LEU:HB2	1:B:131:THR:HG21	1.74	0.70
1:F:235:ASN:ND2	1:F:296:LEU:HB3	2.07	0.70
1:F:250:ASP:O	1:F:252:GLN:N	2.25	0.70
1:D:515:LEU:HD22	1:D:525:ILE:HG23	1.72	0.69
1:D:624:ASP:OD1	1:D:625:ASN:N	2.25	0.69
1:E:439:CYS:HA	1:E:452:ILE:HD13	1.73	0.69
1:F:390:VAL:HG12	1:F:408:LEU:HD21	1.74	0.69
1:A:251:ALA:HB2	1:A:272:GLY:HA2	1.75	0.68
1:C:435:VAL:HG23	1:C:468:GLN:HB2	1.76	0.68
1:E:235:ASN:HD22	1:E:296:LEU:HB3	1.56	0.68
1:E:578:ALA:HA	1:E:581:LEU:HD12	1.75	0.68
1:B:78:ILE:HG12	1:B:98:ALA:HB3	1.73	0.68
1:C:108:LEU:HB2	1:C:131:THR:HG21	1.75	0.68
1:A:134:ARG:HH22	1:A:185:ILE:HA	1.59	0.68
1:F:108:LEU:HB2	1:F:131:THR:HG21	1.76	0.68
1:B:414:LEU:HD21	1:B:418:ARG:HE	1.59	0.67
1:A:214:VAL:HG22	1:A:269:CYS:HB2	1.75	0.67
1:A:326:PHE:CD1	1:A:327:ILE:HG13	2.29	0.67
1:C:535:ARG:NH2	1:C:615:ASP:OD1	2.26	0.67
1:A:515:LEU:HD22	1:A:525:ILE:HG23	1.75	0.67
1:F:588:HIS:HD2	1:F:589:PRO:HD2	1.59	0.67
1:E:16:VAL:HB	1:E:48:GLN:HE22	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:531:GLY:HA2	1:B:574:ILE:HD11	1.77	0.66
1:C:218:HIS:HB2	1:C:247:MET:HB3	1.78	0.66
1:E:535:ARG:HB2	1:E:537:PHE:HE1	1.58	0.66
1:B:535:ARG:NH2	1:B:615:ASP:OD1	2.28	0.66
1:B:64:HIS:CD2	1:E:604:GLU:HG2	2.29	0.66
1:B:375:TRP:HZ2	1:C:375:TRP:CZ2	2.14	0.66
1:D:594:PHE:HE2	1:D:650:LEU:HD22	1.61	0.66
1:A:562:ILE:HD12	1:D:456:VAL:HG21	1.78	0.66
1:A:439:CYS:HA	1:A:452:ILE:HD13	1.78	0.66
1:B:326:PHE:HD2	1:B:327:ILE:HG13	1.61	0.66
1:C:67:TRP:O	1:C:71:ILE:N	2.29	0.66
1:C:299:VAL:HG22	1:C:300:ALA:H	1.59	0.66
1:E:232:PHE:HB3	1:E:241:THR:HG22	1.76	0.66
1:C:615:ASP:OD1	1:C:616:VAL:N	2.28	0.65
1:E:581:LEU:HD23	1:E:642:VAL:HG13	1.78	0.65
1:C:323:VAL:HG22	1:C:353:ILE:HG21	1.78	0.65
1:D:232:PHE:HB3	1:D:241:THR:HG22	1.77	0.65
1:D:509:SER:HB2	1:D:513:THR:HG23	1.78	0.65
1:E:129:GLY:HA3	1:E:149:ARG:HA	1.78	0.65
1:F:394:THR:HG21	1:F:508:SER:HA	1.79	0.65
1:D:108:LEU:HB2	1:D:131:THR:HG21	1.77	0.65
1:A:108:LEU:HB2	1:A:131:THR:HG21	1.77	0.65
1:B:113:GLY:HA2	1:B:197:TYR:CD1	2.32	0.65
1:E:159:LEU:HD12	1:E:227:PRO:HD3	1.79	0.65
1:A:501:LEU:HD13	1:A:649:PHE:CD1	2.32	0.64
1:C:156:ASP:OD2	1:C:164:LYS:NZ	2.28	0.64
1:A:326:PHE:HD1	1:A:327:ILE:H	1.42	0.64
1:B:647:ASP:O	1:B:651:ARG:HG2	1.98	0.64
1:C:113:GLY:HA2	1:C:197:TYR:CD1	2.33	0.64
1:C:277:ILE:HG22	1:C:278:THR:HG23	1.78	0.64
1:D:609:TYR:OH	2:D:1100:UGA:H2A1	1.97	0.64
1:B:59:PRO:HG2	1:B:62:VAL:HG22	1.79	0.64
1:E:515:LEU:HD22	1:E:525:ILE:HG23	1.79	0.64
1:F:277:ILE:HG22	1:F:278:THR:HG23	1.80	0.64
1:B:439:CYS:HA	1:B:452:ILE:HD13	1.80	0.64
1:E:134:ARG:HH21	1:E:187:SER:HB3	1.64	0.64
1:D:417:ILE:HD11	1:D:470:LEU:HD21	1.80	0.63
1:C:434:GLU:HG2	1:C:464:SER:HB2	1.81	0.63
1:D:439:CYS:HA	1:D:452:ILE:HD13	1.80	0.63
1:E:535:ARG:NH2	1:E:615:ASP:OD1	2.30	0.63
1:C:251:ALA:HA	1:C:272:GLY:HA2	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:321:LEU:HB2	1:D:388:PRO:HA	1.79	0.63
1:E:108:LEU:HB2	1:E:131:THR:HG21	1.80	0.63
1:E:326:PHE:CD1	1:E:327:ILE:HG13	2.33	0.63
1:D:299:VAL:HG22	1:D:300:ALA:H	1.62	0.63
1:F:245:SER:HB2	1:F:274:LEU:HD11	1.81	0.63
1:A:19:VAL:HG22	1:A:177:LEU:HD21	1.79	0.63
1:D:265:LEU:HD23	1:D:276:ILE:HB	1.80	0.63
1:D:535:ARG:NH2	1:D:615:ASP:OD1	2.30	0.63
1:E:299:VAL:HG23	1:E:300:ALA:N	2.13	0.63
1:E:588:HIS:HE1	1:E:651:ARG:NH2	1.97	0.63
1:A:371:ILE:HD13	1:C:377:GLU:HG2	1.79	0.63
1:A:438:MET:SD	1:A:614:GLN:NE2	2.71	0.62
1:D:528:ILE:HD13	2:D:1100:UGA:HN3	1.63	0.62
1:F:260:ILE:HB	1:F:266:ARG:HB2	1.80	0.62
1:F:326:PHE:CD2	1:F:327:ILE:HG13	2.33	0.62
1:A:531:GLY:HA2	1:A:574:ILE:HD11	1.81	0.62
1:D:435:VAL:HG23	1:D:468:GLN:HB2	1.80	0.62
1:E:59:PRO:HG2	1:E:62:VAL:HG22	1.81	0.62
1:C:586:ASP:HA	1:C:591:ARG:HD3	1.80	0.62
1:E:117:LEU:HD13	1:E:165:LEU:HD12	1.82	0.62
1:F:332:THR:O	1:F:336:LEU:HB2	1.98	0.62
1:D:438:MET:SD	1:D:614:GLN:NE2	2.73	0.62
1:B:133:HIS:HD2	1:B:142:GLY:H	1.46	0.61
1:E:371:ILE:HD11	1:F:381:LYS:HD2	1.81	0.61
1:E:371:ILE:HD13	1:F:378:TYR:HA	1.81	0.61
1:D:615:ASP:OD1	1:D:616:VAL:N	2.33	0.61
1:A:103:LEU:HD11	1:A:130:VAL:HB	1.82	0.61
1:C:56:VAL:O	1:D:291:GLN:NE2	2.33	0.61
1:D:59:PRO:HG2	1:D:62:VAL:HG22	1.82	0.61
1:F:615:ASP:OD1	1:F:616:VAL:N	2.33	0.61
1:B:235:ASN:HB2	1:B:303:ARG:HH21	1.63	0.61
1:B:385:VAL:HG12	1:B:426:ARG:HB3	1.83	0.61
1:D:596:PRO:HB2	1:E:299:VAL:HG21	1.82	0.61
1:C:121:LEU:O	1:C:219:ASN:HB3	2.00	0.61
1:D:573:SER:HB3	1:D:576:GLU:OE1	2.01	0.61
1:F:354:SER:HA	1:F:357:LEU:HD23	1.81	0.61
1:B:433:SER:OG	2:B:1100:UGA:O'Q	2.19	0.61
1:A:509:SER:OG	1:A:513:THR:HG23	2.00	0.61
1:C:394:THR:HG21	1:C:508:SER:HA	1.82	0.61
1:C:78:ILE:HG12	1:C:98:ALA:HB3	1.83	0.60
1:C:429:PHE:HB3	1:C:487:LEU:HD23	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:LEU:HD13	1:D:165:LEU:HD12	1.82	0.60
1:C:390:VAL:HG12	1:C:408:LEU:HD21	1.83	0.60
1:C:439:CYS:HA	1:C:452:ILE:HD13	1.82	0.60
1:C:153:ALA:O	1:C:222:ARG:NH2	2.33	0.60
1:C:321:LEU:HB2	1:C:388:PRO:HA	1.82	0.60
1:C:509:SER:OG	1:C:513:THR:HG23	2.01	0.60
1:F:299:VAL:HG12	1:F:300:ALA:H	1.67	0.60
1:A:128:THR:HG22	1:A:152:ILE:HD11	1.84	0.60
1:C:24:TYR:HE2	1:C:78:ILE:HD12	1.66	0.60
1:B:129:GLY:HA3	1:B:149:ARG:HA	1.82	0.60
1:D:107:LEU:HB2	1:D:129:GLY:H	1.66	0.60
1:F:71:ILE:HD12	1:F:92:ILE:HD11	1.83	0.60
1:B:435:VAL:HG23	1:B:468:GLN:HB2	1.84	0.60
1:C:647:ASP:OD2	1:C:651:ARG:NH2	2.34	0.60
1:F:478:GLY:HA2	1:F:483:LEU:H	1.67	0.60
1:B:401:ASN:HB3	1:B:404:ARG:HB3	1.83	0.60
1:F:438:MET:SD	1:F:614:GLN:NE2	2.75	0.59
1:A:333:GLU:OE1	1:A:355:ARG:NH2	2.36	0.59
1:A:562:ILE:CD1	1:D:456:VAL:HG21	2.32	0.59
1:A:591:ARG:HH22	1:A:596:PRO:HA	1.67	0.59
1:D:240:PHE:HZ	1:D:292:LEU:HD22	1.67	0.59
1:F:59:PRO:CG	1:F:62:VAL:HG22	2.33	0.59
1:B:343:VAL:HG23	1:B:362:PHE:HD1	1.67	0.59
1:C:103:LEU:HD11	1:C:130:VAL:HB	1.83	0.59
1:F:394:THR:OG1	1:F:510:ARG:NH2	2.35	0.59
1:F:511:ALA:HB2	2:F:1100:UGA:H5A1	1.85	0.59
1:A:4:VAL:HG22	1:A:28:ALA:HB3	1.83	0.59
1:A:232:PHE:HB3	1:A:241:THR:HG22	1.83	0.59
1:B:56:VAL:HG13	1:F:287:VAL:HG12	1.85	0.59
1:B:321:LEU:HB2	1:B:388:PRO:HA	1.84	0.59
1:D:103:LEU:HD11	1:D:130:VAL:HB	1.85	0.59
1:F:78:ILE:HG12	1:F:98:ALA:HB3	1.84	0.59
1:C:90:GLU:HA	1:C:93:LEU:HD23	1.84	0.59
1:E:338:GLU:N	1:E:338:GLU:OE1	2.36	0.59
1:C:355:ARG:HH12	1:C:497:ARG:NH1	2.00	0.59
1:E:435:VAL:HG23	1:E:468:GLN:HB2	1.84	0.59
1:F:235:ASN:HD22	1:F:296:LEU:HB3	1.68	0.59
1:B:284:ASP:OD1	1:B:285:ILE:N	2.35	0.58
1:D:277:ILE:HG22	1:D:278:THR:HG23	1.83	0.58
1:E:153:ALA:O	1:E:222:ARG:NH2	2.35	0.58
1:F:6:PHE:CD1	1:F:30:PHE:HB2	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:LEU:HB3	1:A:531:GLY:HA3	1.84	0.58
1:B:242:ILE:HG23	1:B:276:ILE:HG23	1.84	0.58
1:D:90:GLU:HA	1:D:93:LEU:HD23	1.86	0.58
1:D:431:SER:HB3	1:D:489:ARG:HG2	1.84	0.58
1:F:243:TRP:HD1	1:F:279:GLY:HA2	1.68	0.58
1:A:284:ASP:OD1	1:A:285:ILE:N	2.34	0.58
1:A:606:ARG:HD2	1:A:611:LYS:HD3	1.85	0.58
1:E:615:ASP:OD1	1:E:616:VAL:N	2.36	0.58
1:B:365:VAL:HG22	1:B:375:TRP:HZ3	1.68	0.58
1:C:431:SER:HB3	1:C:489:ARG:HG2	1.85	0.58
1:E:357:LEU:HD23	1:E:362:PHE:HE2	1.68	0.58
1:A:249:PRO:HA	1:A:272:GLY:HA3	1.86	0.58
1:B:291:GLN:NE2	1:F:56:VAL:O	2.37	0.58
1:C:326:PHE:HD1	1:C:327:ILE:H	1.50	0.58
1:C:527:LEU:HB3	1:C:531:GLY:HA3	1.84	0.58
1:C:604:GLU:OE2	1:F:67:TRP:NE1	2.34	0.58
1:F:417:ILE:HD12	1:F:470:LEU:HD21	1.86	0.58
1:D:414:LEU:HD21	1:D:418:ARG:HE	1.69	0.58
1:A:6:PHE:HD1	1:A:30:PHE:HB2	1.69	0.58
1:C:529:ASP:HA	1:F:66:ILE:HD11	1.84	0.57
1:A:71:ILE:HD12	1:A:92:ILE:HD11	1.85	0.57
1:A:586:ASP:HA	1:A:591:ARG:HG2	1.86	0.57
1:D:6:PHE:HD1	1:D:30:PHE:HB2	1.69	0.57
1:F:588:HIS:CD2	1:F:589:PRO:HD2	2.38	0.57
1:C:252:GLN:HG2	1:C:260:ILE:HD13	1.86	0.57
1:E:470:LEU:O	1:E:474:ILE:HG13	2.05	0.57
1:F:157:VAL:N	1:F:160:THR:OG1	2.28	0.57
1:F:331:LEU:HB2	1:F:544:ILE:HD11	1.86	0.57
1:E:243:TRP:HD1	1:E:279:GLY:HA2	1.69	0.57
1:D:486:THR:HG21	1:D:558:CYS:HB3	1.86	0.57
1:E:235:ASN:ND2	1:E:296:LEU:HB3	2.19	0.57
1:A:535:ARG:NH2	1:A:615:ASP:OD1	2.35	0.57
1:B:538:THR:HG23	1:B:567:ASN:HB2	1.84	0.57
1:D:594:PHE:CE2	1:D:650:LEU:HD22	2.39	0.57
1:D:218:HIS:ND1	1:D:247:MET:HG3	2.20	0.57
1:D:460:ARG:HD3	1:D:613:TYR:CE1	2.39	0.57
1:E:212:LYS:HB3	1:E:213:PRO:HD2	1.87	0.57
1:A:330:HIS:HB2	1:A:544:ILE:HD11	1.87	0.56
1:D:148:GLN:HG2	1:D:172:LEU:HD12	1.87	0.56
1:E:537:PHE:HE2	1:E:577:LEU:HD22	1.69	0.56
1:C:490:PRO:HB3	1:C:493:TRP:CE2	2.41	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:130:VAL:HG23	1:A:172:LEU:HD13	1.87	0.56
1:E:529:ASP:OD1	1:E:605:SER:N	2.38	0.56
1:B:6:PHE:CD1	1:B:30:PHE:HB2	2.40	0.56
1:B:71:ILE:HD12	1:B:92:ILE:HD11	1.86	0.56
1:E:343:VAL:HG23	1:E:362:PHE:HD1	1.70	0.56
1:E:414:LEU:HD21	1:E:418:ARG:HE	1.70	0.56
1:F:103:LEU:HD11	1:F:130:VAL:HB	1.86	0.56
1:C:359:HIS:HE1	1:C:361:ARG:HE	1.53	0.56
1:E:566:GLY:HA3	1:E:621:PRO:HG3	1.88	0.56
1:A:280:GLN:NE2	1:A:282:GLY:O	2.39	0.56
1:A:615:ASP:OD1	1:A:616:VAL:N	2.39	0.56
1:E:146:ALA:HB2	1:E:176:ILE:HG12	1.87	0.56
1:A:117:LEU:HD13	1:A:165:LEU:HD12	1.87	0.56
1:A:478:GLY:HA2	1:A:483:LEU:H	1.71	0.56
1:E:4:VAL:HG22	1:E:28:ALA:HB3	1.87	0.56
1:D:606:ARG:NH1	1:D:612:GLY:H	2.03	0.56
1:E:431:SER:HB3	1:E:489:ARG:HG2	1.88	0.56
1:F:512:ILE:HD11	1:F:581:LEU:HD11	1.88	0.56
1:C:72:ALA:HB2	1:C:95:LEU:HD13	1.88	0.55
1:C:134:ARG:O	1:C:142:GLY:HA3	2.05	0.55
1:F:387:LEU:HD11	1:F:551:ILE:HD11	1.88	0.55
1:C:210:TRP:HH2	1:C:233:SER:HB3	1.72	0.55
1:F:243:TRP:HE1	1:F:280:GLN:HG2	1.71	0.55
1:B:615:ASP:OD1	1:B:616:VAL:N	2.39	0.55
1:C:438:MET:SD	1:C:614:GLN:NE2	2.80	0.55
1:A:414:LEU:HD21	1:A:418:ARG:HE	1.70	0.55
1:D:326:PHE:CD2	1:D:327:ILE:HG13	2.36	0.55
1:F:107:LEU:HB2	1:F:129:GLY:H	1.72	0.55
1:A:280:GLN:HB3	1:A:286:THR:HA	1.89	0.55
1:B:19:VAL:HG22	1:B:177:LEU:HD21	1.89	0.55
1:A:117:LEU:HD21	1:A:162:HIS:HB2	1.88	0.54
1:B:466:SER:HA	1:E:469:LEU:HD11	1.88	0.54
1:C:619:ARG:HH12	2:C:1100:UGA:H5'1	1.72	0.54
1:D:655:ILE:HD12	1:D:655:ILE:H	1.71	0.54
1:E:332:THR:O	1:E:336:LEU:HB2	2.07	0.54
1:E:512:ILE:CD1	1:E:581:LEU:HD21	2.37	0.54
1:F:155:ASP:OD1	1:F:155:ASP:N	2.40	0.54
1:A:130:VAL:HG11	1:A:169:ALA:HB2	1.90	0.54
1:A:394:THR:HG21	1:A:508:SER:HA	1.90	0.54
1:C:6:PHE:CD1	1:C:30:PHE:HB2	2.42	0.54
1:C:59:PRO:HG2	1:C:62:VAL:HG22	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:117:LEU:HD21	1:D:162:HIS:HB2	1.90	0.54
1:D:129:GLY:HA3	1:D:149:ARG:HA	1.90	0.54
1:D:417:ILE:HD13	1:D:474:ILE:HG12	1.89	0.54
1:D:260:ILE:HD11	1:D:268:ALA:HB2	1.89	0.54
1:D:542:ASP:HB3	1:D:632:TRP:HZ2	1.73	0.54
1:F:84:TYR:HE2	1:F:86:ASN:HB2	1.73	0.54
1:F:433:SER:OG	1:F:490:PRO:O	2.25	0.54
1:F:439:CYS:HA	1:F:452:ILE:HD13	1.88	0.54
1:F:580:LEU:HD21	1:F:639:ARG:HA	1.90	0.54
1:C:11:MET:HB2	1:C:83:TYR:HB2	1.90	0.54
1:C:208:ILE:HD11	1:C:231:ALA:HB1	1.89	0.54
1:E:375:TRP:HE1	1:F:375:TRP:HE1	1.56	0.54
1:A:242:ILE:HG23	1:A:276:ILE:HG23	1.90	0.54
1:A:540:ILE:HG13	1:A:544:ILE:HD12	1.90	0.54
1:B:31:THR:OG1	1:B:32:HIS:N	2.41	0.54
1:B:114:ARG:NH2	1:B:200:ARG:HH21	2.06	0.54
1:C:387:LEU:HG	1:C:428:VAL:HB	1.89	0.54
1:D:647:ASP:O	1:D:651:ARG:HG2	2.08	0.54
1:F:542:ASP:HB3	1:F:632:TRP:HZ2	1.73	0.54
1:A:357:LEU:HD23	1:A:362:PHE:HE2	1.72	0.53
1:A:549:ARG:HH11	1:A:632:TRP:HB2	1.73	0.53
1:C:332:THR:O	1:C:336:LEU:HB2	2.07	0.53
1:F:156:ASP:O	1:F:222:ARG:NH1	2.37	0.53
1:E:249:PRO:O	1:E:251:ALA:N	2.42	0.53
1:A:146:ALA:HB2	1:A:176:ILE:HG12	1.89	0.53
1:B:130:VAL:HG11	1:B:169:ALA:HB2	1.90	0.53
1:F:338:GLU:HG3	1:F:548:PHE:CZ	2.43	0.53
1:B:14:GLN:HB3	1:B:170:ARG:HD3	1.90	0.53
1:D:213:PRO:HA	1:D:270:ALA:HB3	1.91	0.53
1:A:582:LEU:HD11	1:A:597:PHE:CD2	2.43	0.53
1:D:71:ILE:HD12	1:D:92:ILE:HD11	1.90	0.53
1:E:490:PRO:HB3	1:E:493:TRP:CE2	2.44	0.53
1:F:500:SER:HB3	1:F:503:ALA:HB3	1.91	0.53
1:A:120:VAL:HG23	1:A:121:LEU:HD22	1.89	0.53
1:B:280:GLN:HG2	1:B:286:THR:HA	1.91	0.53
1:E:260:ILE:HD11	1:E:268:ALA:HB2	1.91	0.53
1:E:277:ILE:HG22	1:E:278:THR:HG23	1.91	0.53
1:A:332:THR:HG23	1:A:343:VAL:HG21	1.90	0.53
1:B:134:ARG:O	1:B:142:GLY:HA3	2.09	0.53
1:C:146:ALA:HB2	1:C:176:ILE:HG12	1.91	0.53
1:A:387:LEU:HG	1:A:428:VAL:HB	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:438:MET:HA	1:B:616:VAL:HG13	1.91	0.53
1:D:103:LEU:HD21	1:D:169:ALA:HB1	1.91	0.53
1:A:148:GLN:HG2	1:A:171:GLN:HE21	1.74	0.53
1:A:466:SER:HA	1:D:469:LEU:HD11	1.90	0.53
1:D:596:PRO:HB2	1:E:299:VAL:CG2	2.39	0.53
1:D:487:LEU:HD12	1:D:562:ILE:HG12	1.91	0.53
1:E:246:ARG:HB3	1:E:275:GLU:HB3	1.90	0.53
1:B:155:ASP:OD1	1:B:155:ASP:N	2.37	0.52
1:B:332:THR:O	1:B:336:LEU:HB2	2.09	0.52
1:B:478:GLY:HA2	1:B:483:LEU:H	1.73	0.52
1:C:71:ILE:HD12	1:C:92:ILE:HD11	1.92	0.52
1:E:71:ILE:HD12	1:E:92:ILE:HD11	1.90	0.52
1:B:410:PHE:HA	1:B:470:LEU:HD12	1.92	0.52
1:B:545:GLU:OE2	1:B:549:ARG:NH2	2.42	0.52
1:D:243:TRP:HD1	1:D:279:GLY:HA2	1.75	0.52
1:D:546:ALA:O	1:D:550:ILE:HG13	2.09	0.52
1:E:6:PHE:CD1	1:E:30:PHE:HB2	2.43	0.52
1:F:362:PHE:HE1	1:F:364:PHE:HB2	1.74	0.52
1:B:421:VAL:HG12	1:B:483:LEU:HD13	1.92	0.52
1:E:185:ILE:O	1:E:187:SER:N	2.42	0.52
1:A:494:MET:HA	1:A:498:LEU:HD22	1.92	0.52
1:B:232:PHE:HB3	1:B:241:THR:HG22	1.91	0.52
1:C:212:LYS:HB3	1:C:213:PRO:HD2	1.90	0.52
1:C:287:VAL:HG12	1:D:56:VAL:HG13	1.92	0.52
1:E:326:PHE:HD1	1:E:327:ILE:H	1.57	0.52
1:E:439:CYS:HB3	1:E:444:PHE:CE1	2.43	0.52
1:A:321:LEU:HB2	1:A:388:PRO:HA	1.91	0.52
1:C:458:LYS:NZ	1:C:613:TYR:O	2.42	0.52
1:D:606:ARG:HH12	1:D:612:GLY:H	1.56	0.52
1:E:542:ASP:HB3	1:E:632:TRP:HZ2	1.74	0.52
1:A:56:VAL:HG13	1:E:287:VAL:HG12	1.92	0.52
1:A:343:VAL:HG23	1:A:362:PHE:HD1	1.75	0.52
1:B:376:ILE:HB	1:B:419:TYR:HE2	1.75	0.52
1:C:414:LEU:CD2	1:C:418:ARG:HE	2.23	0.52
1:D:106:SER:HB2	1:D:111:TYR:HB2	1.92	0.52
1:D:287:VAL:CG1	1:D:291:GLN:HB3	2.40	0.52
1:E:118:ASN:ND2	1:E:223:ALA:O	2.39	0.51
1:F:588:HIS:ND1	1:F:650:LEU:HD12	2.26	0.51
1:A:429:PHE:HB3	1:A:487:LEU:HD23	1.92	0.51
1:B:296:LEU:HB3	1:B:298:LEU:HD13	1.93	0.51
1:A:56:VAL:O	1:E:291:GLN:NE2	2.41	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:591:ARG:HH22	1:B:596:PRO:HA	1.74	0.51
1:E:509:SER:OG	1:E:513:THR:HG23	2.11	0.51
1:F:93:LEU:HD22	1:F:100:ALA:HB3	1.91	0.51
1:F:117:LEU:HD21	1:F:162:HIS:HB2	1.92	0.51
1:F:490:PRO:HB3	1:F:493:TRP:CE2	2.45	0.51
1:F:79:ILE:HB	1:F:100:ALA:HB2	1.93	0.51
1:C:117:LEU:HD21	1:C:162:HIS:HB2	1.91	0.51
1:C:250:ASP:O	1:C:252:GLN:N	2.39	0.51
1:E:319:LEU:HD11	1:E:379:HIS:HB3	1.92	0.51
1:F:232:PHE:HB3	1:F:241:THR:HG22	1.90	0.51
1:C:259:VAL:HG22	1:C:267:VAL:HG22	1.93	0.51
1:C:458:LYS:NZ	1:C:606:ARG:HH21	2.09	0.51
1:D:240:PHE:CZ	1:D:292:LEU:HD13	2.46	0.51
1:F:299:VAL:HG12	1:F:300:ALA:N	2.25	0.51
1:F:550:ILE:HD11	1:F:565:ILE:HD11	1.91	0.51
1:B:527:LEU:HB3	1:B:531:GLY:HA3	1.92	0.51
1:F:114:ARG:HD3	1:F:200:ARG:HB3	1.92	0.51
1:B:138:ARG:HB3	1:B:141:ALA:HB3	1.93	0.51
1:B:329:ASN:ND2	1:B:352:ALA:O	2.43	0.51
1:D:410:PHE:CD1	1:D:470:LEU:HB2	2.45	0.51
1:E:68:VAL:HG22	1:E:92:ILE:HG13	1.93	0.51
1:A:543:GLY:HA2	1:A:565:ILE:HG21	1.92	0.51
1:D:412:GLU:O	1:D:415:ARG:HB2	2.10	0.51
1:E:421:VAL:HG12	1:E:483:LEU:HD13	1.93	0.51
1:F:303:ARG:O	1:F:304:LEU:HB2	2.11	0.51
1:E:68:VAL:HG13	1:E:95:LEU:HD11	1.92	0.51
1:F:344:TYR:CD1	1:F:363:HIS:HB2	2.46	0.51
1:B:93:LEU:HD12	1:B:100:ALA:HB3	1.93	0.50
1:C:243:TRP:HD1	1:C:279:GLY:HA2	1.75	0.50
1:E:527:LEU:HB3	1:E:531:GLY:HA3	1.93	0.50
1:A:529:ASP:HA	1:D:66:ILE:HD11	1.92	0.50
1:B:243:TRP:HZ3	1:F:47:ARG:HD2	1.76	0.50
1:B:487:LEU:HD12	1:B:562:ILE:HG12	1.91	0.50
1:C:59:PRO:HB3	1:C:67:TRP:NE1	2.26	0.50
1:E:344:TYR:CD1	1:E:363:HIS:HB2	2.46	0.50
1:E:535:ARG:HB2	1:E:537:PHE:CE1	2.43	0.50
1:F:134:ARG:O	1:F:142:GLY:HA3	2.10	0.50
1:C:387:LEU:HD11	1:C:551:ILE:HD11	1.93	0.50
1:C:543:GLY:HA2	1:C:565:ILE:HG21	1.93	0.50
1:D:512:ILE:HD12	1:D:581:LEU:HD21	1.93	0.50
1:F:321:LEU:HB2	1:F:388:PRO:HA	1.92	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:368:ASP:H	1:F:372:HIS:HD2	1.59	0.50
1:B:9:HIS:CG	1:B:10:ASP:H	2.29	0.50
1:B:224:VAL:HB	1:B:230:GLY:H	1.76	0.50
1:B:359:HIS:CE1	1:B:361:ARG:HB2	2.47	0.50
1:D:346:MET:HE3	1:D:369:ILE:HG22	1.93	0.50
1:F:280:GLN:HB3	1:F:286:THR:HA	1.94	0.50
1:A:469:LEU:HD11	1:D:466:SER:HA	1.93	0.50
1:B:394:THR:HG21	1:B:508:SER:HA	1.93	0.50
1:C:346:MET:SD	1:C:376:ILE:HG12	2.52	0.50
1:C:546:ALA:O	1:C:550:ILE:HG13	2.12	0.50
1:E:414:LEU:CD2	1:E:418:ARG:HE	2.24	0.50
1:A:542:ASP:HB3	1:A:632:TRP:HZ2	1.76	0.50
1:C:218:HIS:O	1:C:222:ARG:HG3	2.12	0.50
1:C:355:ARG:HH12	1:C:497:ARG:HH12	1.58	0.50
1:C:511:ALA:HB2	2:C:1100:UGA:H5A1	1.94	0.50
1:E:588:HIS:CE1	1:E:651:ARG:NH2	2.77	0.50
1:F:327:ILE:HB	1:F:389:LEU:HD13	1.93	0.50
1:A:426:ARG:NH2	1:A:550:ILE:O	2.40	0.50
1:B:454:GLY:O	1:E:472:ARG:NH2	2.44	0.50
1:C:459:PRO:HD2	1:C:612:GLY:HA3	1.94	0.50
1:D:490:PRO:HB3	1:D:493:TRP:CE2	2.46	0.50
1:F:421:VAL:HG12	1:F:483:LEU:HD13	1.94	0.50
1:A:439:CYS:HB3	1:A:444:PHE:CE1	2.47	0.50
1:B:177:LEU:HB3	1:B:178:PRO:HD3	1.94	0.50
1:D:112:ARG:NH2	1:D:195:SER:OG	2.45	0.50
1:D:315:ARG:HH11	1:D:340:ASN:HA	1.77	0.50
1:F:368:ASP:HB3	1:F:371:ILE:HD12	1.94	0.50
1:A:55:PRO:HA	1:E:291:GLN:OE1	2.12	0.49
1:B:79:ILE:O	1:B:100:ALA:HA	2.11	0.49
1:E:221:VAL:HG22	1:E:231:ALA:HB3	1.94	0.49
1:F:431:SER:HB3	1:F:489:ARG:HG2	1.94	0.49
1:A:535:ARG:HH12	1:A:616:VAL:HB	1.76	0.49
1:E:546:ALA:O	1:E:550:ILE:HG13	2.12	0.49
1:F:29:ILE:HD12	1:F:49:ALA:HB2	1.94	0.49
1:F:369:ILE:HA	1:F:376:ILE:HD11	1.94	0.49
1:B:56:VAL:O	1:F:291:GLN:NE2	2.37	0.49
1:C:588:HIS:NE2	1:C:647:ASP:OD1	2.45	0.49
1:D:146:ALA:HB2	1:D:176:ILE:HG12	1.94	0.49
1:D:521:GLU:HG3	1:D:523:THR:OG1	2.12	0.49
1:A:28:ALA:HB1	1:A:30:PHE:HE1	1.77	0.49
1:B:285:ILE:HB	1:F:46:SER:HB2	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:528:ILE:HG21	1:C:609:TYR:CE2	2.47	0.49
1:D:120:VAL:HG23	1:D:121:LEU:HD22	1.95	0.49
1:A:456:VAL:HG21	1:D:562:ILE:HD13	1.94	0.49
1:B:64:HIS:H	1:B:68:VAL:HG23	1.77	0.49
1:C:339:GLU:HG2	1:C:340:ASN:N	2.28	0.49
1:E:255:LEU:CD1	1:E:256:PRO:HD2	2.41	0.49
1:E:627:ARG:HD3	1:E:633:GLU:CG	2.39	0.49
1:B:121:LEU:O	1:B:219:ASN:HB3	2.12	0.49
1:C:609:TYR:OH	2:C:1100:UGA:H2A1	2.12	0.49
1:E:321:LEU:HB2	1:E:388:PRO:HA	1.95	0.49
1:F:106:SER:HB2	1:F:111:TYR:HB2	1.94	0.49
1:F:458:LYS:NZ	1:F:606:ARG:HH21	2.10	0.49
1:D:271:ASP:CG	1:D:272:GLY:H	2.15	0.49
1:A:338:GLU:HG3	1:A:548:PHE:CZ	2.48	0.49
1:B:143:GLU:HB3	1:B:187:SER:HB2	1.94	0.49
1:B:574:ILE:CD1	2:B:1100:UGA:H1A1	2.43	0.49
1:C:177:LEU:HB3	1:C:178:PRO:HD3	1.93	0.49
1:C:515:LEU:HD22	1:C:525:ILE:HG23	1.94	0.49
1:D:627:ARG:HD3	1:D:633:GLU:HG3	1.93	0.49
1:E:586:ASP:O	1:E:591:ARG:HD3	2.13	0.49
1:D:497:ARG:HD2	1:D:648:PHE:CZ	2.47	0.49
1:D:619:ARG:HH12	2:D:1100:UGA:H5'1	1.77	0.49
1:B:326:PHE:CD2	1:B:327:ILE:HG13	2.45	0.49
1:C:546:ALA:HB2	1:C:632:TRP:CE2	2.48	0.49
1:E:128:THR:HG22	1:E:152:ILE:HD11	1.94	0.49
1:C:19:VAL:HG22	1:C:177:LEU:HD21	1.95	0.48
1:C:46:SER:HB2	1:D:285:ILE:HB	1.95	0.48
1:C:185:ILE:O	1:C:187:SER:N	2.45	0.48
1:D:259:VAL:HG21	1:D:298:LEU:HD23	1.95	0.48
1:C:478:GLY:HA2	1:C:483:LEU:H	1.78	0.48
1:A:6:PHE:CD1	1:A:30:PHE:HB2	2.47	0.48
1:B:369:ILE:O	1:B:415:ARG:NH2	2.47	0.48
1:B:393:ALA:HB1	2:B:1100:UGA:O3'	2.12	0.48
1:D:6:PHE:CD1	1:D:30:PHE:HB2	2.48	0.48
1:E:619:ARG:HH12	2:E:1100:UGA:H5'1	1.77	0.48
1:F:619:ARG:NH1	2:F:1100:UGA:H5'1	2.26	0.48
1:A:338:GLU:HB2	1:A:341:TYR:HD2	1.78	0.48
1:B:318:VAL:HG13	1:B:385:VAL:HG23	1.94	0.48
1:B:431:SER:HB3	1:B:489:ARG:HG2	1.95	0.48
1:C:31:THR:OG1	1:C:32:HIS:N	2.47	0.48
1:F:157:VAL:HG12	1:F:222:ARG:HG2	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:249:PRO:O	1:F:251:ALA:N	2.46	0.48
1:A:421:VAL:HG12	1:A:483:LEU:HD13	1.95	0.48
1:B:133:HIS:CD2	1:B:142:GLY:H	2.29	0.48
1:C:499:ASP:OD1	1:C:510:ARG:NH1	2.47	0.48
1:D:134:ARG:O	1:D:142:GLY:HA3	2.12	0.48
1:E:113:GLY:HA2	1:E:197:TYR:CD1	2.47	0.48
1:E:218:HIS:CD2	1:E:245:SER:HB3	2.49	0.48
1:E:220:LEU:O	1:E:224:VAL:HG22	2.13	0.48
1:F:146:ALA:HB2	1:F:176:ILE:HG12	1.95	0.48
1:A:277:ILE:O	1:A:289:GLY:N	2.45	0.48
1:A:470:LEU:O	1:A:474:ILE:HG13	2.13	0.48
1:B:509:SER:OG	1:B:513:THR:HG23	2.13	0.48
1:B:573:SER:O	1:B:577:LEU:N	2.38	0.48
1:C:469:LEU:HD11	1:F:466:SER:HA	1.94	0.48
1:F:112:ARG:HE	1:F:195:SER:HB2	1.77	0.48
1:A:326:PHE:HD1	1:A:327:ILE:N	2.11	0.48
1:A:332:THR:O	1:A:336:LEU:HB2	2.13	0.48
1:A:497:ARG:HD2	1:A:648:PHE:CZ	2.49	0.48
1:B:321:LEU:HD22	1:B:346:MET:HE1	1.96	0.48
1:F:494:MET:HA	1:F:498:LEU:HD22	1.96	0.48
1:E:549:ARG:HD2	1:E:630:LEU:O	2.14	0.48
1:B:563:ILE:HG22	1:B:564:ASN:H	1.79	0.48
1:E:487:LEU:HD12	1:E:562:ILE:HG12	1.94	0.48
1:A:103:LEU:HD21	1:A:169:ALA:HB1	1.96	0.47
1:B:146:ALA:HB2	1:B:176:ILE:HG12	1.95	0.47
1:E:84:TYR:HE2	1:E:86:ASN:HB2	1.79	0.47
1:F:6:PHE:HB3	1:F:84:TYR:CD1	2.49	0.47
1:D:31:THR:OG1	1:D:32:HIS:N	2.45	0.47
1:E:6:PHE:HD1	1:E:30:PHE:HB2	1.80	0.47
1:A:24:TYR:HE2	1:A:78:ILE:HD12	1.79	0.47
1:A:134:ARG:O	1:A:142:GLY:HA3	2.14	0.47
1:C:470:LEU:O	1:C:474:ILE:HG13	2.13	0.47
1:E:117:LEU:HD21	1:E:162:HIS:HB2	1.96	0.47
1:F:81:SER:HB3	1:F:102:ASN:HA	1.96	0.47
1:F:431:SER:OG	1:F:432:THR:N	2.45	0.47
1:B:112:ARG:NH1	1:B:140:ASP:O	2.47	0.47
1:B:112:ARG:N	1:B:196:THR:O	2.48	0.47
1:B:130:VAL:HG23	1:B:172:LEU:HD13	1.96	0.47
1:C:478:GLY:HA2	1:C:483:LEU:N	2.29	0.47
1:A:434:GLU:HG2	1:A:464:SER:HB2	1.95	0.47
1:D:111:TYR:CE2	1:D:120:VAL:HG12	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:470:LEU:O	1:D:474:ILE:HG13	2.14	0.47
1:F:79:ILE:HB	1:F:100:ALA:CB	2.45	0.47
1:B:439:CYS:HB3	1:B:444:PHE:CE1	2.49	0.47
1:C:6:PHE:HD1	1:C:30:PHE:HB2	1.80	0.47
1:C:417:ILE:HD12	1:C:470:LEU:HD21	1.96	0.47
1:A:143:GLU:CB	1:A:187:SER:HB2	2.45	0.47
1:B:353:ILE:HB	1:B:356:PHE:CE1	2.50	0.47
1:B:469:LEU:HD11	1:E:466:SER:HA	1.95	0.47
1:C:55:PRO:HA	1:D:291:GLN:OE1	2.15	0.47
1:C:534:LYS:HD3	1:C:571:GLU:HG2	1.96	0.47
1:D:130:VAL:HG11	1:D:169:ALA:HB2	1.96	0.47
1:E:333:GLU:OE1	1:E:355:ARG:NH2	2.46	0.47
1:B:422:LYS:HG2	1:B:423:TYR:CE1	2.49	0.47
1:E:134:ARG:O	1:E:142:GLY:HA3	2.13	0.47
1:E:433:SER:HB3	1:E:491:PHE:CD1	2.49	0.47
1:D:212:LYS:HB3	1:D:213:PRO:HD2	1.97	0.47
1:D:346:MET:SD	1:D:376:ILE:HG22	2.55	0.47
1:E:119:TRP:CZ2	1:E:201:ARG:HG2	2.49	0.47
1:F:535:ARG:HB2	1:F:537:PHE:CE1	2.49	0.47
1:A:285:ILE:HD13	1:E:58:ALA:HB2	1.97	0.47
1:B:365:VAL:HG22	1:B:375:TRP:CZ3	2.48	0.47
1:B:375:TRP:CZ2	1:C:375:TRP:CZ2	3.01	0.47
1:B:542:ASP:HB3	1:B:632:TRP:HZ2	1.79	0.46
1:C:143:GLU:HB3	1:C:187:SER:HB2	1.97	0.46
1:C:369:ILE:HA	1:C:376:ILE:CD1	2.45	0.46
1:C:374:GLU:HG3	1:C:375:TRP:N	2.30	0.46
1:D:102:ASN:HB2	1:D:135:MET:SD	2.55	0.46
1:F:6:PHE:HD1	1:F:30:PHE:HB2	1.79	0.46
1:F:324:ASN:OD1	1:F:352:ALA:HB3	2.15	0.46
1:A:330:HIS:HB2	1:A:544:ILE:CD1	2.45	0.46
1:C:280:GLN:HB2	1:C:284:ASP:O	2.15	0.46
1:D:332:THR:O	1:D:336:LEU:HB2	2.15	0.46
1:B:585:PHE:HA	1:B:646:LEU:HD21	1.97	0.46
1:C:79:ILE:O	1:C:100:ALA:HA	2.16	0.46
1:F:120:VAL:HG23	1:F:121:LEU:HD13	1.97	0.46
1:F:459:PRO:HD2	1:F:612:GLY:HA3	1.97	0.46
1:F:567:ASN:HA	1:F:634:PRO:HG3	1.96	0.46
1:B:321:LEU:HD22	1:B:346:MET:CE	2.46	0.46
1:B:344:TYR:CD1	1:B:363:HIS:HB2	2.50	0.46
1:B:7:ALA:HB1	1:B:12:GLY:HA3	1.98	0.46
1:B:417:ILE:HD12	1:B:470:LEU:HD21	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:528:ILE:HG21	1:C:609:TYR:HE2	1.80	0.46
1:D:185:ILE:HD12	1:D:185:ILE:O	2.15	0.46
1:E:206:GLY:O	1:E:231:ALA:HA	2.15	0.46
1:A:78:ILE:HG12	1:A:98:ALA:HB3	1.98	0.46
1:A:118:ASN:O	1:A:122:VAL:HG23	2.14	0.46
1:A:143:GLU:HB3	1:A:187:SER:HB2	1.98	0.46
1:B:490:PRO:HB3	1:B:493:TRP:CE2	2.51	0.46
1:C:458:LYS:HZ3	1:C:606:ARG:HH21	1.63	0.46
1:A:7:ALA:HA	1:A:82:PHE:O	2.15	0.46
1:A:260:ILE:HD11	1:A:268:ALA:HB2	1.97	0.46
1:A:326:PHE:CD1	1:A:327:ILE:N	2.78	0.46
1:B:567:ASN:HD21	1:B:569:ASP:HB2	1.81	0.46
1:D:285:ILE:O	1:D:287:VAL:HG23	2.15	0.46
1:E:31:THR:OG1	1:E:32:HIS:N	2.49	0.46
1:B:235:ASN:HB2	1:B:303:ARG:NH2	2.31	0.46
1:C:120:VAL:HG23	1:C:121:LEU:HD22	1.98	0.46
1:C:520:VAL:HG13	1:C:594:PHE:CE1	2.51	0.46
1:D:85:ARG:HH11	1:D:200:ARG:HH22	1.63	0.46
1:D:177:LEU:HA	1:D:180:MET:HE2	1.98	0.46
1:F:435:VAL:HG23	1:F:468:GLN:HB2	1.98	0.46
1:A:220:LEU:O	1:A:224:VAL:HG22	2.16	0.46
1:B:470:LEU:O	1:B:474:ILE:HG13	2.15	0.46
1:E:76:PRO:O	1:E:97:PRO:HD2	2.15	0.46
1:E:394:THR:HG21	1:E:509:SER:H	1.80	0.46
1:E:429:PHE:HB3	1:E:487:LEU:HD23	1.97	0.46
1:F:456:VAL:C	1:F:458:LYS:H	2.19	0.46
1:F:488:PHE:HA	1:F:563:ILE:O	2.15	0.46
1:A:490:PRO:HB3	1:A:493:TRP:CE2	2.51	0.45
1:A:546:ALA:O	1:A:550:ILE:HG13	2.17	0.45
1:B:319:LEU:HD11	1:B:379:HIS:HB3	1.98	0.45
1:B:458:LYS:HD2	1:B:614:GLN:HB2	1.98	0.45
1:E:72:ALA:HB2	1:E:95:LEU:HD13	1.98	0.45
1:A:114:ARG:HD3	1:A:200:ARG:HB2	1.98	0.45
1:A:388:PRO:HB3	1:A:416:ILE:HG21	1.99	0.45
1:C:208:ILE:HD11	1:C:220:LEU:HD22	1.98	0.45
1:C:452:ILE:HG13	1:F:452:ILE:HG23	1.99	0.45
1:D:138:ARG:HB3	1:D:141:ALA:HB3	1.98	0.45
1:D:177:LEU:HB3	1:D:178:PRO:HD3	1.97	0.45
1:D:185:ILE:O	1:D:187:SER:N	2.47	0.45
1:F:353:ILE:HD11	1:F:364:PHE:HE2	1.82	0.45
1:B:14:GLN:OE1	1:B:170:ARG:NH1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:VAL:HG22	1:B:269:CYS:SG	2.56	0.45
1:B:356:PHE:HD1	1:B:362:PHE:CD2	2.34	0.45
1:B:387:LEU:HG	1:B:428:VAL:HB	1.98	0.45
1:E:410:PHE:HA	1:E:470:LEU:HD12	1.98	0.45
1:C:516:ILE:HG12	1:C:581:LEU:HD11	1.97	0.45
1:E:299:VAL:CG2	1:E:300:ALA:H	2.18	0.45
1:A:353:ILE:HD11	1:A:364:PHE:CD1	2.51	0.45
1:A:519:LEU:HB3	1:A:585:PHE:CE2	2.51	0.45
1:A:536:CYS:SG	1:A:568:PRO:HA	2.56	0.45
1:B:252:GLN:HG2	1:B:260:ILE:CG2	2.47	0.45
1:C:159:LEU:HD23	1:C:227:PRO:HD2	1.98	0.45
1:C:421:VAL:HG12	1:C:483:LEU:HD13	1.99	0.45
1:D:395:PRO:HA	1:D:398:TYR:CD2	2.52	0.45
1:D:414:LEU:CD2	1:D:418:ARG:HE	2.30	0.45
1:A:134:ARG:HH12	1:A:185:ILE:HB	1.82	0.45
1:B:567:ASN:HA	1:B:634:PRO:HG3	1.99	0.45
1:C:150:VAL:HG11	1:C:164:LYS:HG2	1.99	0.45
1:C:492:ASN:H	2:C:1100:UGA:C6'	2.29	0.45
1:F:111:TYR:CE1	1:F:198:TYR:HE2	2.34	0.45
1:A:299:VAL:HG22	1:A:300:ALA:N	2.23	0.45
1:C:334:ARG:NH1	1:C:338:GLU:OE2	2.50	0.45
1:D:19:VAL:HA	1:D:177:LEU:HD21	1.99	0.45
1:D:218:HIS:CD2	1:D:245:SER:HB3	2.52	0.45
1:E:344:TYR:HD2	1:E:383:CYS:SG	2.39	0.45
1:E:365:VAL:HG21	1:E:379:HIS:NE2	2.32	0.45
1:F:185:ILE:O	1:F:187:SER:N	2.48	0.45
1:F:234:TYR:CD2	1:F:304:LEU:HD21	2.42	0.45
1:F:235:ASN:ND2	1:F:298:LEU:HD21	2.32	0.45
1:F:319:LEU:HD11	1:F:379:HIS:HB3	1.97	0.45
1:B:214:VAL:HG23	1:B:271:ASP:O	2.16	0.45
1:B:478:GLY:HA2	1:B:483:LEU:N	2.31	0.45
1:D:426:ARG:HA	1:D:484:ARG:O	2.16	0.45
1:E:102:ASN:HD22	1:E:133:HIS:CE1	2.25	0.45
1:B:435:VAL:HG11	1:B:489:ARG:CZ	2.46	0.45
1:C:210:TRP:HH2	1:C:233:SER:CB	2.30	0.45
1:C:488:PHE:HD1	1:C:490:PRO:HD3	1.82	0.45
1:C:519:LEU:HD11	1:C:581:LEU:HG	1.99	0.45
1:E:120:VAL:HG11	1:E:128:THR:HG21	1.99	0.45
1:A:324:ASN:OD1	1:A:352:ALA:HB3	2.17	0.45
1:A:348:ILE:HD12	1:C:378:TYR:CZ	2.52	0.45
1:E:103:LEU:HD11	1:E:130:VAL:HB	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:65:PRO:O	1:C:69:ASP:HB3	2.17	0.44
1:D:92:ILE:HA	1:D:95:LEU:HG	1.98	0.44
1:D:218:HIS:O	1:D:222:ARG:HG3	2.17	0.44
1:D:446:GLU:H	1:D:446:GLU:CD	2.21	0.44
1:F:504:ALA:HA	1:F:509:SER:HB3	1.99	0.44
1:A:10:ASP:HB3	1:A:166:CYS:SG	2.58	0.44
1:E:68:VAL:HG11	1:E:91:GLU:OE1	2.17	0.44
1:E:243:TRP:HE1	1:E:280:GLN:HG2	1.82	0.44
1:E:459:PRO:HD2	1:E:612:GLY:HA3	1.99	0.44
1:F:32:HIS:NE2	1:F:85:ARG:HB2	2.32	0.44
1:A:427:VAL:HG23	1:A:485:PHE:HB2	2.00	0.44
1:C:369:ILE:HA	1:C:376:ILE:HD11	1.99	0.44
1:E:177:LEU:HB3	1:E:178:PRO:HD3	1.98	0.44
1:E:499:ASP:OD2	1:E:510:ARG:NH1	2.43	0.44
1:F:355:ARG:H	1:F:355:ARG:HG2	1.64	0.44
1:A:417:ILE:HD13	1:A:474:ILE:HG12	2.00	0.44
1:C:529:ASP:OD2	1:C:605:SER:HB3	2.18	0.44
1:D:536:CYS:SG	1:D:568:PRO:HA	2.58	0.44
1:F:417:ILE:O	1:F:421:VAL:HG13	2.18	0.44
1:F:580:LEU:HD23	1:F:642:VAL:HG21	2.00	0.44
1:B:64:HIS:CD2	1:B:66:ILE:HB	2.52	0.44
1:B:500:SER:O	1:B:504:ALA:N	2.51	0.44
1:D:138:ARG:NH1	1:D:192:GLU:OE2	2.51	0.44
1:F:212:LYS:HB3	1:F:213:PRO:HD2	2.00	0.44
1:A:329:ASN:ND2	1:A:352:ALA:O	2.51	0.44
1:A:417:ILE:HD11	1:A:429:PHE:CD1	2.53	0.44
1:A:550:ILE:HG12	1:A:563:ILE:HD12	2.00	0.44
1:B:429:PHE:CZ	1:B:470:LEU:HD22	2.53	0.44
1:B:494:MET:HG3	1:B:641:THR:HG21	1.99	0.44
1:B:574:ILE:HD13	2:B:1100:UGA:H1A1	1.99	0.44
1:A:31:THR:OG1	1:A:32:HIS:N	2.50	0.44
1:B:76:PRO:O	1:B:97:PRO:HD2	2.17	0.44
1:B:90:GLU:HA	1:B:93:LEU:HD23	2.00	0.44
1:B:214:VAL:HG21	1:B:273:ALA:N	2.33	0.44
1:B:324:ASN:OD1	1:B:352:ALA:HB3	2.18	0.44
1:E:456:VAL:C	1:E:458:LYS:H	2.21	0.44
1:E:486:THR:HG21	1:E:558:CYS:HB3	2.00	0.44
1:F:157:VAL:HA	1:F:222:ARG:HB3	2.00	0.44
1:F:426:ARG:NH2	1:F:550:ILE:O	2.45	0.44
1:A:176:ILE:O	1:A:180:MET:HG3	2.18	0.44
1:C:239:LYS:HE2	1:C:241:THR:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:509:SER:HB2	1:D:513:THR:CG2	2.47	0.44
1:D:539:ASP:OD2	1:D:641:THR:OG1	2.32	0.44
1:E:344:TYR:HD1	1:E:363:HIS:HB2	1.82	0.44
1:F:546:ALA:O	1:F:550:ILE:HG13	2.18	0.44
1:A:433:SER:OG	2:A:1100:UGA:O'Q	2.33	0.44
1:A:478:GLY:HA2	1:A:483:LEU:N	2.32	0.44
1:A:567:ASN:HD21	1:A:569:ASP:HB2	1.83	0.44
1:B:6:PHE:HD1	1:B:30:PHE:HB2	1.79	0.44
1:B:288:GLN:O	1:B:292:LEU:N	2.45	0.44
1:C:648:PHE:HA	1:C:651:ARG:HE	1.83	0.44
1:E:102:ASN:HB2	1:E:135:MET:SD	2.58	0.44
1:F:353:ILE:HD11	1:F:364:PHE:CE2	2.53	0.44
1:D:112:ARG:NH1	1:D:140:ASP:O	2.51	0.43
1:B:58:ALA:HB2	1:F:285:ILE:HG12	2.00	0.43
1:C:539:ASP:OD1	1:C:540:ILE:N	2.51	0.43
1:D:192:GLU:O	1:D:192:GLU:HG3	2.18	0.43
1:E:12:GLY:HA2	1:E:82:PHE:HB2	1.99	0.43
1:E:67:TRP:O	1:E:71:ILE:N	2.51	0.43
1:E:394:THR:HG21	1:E:508:SER:HA	2.00	0.43
1:A:353:ILE:HB	1:A:356:PHE:CE1	2.52	0.43
1:B:317:ARG:HB2	1:B:383:CYS:HA	2.00	0.43
1:C:398:TYR:HD2	1:C:460:ARG:HD2	1.83	0.43
1:C:455:PRO:HB2	1:C:457:ASN:OD1	2.18	0.43
1:D:550:ILE:HG12	1:D:630:LEU:HD21	2.01	0.43
1:F:430:PRO:HB3	1:F:488:PHE:CZ	2.53	0.43
1:A:582:LEU:HD21	1:A:597:PHE:CG	2.54	0.43
1:B:426:ARG:HB2	1:B:484:ARG:NH1	2.33	0.43
1:D:243:TRP:HE1	1:D:280:GLN:HG2	1.83	0.43
1:D:292:LEU:HD12	1:D:293:ALA:N	2.32	0.43
1:E:549:ARG:CB	1:E:630:LEU:HD22	2.48	0.43
1:F:79:ILE:HG13	1:F:96:ALA:HB2	2.00	0.43
1:A:9:HIS:CG	1:A:10:ASP:H	2.36	0.43
1:C:185:ILE:O	1:C:185:ILE:HD12	2.19	0.43
1:C:439:CYS:HB3	1:C:444:PHE:CE1	2.54	0.43
1:F:77:ASP:HA	1:F:97:PRO:HD2	2.00	0.43
1:F:247:MET:O	1:F:249:PRO:HD3	2.18	0.43
1:F:414:LEU:HD21	1:F:418:ARG:HE	1.82	0.43
1:F:527:LEU:HB3	1:F:531:GLY:HA3	2.00	0.43
1:F:549:ARG:HD2	1:F:630:LEU:O	2.18	0.43
1:B:284:ASP:OD1	1:B:285:ILE:HG12	2.18	0.43
1:C:329:ASN:ND2	1:C:352:ALA:O	2.43	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:445:ASP:O	1:B:449:SER:HB2	2.18	0.43
1:C:353:ILE:HB	1:C:356:PHE:CE1	2.53	0.43
1:C:546:ALA:HB2	1:C:632:TRP:CD2	2.53	0.43
1:C:594:PHE:HB3	1:C:595:PRO:HD2	2.01	0.43
1:D:93:LEU:HD12	1:D:100:ALA:HB3	2.01	0.43
1:D:418:ARG:HA	1:D:421:VAL:HG22	2.00	0.43
1:E:339:GLU:HA	1:E:361:ARG:NE	2.34	0.43
1:F:415:ARG:HE	1:F:415:ARG:HB3	1.67	0.43
1:A:451:LEU:HB2	1:D:453:VAL:HG23	2.01	0.43
1:D:549:ARG:HB3	1:D:630:LEU:HD22	2.00	0.43
1:E:243:TRP:CD1	1:E:279:GLY:HA2	2.52	0.43
1:E:417:ILE:HD12	1:E:470:LEU:HD21	2.00	0.43
1:B:78:ILE:HG21	1:B:80:PHE:CZ	2.54	0.43
1:C:339:GLU:HG2	1:C:340:ASN:H	1.83	0.43
1:C:497:ARG:HG3	1:C:648:PHE:CZ	2.54	0.43
1:D:84:TYR:CE2	1:D:86:ASN:HB2	2.54	0.43
1:E:435:VAL:HG11	1:E:489:ARG:CZ	2.49	0.43
1:F:512:ILE:CD1	1:F:581:LEU:HD11	2.48	0.43
1:A:426:ARG:HA	1:A:484:ARG:O	2.18	0.43
1:C:112:ARG:NH1	1:C:140:ASP:O	2.52	0.43
1:C:150:VAL:HG21	1:C:168:ALA:HB2	2.01	0.43
1:C:184:ASP:CG	1:C:186:PRO:HD3	2.40	0.43
1:D:81:SER:HB3	1:D:102:ASN:HA	2.01	0.43
1:D:586:ASP:O	1:D:591:ARG:HD2	2.19	0.42
1:A:204:GLU:O	1:A:204:GLU:HG2	2.19	0.42
1:C:48:GLN:O	1:C:52:LEU:HG	2.19	0.42
1:C:133:HIS:HD2	1:C:142:GLY:H	1.66	0.42
1:E:120:VAL:HG23	1:E:121:LEU:HD22	2.01	0.42
1:E:324:ASN:OD1	1:E:352:ALA:HB3	2.19	0.42
1:F:429:PHE:HB3	1:F:487:LEU:HD23	2.01	0.42
1:A:109:PRO:O	1:A:195:SER:HA	2.19	0.42
1:A:417:ILE:HD12	1:A:470:LEU:HD21	2.00	0.42
1:A:546:ALA:HB2	1:A:632:TRP:CE2	2.54	0.42
1:C:84:TYR:CE2	1:C:86:ASN:HB2	2.54	0.42
1:D:202:ARG:HB2	1:D:203:PRO:HD2	2.01	0.42
1:D:418:ARG:HD3	1:D:477:TYR:OH	2.18	0.42
1:E:211:HIS:HD2	1:E:256:PRO:HB2	1.84	0.42
1:F:344:TYR:HD1	1:F:363:HIS:HB2	1.85	0.42
1:F:369:ILE:HA	1:F:376:ILE:CD1	2.49	0.42
1:F:566:GLY:HA3	1:F:621:PRO:HG3	2.01	0.42
1:A:287:VAL:HG12	1:E:56:VAL:HG13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:431:SER:HB3	1:A:489:ARG:HG2	2.00	0.42
1:E:504:ALA:HA	1:E:509:SER:HB2	2.02	0.42
1:F:121:LEU:HD23	1:F:223:ALA:HA	2.00	0.42
1:A:430:PRO:HB3	1:A:488:PHE:CZ	2.54	0.42
1:B:549:ARG:HH11	1:B:632:TRP:HB2	1.85	0.42
1:B:605:SER:HB2	1:B:613:TYR:HD2	1.84	0.42
1:C:2:LYS:HG2	1:C:25:GLU:OE1	2.19	0.42
1:C:84:TYR:HE2	1:C:86:ASN:HB2	1.84	0.42
1:D:76:PRO:O	1:D:97:PRO:HD2	2.19	0.42
1:D:205:ASP:C	1:D:207:LEU:H	2.23	0.42
1:D:279:GLY:O	1:D:287:VAL:N	2.51	0.42
1:E:121:LEU:O	1:E:219:ASN:HB3	2.20	0.42
1:E:394:THR:HG21	1:E:509:SER:N	2.35	0.42
1:A:395:PRO:HA	1:A:398:TYR:CD2	2.55	0.42
1:A:398:TYR:HD2	1:A:460:ARG:HD2	1.85	0.42
1:C:344:TYR:CD1	1:C:363:HIS:HB2	2.55	0.42
1:C:415:ARG:HE	1:C:415:ARG:HB3	1.69	0.42
1:D:277:ILE:O	1:D:289:GLY:N	2.49	0.42
1:A:157:VAL:HG12	1:A:160:THR:HG23	2.01	0.42
1:A:407:GLU:O	1:A:412:GLU:HG2	2.19	0.42
1:B:422:LYS:HG2	1:B:423:TYR:CD1	2.55	0.42
1:D:19:VAL:HG22	1:D:177:LEU:HD21	2.01	0.42
1:D:374:GLU:HG3	1:D:375:TRP:N	2.35	0.42
1:E:185:ILE:O	1:E:185:ILE:HD12	2.19	0.42
1:E:512:ILE:HD11	1:E:581:LEU:HD21	2.01	0.42
1:A:505:ARG:HE	1:A:505:ARG:HB2	1.68	0.42
1:B:194:ASP:OD1	1:B:194:ASP:N	2.53	0.42
1:C:59:PRO:CG	1:C:62:VAL:HG22	2.50	0.42
1:C:208:ILE:CD1	1:C:220:LEU:HD22	2.50	0.42
1:C:410:PHE:HA	1:C:470:LEU:HD12	2.02	0.42
1:D:359:HIS:CE1	1:D:361:ARG:HB2	2.54	0.42
1:E:549:ARG:HB2	1:E:630:LEU:HD22	2.01	0.42
1:F:427:VAL:HG23	1:F:485:PHE:HB2	2.01	0.42
1:A:334:ARG:O	1:A:338:GLU:HG2	2.20	0.42
1:A:431:SER:O	1:A:489:ARG:HA	2.19	0.42
1:B:435:VAL:HG11	1:B:489:ARG:NE	2.35	0.42
1:C:208:ILE:HD12	1:C:217:VAL:HG13	2.01	0.42
1:C:355:ARG:HG3	1:C:356:PHE:CD2	2.54	0.42
1:F:543:GLY:HA2	1:F:565:ILE:HG21	2.01	0.42
1:B:121:LEU:HD21	1:B:161:LEU:HD23	2.01	0.42
1:D:248:CYS:O	1:D:273:ALA:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:90:GLU:HA	1:E:93:LEU:HD23	2.02	0.42
1:F:4:VAL:O	1:F:79:ILE:HA	2.20	0.42
1:F:368:ASP:H	1:F:372:HIS:CD2	2.38	0.42
1:A:417:ILE:O	1:A:421:VAL:HG13	2.19	0.41
1:A:444:PHE:O	1:A:622:SER:HB3	2.19	0.41
1:A:655:ILE:HD12	1:A:655:ILE:O	2.20	0.41
1:C:32:HIS:NE2	1:C:85:ARG:HB2	2.35	0.41
1:C:260:ILE:HG13	1:C:266:ARG:O	2.20	0.41
1:D:200:ARG:HG2	1:D:201:ARG:N	2.35	0.41
1:F:470:LEU:O	1:F:474:ILE:HG13	2.20	0.41
1:A:93:LEU:HD12	1:A:100:ALA:HB3	2.02	0.41
1:B:288:GLN:HG2	1:B:289:GLY:N	2.34	0.41
1:D:468:GLN:O	1:D:472:ARG:HG3	2.20	0.41
1:F:9:HIS:CG	1:F:10:ASP:H	2.37	0.41
1:F:31:THR:OG1	1:F:32:HIS:N	2.51	0.41
1:F:334:ARG:HD2	1:F:334:ARG:HA	1.89	0.41
1:F:535:ARG:NH2	1:F:615:ASP:OD1	2.52	0.41
1:B:427:VAL:HG12	1:B:429:PHE:HB2	2.01	0.41
1:C:426:ARG:HA	1:C:484:ARG:O	2.21	0.41
1:C:613:TYR:CE2	1:C:615:ASP:HB2	2.55	0.41
1:D:390:VAL:HG12	1:D:408:LEU:HD21	2.02	0.41
1:D:421:VAL:HG12	1:D:483:LEU:HD13	2.03	0.41
1:E:250:ASP:O	1:E:252:GLN:N	2.46	0.41
1:F:2:LYS:O	1:F:77:ASP:HB2	2.20	0.41
1:F:299:VAL:O	1:F:301:GLY:N	2.53	0.41
1:A:604:GLU:HB3	1:D:64:HIS:CD2	2.56	0.41
1:B:64:HIS:ND1	1:B:65:PRO:HD2	2.36	0.41
1:B:368:ASP:HB3	1:B:371:ILE:HD12	2.03	0.41
1:B:519:LEU:HD13	1:B:585:PHE:CD2	2.55	0.41
1:B:605:SER:HB2	1:B:613:TYR:CD2	2.55	0.41
1:C:339:GLU:O	1:C:361:ARG:NH1	2.54	0.41
1:C:394:THR:HG22	1:C:396:ILE:HG22	2.01	0.41
1:A:374:GLU:HG3	1:A:375:TRP:N	2.35	0.41
1:B:220:LEU:O	1:B:224:VAL:HG22	2.20	0.41
1:D:6:PHE:HE1	1:D:30:PHE:CD2	2.38	0.41
1:F:84:TYR:CE2	1:F:86:ASN:HB2	2.54	0.41
1:A:177:LEU:HB3	1:A:178:PRO:HD3	2.03	0.41
1:B:416:ILE:O	1:B:419:TYR:HB2	2.20	0.41
1:C:148:GLN:HG2	1:C:172:LEU:HD12	2.02	0.41
1:D:353:ILE:HB	1:D:356:PHE:CE1	2.54	0.41
1:E:93:LEU:HD12	1:E:100:ALA:CB	2.51	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:638:MET:O	1:E:642:VAL:HG23	2.21	0.41
1:F:30:PHE:HA	1:F:57:TYR:O	2.20	0.41
1:A:62:VAL:O	1:A:64:HIS:N	2.54	0.41
1:A:242:ILE:HD13	1:A:276:ILE:HG12	2.02	0.41
1:A:288:GLN:HG2	1:A:289:GLY:N	2.35	0.41
1:C:77:ASP:HA	1:C:97:PRO:HD2	2.01	0.41
1:C:112:ARG:NH1	1:C:141:ALA:HA	2.36	0.41
1:C:429:PHE:CZ	1:C:470:LEU:HD22	2.56	0.41
1:D:456:VAL:H	1:D:456:VAL:HG22	1.58	0.41
2:E:1100:UGA:PB	2:E:1100:UGA:H5'2	2.60	0.41
1:F:536:CYS:SG	1:F:568:PRO:HA	2.60	0.41
1:A:536:CYS:SG	1:A:620:LYS:HA	2.61	0.41
1:D:78:ILE:HG12	1:D:98:ALA:HB3	2.02	0.41
1:F:386:VAL:HG12	1:F:388:PRO:HD3	2.02	0.41
1:F:534:LYS:HD3	1:F:571:GLU:HG2	2.02	0.41
1:A:112:ARG:HE	1:A:195:SER:HB2	1.86	0.41
1:A:118:ASN:ND2	1:A:223:ALA:O	2.48	0.41
1:A:493:TRP:CD1	1:A:538:THR:HB	2.55	0.41
1:B:118:ASN:O	1:B:122:VAL:HG23	2.21	0.41
1:B:120:VAL:HG23	1:B:121:LEU:HD22	2.02	0.41
1:B:204:GLU:HG3	1:B:204:GLU:O	2.21	0.41
1:B:332:THR:HG21	1:B:356:PHE:CE1	2.56	0.41
1:C:111:TYR:HE1	1:C:198:TYR:HE2	1.69	0.41
1:C:426:ARG:NH2	1:C:550:ILE:O	2.49	0.41
1:C:466:SER:HA	1:F:469:LEU:HD11	2.01	0.41
1:C:471:ASP:HA	1:C:474:ILE:HD12	2.03	0.41
1:C:647:ASP:C	1:C:651:ARG:HH21	2.24	0.41
1:D:72:ALA:HB2	1:D:95:LEU:HD13	2.03	0.41
1:D:321:LEU:HD22	1:D:346:MET:CE	2.51	0.41
1:D:375:TRP:CZ2	1:E:375:TRP:HZ2	2.39	0.41
1:F:7:ALA:HB1	1:F:12:GLY:CA	2.51	0.41
1:F:78:ILE:HG21	1:F:80:PHE:CZ	2.56	0.41
1:A:609:TYR:OH	2:A:1100:UGA:H2A1	2.20	0.41
1:B:445:ASP:HA	1:B:622:SER:HB3	2.03	0.41
1:D:353:ILE:HD11	1:D:364:PHE:CE2	2.56	0.41
1:D:410:PHE:HD1	1:D:470:LEU:HB2	1.86	0.41
1:E:577:LEU:O	1:E:581:LEU:HG	2.21	0.41
1:E:581:LEU:HD23	1:E:642:VAL:CG1	2.49	0.41
1:F:549:ARG:HB3	1:F:630:LEU:HD22	2.03	0.41
1:B:429:PHE:HB3	1:B:487:LEU:HD23	2.02	0.40
1:C:143:GLU:CB	1:C:187:SER:HB2	2.50	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:431:SER:CB	1:C:489:ARG:HG2	2.50	0.40
1:F:192:GLU:O	1:F:192:GLU:HG3	2.22	0.40
1:A:446:GLU:OE1	1:A:446:GLU:N	2.43	0.40
1:A:533:GLN:HB2	1:A:617:ALA:O	2.22	0.40
1:B:343:VAL:HG23	1:B:362:PHE:CD1	2.52	0.40
1:B:365:VAL:HG21	1:B:379:HIS:CE1	2.57	0.40
1:C:2:LYS:O	1:C:77:ASP:HB2	2.21	0.40
1:C:184:ASP:OD1	1:C:185:ILE:N	2.54	0.40
1:E:417:ILE:HD11	1:E:429:PHE:CD1	2.55	0.40
1:F:64:HIS:ND1	1:F:65:PRO:HD2	2.36	0.40
1:F:65:PRO:O	1:F:69:ASP:HB2	2.21	0.40
1:A:460:ARG:NH1	1:A:613:TYR:OH	2.54	0.40
1:B:417:ILE:O	1:B:421:VAL:HG13	2.20	0.40
1:B:581:LEU:HA	1:B:642:VAL:HG11	2.03	0.40
1:C:129:GLY:HA2	1:C:165:LEU:HD11	2.03	0.40
1:C:357:LEU:HD23	1:C:357:LEU:HA	1.87	0.40
1:C:528:ILE:HD13	2:C:1100:UGA:N3	2.37	0.40
1:D:111:TYR:HD1	1:D:198:TYR:CE2	2.39	0.40
1:D:421:VAL:HG12	1:D:483:LEU:HD22	2.02	0.40
1:E:30:PHE:HA	1:E:57:TYR:O	2.22	0.40
1:E:143:GLU:HB3	1:E:187:SER:HB2	2.02	0.40
1:E:336:LEU:HA	1:E:336:LEU:HD12	1.83	0.40
1:A:72:ALA:HB2	1:A:95:LEU:HD13	2.03	0.40
1:B:346:MET:HA	1:B:365:VAL:O	2.21	0.40
1:B:546:ALA:O	1:B:550:ILE:HG13	2.22	0.40
1:D:429:PHE:CZ	1:D:470:LEU:HD22	2.57	0.40
1:D:446:GLU:HG2	1:D:564:ASN:HB2	2.03	0.40
1:D:597:PHE:HZ	1:D:600:PHE:CE1	2.40	0.40
1:E:67:TRP:O	1:E:71:ILE:HG13	2.20	0.40
1:E:258:SER:HA	1:E:302:ALA:HA	2.03	0.40
1:A:647:ASP:OD1	1:A:651:ARG:NH2	2.53	0.40
1:B:468:GLN:O	1:B:471:ASP:HB2	2.21	0.40
1:C:317:ARG:HB2	1:C:383:CYS:HA	2.03	0.40
1:E:111:TYR:CE1	1:E:198:TYR:HE2	2.40	0.40
1:E:218:HIS:CD2	1:E:222:ARG:HG3	2.56	0.40
1:E:458:LYS:HZ3	1:E:606:ARG:HH21	1.70	0.40
1:F:177:LEU:HB3	1:F:178:PRO:HD3	2.03	0.40

There are no symmetry-related clashes.

## 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	633/660 (96%)	578 (91%)	52 (8%)	3 (0%)	29	68
1	B	632/660 (96%)	574 (91%)	55 (9%)	3 (0%)	29	68
1	C	633/660 (96%)	568 (90%)	61 (10%)	4 (1%)	25	64
1	D	632/660 (96%)	564 (89%)	64 (10%)	4 (1%)	25	64
1	E	632/660 (96%)	571 (90%)	57 (9%)	4 (1%)	25	64
1	F	633/660 (96%)	567 (90%)	60 (10%)	6 (1%)	17	57
All	All	3795/3960 (96%)	3422 (90%)	349 (9%)	24 (1%)	25	64

All (24) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	253	GLY
1	E	250	ASP
1	F	251	ALA
1	F	300	ALA
1	A	63	ASN
1	C	253	GLY
1	D	253	GLY
1	D	300	ALA
1	E	63	ASN
1	F	63	ASN
1	F	250	ASP
1	B	300	ALA
1	C	252	GLN
1	D	63	ASN
1	E	113	GLY
1	F	183	GLY
1	C	251	ALA
1	C	299	VAL
1	B	236	GLY
1	F	589	PRO

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Mol	Chain	Res	Type
1	E	253	GLY
1	A	297	GLY
1	A	299	VAL
1	D	299	VAL

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	538/555 (97%)	528 (98%)	10 (2%)	57	80
1	B	538/555 (97%)	531 (99%)	7 (1%)	69	86
1	C	538/555 (97%)	534 (99%)	4 (1%)	84	93
1	D	538/555 (97%)	532 (99%)	6 (1%)	73	88
1	E	538/555 (97%)	535 (99%)	3 (1%)	86	94
1	F	538/555 (97%)	537 (100%)	1 (0%)	93	98
All	All	3228/3330 (97%)	3197 (99%)	31 (1%)	76	88

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	ARG
1	A	134	ARG
1	A	155	ASP
1	A	182	CYS
1	A	252	GLN
1	A	304	LEU
1	A	450	ASN
1	A	556	ASP
1	A	567	ASN
1	A	606	ARG
1	B	112	ARG
1	B	194	ASP
1	B	271	ASP
1	B	460	ARG

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	B	514	GLN
1	B	564	ASN
1	B	567	ASN
1	C	64	HIS
1	C	112	ARG
1	C	326	PHE
1	C	510	ARG
1	D	112	ARG
1	D	125	GLU
1	D	138	ARG
1	D	351	ASN
1	D	356	PHE
1	D	514	GLN
1	E	356	PHE
1	E	409	ASP
1	E	529	ASP
1	F	497	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	171	GLN
1	A	174	ASN
1	A	252	GLN
1	A	363	HIS
1	A	567	ASN
1	A	570	ASN
1	B	174	ASN
1	B	280	GLN
1	B	372	HIS
1	B	518	ASN
1	B	567	ASN
1	B	588	HIS
1	B	614	GLN
1	C	102	ASN
1	C	174	ASN
1	C	238	GLN
1	C	379	HIS
1	C	450	ASN
1	C	518	ASN
1	C	614	GLN
1	D	123	ASN

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Mol	Chain	Res	Type
1	D	174	ASN
1	D	450	ASN
1	D	625	ASN
1	E	48	GLN
1	E	102	ASN
1	E	211	HIS
1	E	218	HIS
1	E	330	HIS
1	E	518	ASN
1	E	593	HIS
1	E	601	GLN
1	E	625	ASN
1	F	61	ASN
1	F	174	ASN
1	F	235	ASN
1	F	372	HIS
1	F	450	ASN
1	F	518	ASN
1	F	625	ASN

### 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](#)

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	UGA	B	1100	-	32,39,39	1.52	6 (18%)	42,60,60	1.82	7 (16%)
2	UGA	C	1100	-	32,39,39	1.48	6 (18%)	42,60,60	1.63	5 (11%)
2	UGA	D	1100	-	32,39,39	1.47	6 (18%)	42,60,60	1.74	5 (11%)
2	UGA	F	1100	-	32,39,39	1.43	5 (15%)	42,60,60	1.71	7 (16%)
2	UGA	A	1100	-	32,39,39	1.49	6 (18%)	42,60,60	1.77	7 (16%)
2	UGA	E	1100	-	32,39,39	1.50	6 (18%)	42,60,60	1.63	6 (14%)

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	UGA	B	1100	-	-	0/23/61/61	0/3/3/3
2	UGA	C	1100	-	-	6/23/61/61	0/3/3/3
2	UGA	D	1100	-	-	1/23/61/61	0/3/3/3
2	UGA	F	1100	-	-	6/23/61/61	0/3/3/3
2	UGA	A	1100	-	-	5/23/61/61	0/3/3/3
2	UGA	E	1100	-	-	4/23/61/61	0/3/3/3

All (35) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1100	UGA	O5'-C5'	-3.21	1.38	1.43
2	C	1100	UGA	O5'-C5'	-3.11	1.38	1.43
2	D	1100	UGA	O5'-C5'	-3.10	1.38	1.43
2	B	1100	UGA	O5'-C5'	-3.04	1.38	1.43
2	A	1100	UGA	O5'-C5'	-2.99	1.38	1.43
2	B	1100	UGA	C2D-C1D	-2.95	1.49	1.53
2	D	1100	UGA	C2D-C1D	-2.94	1.49	1.53
2	C	1100	UGA	C2D-C1D	-2.92	1.49	1.53
2	A	1100	UGA	C2D-C1D	-2.91	1.49	1.53
2	F	1100	UGA	C2D-C1D	-2.90	1.49	1.53
2	E	1100	UGA	C2D-C1D	-2.90	1.49	1.53
2	F	1100	UGA	O5'-C5'	-2.85	1.38	1.43
2	B	1100	UGA	C4'-C5'	-2.68	1.48	1.53
2	E	1100	UGA	C4'-C5'	-2.56	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1100	UGA	C4'-C5'	-2.51	1.49	1.53
2	B	1100	UGA	O3D-C3D	-2.40	1.37	1.43
2	C	1100	UGA	O3D-C3D	-2.40	1.37	1.43
2	F	1100	UGA	O3D-C3D	-2.38	1.37	1.43
2	A	1100	UGA	O3D-C3D	-2.34	1.37	1.43
2	D	1100	UGA	O3D-C3D	-2.32	1.37	1.43
2	E	1100	UGA	O3D-C3D	-2.32	1.37	1.43
2	B	1100	UGA	C2D-C3D	-2.28	1.47	1.53
2	C	1100	UGA	C2D-C3D	-2.27	1.47	1.53
2	C	1100	UGA	C4'-C5'	-2.25	1.49	1.53
2	E	1100	UGA	C2D-C3D	-2.21	1.47	1.53
2	F	1100	UGA	C2D-C3D	-2.19	1.47	1.53
2	D	1100	UGA	C4'-C5'	-2.19	1.49	1.53
2	D	1100	UGA	C2D-C3D	-2.18	1.47	1.53
2	C	1100	UGA	O4D-C4D	-2.18	1.40	1.45
2	E	1100	UGA	O4D-C4D	-2.16	1.40	1.45
2	A	1100	UGA	C2D-C3D	-2.16	1.47	1.53
2	A	1100	UGA	O4D-C4D	-2.16	1.40	1.45
2	B	1100	UGA	O4D-C4D	-2.14	1.40	1.45
2	F	1100	UGA	O4D-C4D	-2.14	1.40	1.45
2	D	1100	UGA	O4D-C4D	-2.12	1.40	1.45

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1100	UGA	O'Q-C6'-O'P	7.54	141.21	124.09
2	E	1100	UGA	O'Q-C6'-O'P	7.46	141.03	124.09
2	A	1100	UGA	O'Q-C6'-O'P	7.40	140.88	124.09
2	B	1100	UGA	O'Q-C6'-O'P	7.39	140.87	124.09
2	C	1100	UGA	O'Q-C6'-O'P	7.33	140.74	124.09
2	F	1100	UGA	O'Q-C6'-O'P	7.32	140.70	124.09
2	B	1100	UGA	C1'-O5'-C5'	4.55	119.70	112.20
2	A	1100	UGA	C1'-O5'-C5'	3.83	118.50	112.20
2	B	1100	UGA	O5'-C1'-C2'	3.62	118.02	110.35
2	D	1100	UGA	C3D-C2D-C1D	3.36	106.03	100.98
2	F	1100	UGA	PA-O3A-PB	-3.24	121.69	132.83
2	B	1100	UGA	C1'-C2'-C3'	3.15	116.57	110.00
2	F	1100	UGA	O'P-C6'-C5'	-3.14	109.30	120.81
2	D	1100	UGA	O'P-C6'-C5'	-3.13	109.32	120.81
2	F	1100	UGA	C3'-C4'-C5'	3.11	114.56	109.25
2	C	1100	UGA	O'P-C6'-C5'	-3.04	109.66	120.81
2	B	1100	UGA	PA-O3A-PB	-3.03	122.42	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1100	UGA	O'P-C6'-C5'	-3.01	109.78	120.81
2	E	1100	UGA	O'P-C6'-C5'	-3.00	109.81	120.81
2	E	1100	UGA	O3A-PB-O3B	2.97	108.48	102.48
2	B	1100	UGA	O'P-C6'-C5'	-2.94	110.01	120.81
2	A	1100	UGA	PA-O3A-PB	-2.91	122.83	132.83
2	C	1100	UGA	PA-O3A-PB	-2.79	123.24	132.83
2	F	1100	UGA	O5'-C5'-C4'	2.72	114.43	109.57
2	A	1100	UGA	C3D-C2D-C1D	2.58	104.86	100.98
2	A	1100	UGA	O3A-PB-O3B	2.58	107.68	102.48
2	E	1100	UGA	PA-O3A-PB	-2.55	124.08	132.83
2	F	1100	UGA	O3A-PB-O3B	2.51	107.55	102.48
2	D	1100	UGA	PA-O3A-PB	-2.50	124.24	132.83
2	C	1100	UGA	C1'-O5'-C5'	2.46	116.25	112.20
2	C	1100	UGA	C1'-C2'-C3'	2.34	114.88	110.00
2	D	1100	UGA	O3A-PB-O3B	2.27	107.06	102.48
2	E	1100	UGA	C1'-C2'-C3'	2.23	114.64	110.00
2	A	1100	UGA	O5'-C1'-C2'	2.18	114.97	110.35
2	B	1100	UGA	O3A-PB-O3B	2.18	106.87	102.48
2	F	1100	UGA	C1'-O5'-C5'	2.05	115.57	112.20
2	E	1100	UGA	C3D-C2D-C1D	2.01	104.00	100.98

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1100	UGA	C5D-O5D-PA-O2A
2	D	1100	UGA	C2D-C1D-N1-C6
2	E	1100	UGA	O4D-C1D-N1-C6
2	E	1100	UGA	C2D-C1D-N1-C6
2	F	1100	UGA	C1'-O3B-PB-O3A
2	F	1100	UGA	C5D-O5D-PA-O1A
2	F	1100	UGA	C5D-O5D-PA-O2A
2	F	1100	UGA	O4D-C4D-C5D-O5D
2	F	1100	UGA	C3D-C4D-C5D-O5D
2	C	1100	UGA	C3D-C4D-C5D-O5D
2	C	1100	UGA	O4D-C4D-C5D-O5D
2	C	1100	UGA	C1'-O3B-PB-O3A
2	C	1100	UGA	C5D-O5D-PA-O3A
2	E	1100	UGA	C5D-O5D-PA-O3A
2	A	1100	UGA	PA-O3A-PB-O1B
2	C	1100	UGA	C5D-O5D-PA-O1A
2	A	1100	UGA	O4D-C4D-C5D-O5D

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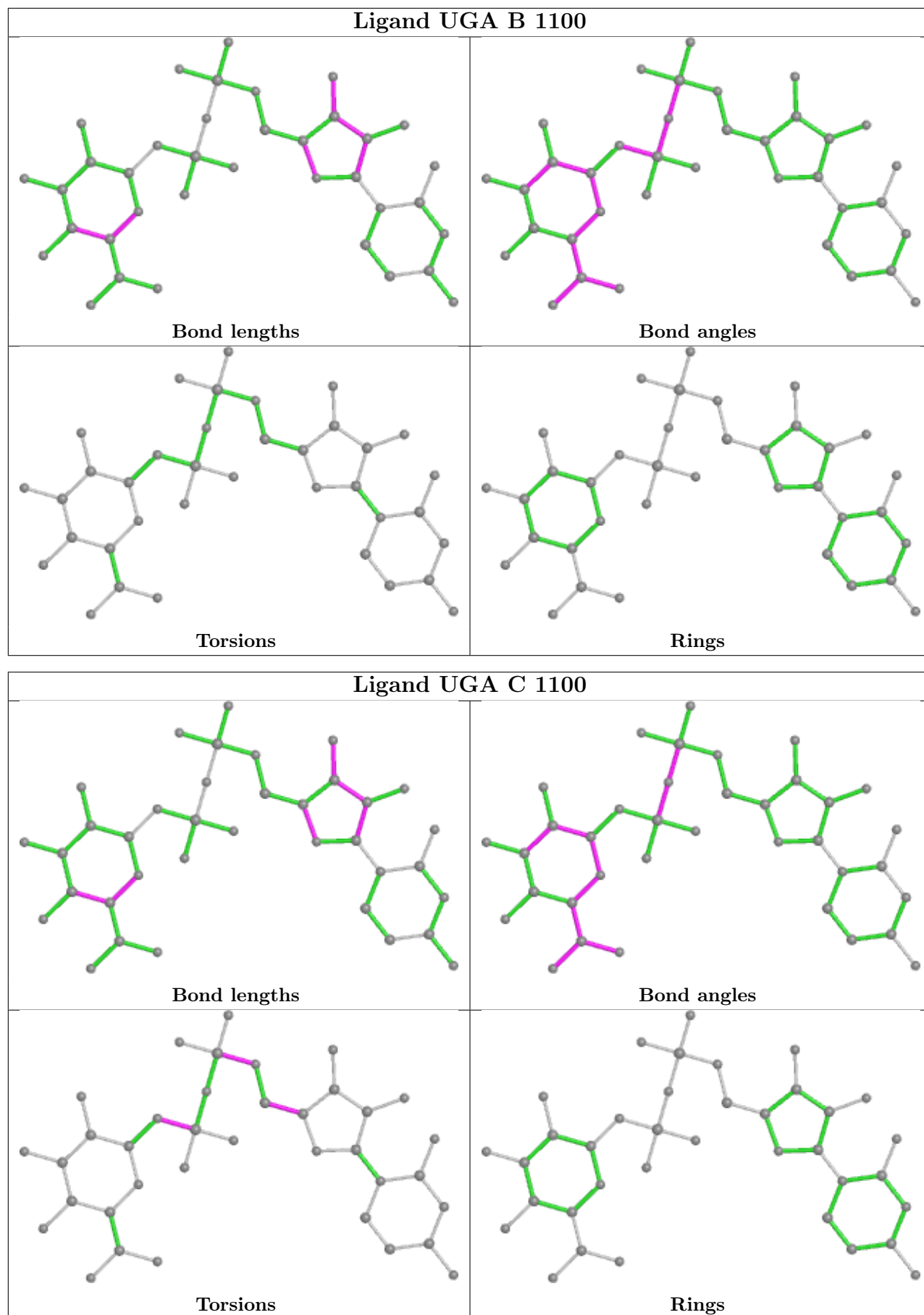
Mol	Chain	Res	Type	Atoms
2	A	1100	UGA	C3D-C4D-C5D-O5D
2	F	1100	UGA	C5D-O5D-PA-O3A
2	A	1100	UGA	O5'-C5'-C6'-O'P
2	A	1100	UGA	O5'-C5'-C6'-O'Q
2	E	1100	UGA	C5D-O5D-PA-O2A

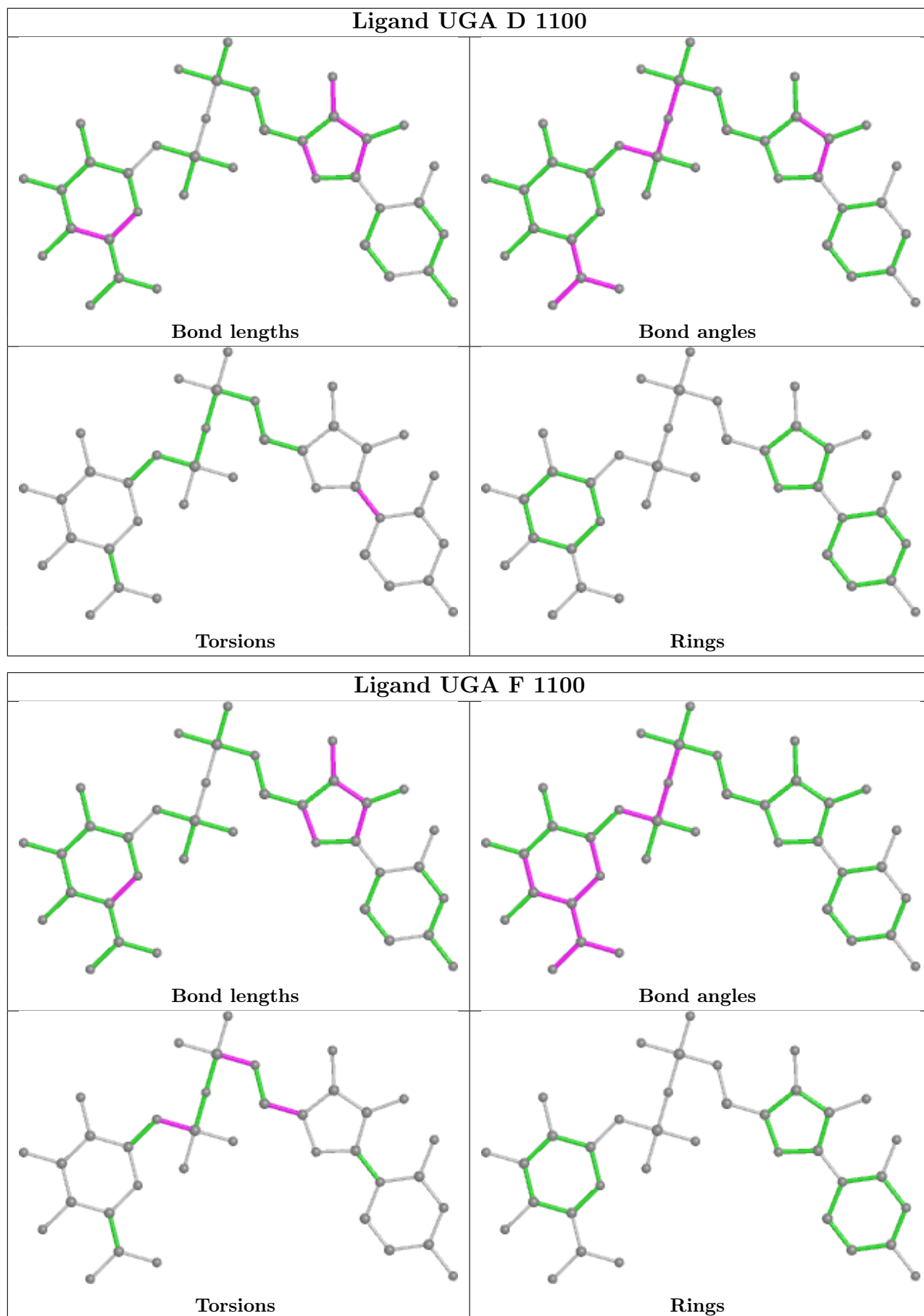
There are no ring outliers.

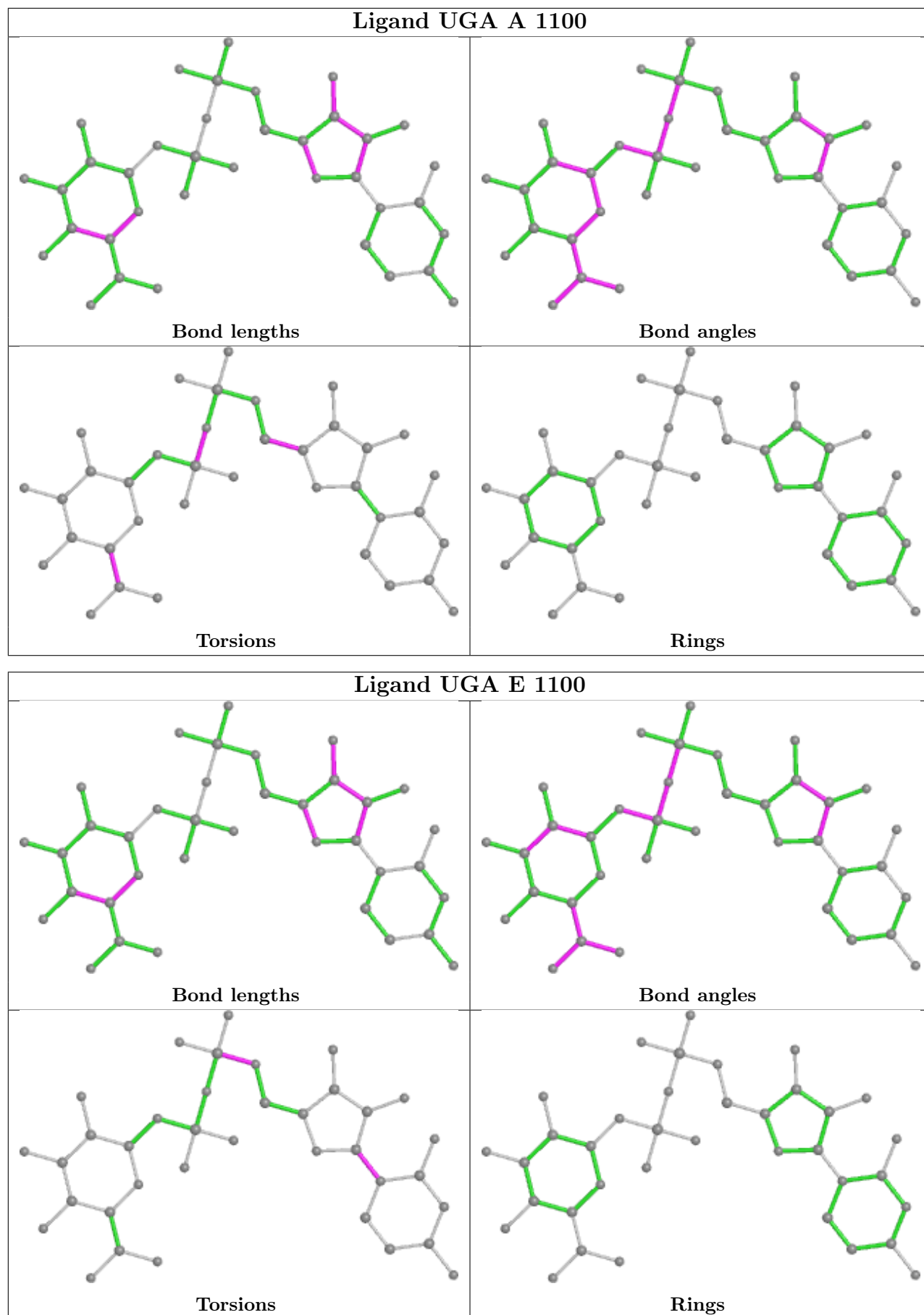
6 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1100	UGA	4	0
2	C	1100	UGA	5	0
2	D	1100	UGA	3	0
2	F	1100	UGA	3	0
2	A	1100	UGA	2	0
2	E	1100	UGA	2	0

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

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	639/660 (96%)	-0.17	12 (1%) 66 51	63, 124, 164, 193	0
1	B	638/660 (96%)	-0.27	8 (1%) 77 63	61, 116, 158, 177	0
1	C	639/660 (96%)	-0.29	5 (0%) 86 75	61, 108, 162, 176	0
1	D	638/660 (96%)	-0.33	2 (0%) 94 88	66, 110, 140, 181	0
1	E	638/660 (96%)	-0.36	3 (0%) 91 83	60, 106, 136, 158	0
1	F	639/660 (96%)	-0.27	7 (1%) 80 68	60, 106, 136, 171	0
All	All	3831/3960 (96%)	-0.28	37 (0%) 82 70	60, 111, 155, 193	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	102	ASN	5.8
1	B	81	SER	3.8
1	A	182	CYS	3.6
1	B	102	ASN	3.6
1	D	43	GLY	3.2
1	C	283	ASP	3.1
1	B	109	PRO	2.9
1	B	195	SER	2.9
1	F	102	ASN	2.9
1	F	492	ASN	2.7
1	F	433	SER	2.7
1	F	656	ALA	2.6
1	A	104	HIS	2.6
1	A	252	GLN	2.5
1	C	254	ALA	2.5
1	C	195	SER	2.5
1	A	432	THR	2.5
1	A	433	SER	2.4
1	E	253	GLY	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	192	GLU	2.4
1	F	490	PRO	2.3
1	A	197	TYR	2.3
1	C	102	ASN	2.3
1	F	339	GLU	2.2
1	B	431	SER	2.2
1	F	254	ALA	2.2
1	C	24	TYR	2.2
1	E	611	LYS	2.2
1	E	196	THR	2.2
1	A	194	ASP	2.2
1	D	252	GLN	2.2
1	A	492	ASN	2.2
1	B	170	ARG	2.1
1	A	81	SER	2.1
1	A	655	ILE	2.1
1	A	195	SER	2.1
1	B	104	HIS	2.0

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

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

## 6.3 Carbohydrates [i](#)

There are no 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(Å <sup>2</sup> )	Q<0.9
2	UGA	A	1100	37/37	0.88	0.31	102,109,128,132	0
2	UGA	F	1100	37/37	0.88	0.26	101,114,123,130	0
2	UGA	C	1100	37/37	0.91	0.27	84,94,107,110	0
2	UGA	B	1100	37/37	0.91	0.24	95,105,114,119	0
2	UGA	E	1100	37/37	0.92	0.23	87,100,112,115	0

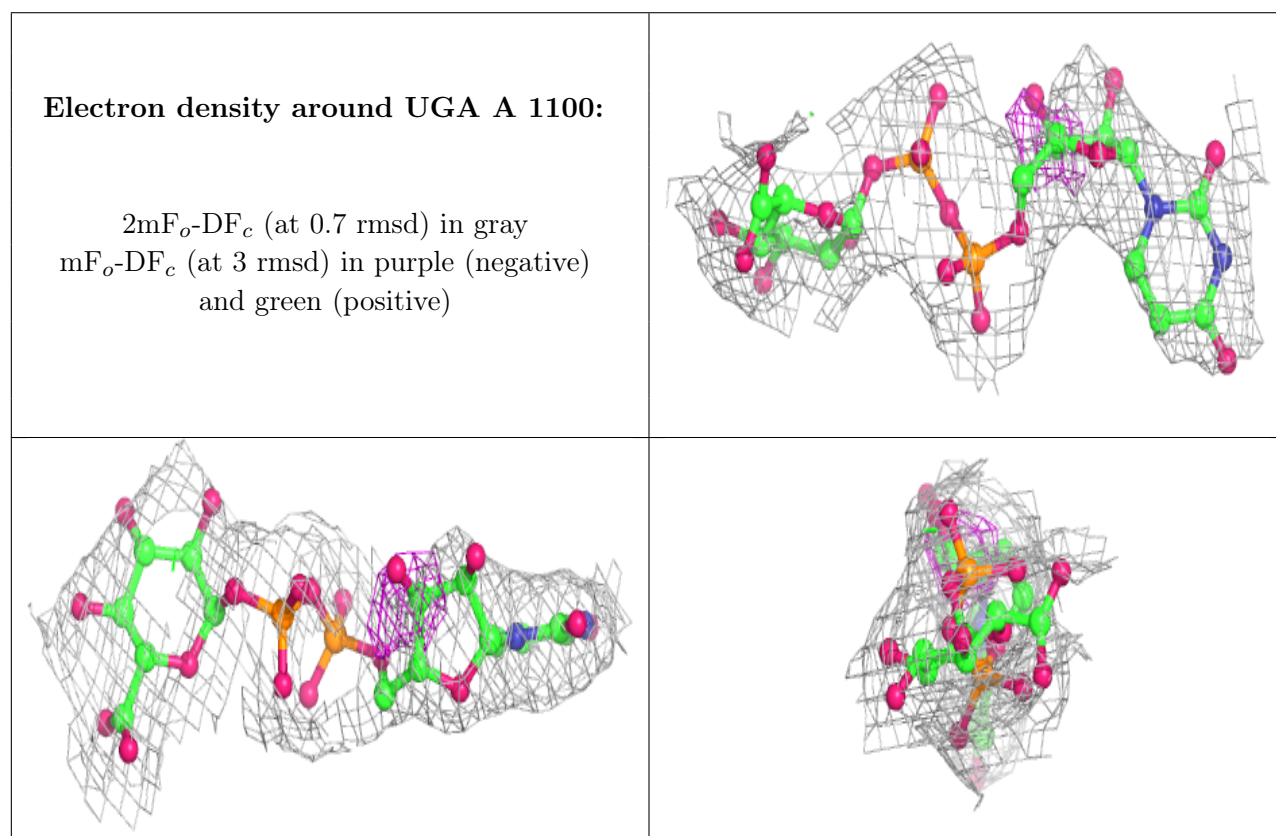
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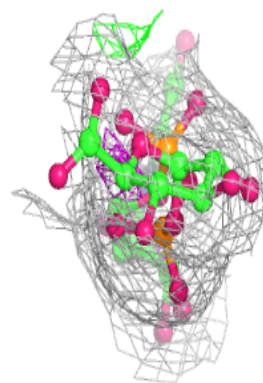
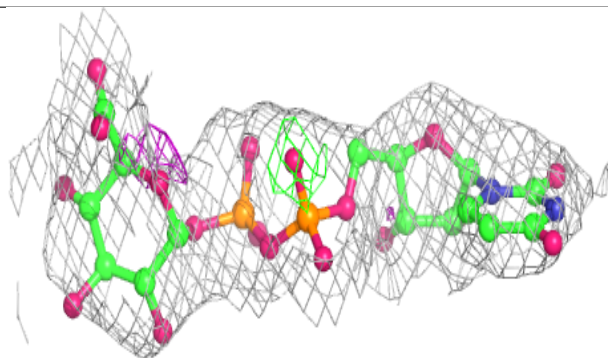
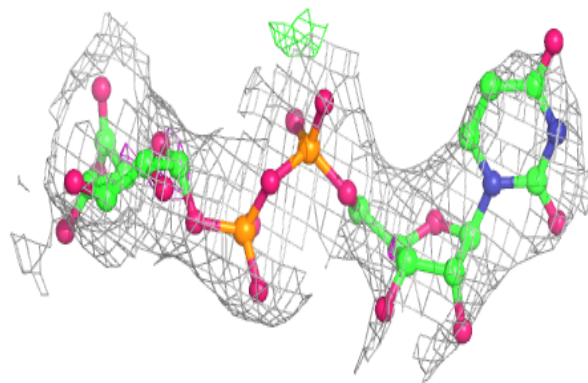
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	UGA	D	1100	37/37	0.92	0.28	98,111,129,138	0

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.

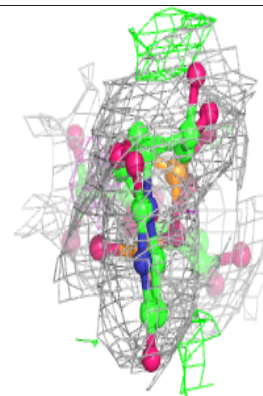
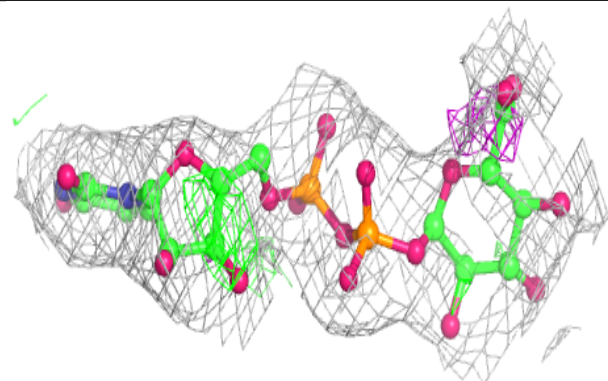
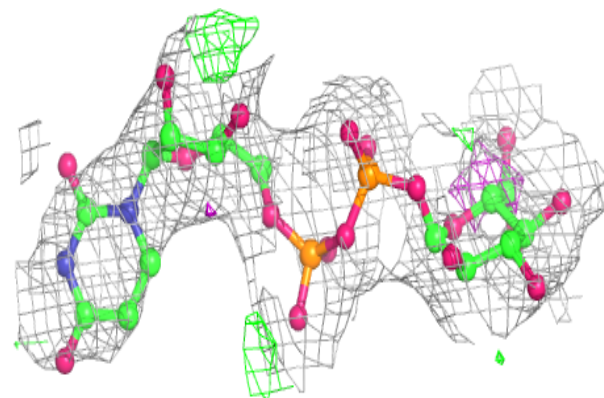


**Electron density around UGA F 1100:**

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

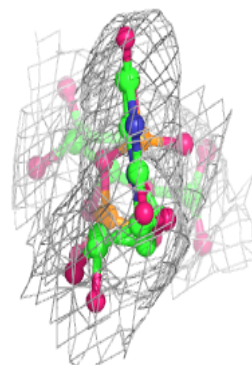
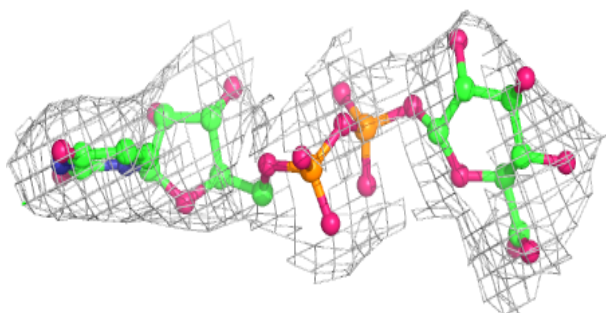
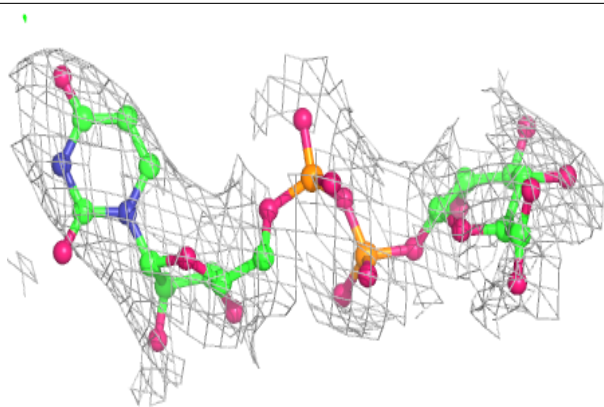
**Electron density around UGA C 1100:**

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

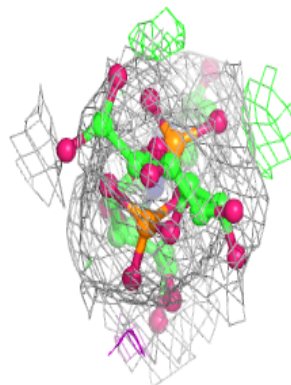
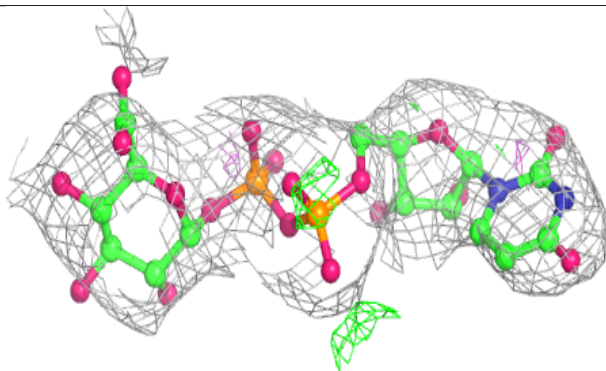
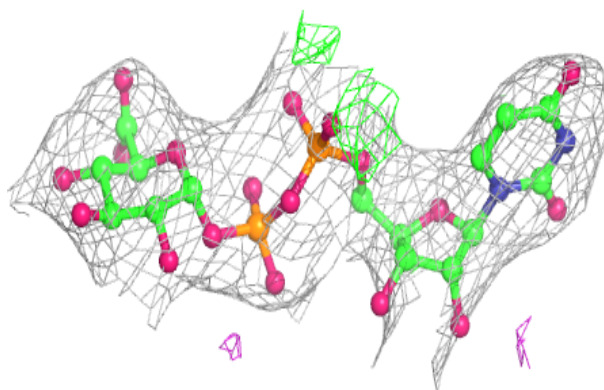


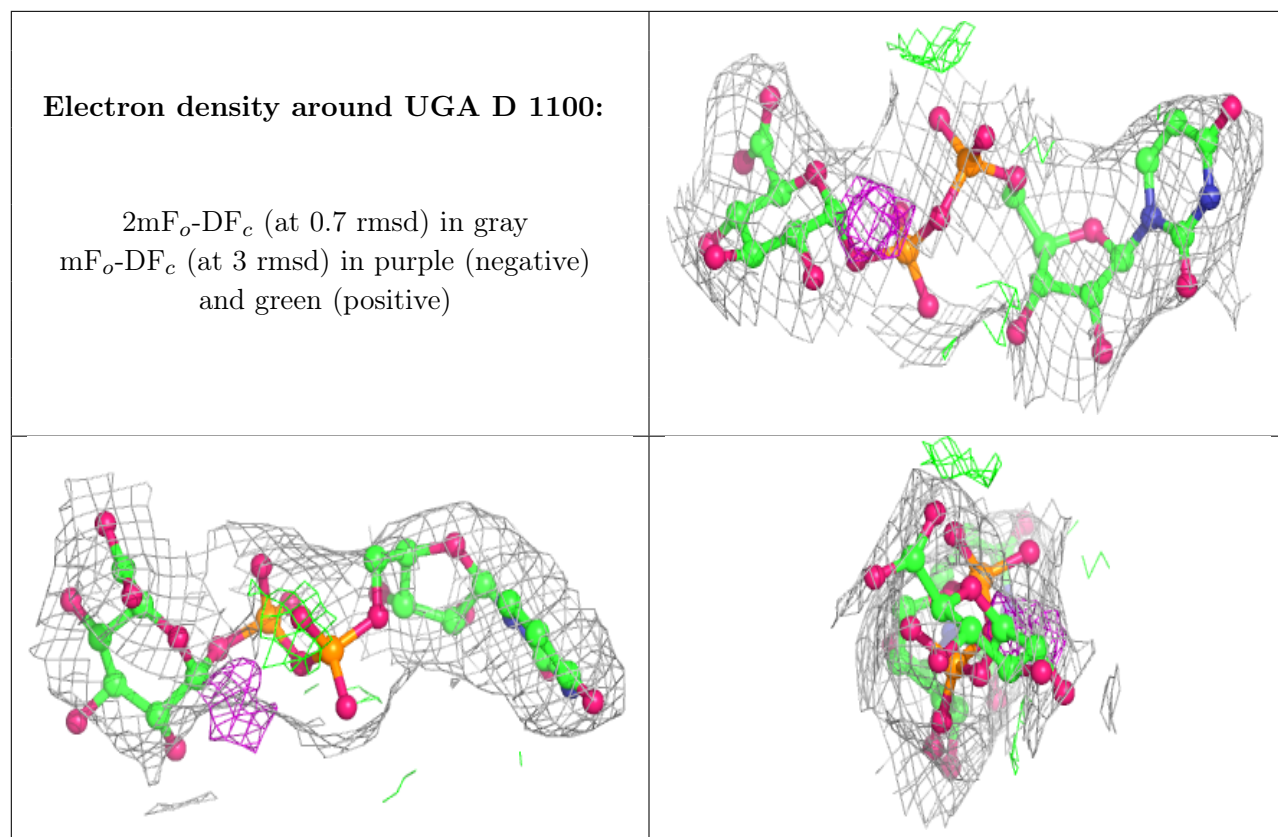
**Electron density around UGA B 1100:**

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

**Electron density around UGA E 1100:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.