



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2021 – 08:47 PM EDT

PDB ID : 1Q3G  
Title : MurA (Asp305Ala) liganded with tetrahedral reaction intermediate  
Authors : Eschenburg, S.; Kabsch, W.; Healy, M.L.; Schonbrunn, E.  
Deposited on : 2003-07-29  
Resolution : 2.65 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

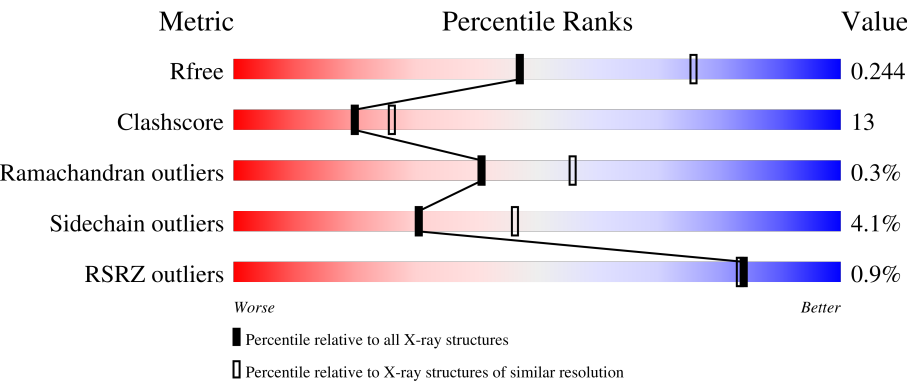
MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.23.2  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.23.2

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 2.65 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.




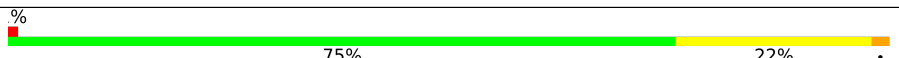

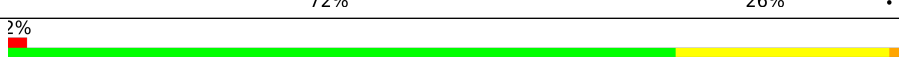


Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	419	<div><div>%</div><div><div></div><div>72%</div><div>26%</div><div>.</div></div></div>
1	B	419	<div><div>%</div><div><div></div><div>74%</div><div>25%</div><div>.</div></div></div>
1	C	419	<div><div></div><div><div></div><div>79%</div><div>19%</div><div>.</div></div></div>
1	D	419	<div><div>%</div><div><div></div><div>73%</div><div>26%</div><div>.</div></div></div>
1	E	419	<div><div></div><div><div></div><div>77%</div><div>22%</div><div>.</div></div></div>

Continued on next page...

*Continued from previous page...*

Mol	Chain	Length	Quality of chain
1	F	419	
1	G	419	
1	H	419	
1	I	419	
1	J	419	
1	K	419	
1	L	419	
1	W	419	
1	X	419	
1	Y	419	
1	Z	419	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 52519 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.

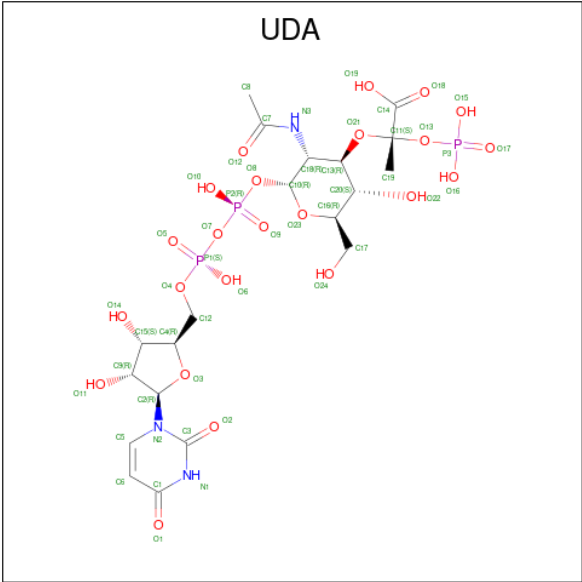
- Molecule 1 is a protein called UDP-N-acetylglucosamine 1-carboxyvinyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	419	Total	C	N	O	S	0	0	0
			3140	1975	554	597	14			
1	B	419	Total	C	N	O	S	0	0	0
			3140	1975	554	597	14			
1	C	419	Total	C	N	O	S	0	0	0
			3140	1975	554	597	14			
1	D	419	Total	C	N	O	S	0	0	0
			3140	1975	554	597	14			
1	E	419	Total	C	N	O	S	0	0	0
			3140	1975	554	597	14			
1	F	419	Total	C	N	O	S	0	0	0
			3140	1975	554	597	14			
1	G	419	Total	C	N	O	S	0	0	0
			3140	1975	554	597	14			
1	H	419	Total	C	N	O	S	0	0	0
			3140	1975	554	597	14			
1	I	419	Total	C	N	O	S	0	0	0
			3140	1975	554	597	14			
1	J	419	Total	C	N	O	S	0	0	0
			3140	1975	554	597	14			
1	K	419	Total	C	N	O	S	0	0	0
			3140	1975	554	597	14			
1	L	419	Total	C	N	O	S	0	0	0
			3140	1975	554	597	14			
1	W	419	Total	C	N	O	S	0	0	0
			3140	1975	554	597	14			
1	X	419	Total	C	N	O	S	0	0	0
			3140	1975	554	597	14			
1	Y	419	Total	C	N	O	S	0	0	0
			3140	1975	554	597	14			
1	Z	419	Total	C	N	O	S	0	0	0
			3140	1975	554	597	14			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	67	IAS	ASN	engineered mutation	UNP P33038
A	305	ALA	ASP	engineered mutation	UNP P33038
B	67	IAS	ASN	engineered mutation	UNP P33038
B	305	ALA	ASP	engineered mutation	UNP P33038
C	67	IAS	ASN	engineered mutation	UNP P33038
C	305	ALA	ASP	engineered mutation	UNP P33038
D	67	IAS	ASN	engineered mutation	UNP P33038
D	305	ALA	ASP	engineered mutation	UNP P33038
E	67	IAS	ASN	engineered mutation	UNP P33038
E	305	ALA	ASP	engineered mutation	UNP P33038
F	67	IAS	ASN	engineered mutation	UNP P33038
F	305	ALA	ASP	engineered mutation	UNP P33038
G	67	IAS	ASN	engineered mutation	UNP P33038
G	305	ALA	ASP	engineered mutation	UNP P33038
H	67	IAS	ASN	engineered mutation	UNP P33038
H	305	ALA	ASP	engineered mutation	UNP P33038
I	67	IAS	ASN	engineered mutation	UNP P33038
I	305	ALA	ASP	engineered mutation	UNP P33038
J	67	IAS	ASN	engineered mutation	UNP P33038
J	305	ALA	ASP	engineered mutation	UNP P33038
K	67	IAS	ASN	engineered mutation	UNP P33038
K	305	ALA	ASP	engineered mutation	UNP P33038
L	67	IAS	ASN	engineered mutation	UNP P33038
L	305	ALA	ASP	engineered mutation	UNP P33038
W	67	IAS	ASN	engineered mutation	UNP P33038
W	305	ALA	ASP	engineered mutation	UNP P33038
X	67	IAS	ASN	engineered mutation	UNP P33038
X	305	ALA	ASP	engineered mutation	UNP P33038
Y	67	IAS	ASN	engineered mutation	UNP P33038
Y	305	ALA	ASP	engineered mutation	UNP P33038
Z	67	IAS	ASN	engineered mutation	UNP P33038
Z	305	ALA	ASP	engineered mutation	UNP P33038

- Molecule 2 is 3'-1-CARBOXY-1-PHOSPHONOOXY-ETHOXY-URIDINE-DIPHOSPHAT E-N-ACETYLGLUCOSAMINE (three-letter code: UDA) (formula: C<sub>20</sub>H<sub>32</sub>N<sub>3</sub>O<sub>23</sub>P<sub>3</sub>).



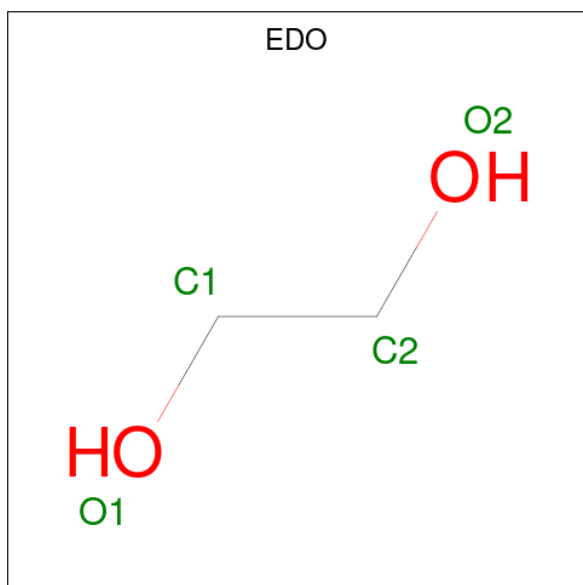
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			49	20	3	23	3		
2	B	1	Total	C	N	O	P	0	0
			49	20	3	23	3		
2	C	1	Total	C	N	O	P	0	0
			49	20	3	23	3		
2	D	1	Total	C	N	O	P	0	0
			49	20	3	23	3		
2	E	1	Total	C	N	O	P	0	0
			49	20	3	23	3		
2	F	1	Total	C	N	O	P	0	0
			49	20	3	23	3		
2	G	1	Total	C	N	O	P	0	0
			49	20	3	23	3		
2	H	1	Total	C	N	O	P	0	0
			49	20	3	23	3		
2	I	1	Total	C	N	O	P	0	0
			49	20	3	23	3		
2	J	1	Total	C	N	O	P	0	0
			49	20	3	23	3		
2	K	1	Total	C	N	O	P	0	0
			49	20	3	23	3		
2	L	1	Total	C	N	O	P	0	0
			49	20	3	23	3		
2	W	1	Total	C	N	O	P	0	0
			49	20	3	23	3		
2	X	1	Total	C	N	O	P	0	0
			49	20	3	23	3		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	
2	Y	1	Total 49	C 20	N 3	O 23	P 3	0	0
2	Z	1	Total 49	C 20	N 3	O 23	P 3	0	0

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		
3	E	1	Total	C	O	0	0
			4	2	2		
3	F	1	Total	C	O	0	0
			4	2	2		
3	G	1	Total	C	O	0	0
			4	2	2		
3	H	1	Total	C	O	0	0
			4	2	2		
3	I	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

*Continued from previous page...*

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	J	1	Total C O 4 2 2	0	0
3	K	1	Total C O 4 2 2	0	0
3	L	1	Total C O 4 2 2	0	0
3	W	1	Total C O 4 2 2	0	0
3	X	1	Total C O 4 2 2	0	0
3	Y	1	Total C O 4 2 2	0	0
3	Z	1	Total C O 4 2 2	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	93	Total O 93 93	0	0
4	B	100	Total O 100 100	0	0
4	C	124	Total O 124 124	0	0
4	D	123	Total O 123 123	0	0
4	E	116	Total O 116 116	0	0
4	F	106	Total O 106 106	0	0
4	G	136	Total O 136 136	0	0
4	H	111	Total O 111 111	0	0
4	I	76	Total O 76 76	0	0
4	J	76	Total O 76 76	0	0
4	K	67	Total O 67 67	0	0
4	L	68	Total O 68 68	0	0

*Continued on next page...*

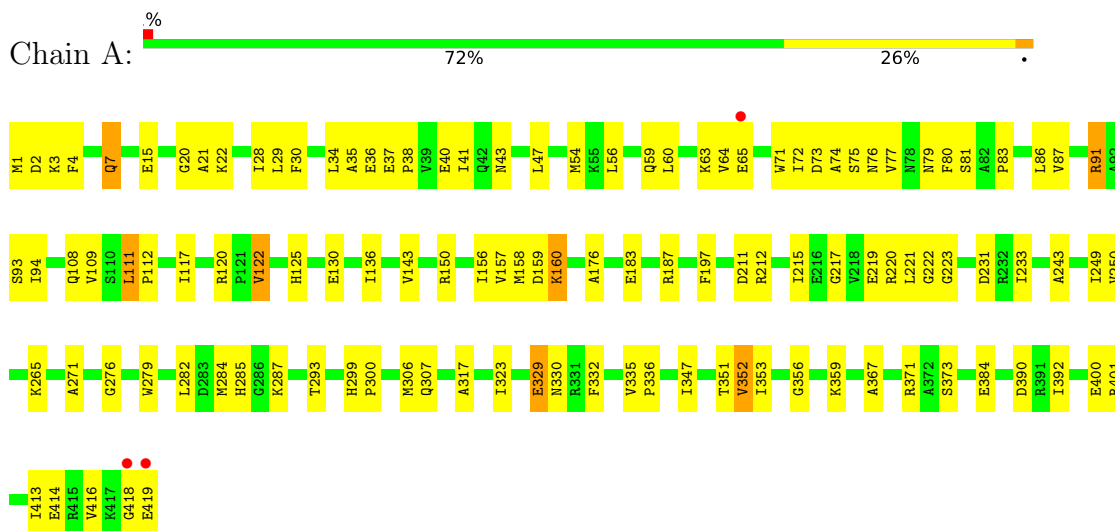
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	W	70	Total 70	O 70	0	0
4	X	52	Total 52	O 52	0	0
4	Y	67	Total 67	O 67	0	0
4	Z	46	Total 46	O 46	0	0

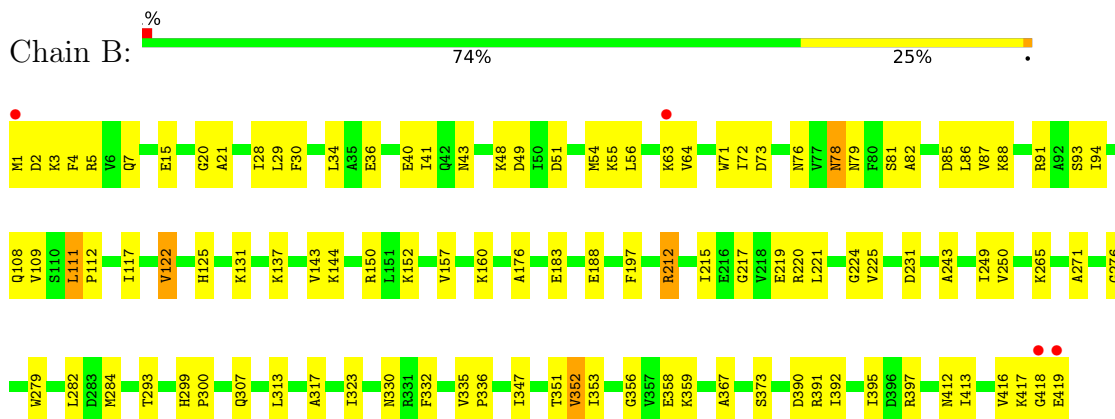
### 3 Residue-property plots [i](#)

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.

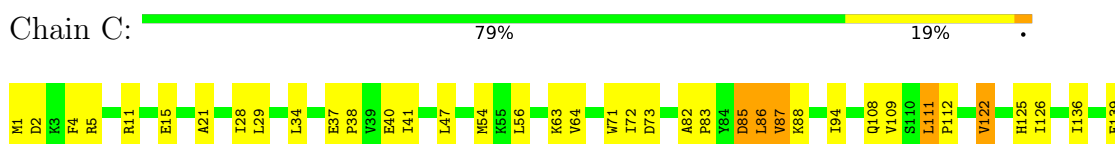
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

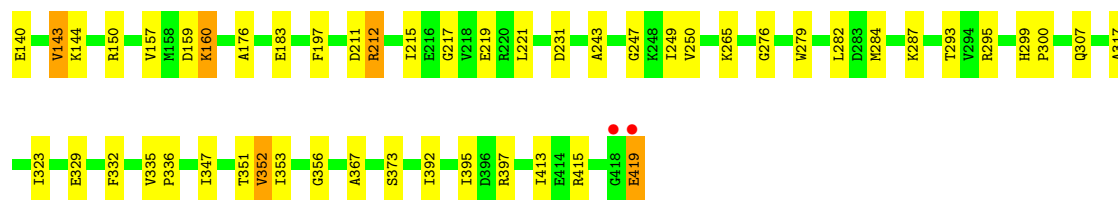


- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

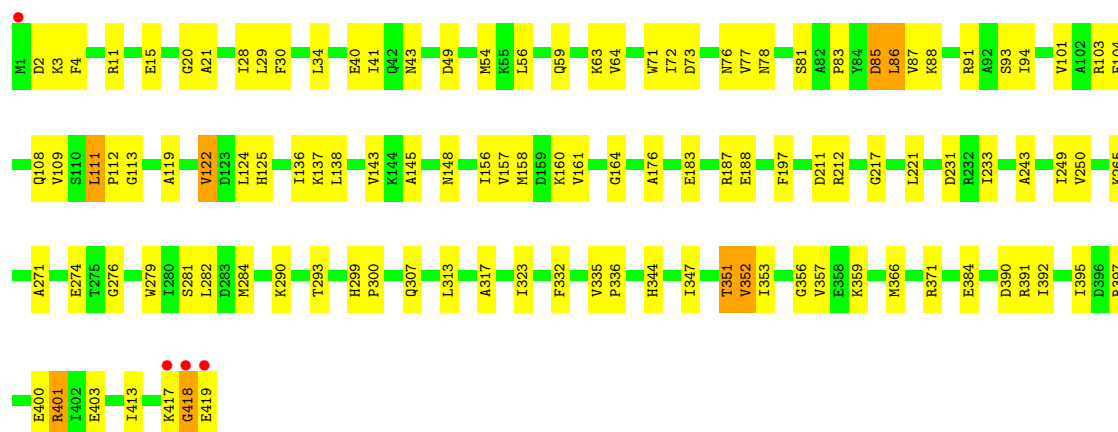


- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

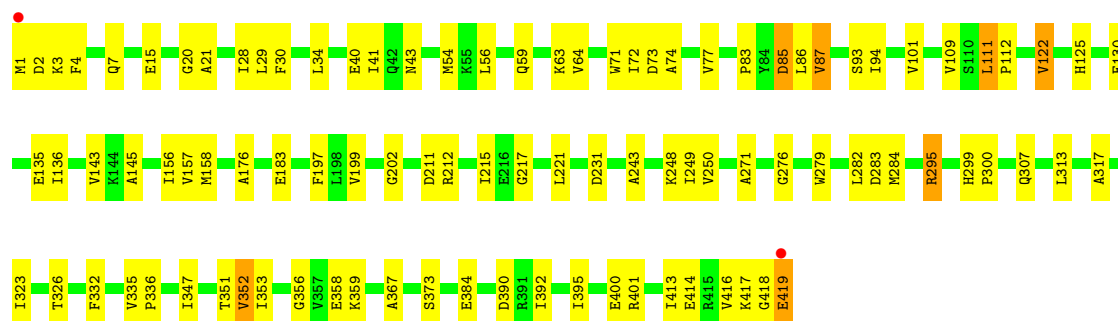




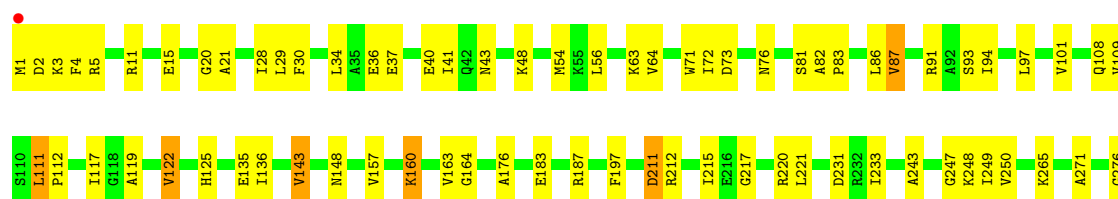
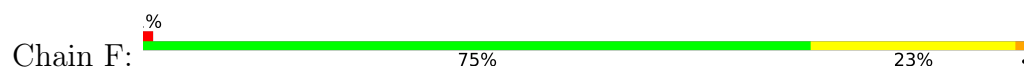
• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

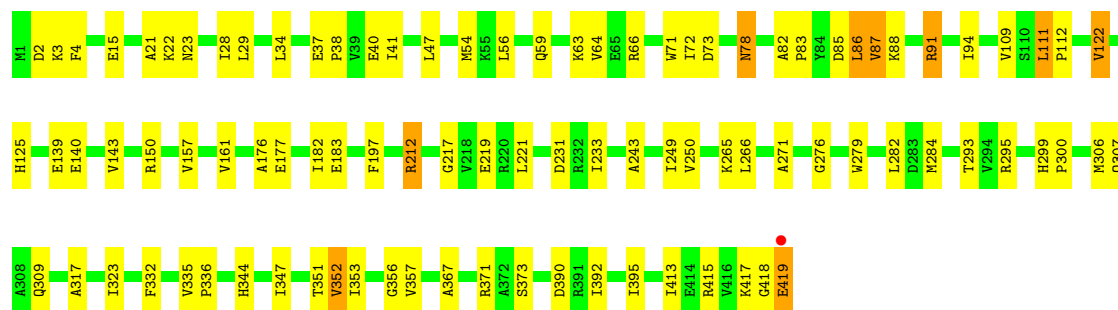
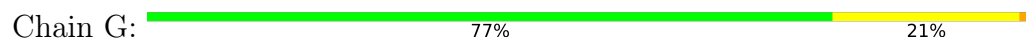


• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

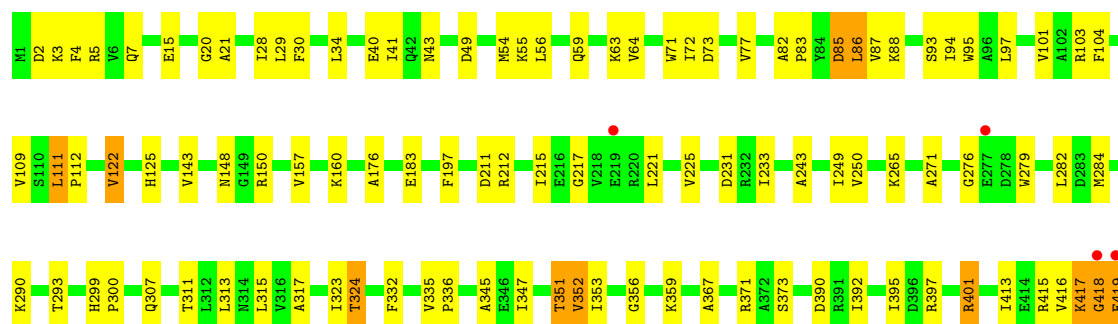
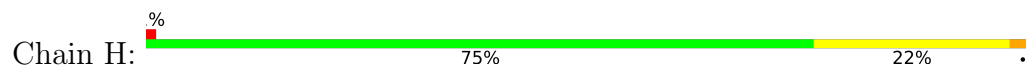




- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



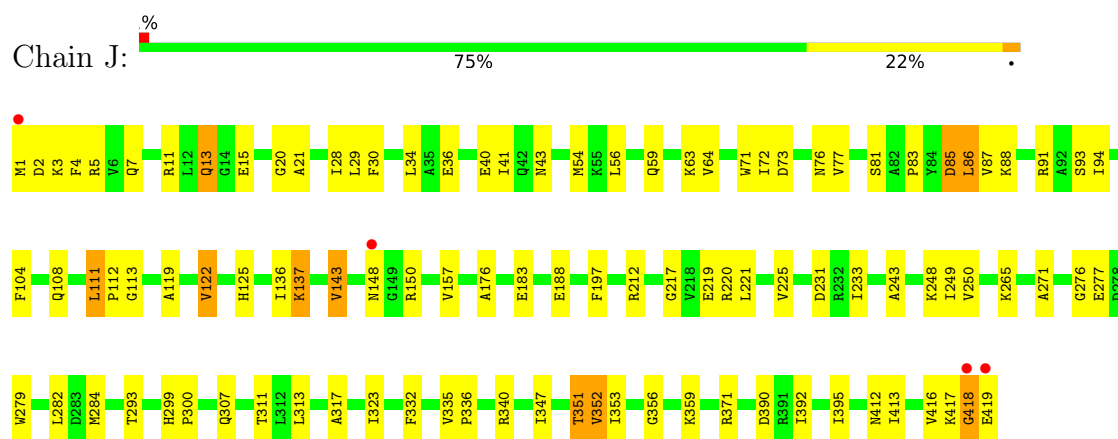
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



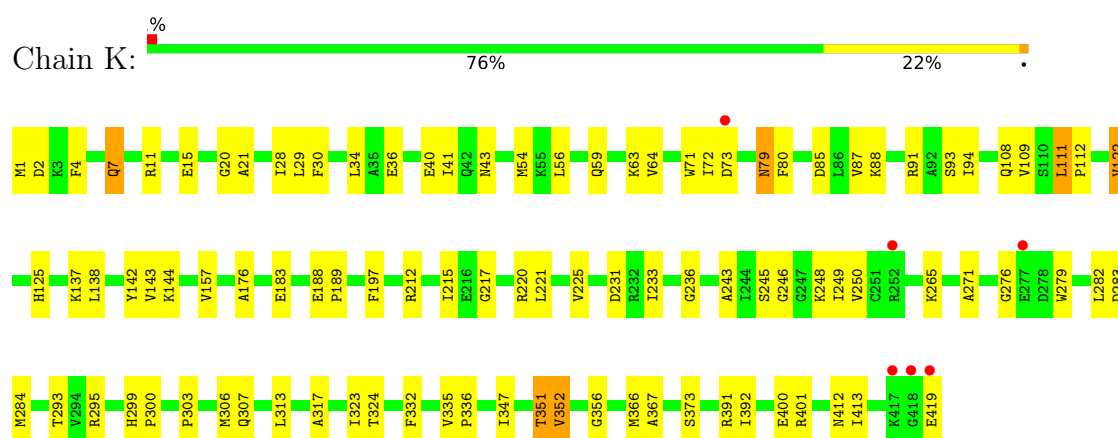
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



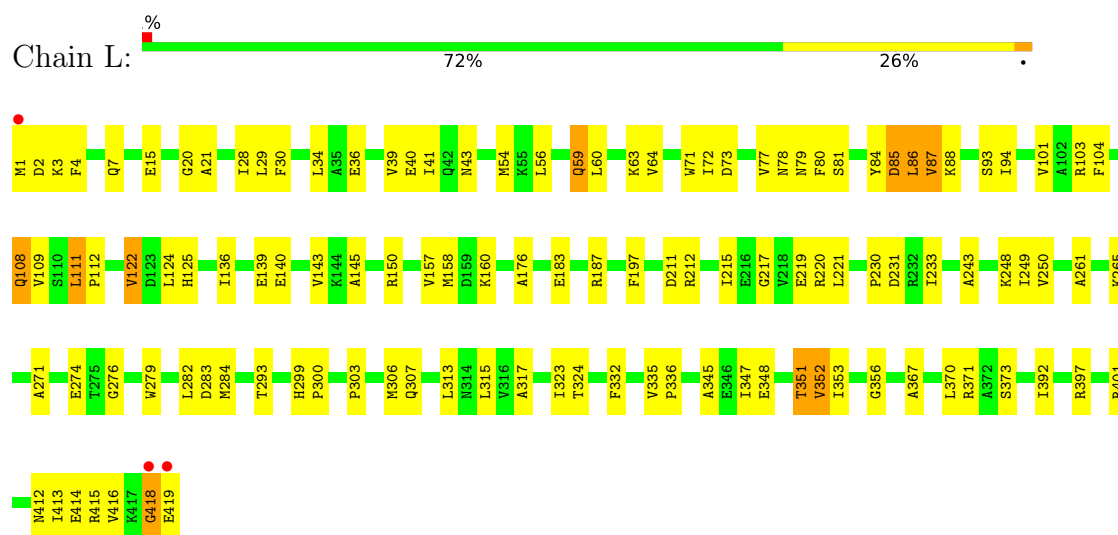
- Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

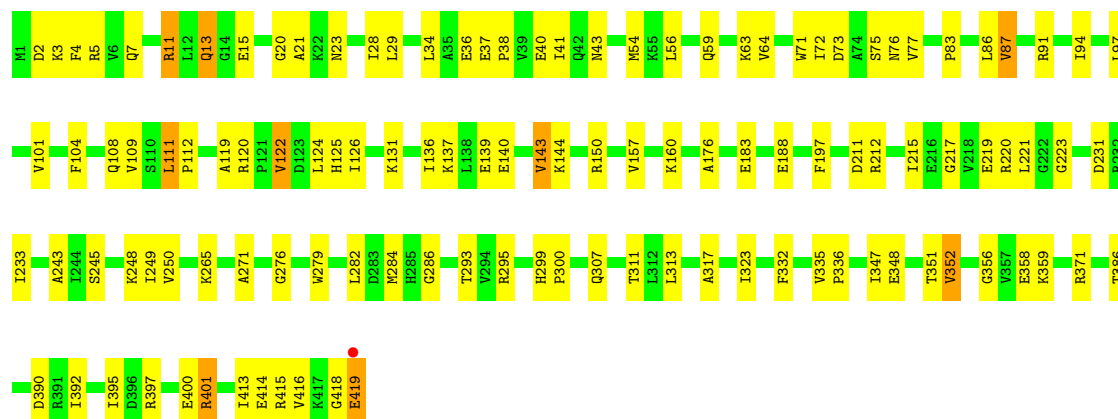


• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

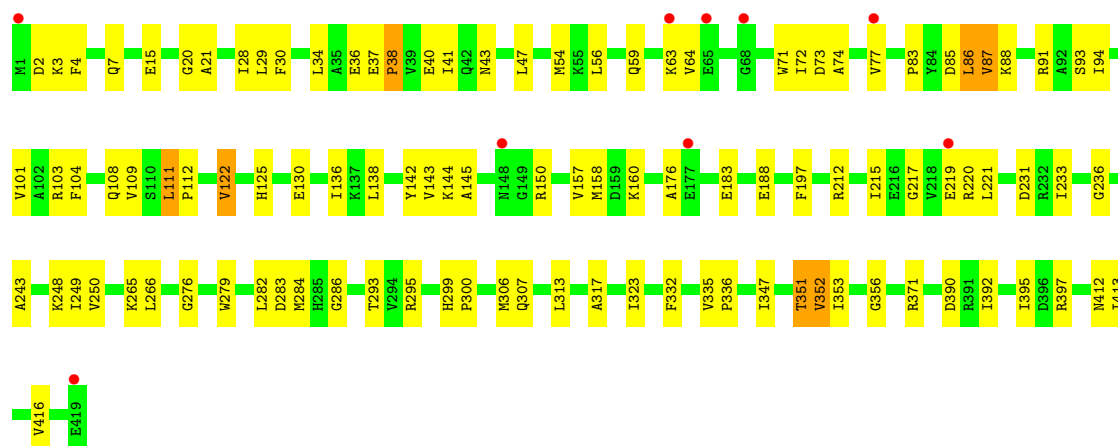
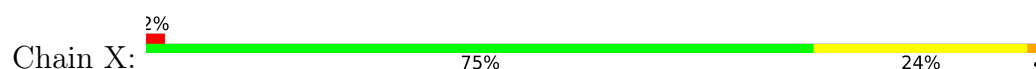


• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

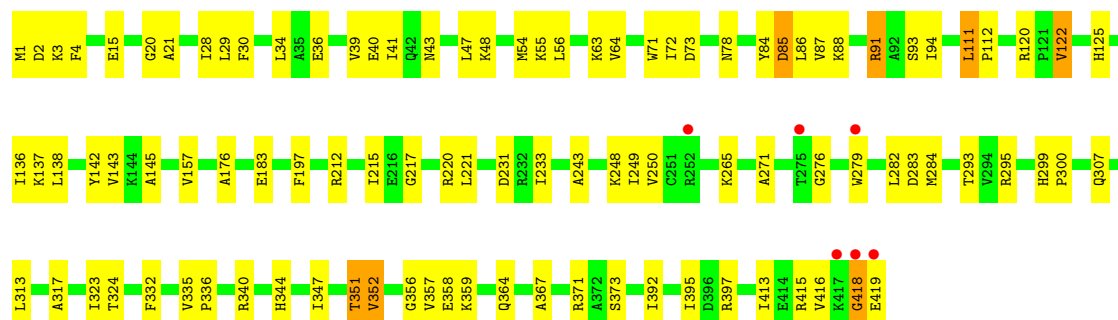
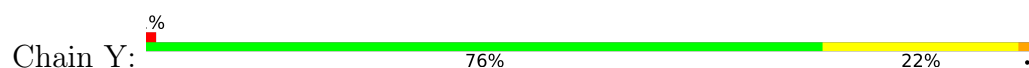




• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase

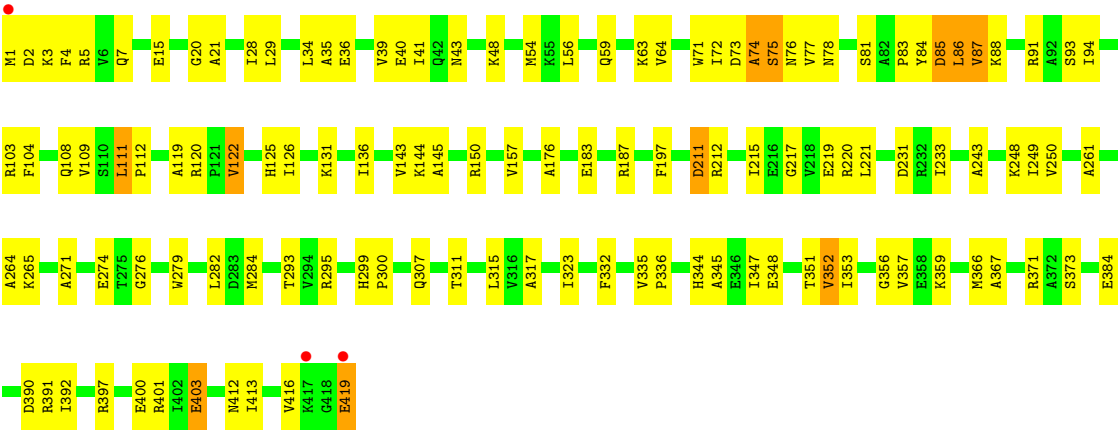


• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase



• Molecule 1: UDP-N-acetylglucosamine 1-carboxyvinyltransferase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	139.46Å 153.93Å 167.48Å 90.00° 112.95° 90.00°	Depositor
Resolution (Å)	20.00 – 2.65 29.94 – 2.65	Depositor EDS
% Data completeness (in resolution range)	(Not available) (20.00-2.65) 98.7 (29.94-2.65)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.78 (at 2.64Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.217 , 0.253 0.209 , 0.244	Depositor DCC
$R_{free}$ test set	3721 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.4	Xtriage
Anisotropy	0.360	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 47.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	52519	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 45.13 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.3816e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: IAS, UDA, EDO

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	0.36	0/3176	0.60	0/4301
1	B	0.36	0/3176	0.60	0/4301
1	C	0.38	0/3176	0.60	0/4301
1	D	0.36	0/3176	0.60	0/4301
1	E	0.37	0/3176	0.60	0/4301
1	F	0.37	0/3176	0.60	0/4301
1	G	0.38	0/3176	0.61	0/4301
1	H	0.36	0/3176	0.59	0/4301
1	I	0.36	0/3176	0.61	0/4301
1	J	0.35	0/3176	0.59	0/4301
1	K	0.36	0/3176	0.60	0/4301
1	L	0.36	0/3176	0.60	0/4301
1	W	0.36	0/3176	0.60	0/4301
1	X	0.35	0/3176	0.60	0/4301
1	Y	0.36	0/3176	0.60	0/4301
1	Z	0.36	0/3176	0.59	0/4301
All	All	0.36	0/50816	0.60	0/68816

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

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	3140	0	3217	90	0
1	B	3140	0	3217	77	0
1	C	3140	0	3217	68	0
1	D	3140	0	3217	83	0
1	E	3140	0	3217	81	0
1	F	3140	0	3217	79	0
1	G	3140	0	3217	72	0
1	H	3140	0	3217	88	0
1	I	3140	0	3217	91	0
1	J	3140	0	3217	81	0
1	K	3140	0	3217	78	0
1	L	3140	0	3217	95	0
1	W	3140	0	3217	101	0
1	X	3140	0	3217	84	0
1	Y	3140	0	3217	82	0
1	Z	3140	0	3217	101	0
2	A	49	0	28	1	0
2	B	49	0	28	0	0
2	C	49	0	28	1	0
2	D	49	0	28	0	0
2	E	49	0	28	0	0
2	F	49	0	28	0	0
2	G	49	0	28	0	0
2	H	49	0	28	0	0
2	I	49	0	28	2	0
2	J	49	0	28	0	0
2	K	49	0	28	0	0
2	L	49	0	28	0	0
2	W	49	0	28	1	0
2	X	49	0	28	0	0
2	Y	49	0	28	1	0
2	Z	49	0	28	1	0
3	A	4	0	6	0	0
3	B	4	0	6	1	0
3	C	4	0	6	0	0
3	D	4	0	6	3	0
3	E	4	0	6	0	0
3	F	4	0	6	2	0
3	G	4	0	6	0	0
3	H	4	0	6	0	0
3	I	4	0	6	0	0
3	J	4	0	6	0	0
3	K	4	0	6	0	0

Continued on next page...

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	L	4	0	6	0	0
3	W	4	0	6	0	0
3	X	4	0	6	1	0
3	Y	4	0	6	0	0
3	Z	4	0	6	0	0
4	A	93	0	0	2	0
4	B	100	0	0	2	0
4	C	124	0	0	1	0
4	D	123	0	0	7	0
4	E	116	0	0	0	0
4	F	106	0	0	5	0
4	G	136	0	0	5	0
4	H	111	0	0	5	0
4	I	76	0	0	0	0
4	J	76	0	0	3	0
4	K	67	0	0	2	0
4	L	68	0	0	1	0
4	W	70	0	0	2	0
4	X	52	0	0	3	0
4	Y	67	0	0	3	0
4	Z	46	0	0	2	0
All	All	52519	0	52016	1303	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 13.

All (1303) 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:G:233:ILE:HG23	1:G:306:MET:HE3	1.41	0.99
1:W:5:ARG:HH12	1:W:7:GLN:HE21	1.13	0.95
1:E:1:MET:HB3	1:E:419:GLU:HA	1.49	0.91
1:H:401:ARG:HB3	1:H:401:ARG:NH1	1.85	0.90
1:D:401:ARG:HB3	1:D:401:ARG:HH11	1.35	0.89
1:L:150:ARG:HH12	1:L:219:GLU:HA	1.36	0.89
1:F:233:ILE:HA	1:F:306:MET:HE1	1.55	0.88
1:W:59:GLN:HE22	1:W:83:PRO:CD	1.86	0.88
1:X:91:ARG:HD3	4:X:885:HOH:O	1.74	0.88
1:W:59:GLN:HE22	1:W:83:PRO:HD3	1.40	0.87
1:I:150:ARG:HH12	1:I:219:GLU:HA	1.40	0.87
1:F:3:LYS:HE3	1:F:419:GLU:HA	1.55	0.86

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:5:ARG:HH22	1:H:7:GLN:HE21	1.16	0.86
1:E:295:ARG:HD2	1:H:160:LYS:HZ3	1.42	0.85
1:D:164:GLY:HA3	3:D:1473:EDO:H11	1.59	0.84
1:W:150:ARG:HH12	1:W:219:GLU:HA	1.43	0.84
1:A:233:ILE:HG23	1:A:306:MET:HE2	1.58	0.84
1:D:401:ARG:HB3	1:D:401:ARG:NH1	1.92	0.83
1:A:65:GLU:HG2	1:A:71:TRP:HB2	1.60	0.83
1:Z:108:GLN:HG2	1:Z:144:LYS:HG2	1.58	0.83
1:C:83:PRO:HG2	1:C:86:LEU:HB2	1.60	0.82
1:X:150:ARG:NH1	1:X:219:GLU:HA	1.95	0.82
1:Z:4:PHE:CZ	1:Z:403:GLU:HG2	2.16	0.81
1:C:150:ARG:HH12	1:C:219:GLU:HA	1.45	0.81
1:H:150:ARG:HD3	4:H:663:HOH:O	1.83	0.79
1:L:150:ARG:NH1	1:L:219:GLU:HA	1.97	0.79
1:D:109:VAL:O	1:D:143:VAL:HG12	1.82	0.78
1:E:295:ARG:HD2	1:H:160:LYS:NZ	1.97	0.78
1:G:306:MET:HE2	1:G:309:GLN:NE2	1.97	0.78
1:L:109:VAL:O	1:L:143:VAL:HG12	1.84	0.78
1:B:94:ILE:HG12	1:B:122:VAL:HG21	1.66	0.77
1:G:233:ILE:HG23	1:G:306:MET:CE	2.15	0.77
1:K:109:VAL:O	1:K:143:VAL:HG12	1.84	0.76
1:F:94:ILE:HG12	1:F:122:VAL:HG21	1.67	0.76
1:H:401:ARG:HB3	1:H:401:ARG:HH11	1.49	0.76
1:C:126:ILE:HG23	1:C:136:ILE:HD12	1.68	0.76
1:E:94:ILE:HG12	1:E:122:VAL:HG21	1.68	0.76
1:C:150:ARG:NH1	1:C:219:GLU:HA	2.00	0.76
1:E:400:GLU:HG2	1:E:401:ARG:HG2	1.68	0.76
1:A:94:ILE:HG12	1:A:122:VAL:HG21	1.68	0.75
1:J:1:MET:HB3	1:J:419:GLU:HB3	1.69	0.75
1:W:2:ASP:HB3	1:W:392:ILE:HD11	1.68	0.75
1:E:130:GLU:HG3	1:E:136:ILE:HD13	1.68	0.74
1:I:2:ASP:HB3	1:I:392:ILE:HD11	1.69	0.74
1:H:290:LYS:HZ3	1:W:286:GLY:HA3	1.52	0.74
1:W:94:ILE:HG12	1:W:122:VAL:HG21	1.69	0.74
1:K:94:ILE:HG12	1:K:122:VAL:HG21	1.70	0.74
1:Y:94:ILE:HG12	1:Y:122:VAL:HG21	1.70	0.74
1:I:94:ILE:HG12	1:I:122:VAL:HG21	1.69	0.74
1:H:5:ARG:HH22	1:H:7:GLN:NE2	1.83	0.74
1:W:150:ARG:NH1	1:W:219:GLU:HA	2.02	0.74
1:I:150:ARG:NH1	1:I:219:GLU:HA	2.02	0.74
1:X:150:ARG:HH12	1:X:219:GLU:HA	1.53	0.74

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:94:ILE:HG12	1:G:122:VAL:HG21	1.69	0.74
1:W:348:GLU:HG2	1:Y:351:THR:HG21	1.69	0.73
1:G:306:MET:HE2	1:G:306:MET:HA	1.70	0.73
1:C:94:ILE:HG12	1:C:122:VAL:HG21	1.70	0.73
1:Z:109:VAL:O	1:Z:143:VAL:HG12	1.89	0.73
1:H:109:VAL:O	1:H:143:VAL:HG12	1.87	0.73
1:X:94:ILE:HG12	1:X:122:VAL:HG21	1.70	0.72
1:G:2:ASP:HB3	1:G:392:ILE:HD11	1.71	0.72
1:L:94:ILE:HG12	1:L:122:VAL:HG21	1.68	0.72
1:D:94:ILE:HG12	1:D:122:VAL:HG21	1.70	0.72
1:H:85:ASP:HB3	4:H:976:HOH:O	1.89	0.72
1:C:2:ASP:HB3	1:C:392:ILE:HD11	1.72	0.72
1:D:290:LYS:HZ3	1:I:286:GLY:HA3	1.56	0.71
1:J:94:ILE:HG12	1:J:122:VAL:HG21	1.72	0.71
1:B:225:VAL:HG21	1:E:202:GLY:HA2	1.71	0.71
1:X:83:PRO:HG2	1:X:86:LEU:HB2	1.72	0.71
1:A:2:ASP:HB3	1:A:392:ILE:HD11	1.72	0.71
1:Z:94:ILE:HG12	1:Z:122:VAL:HG21	1.70	0.71
1:E:2:ASP:HB3	1:E:392:ILE:HD11	1.71	0.70
1:Y:2:ASP:HB3	1:Y:392:ILE:HD11	1.71	0.70
1:D:2:ASP:HB3	1:D:392:ILE:HD11	1.73	0.70
1:W:5:ARG:NH1	1:W:7:GLN:HE21	1.88	0.70
1:B:78:ASN:HD22	1:B:79:ASN:N	1.88	0.70
1:F:2:ASP:HB3	1:F:392:ILE:HD11	1.72	0.70
1:H:2:ASP:HB3	1:H:392:ILE:HD11	1.73	0.70
1:K:2:ASP:HB3	1:K:392:ILE:HD11	1.72	0.70
1:J:2:ASP:HB3	1:J:392:ILE:HD11	1.74	0.70
1:F:48:LYS:HB3	1:F:397:ARG:HD3	1.74	0.70
1:H:94:ILE:HG12	1:H:122:VAL:HG21	1.74	0.69
1:K:11:ARG:HD3	1:K:245:SER:O	1.91	0.69
1:L:2:ASP:HB3	1:L:392:ILE:HD11	1.73	0.69
1:X:2:ASP:HB3	1:X:392:ILE:HD11	1.75	0.69
1:B:160:LYS:NZ	1:C:295:ARG:HD2	2.08	0.69
1:C:139:GLU:O	1:C:140:GLU:HG2	1.93	0.69
1:I:277:GLU:HG2	1:X:37:GLU:OE2	1.92	0.69
1:G:306:MET:CE	1:G:309:GLN:NE2	2.56	0.68
1:B:2:ASP:HB3	1:B:392:ILE:HD11	1.73	0.68
1:L:85:ASP:HA	1:L:88:LYS:HE2	1.76	0.68
1:K:248:LYS:HD2	1:K:283:ASP:OD2	1.94	0.68
1:I:83:PRO:HG2	1:I:86:LEU:HB2	1.75	0.68
1:L:139:GLU:O	1:L:140:GLU:HG2	1.94	0.68

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:77:VAL:HB	1:H:104:PHE:CZ	2.29	0.68
1:B:417:LYS:HE2	1:B:417:LYS:HA	1.76	0.67
1:W:2:ASP:OD2	1:W:415:ARG:HD3	1.93	0.67
1:Z:2:ASP:HB3	1:Z:392:ILE:HD11	1.76	0.67
1:W:157:VAL:HA	1:W:183:GLU:HB2	1.77	0.67
1:Y:344:HIS:HD2	1:Y:357:VAL:CG1	2.08	0.66
1:W:5:ARG:HH12	1:W:7:GLN:NE2	1.89	0.66
1:I:157:VAL:HA	1:I:183:GLU:HB2	1.78	0.66
1:D:3:LYS:HE3	1:D:419:GLU:HA	1.78	0.65
1:I:15:GLU:HG2	1:I:250:VAL:HB	1.79	0.65
1:F:5:ARG:HD2	4:F:738:HOH:O	1.95	0.65
1:Y:2:ASP:OD2	1:Y:415:ARG:HD3	1.97	0.65
1:A:37:GLU:HB3	1:A:38:PRO:CD	2.26	0.65
1:W:15:GLU:HG2	1:W:250:VAL:HB	1.79	0.65
1:Y:344:HIS:HD2	1:Y:357:VAL:HG11	1.62	0.65
1:B:109:VAL:O	1:B:143:VAL:HG12	1.96	0.65
1:K:157:VAL:HA	1:K:183:GLU:HB2	1.79	0.65
1:H:157:VAL:HA	1:H:183:GLU:HB2	1.79	0.65
1:E:130:GLU:CG	1:E:136:ILE:HD13	2.27	0.64
1:F:135:GLU:C	1:F:136:ILE:HD12	2.18	0.64
1:J:157:VAL:HA	1:J:183:GLU:HB2	1.79	0.64
1:L:15:GLU:HG2	1:L:250:VAL:HB	1.79	0.64
1:C:2:ASP:OD2	1:C:415:ARG:HD3	1.98	0.64
1:G:157:VAL:HA	1:G:183:GLU:HB2	1.79	0.64
1:X:416:VAL:HG23	1:X:416:VAL:O	1.98	0.64
1:Z:15:GLU:HG2	1:Z:250:VAL:HB	1.80	0.64
1:K:236:GLY:HA3	1:K:306:MET:HE3	1.79	0.63
1:A:109:VAL:O	1:A:143:VAL:HG12	1.97	0.63
1:X:157:VAL:HA	1:X:183:GLU:HB2	1.80	0.63
1:Z:295:ARG:HB2	1:Z:295:ARG:HH11	1.63	0.63
1:D:157:VAL:HA	1:D:183:GLU:HB2	1.81	0.63
1:G:15:GLU:HG2	1:G:250:VAL:HB	1.81	0.63
1:L:157:VAL:HA	1:L:183:GLU:HB2	1.80	0.63
1:W:401:ARG:HB3	1:W:401:ARG:NH1	2.13	0.63
1:D:15:GLU:HG2	1:D:250:VAL:HB	1.80	0.63
1:F:108:GLN:HG2	4:F:427:HOH:O	1.97	0.63
1:I:348:GLU:OE1	1:K:295:ARG:NH2	2.32	0.63
1:Y:157:VAL:HA	1:Y:183:GLU:HB2	1.81	0.63
1:Z:157:VAL:HA	1:Z:183:GLU:HB2	1.80	0.63
1:C:15:GLU:HG2	1:C:250:VAL:HB	1.81	0.63
1:E:136:ILE:HD12	1:E:136:ILE:N	2.13	0.63

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:156:ILE:HG22	1:E:158:MET:HE1	1.81	0.63
1:G:243:ALA:HA	1:G:284:MET:CG	2.29	0.63
1:H:83:PRO:HG2	1:H:86:LEU:HB2	1.81	0.63
1:B:157:VAL:HA	1:B:183:GLU:HB2	1.81	0.62
1:H:97:LEU:O	1:H:101:VAL:HG12	1.99	0.62
1:I:243:ALA:HA	1:I:284:MET:CG	2.29	0.62
1:W:243:ALA:HA	1:W:284:MET:CG	2.29	0.62
1:H:243:ALA:HA	1:H:284:MET:CG	2.29	0.62
1:L:243:ALA:HA	1:L:284:MET:CG	2.30	0.62
1:D:274:GLU:HB2	1:D:281:SER:OG	2.00	0.62
1:F:136:ILE:HD12	1:F:136:ILE:N	2.15	0.62
1:A:150:ARG:NH1	1:A:219:GLU:HA	2.15	0.62
1:E:63:LYS:HB2	1:E:73:ASP:HB3	1.81	0.62
1:B:15:GLU:HG2	1:B:250:VAL:HB	1.81	0.62
1:E:15:GLU:HG2	1:E:250:VAL:HB	1.80	0.62
1:E:157:VAL:HA	1:E:183:GLU:HB2	1.80	0.62
1:J:15:GLU:HG2	1:J:250:VAL:HB	1.82	0.62
1:Z:243:ALA:HA	1:Z:284:MET:CG	2.30	0.62
1:B:78:ASN:HD22	1:B:78:ASN:C	2.00	0.61
1:E:59:GLN:HE22	1:E:83:PRO:HG3	1.65	0.61
1:C:243:ALA:HA	1:C:284:MET:CG	2.30	0.61
1:F:243:ALA:HA	1:F:284:MET:CG	2.30	0.61
1:A:63:LYS:HB2	1:A:73:ASP:HB3	1.82	0.61
1:H:15:GLU:HG2	1:H:250:VAL:HB	1.82	0.61
1:K:15:GLU:HG2	1:K:250:VAL:HB	1.81	0.61
1:L:7:GLN:HB2	1:L:412:ASN:HB3	1.82	0.61
1:L:139:GLU:O	1:L:140:GLU:CG	2.49	0.61
1:A:243:ALA:HA	1:A:284:MET:CG	2.31	0.61
1:C:157:VAL:HA	1:C:183:GLU:HB2	1.82	0.61
1:I:59:GLN:O	1:I:59:GLN:HG2	1.99	0.61
1:W:63:LYS:HB2	1:W:73:ASP:HB3	1.81	0.61
1:Z:48:LYS:HB3	1:Z:397:ARG:HD3	1.82	0.61
1:A:15:GLU:HG2	1:A:250:VAL:HB	1.81	0.61
1:X:63:LYS:HB2	1:X:73:ASP:HB3	1.82	0.61
1:X:243:ALA:HA	1:X:284:MET:CG	2.30	0.61
1:Z:75:SER:HA	1:Z:103:ARG:HH22	1.66	0.61
1:F:15:GLU:HG2	1:F:250:VAL:HB	1.83	0.61
1:X:15:GLU:HG2	1:X:250:VAL:HB	1.83	0.60
1:L:3:LYS:HE3	1:L:419:GLU:HA	1.83	0.60
1:X:85:ASP:HA	1:X:88:LYS:HE2	1.82	0.60
1:Y:243:ALA:HA	1:Y:284:MET:CG	2.31	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:ALA:HA	1:B:284:MET:CG	2.30	0.60
1:E:243:ALA:HA	1:E:284:MET:CG	2.31	0.60
1:H:324:THR:HB	1:H:351:THR:HB	1.82	0.60
1:K:243:ALA:HA	1:K:284:MET:CG	2.31	0.60
1:C:1:MET:HB3	1:C:419:GLU:HA	1.83	0.60
1:C:317:ALA:O	1:C:356:GLY:HA3	2.01	0.60
1:F:48:LYS:HD2	1:F:397:ARG:CZ	2.30	0.60
1:J:243:ALA:HA	1:J:284:MET:CG	2.31	0.60
1:J:353:ILE:HD12	1:L:353:ILE:HD12	1.82	0.60
1:Y:15:GLU:HG2	1:Y:250:VAL:HB	1.83	0.60
1:D:243:ALA:HA	1:D:284:MET:CG	2.31	0.60
1:H:3:LYS:HE3	1:H:419:GLU:HA	1.84	0.60
1:Y:364:GLN:HB3	4:Y:767:HOH:O	2.00	0.60
1:F:157:VAL:HA	1:F:183:GLU:HB2	1.84	0.60
1:J:77:VAL:HB	1:J:104:PHE:CZ	2.36	0.60
1:D:397:ARG:HD2	4:D:757:HOH:O	2.01	0.59
1:J:85:ASP:HA	1:J:88:LYS:HE2	1.84	0.59
1:K:63:LYS:HB2	1:K:73:ASP:HB3	1.83	0.59
1:G:63:LYS:HB2	1:G:73:ASP:HB3	1.84	0.59
1:Z:84:TYR:CE2	1:Z:88:LYS:HD3	2.37	0.59
1:F:82:ALA:HB3	1:F:109:VAL:HG13	1.84	0.59
1:J:3:LYS:HE3	1:J:419:GLU:HA	1.83	0.59
1:J:13:GLN:HB2	1:J:248:LYS:O	2.02	0.59
1:J:137:LYS:HD3	1:J:137:LYS:N	2.18	0.59
1:Z:108:GLN:HE21	1:Z:144:LYS:HE2	1.68	0.59
1:J:111:LEU:HD23	1:J:112:PRO:HD2	1.83	0.59
1:Z:359:LYS:CD	1:Z:384:GLU:HB2	2.32	0.59
1:G:59:GLN:HE22	1:G:83:PRO:HG3	1.67	0.59
1:K:233:ILE:HA	1:K:306:MET:HE2	1.85	0.59
1:I:63:LYS:HB2	1:I:73:ASP:HB3	1.83	0.59
1:Y:39:VAL:CG2	1:Y:72:ILE:HB	2.33	0.58
1:Z:29:LEU:HD23	1:Z:41:ILE:HD12	1.84	0.58
1:A:59:GLN:HE22	1:A:83:PRO:HD3	1.67	0.58
1:G:317:ALA:O	1:G:356:GLY:HA3	2.03	0.58
1:X:351:THR:HG21	1:Z:348:GLU:HG3	1.84	0.58
1:C:63:LYS:HB2	1:C:73:ASP:HB3	1.84	0.58
1:D:359:LYS:NZ	1:D:359:LYS:HB2	2.18	0.58
1:E:1:MET:CB	1:E:419:GLU:HA	2.30	0.58
1:F:37:GLU:OE1	1:F:37:GLU:HA	2.02	0.58
1:W:124:LEU:HD11	1:W:160:LYS:HB3	1.86	0.58
1:A:29:LEU:HD23	1:A:41:ILE:HD12	1.86	0.58

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:VAL:HA	1:A:183:GLU:HB2	1.83	0.58
1:C:21:ALA:HA	1:C:231:ASP:HB2	1.85	0.58
1:C:109:VAL:O	1:C:143:VAL:HG13	2.04	0.58
1:I:317:ALA:O	1:I:356:GLY:HA3	2.03	0.58
1:J:29:LEU:HD23	1:J:41:ILE:HD12	1.85	0.58
1:Z:143:VAL:HG13	1:Z:143:VAL:O	2.04	0.58
1:J:63:LYS:HB2	1:J:73:ASP:HB3	1.84	0.58
1:H:63:LYS:HB2	1:H:73:ASP:HB3	1.84	0.58
1:B:417:LYS:HE2	1:B:417:LYS:CA	2.34	0.58
1:W:54:MET:HG2	1:W:64:VAL:HG11	1.86	0.58
1:X:29:LEU:HD23	1:X:41:ILE:HD12	1.86	0.58
1:Z:295:ARG:HB2	1:Z:295:ARG:NH1	2.18	0.58
1:H:54:MET:HG2	1:H:64:VAL:HG11	1.85	0.58
1:X:83:PRO:O	1:X:87:VAL:HG13	2.04	0.58
1:B:150:ARG:NH1	1:B:219:GLU:HA	2.18	0.58
1:Z:317:ALA:O	1:Z:356:GLY:HA3	2.04	0.57
1:F:391:ARG:HD2	1:F:393:TYR:HE2	1.69	0.57
1:I:124:LEU:HD11	1:I:160:LYS:HB3	1.86	0.57
1:X:353:ILE:HD12	1:Z:353:ILE:CD1	2.34	0.57
1:D:366:MET:HG3	1:D:391:ARG:HD2	1.85	0.57
1:E:54:MET:HG2	1:E:64:VAL:HG11	1.85	0.57
1:H:290:LYS:HZ3	1:W:286:GLY:CA	2.17	0.57
1:J:353:ILE:HD12	1:L:353:ILE:CD1	2.34	0.57
1:X:108:GLN:NE2	1:X:144:LYS:HE2	2.20	0.57
1:Y:48:LYS:HB3	1:Y:397:ARG:HD3	1.85	0.57
1:L:29:LEU:HD23	1:L:41:ILE:HD12	1.86	0.57
1:W:83:PRO:HG2	1:W:86:LEU:HB2	1.85	0.57
1:Z:59:GLN:HE22	1:Z:83:PRO:HG3	1.70	0.57
1:B:48:LYS:HB3	1:B:397:ARG:HD3	1.86	0.57
1:J:150:ARG:NH1	1:J:219:GLU:HA	2.20	0.57
1:L:81:SER:HB3	1:L:108:GLN:HG3	1.86	0.57
1:X:317:ALA:O	1:X:356:GLY:HA3	2.04	0.57
1:Z:416:VAL:HG23	1:Z:416:VAL:O	2.04	0.57
1:A:130:GLU:HG3	1:A:136:ILE:HD13	1.85	0.57
1:C:29:LEU:HD23	1:C:41:ILE:HD12	1.86	0.57
1:C:111:LEU:HD23	1:C:112:PRO:HD2	1.86	0.57
1:Y:47:LEU:HB3	1:Y:397:ARG:O	2.05	0.57
1:I:347:ILE:HG12	1:I:352:VAL:HG13	1.86	0.57
1:D:317:ALA:O	1:D:356:GLY:HA3	2.05	0.57
1:G:23:ASN:HB3	4:G:956:HOH:O	2.05	0.57
1:W:137:LYS:HE2	1:W:139:GLU:OE1	2.04	0.57

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:285:HIS:O	1:A:287:LYS:HD2	2.05	0.57
1:D:137:LYS:HE3	4:D:576:HOH:O	2.03	0.57
1:F:63:LYS:HB2	1:F:73:ASP:HB3	1.86	0.57
1:I:29:LEU:HD23	1:I:41:ILE:HD12	1.87	0.57
1:Y:317:ALA:O	1:Y:356:GLY:HA3	2.05	0.57
1:F:111:LEU:HD23	1:F:112:PRO:HD2	1.86	0.57
1:B:63:LYS:HB2	1:B:73:ASP:HB3	1.86	0.56
1:J:317:ALA:O	1:J:356:GLY:HA3	2.05	0.56
1:Z:63:LYS:HB2	1:Z:73:ASP:HB3	1.87	0.56
1:W:28:ILE:HG23	1:W:197:PHE:CD2	2.40	0.56
1:G:29:LEU:HD23	1:G:41:ILE:HD12	1.87	0.56
1:H:29:LEU:HD23	1:H:41:ILE:HD12	1.87	0.56
1:I:119:ALA:HB1	1:J:336:PRO:HG3	1.87	0.56
1:L:248:LYS:HD2	1:L:283:ASP:OD2	2.05	0.56
1:W:109:VAL:O	1:W:143:VAL:HG13	2.05	0.56
1:X:77:VAL:HB	1:X:104:PHE:CZ	2.39	0.56
1:Z:359:LYS:HD2	1:Z:384:GLU:HB2	1.87	0.56
1:A:233:ILE:HA	1:A:306:MET:HE3	1.86	0.56
1:D:111:LEU:HD23	1:D:112:PRO:HD2	1.88	0.56
1:L:63:LYS:HB2	1:L:73:ASP:HB3	1.87	0.56
1:D:63:LYS:HB2	1:D:73:ASP:HB3	1.86	0.56
1:E:417:LYS:N	1:E:417:LYS:HD2	2.19	0.56
1:J:347:ILE:HG12	1:J:352:VAL:HG13	1.88	0.56
1:K:29:LEU:HD23	1:K:41:ILE:HD12	1.86	0.56
1:G:2:ASP:OD2	1:G:415:ARG:HD3	2.04	0.56
1:K:400:GLU:HG2	1:K:401:ARG:HG2	1.86	0.56
1:A:359:LYS:HD2	1:A:384:GLU:HB2	1.88	0.56
1:W:317:ALA:O	1:W:356:GLY:HA3	2.06	0.56
1:A:35:ALA:O	1:A:74:ALA:HB3	2.05	0.56
1:C:336:PRO:HG3	1:D:119:ALA:HB1	1.87	0.56
1:E:156:ILE:CG2	1:E:158:MET:HE1	2.36	0.56
1:E:353:ILE:HD12	1:G:353:ILE:HD12	1.88	0.56
1:K:7:GLN:HB2	1:K:412:ASN:HB3	1.88	0.56
1:A:54:MET:HG2	1:A:64:VAL:HG11	1.87	0.56
1:A:65:GLU:CG	1:A:71:TRP:HB2	2.33	0.55
1:D:54:MET:HG2	1:D:64:VAL:HG11	1.87	0.55
1:W:29:LEU:HD23	1:W:41:ILE:HD12	1.89	0.55
1:W:401:ARG:HB3	1:W:401:ARG:HH11	1.70	0.55
1:B:111:LEU:HD23	1:B:112:PRO:HD2	1.88	0.55
1:H:5:ARG:NH2	1:H:7:GLN:HE21	1.96	0.55
1:J:7:GLN:HB2	1:J:412:ASN:HB3	1.88	0.55

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:40:GLU:HG3	1:X:71:TRP:NE1	2.21	0.55
1:L:1:MET:N	1:L:418:GLY:HA2	2.22	0.55
1:X:54:MET:HG2	1:X:64:VAL:HG11	1.88	0.55
1:Y:29:LEU:HD23	1:Y:41:ILE:HD12	1.87	0.55
1:F:29:LEU:HD23	1:F:41:ILE:HD12	1.88	0.55
1:W:37:GLU:OE1	1:W:220:ARG:NH2	2.39	0.55
1:J:5:ARG:HH12	1:J:7:GLN:NE2	2.05	0.55
1:X:4:PHE:CD1	1:X:413:ILE:HD11	2.41	0.55
1:Z:21:ALA:HA	1:Z:231:ASP:HB2	1.88	0.55
1:I:28:ILE:HG23	1:I:197:PHE:CD2	2.42	0.55
1:C:159:ASP:O	1:C:160:LYS:HB2	2.07	0.55
1:F:21:ALA:HA	1:F:231:ASP:HB2	1.89	0.55
1:X:130:GLU:HG3	1:X:136:ILE:HD12	1.88	0.55
1:Y:347:ILE:HG12	1:Y:352:VAL:HG13	1.88	0.55
1:E:59:GLN:NE2	1:E:86:LEU:HD12	2.21	0.55
1:I:54:MET:HG2	1:I:64:VAL:HG11	1.89	0.55
1:W:348:GLU:CG	1:Y:351:THR:HG21	2.36	0.55
1:Y:63:LYS:HB2	1:Y:73:ASP:HB3	1.89	0.55
1:D:81:SER:HB3	4:D:427:HOH:O	2.07	0.54
1:G:40:GLU:HG3	1:G:71:TRP:NE1	2.22	0.54
1:Y:111:LEU:HD23	1:Y:112:PRO:HD2	1.87	0.54
1:Y:122:VAL:HG22	1:Y:125:HIS:CD2	2.42	0.54
1:B:224:GLY:HA2	1:E:199:VAL:CG1	2.38	0.54
1:H:176:ALA:O	1:H:217:GLY:HA3	2.07	0.54
1:J:122:VAL:HG22	1:J:125:HIS:CD2	2.42	0.54
1:K:143:VAL:O	1:K:143:VAL:HG13	2.06	0.54
1:W:358:GLU:O	1:W:359:LYS:HD2	2.07	0.54
1:Z:84:TYR:O	1:Z:86:LEU:N	2.40	0.54
1:A:30:PHE:CZ	1:A:93:SER:HA	2.42	0.54
1:F:347:ILE:HG12	1:F:352:VAL:HG13	1.89	0.54
1:W:176:ALA:O	1:W:217:GLY:HA3	2.07	0.54
1:W:347:ILE:HG12	1:W:352:VAL:HG13	1.89	0.54
1:X:138:LEU:HD12	1:X:142:TYR:O	2.07	0.54
1:H:59:GLN:HG2	1:H:59:GLN:O	2.06	0.54
1:H:290:LYS:NZ	1:W:286:GLY:HA3	2.22	0.54
1:J:4:PHE:CD1	1:J:413:ILE:HD11	2.42	0.54
1:J:21:ALA:HA	1:J:231:ASP:HB2	1.90	0.54
1:G:66:ARG:NH1	4:G:420:HOH:O	2.41	0.54
1:I:21:ALA:HA	1:I:231:ASP:HB2	1.89	0.54
1:L:317:ALA:O	1:L:356:GLY:HA3	2.07	0.54
1:Z:176:ALA:O	1:Z:217:GLY:HA3	2.07	0.54

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:176:ALA:O	1:D:217:GLY:HA3	2.07	0.54
1:D:401:ARG:NH1	1:D:401:ARG:CB	2.69	0.54
1:E:111:LEU:HD23	1:E:112:PRO:HD2	1.89	0.54
1:H:55:LYS:HG3	4:H:1283:HOH:O	2.07	0.54
1:B:29:LEU:HD23	1:B:41:ILE:HD12	1.89	0.54
1:E:136:ILE:CG2	1:E:143:VAL:HG23	2.38	0.54
1:J:54:MET:HG2	1:J:64:VAL:HG11	1.90	0.54
1:X:347:ILE:HG12	1:X:352:VAL:HG13	1.90	0.54
1:G:176:ALA:O	1:G:217:GLY:HA3	2.08	0.54
1:Z:366:MET:HG3	1:Z:391:ARG:HD2	1.90	0.54
1:D:29:LEU:HD23	1:D:41:ILE:HD12	1.89	0.54
1:X:74:ALA:O	1:X:77:VAL:HG23	2.08	0.54
1:I:122:VAL:HG22	1:I:125:HIS:CD2	2.43	0.53
1:H:317:ALA:O	1:H:356:GLY:HA3	2.08	0.53
1:W:3:LYS:HE3	1:W:418:GLY:HA2	1.91	0.53
1:G:83:PRO:O	1:G:87:VAL:HG13	2.09	0.53
1:I:4:PHE:CD1	1:I:413:ILE:HD11	2.42	0.53
1:W:400:GLU:C	1:W:401:ARG:HG2	2.29	0.53
1:Z:150:ARG:NH2	1:Z:219:GLU:HA	2.24	0.53
1:E:414:GLU:HG2	1:E:416:VAL:HG13	1.90	0.53
1:H:30:PHE:CZ	1:H:93:SER:HA	2.44	0.53
1:L:176:ALA:O	1:L:217:GLY:HA3	2.08	0.53
1:X:353:ILE:HD12	1:Z:353:ILE:HD12	1.91	0.53
1:A:1:MET:O	1:A:418:GLY:CA	2.57	0.53
1:L:111:LEU:HD23	1:L:112:PRO:HD2	1.90	0.53
1:Y:344:HIS:CD2	1:Y:357:VAL:HG11	2.42	0.53
1:A:117:ILE:HA	1:A:330:ASN:O	2.08	0.53
1:A:143:VAL:HG13	1:A:143:VAL:O	2.09	0.53
1:B:317:ALA:O	1:B:356:GLY:HA3	2.08	0.53
1:B:54:MET:HG2	1:B:64:VAL:HG11	1.90	0.53
1:E:83:PRO:HG2	1:E:86:LEU:HB2	1.90	0.53
1:H:111:LEU:HD23	1:H:112:PRO:HD2	1.91	0.53
1:I:40:GLU:HG3	1:I:71:TRP:NE1	2.24	0.53
1:Z:48:LYS:HD2	1:Z:397:ARG:CZ	2.39	0.53
1:G:83:PRO:HG2	1:G:86:LEU:HB2	1.90	0.53
1:K:351:THR:HG23	4:K:1177:HOH:O	2.09	0.52
1:W:4:PHE:CD1	1:W:413:ILE:HD11	2.43	0.52
1:X:111:LEU:HD23	1:X:112:PRO:HD2	1.90	0.52
1:Y:138:LEU:HD12	1:Y:142:TYR:O	2.08	0.52
1:D:83:PRO:HG2	1:D:86:LEU:HB2	1.91	0.52
1:H:40:GLU:HG3	1:H:71:TRP:NE1	2.25	0.52

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:83:PRO:O	1:I:87:VAL:HG13	2.07	0.52
1:X:109:VAL:O	1:X:143:VAL:HG12	2.09	0.52
1:Z:85:ASP:HA	1:Z:88:LYS:HE2	1.92	0.52
1:A:40:GLU:HG3	1:A:71:TRP:NE1	2.25	0.52
1:Y:340:ARG:NH1	1:Z:111:LEU:O	2.37	0.52
1:D:77:VAL:HB	1:D:104:PHE:CZ	2.45	0.52
1:D:122:VAL:HG22	1:D:125:HIS:CD2	2.44	0.52
1:G:21:ALA:HA	1:G:231:ASP:HB2	1.91	0.52
1:J:83:PRO:HG2	1:J:86:LEU:HB2	1.91	0.52
1:L:21:ALA:HA	1:L:231:ASP:HB2	1.90	0.52
1:X:7:GLN:HB2	1:X:412:ASN:HB3	1.92	0.52
1:Y:54:MET:HG2	1:Y:64:VAL:HG11	1.91	0.52
1:A:176:ALA:O	1:A:217:GLY:HA3	2.10	0.52
1:L:347:ILE:HG12	1:L:352:VAL:HG13	1.92	0.52
1:B:4:PHE:CD1	1:B:413:ILE:HD11	2.45	0.52
1:X:143:VAL:HG13	1:X:143:VAL:O	2.10	0.52
1:C:11:ARG:HD3	1:C:247:GLY:HA2	1.91	0.52
1:C:347:ILE:HG12	1:C:352:VAL:HG13	1.92	0.52
1:G:347:ILE:HG12	1:G:352:VAL:HG13	1.92	0.52
1:I:3:LYS:HB2	1:I:416:VAL:CG2	2.40	0.52
1:I:176:ALA:O	1:I:217:GLY:HA3	2.09	0.52
1:Z:54:MET:HG2	1:Z:64:VAL:HG11	1.90	0.52
1:A:28:ILE:HG23	1:A:197:PHE:CD2	2.44	0.52
1:E:29:LEU:HD23	1:E:41:ILE:HD12	1.92	0.52
1:L:40:GLU:HG3	1:L:71:TRP:NE1	2.25	0.52
1:Z:39:VAL:HG23	1:Z:72:ILE:HB	1.92	0.52
1:G:111:LEU:HD23	1:G:112:PRO:HD2	1.91	0.52
1:X:101:VAL:HG21	1:X:145:ALA:HB3	1.90	0.52
1:X:176:ALA:O	1:X:217:GLY:HA3	2.10	0.52
1:X:248:LYS:HD2	1:X:283:ASP:OD2	2.10	0.52
1:A:111:LEU:HD23	1:A:112:PRO:HD2	1.91	0.51
1:F:4:PHE:CD1	1:F:413:ILE:HD11	2.45	0.51
1:F:176:ALA:O	1:F:217:GLY:HA3	2.10	0.51
1:A:83:PRO:HG2	1:A:86:LEU:HB2	1.92	0.51
1:B:131:LYS:HE2	4:B:926:HOH:O	2.10	0.51
1:D:347:ILE:HG12	1:D:352:VAL:HG13	1.91	0.51
1:G:243:ALA:HA	1:G:284:MET:HG2	1.92	0.51
1:H:299:HIS:CG	1:H:300:PRO:HA	2.46	0.51
1:W:400:GLU:HG2	1:W:401:ARG:HG2	1.92	0.51
1:X:59:GLN:O	1:X:59:GLN:HG2	2.10	0.51
1:Z:111:LEU:HD23	1:Z:112:PRO:HD2	1.91	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:78:ASN:C	1:B:78:ASN:ND2	2.63	0.51
1:E:176:ALA:O	1:E:217:GLY:HA3	2.10	0.51
1:K:236:GLY:CA	1:K:306:MET:HE3	2.39	0.51
1:Y:3:LYS:HE3	1:Y:419:GLU:HA	1.93	0.51
1:E:400:GLU:C	1:E:401:ARG:HG2	2.29	0.51
1:W:40:GLU:HG3	1:W:71:TRP:NE1	2.26	0.51
1:Z:74:ALA:O	1:Z:76:ASN:N	2.36	0.51
1:A:347:ILE:HG12	1:A:352:VAL:HG13	1.92	0.51
1:D:335:VAL:HB	1:D:336:PRO:HD3	1.92	0.51
1:E:21:ALA:HA	1:E:231:ASP:HB2	1.93	0.51
1:F:28:ILE:HG23	1:F:197:PHE:CD2	2.45	0.51
1:F:40:GLU:HG3	1:F:71:TRP:NE1	2.26	0.51
1:G:4:PHE:CD1	1:G:413:ILE:HD11	2.45	0.51
1:I:108:GLN:OE1	1:I:144:LYS:HE2	2.11	0.51
1:X:85:ASP:HA	1:X:88:LYS:CD	2.40	0.51
1:Z:35:ALA:O	1:Z:74:ALA:HB3	2.10	0.51
1:C:40:GLU:HG3	1:C:71:TRP:NE1	2.26	0.51
1:B:176:ALA:O	1:B:217:GLY:HA3	2.11	0.51
1:E:28:ILE:HG23	1:E:197:PHE:CD2	2.45	0.51
1:E:295:ARG:CD	1:H:160:LYS:NZ	2.71	0.51
1:F:122:VAL:HG22	1:F:125:HIS:CD2	2.46	0.51
1:K:317:ALA:O	1:K:356:GLY:HA3	2.10	0.51
1:W:59:GLN:NE2	1:W:83:PRO:HD3	2.19	0.51
1:X:299:HIS:CG	1:X:300:PRO:HA	2.46	0.51
1:Z:39:VAL:CG2	1:Z:72:ILE:HB	2.41	0.51
1:Z:347:ILE:HG12	1:Z:352:VAL:HG13	1.93	0.51
1:C:108:GLN:NE2	1:C:144:LYS:HE2	2.25	0.51
1:I:1:MET:O	1:I:418:GLY:CA	2.59	0.51
1:I:111:LEU:HD23	1:I:112:PRO:HD2	1.93	0.51
1:K:54:MET:HG2	1:K:64:VAL:HG11	1.92	0.51
1:K:122:VAL:HG22	1:K:125:HIS:CD2	2.46	0.51
1:W:108:GLN:OE1	1:W:144:LYS:HE2	2.11	0.51
1:W:126:ILE:HG23	1:W:136:ILE:HD13	1.92	0.51
1:Z:7:GLN:HB2	1:Z:412:ASN:HB3	1.93	0.51
1:B:91:ARG:HG3	3:B:1471:EDO:H11	1.92	0.51
1:C:176:ALA:O	1:C:217:GLY:HA3	2.11	0.51
1:D:91:ARG:NH2	1:D:113:GLY:O	2.44	0.51
1:F:243:ALA:HA	1:F:284:MET:HG3	1.93	0.51
1:G:34:LEU:HB3	1:G:221:LEU:HD12	1.92	0.51
1:J:28:ILE:HG23	1:J:197:PHE:CD2	2.46	0.51
1:L:54:MET:HG2	1:L:64:VAL:HG11	1.91	0.51

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:84:TYR:O	1:L:86:LEU:N	2.44	0.51
1:L:122:VAL:HG22	1:L:125:HIS:CD2	2.46	0.51
1:X:28:ILE:HG23	1:X:197:PHE:CD2	2.46	0.51
1:G:150:ARG:HH21	1:G:177:GLU:HA	1.76	0.51
1:I:348:GLU:HG2	1:K:351:THR:HG21	1.93	0.51
1:L:34:LEU:HB3	1:L:221:LEU:HD12	1.93	0.51
1:Y:78:ASN:HB2	4:Y:1296:HOH:O	2.10	0.51
1:D:136:ILE:HG13	1:D:145:ALA:HB2	1.93	0.50
1:G:306:MET:HE2	1:G:309:GLN:HE22	1.73	0.50
1:G:332:PHE:CZ	1:G:352:VAL:HG22	2.46	0.50
1:K:347:ILE:HG12	1:K:352:VAL:HG13	1.91	0.50
1:L:397:ARG:HB3	1:L:397:ARG:CZ	2.41	0.50
1:Z:34:LEU:HB3	1:Z:221:LEU:HD12	1.93	0.50
1:H:28:ILE:HG23	1:H:197:PHE:CD2	2.47	0.50
1:W:38:PRO:O	1:W:223:GLY:HA3	2.11	0.50
1:X:34:LEU:HB3	1:X:221:LEU:HD12	1.93	0.50
1:Z:4:PHE:CD1	1:Z:413:ILE:HD11	2.46	0.50
1:A:276:GLY:HA3	1:A:279:TRP:CE2	2.46	0.50
1:B:335:VAL:HB	1:B:336:PRO:HD3	1.94	0.50
1:D:21:ALA:HA	1:D:231:ASP:HB2	1.92	0.50
1:F:164:GLY:HA3	3:F:1475:EDO:H22	1.92	0.50
1:K:111:LEU:HD23	1:K:112:PRO:HD2	1.91	0.50
1:W:34:LEU:HB3	1:W:221:LEU:HD12	1.93	0.50
1:Z:419:GLU:OXT	1:Z:419:GLU:HG3	2.11	0.50
1:B:276:GLY:HA3	1:B:279:TRP:CE2	2.47	0.50
1:C:34:LEU:HB3	1:C:221:LEU:HD12	1.92	0.50
1:E:122:VAL:HG22	1:E:125:HIS:CD2	2.46	0.50
1:H:4:PHE:CD1	1:H:413:ILE:HD11	2.47	0.50
1:K:40:GLU:HG3	1:K:71:TRP:NE1	2.27	0.50
1:X:85:ASP:HA	1:X:88:LYS:CE	2.40	0.50
1:F:54:MET:HG2	1:F:64:VAL:HG11	1.93	0.50
1:L:139:GLU:C	1:L:140:GLU:HG2	2.30	0.50
1:L:370:LEU:HD22	1:L:397:ARG:HH12	1.76	0.50
1:W:139:GLU:O	1:W:140:GLU:CG	2.60	0.50
1:Z:122:VAL:HG22	1:Z:125:HIS:CD2	2.46	0.50
1:C:243:ALA:HA	1:C:284:MET:HG2	1.94	0.50
1:G:28:ILE:HG23	1:G:197:PHE:CD2	2.46	0.50
1:K:4:PHE:CD1	1:K:413:ILE:HD11	2.47	0.50
1:W:122:VAL:HG22	1:W:125:HIS:CD2	2.46	0.50
1:Y:34:LEU:HB3	1:Y:221:LEU:HD12	1.94	0.50
1:Z:5:ARG:NH2	1:Z:416:VAL:HG11	2.27	0.50

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:317:ALA:O	1:A:356:GLY:HA3	2.11	0.50
1:B:51:ASP:O	1:B:55:LYS:HG3	2.12	0.50
1:F:332:PHE:CZ	1:F:352:VAL:HG22	2.46	0.50
1:K:176:ALA:O	1:K:217:GLY:HA3	2.11	0.50
1:Y:21:ALA:HA	1:Y:231:ASP:HB2	1.93	0.50
1:A:359:LYS:NZ	1:A:384:GLU:HB2	2.26	0.50
1:H:34:LEU:HB3	1:H:221:LEU:HD12	1.94	0.50
1:I:276:GLY:HA3	1:I:279:TRP:CE2	2.47	0.50
1:J:335:VAL:HB	1:J:336:PRO:HD3	1.93	0.50
1:W:126:ILE:HG23	1:W:136:ILE:CD1	2.41	0.50
1:X:122:VAL:HG22	1:X:125:HIS:CD2	2.47	0.50
1:F:83:PRO:HG2	1:F:86:LEU:HB2	1.94	0.50
1:G:417:LYS:O	1:G:418:GLY:C	2.51	0.50
1:H:401:ARG:NH1	1:H:401:ARG:CB	2.69	0.50
1:I:120:ARG:HA	2:I:1458:UDA:O11	2.11	0.50
1:K:335:VAL:HB	1:K:336:PRO:HD3	1.94	0.50
1:L:416:VAL:HG23	1:L:416:VAL:O	2.12	0.50
1:W:335:VAL:HB	1:W:336:PRO:HD3	1.94	0.50
1:X:30:PHE:CZ	1:X:93:SER:HA	2.46	0.50
1:B:332:PHE:CZ	1:B:352:VAL:HG22	2.46	0.49
1:C:160:LYS:NZ	4:C:853:HOH:O	2.44	0.49
1:F:317:ALA:O	1:F:356:GLY:HA3	2.11	0.49
1:I:335:VAL:HB	1:I:336:PRO:HD3	1.94	0.49
1:L:4:PHE:CD1	1:L:413:ILE:HD11	2.47	0.49
1:Z:243:ALA:HA	1:Z:284:MET:HG3	1.94	0.49
1:I:74:ALA:O	1:I:77:VAL:HG23	2.11	0.49
1:K:28:ILE:HG23	1:K:197:PHE:CD2	2.47	0.49
1:Y:176:ALA:O	1:Y:217:GLY:HA3	2.11	0.49
1:W:111:LEU:HD23	1:W:112:PRO:HD2	1.95	0.49
1:Y:4:PHE:CD1	1:Y:413:ILE:HD11	2.48	0.49
1:Y:40:GLU:HG3	1:Y:71:TRP:NE1	2.28	0.49
1:Z:136:ILE:CD1	1:Z:145:ALA:HB2	2.43	0.49
1:D:4:PHE:CD1	1:D:413:ILE:HD11	2.48	0.49
1:L:81:SER:HB3	1:L:108:GLN:CG	2.42	0.49
1:W:188:GLU:N	1:W:188:GLU:OE2	2.45	0.49
1:A:156:ILE:HG22	1:A:158:MET:CE	2.43	0.49
1:D:3:LYS:HE3	1:D:419:GLU:CA	2.42	0.49
1:D:344:HIS:HD2	1:D:357:VAL:CG1	2.25	0.49
1:E:317:ALA:O	1:E:356:GLY:HA3	2.11	0.49
1:K:233:ILE:O	1:K:306:MET:CE	2.61	0.49
1:L:243:ALA:HA	1:L:284:MET:HG3	1.95	0.49

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Y:1:MET:O	1:Y:419:GLU:HA	2.12	0.49
1:Y:39:VAL:HG23	1:Y:72:ILE:HB	1.93	0.49
1:Z:211:ASP:HB3	4:Z:559:HOH:O	2.12	0.49
1:B:122:VAL:HG22	1:B:125:HIS:CD2	2.48	0.49
1:H:243:ALA:HA	1:H:284:MET:HG2	1.94	0.49
1:J:265:LYS:CE	1:J:293:THR:O	2.60	0.49
1:A:1:MET:O	1:A:418:GLY:HA3	2.13	0.49
1:A:233:ILE:HG23	1:A:306:MET:CE	2.37	0.49
1:B:299:HIS:CG	1:B:300:PRO:HA	2.47	0.49
1:J:176:ALA:O	1:J:217:GLY:HA3	2.13	0.49
1:W:21:ALA:HA	1:W:231:ASP:HB2	1.95	0.49
1:Z:40:GLU:HG3	1:Z:71:TRP:NE1	2.28	0.49
1:Z:150:ARG:HH11	1:Z:150:ARG:HG3	1.78	0.49
1:I:109:VAL:O	1:I:143:VAL:HG12	2.13	0.49
1:L:335:VAL:HB	1:L:336:PRO:HD3	1.95	0.49
1:A:233:ILE:O	1:A:306:MET:CE	2.61	0.49
1:C:4:PHE:CD1	1:C:413:ILE:HD11	2.48	0.49
1:E:109:VAL:O	1:E:143:VAL:HG12	2.13	0.49
1:L:59:GLN:HE21	1:L:59:GLN:HB3	1.43	0.49
1:Y:332:PHE:CZ	1:Y:352:VAL:HG22	2.48	0.49
1:B:5:ARG:HD2	4:B:750:HOH:O	2.13	0.49
1:D:40:GLU:HG3	1:D:71:TRP:NE1	2.28	0.49
1:I:77:VAL:HB	1:I:104:PHE:CZ	2.48	0.49
1:J:332:PHE:CZ	1:J:352:VAL:HG22	2.48	0.49
1:K:366:MET:HG3	1:K:391:ARG:HD2	1.95	0.49
1:B:40:GLU:HG3	1:B:71:TRP:NE1	2.28	0.48
1:J:91:ARG:NH2	1:J:113:GLY:O	2.46	0.48
1:W:3:LYS:HB2	1:W:416:VAL:CG2	2.42	0.48
1:W:323:ILE:HB	1:W:352:VAL:HG23	1.95	0.48
1:B:160:LYS:HZ3	1:C:295:ARG:HD2	1.78	0.48
1:C:122:VAL:HG22	1:C:125:HIS:CD2	2.48	0.48
1:E:30:PHE:CZ	1:E:93:SER:HA	2.47	0.48
1:H:3:LYS:HE3	1:H:419:GLU:C	2.34	0.48
1:H:3:LYS:HE3	1:H:419:GLU:CA	2.42	0.48
1:I:85:ASP:HA	1:I:88:LYS:HE2	1.94	0.48
1:G:109:VAL:O	1:G:143:VAL:HG13	2.13	0.48
1:L:299:HIS:CG	1:L:300:PRO:HA	2.48	0.48
1:W:276:GLY:HA3	1:W:279:TRP:CE2	2.49	0.48
1:Y:335:VAL:HB	1:Y:336:PRO:HD3	1.95	0.48
1:A:21:ALA:HA	1:A:231:ASP:HB2	1.96	0.48
1:E:347:ILE:HG12	1:E:352:VAL:HG13	1.93	0.48

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:299:HIS:CG	1:F:300:PRO:HA	2.48	0.48
1:K:21:ALA:HA	1:K:231:ASP:HB2	1.95	0.48
1:B:353:ILE:HD12	1:D:353:ILE:HD12	1.94	0.48
1:I:47:LEU:HB3	1:I:397:ARG:O	2.13	0.48
1:I:59:GLN:OE1	1:I:83:PRO:HD3	2.12	0.48
1:Z:264:ALA:HA	4:Z:431:HOH:O	2.13	0.48
1:C:28:ILE:HG23	1:C:197:PHE:CD2	2.48	0.48
1:J:34:LEU:HB3	1:J:221:LEU:HD12	1.95	0.48
1:K:276:GLY:HA3	1:K:279:TRP:CE2	2.48	0.48
1:W:59:GLN:HE22	1:W:83:PRO:HD2	1.74	0.48
1:W:397:ARG:HG3	1:W:397:ARG:HH11	1.78	0.48
1:A:4:PHE:CD1	1:A:413:ILE:HD11	2.48	0.48
1:E:4:PHE:CD1	1:E:413:ILE:HD11	2.48	0.48
1:E:34:LEU:HB3	1:E:221:LEU:HD12	1.95	0.48
1:G:276:GLY:HA3	1:G:279:TRP:CE2	2.48	0.48
1:Z:84:TYR:C	1:Z:86:LEU:H	2.16	0.48
1:A:74:ALA:O	1:A:76:ASN:N	2.47	0.48
1:W:299:HIS:CG	1:W:300:PRO:HA	2.49	0.48
1:Z:87:VAL:HB	1:Z:93:SER:OG	2.14	0.48
1:B:122:VAL:HG13	1:B:122:VAL:O	2.13	0.48
1:C:332:PHE:CZ	1:C:352:VAL:HG22	2.49	0.48
1:H:335:VAL:HB	1:H:336:PRO:HD3	1.95	0.48
1:K:7:GLN:HA	1:K:7:GLN:HE21	1.78	0.48
1:A:56:LEU:O	1:A:59:GLN:HG2	2.13	0.48
1:A:120:ARG:HA	2:A:1450:UDA:O11	2.14	0.48
1:K:34:LEU:HB3	1:K:221:LEU:HD12	1.96	0.48
1:K:56:LEU:C	1:K:56:LEU:HD23	2.34	0.48
1:K:243:ALA:HA	1:K:284:MET:HG3	1.94	0.48
1:Y:20:GLY:HA3	1:Y:43:ASN:O	2.14	0.48
1:B:34:LEU:HB3	1:B:221:LEU:HD12	1.96	0.47
1:F:34:LEU:HB3	1:F:221:LEU:HD12	1.96	0.47
1:F:353:ILE:HD12	1:H:353:ILE:HD12	1.96	0.47
1:H:21:ALA:HA	1:H:231:ASP:HB2	1.95	0.47
1:J:417:LYS:O	1:J:418:GLY:O	2.32	0.47
1:W:243:ALA:HA	1:W:284:MET:HG3	1.96	0.47
1:X:353:ILE:CD1	1:Z:353:ILE:HD11	2.44	0.47
1:Y:276:GLY:HA3	1:Y:279:TRP:CE2	2.49	0.47
1:A:243:ALA:HA	1:A:284:MET:HG3	1.95	0.47
1:C:21:ALA:HA	1:C:231:ASP:CB	2.43	0.47
1:D:28:ILE:HG23	1:D:197:PHE:CD2	2.50	0.47
1:E:332:PHE:CZ	1:E:352:VAL:HG22	2.49	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:233:ILE:CG2	1:G:306:MET:HE3	2.28	0.47
1:H:347:ILE:HG12	1:H:352:VAL:HG13	1.95	0.47
1:K:11:ARG:HD2	1:K:246:GLY:C	2.34	0.47
1:D:34:LEU:HB3	1:D:221:LEU:HD12	1.96	0.47
1:F:276:GLY:HA3	1:F:279:TRP:CE2	2.50	0.47
1:H:2:ASP:OD2	1:H:415:ARG:HD3	2.14	0.47
1:I:348:GLU:CG	1:K:351:THR:HG21	2.44	0.47
1:K:299:HIS:CG	1:K:300:PRO:HA	2.49	0.47
1:K:332:PHE:CZ	1:K:352:VAL:HG22	2.50	0.47
1:L:28:ILE:HG23	1:L:197:PHE:CD2	2.49	0.47
1:W:139:GLU:O	1:W:140:GLU:HG3	2.14	0.47
1:X:21:ALA:HA	1:X:231:ASP:HB2	1.97	0.47
1:A:400:GLU:HG2	1:A:401:ARG:HG2	1.96	0.47
1:D:403:GLU:HB2	4:D:807:HOH:O	2.15	0.47
1:G:54:MET:HG2	1:G:64:VAL:HG11	1.96	0.47
1:H:359:LYS:HB2	1:H:359:LYS:HE3	1.72	0.47
1:I:299:HIS:CG	1:I:300:PRO:HA	2.49	0.47
1:J:85:ASP:HA	1:J:88:LYS:CE	2.44	0.47
1:Z:215:ILE:N	1:Z:215:ILE:HD12	2.29	0.47
1:B:243:ALA:HA	1:B:284:MET:HG3	1.96	0.47
1:C:82:ALA:HB3	1:C:109:VAL:HG13	1.97	0.47
1:J:243:ALA:HA	1:J:284:MET:HG3	1.96	0.47
1:L:7:GLN:HB2	1:L:412:ASN:CB	2.44	0.47
1:L:332:PHE:CZ	1:L:352:VAL:HG22	2.49	0.47
1:X:335:VAL:HB	1:X:336:PRO:HD3	1.95	0.47
1:Z:28:ILE:HG23	1:Z:197:PHE:CD2	2.48	0.47
1:A:56:LEU:CD1	1:A:93:SER:HB2	2.44	0.47
1:C:83:PRO:O	1:C:87:VAL:HG13	2.14	0.47
1:F:335:VAL:HB	1:F:336:PRO:HD3	1.97	0.47
1:H:417:LYS:HG3	1:H:418:GLY:H	1.80	0.47
1:L:323:ILE:HB	1:L:352:VAL:HG23	1.96	0.47
1:C:108:GLN:HE22	1:C:144:LYS:HE2	1.80	0.47
1:C:323:ILE:HB	1:C:352:VAL:HG23	1.96	0.47
1:E:64:VAL:HG13	1:E:72:ILE:HD13	1.97	0.47
1:F:81:SER:HA	1:F:108:GLN:O	2.15	0.47
1:G:299:HIS:CG	1:G:300:PRO:HA	2.50	0.47
1:H:85:ASP:HA	1:H:88:LYS:HE2	1.96	0.47
1:H:95:TRP:HA	4:H:726:HOH:O	2.14	0.47
1:K:64:VAL:HG13	1:K:72:ILE:HD13	1.96	0.47
1:K:108:GLN:NE2	1:K:144:LYS:HE2	2.29	0.47
1:L:20:GLY:HA3	1:L:43:ASN:O	2.15	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:87:VAL:HB	1:L:93:SER:OG	2.14	0.47
1:W:265:LYS:CE	1:W:293:THR:O	2.63	0.47
1:X:332:PHE:CZ	1:X:352:VAL:HG22	2.50	0.47
1:Z:276:GLY:HA3	1:Z:279:TRP:CE2	2.49	0.47
1:Z:299:HIS:CG	1:Z:300:PRO:HA	2.49	0.47
1:A:332:PHE:CZ	1:A:352:VAL:HG22	2.49	0.47
1:E:83:PRO:O	1:E:87:VAL:HG13	2.14	0.47
1:H:323:ILE:HB	1:H:352:VAL:HG23	1.97	0.47
1:L:1:MET:H2	1:L:418:GLY:HA2	1.79	0.47
1:A:7:GLN:HG2	4:A:737:HOH:O	2.14	0.47
1:B:28:ILE:HG23	1:B:197:PHE:CD2	2.49	0.47
1:E:85:ASP:OD1	1:E:85:ASP:N	2.35	0.47
1:H:243:ALA:HA	1:H:284:MET:HG3	1.97	0.47
1:I:139:GLU:O	1:I:140:GLU:HG3	2.14	0.47
1:I:397:ARG:NH1	1:I:397:ARG:HB3	2.30	0.47
1:K:30:PHE:CZ	1:K:93:SER:HA	2.50	0.47
1:Y:299:HIS:CG	1:Y:300:PRO:HA	2.50	0.47
1:Z:248:LYS:HG2	1:Z:249:ILE:N	2.29	0.47
1:C:5:ARG:NH1	1:C:5:ARG:HG2	2.30	0.47
1:C:276:GLY:HA3	1:C:279:TRP:CE2	2.49	0.47
1:D:290:LYS:HZ3	1:I:286:GLY:CA	2.27	0.47
1:G:419:GLU:CD	1:G:419:GLU:O	2.53	0.47
1:H:122:VAL:HG22	1:H:125:HIS:CD2	2.50	0.47
1:H:416:VAL:HG23	1:H:416:VAL:O	2.14	0.47
1:J:282:LEU:C	1:J:282:LEU:HD23	2.36	0.47
1:W:64:VAL:HG13	1:W:72:ILE:HD13	1.97	0.47
1:W:243:ALA:HA	1:W:284:MET:HG2	1.96	0.47
1:Z:323:ILE:HB	1:Z:352:VAL:HG23	1.97	0.47
1:Z:332:PHE:CZ	1:Z:352:VAL:HG22	2.50	0.47
1:B:21:ALA:HA	1:B:231:ASP:HB2	1.97	0.46
1:D:243:ALA:HA	1:D:284:MET:HG2	1.97	0.46
1:F:233:ILE:HD12	1:F:306:MET:HE2	1.98	0.46
1:G:122:VAL:HG22	1:G:125:HIS:CD2	2.50	0.46
1:I:34:LEU:HB3	1:I:221:LEU:HD12	1.97	0.46
1:I:392:ILE:O	1:I:395:ILE:HG22	2.15	0.46
1:L:143:VAL:O	1:L:143:VAL:HG13	2.14	0.46
1:W:313:LEU:C	1:W:313:LEU:HD23	2.36	0.46
1:Y:64:VAL:HG13	1:Y:72:ILE:HD13	1.97	0.46
1:A:64:VAL:HG13	1:A:72:ILE:HD13	1.98	0.46
1:E:248:LYS:HD2	1:E:283:ASP:OD2	2.15	0.46
1:E:299:HIS:CG	1:E:300:PRO:HA	2.50	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:401:ARG:CB	1:H:401:ARG:CZ	2.93	0.46
1:I:243:ALA:HA	1:I:284:MET:HG2	1.95	0.46
1:I:282:LEU:HD23	1:I:282:LEU:C	2.36	0.46
1:L:84:TYR:CE2	1:L:88:LYS:HD3	2.51	0.46
1:X:276:GLY:HA3	1:X:279:TRP:CE2	2.50	0.46
1:G:344:HIS:HD2	1:G:357:VAL:CG1	2.28	0.46
1:I:397:ARG:NH2	2:I:1458:UDA:O15	2.49	0.46
1:W:120:ARG:HA	2:W:1462:UDA:O11	2.16	0.46
1:D:56:LEU:HD23	1:D:56:LEU:C	2.36	0.46
1:D:276:GLY:HA3	1:D:279:TRP:CE2	2.50	0.46
1:A:122:VAL:HG22	1:A:125:HIS:CD2	2.50	0.46
1:C:284:MET:O	1:C:287:LYS:HG3	2.14	0.46
1:H:276:GLY:HA3	1:H:279:TRP:CE2	2.50	0.46
1:I:81:SER:HB2	1:I:108:GLN:HE21	1.79	0.46
1:J:5:ARG:HH11	1:J:5:ARG:HG2	1.81	0.46
1:J:299:HIS:CG	1:J:300:PRO:HA	2.51	0.46
1:K:351:THR:CG2	4:K:1177:HOH:O	2.64	0.46
1:X:323:ILE:HB	1:X:352:VAL:HG23	1.97	0.46
1:Y:367:ALA:HB1	1:Y:373:SER:HB3	1.96	0.46
1:Z:21:ALA:HA	1:Z:231:ASP:CB	2.45	0.46
1:Z:126:ILE:HG23	1:Z:136:ILE:HG13	1.98	0.46
1:B:347:ILE:HG12	1:B:352:VAL:HG13	1.97	0.46
1:D:85:ASP:HA	1:D:88:LYS:HE2	1.97	0.46
1:D:265:LYS:CE	1:D:293:THR:O	2.64	0.46
1:J:30:PHE:CZ	1:J:93:SER:HA	2.50	0.46
1:K:56:LEU:HD23	1:K:56:LEU:O	2.15	0.46
1:X:36:GLU:OE1	1:X:220:ARG:HD2	2.16	0.46
1:Y:243:ALA:HA	1:Y:284:MET:HG3	1.96	0.46
1:Y:392:ILE:O	1:Y:395:ILE:HG22	2.16	0.46
1:A:37:GLU:HB2	1:A:223:GLY:N	2.31	0.46
1:A:37:GLU:HB2	1:A:222:GLY:C	2.36	0.46
1:E:243:ALA:HA	1:E:284:MET:HG3	1.97	0.46
1:E:276:GLY:HA3	1:E:279:TRP:CE2	2.51	0.46
1:K:215:ILE:HD12	1:K:215:ILE:N	2.31	0.46
1:L:84:TYR:C	1:L:86:LEU:N	2.68	0.46
1:Y:28:ILE:HG23	1:Y:197:PHE:CD2	2.50	0.46
1:Y:91:ARG:HG2	4:Y:850:HOH:O	2.15	0.46
1:Y:323:ILE:HB	1:Y:352:VAL:HG23	1.97	0.46
1:A:299:HIS:CG	1:A:300:PRO:HA	2.51	0.46
1:C:335:VAL:HB	1:C:336:PRO:HD3	1.97	0.46
1:D:243:ALA:HA	1:D:284:MET:HG3	1.98	0.46

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:299:HIS:CG	1:D:300:PRO:HA	2.51	0.46
1:E:20:GLY:HA3	1:E:43:ASN:O	2.15	0.46
1:I:370:LEU:HB2	1:I:397:ARG:HH12	1.80	0.46
1:Y:55:LYS:HE3	1:Y:55:LYS:HB2	1.79	0.46
1:Z:366:MET:CG	1:Z:391:ARG:HD2	2.45	0.46
1:A:56:LEU:C	1:A:56:LEU:HD23	2.36	0.46
1:D:161:VAL:HA	4:D:1012:HOH:O	2.16	0.46
1:I:11:ARG:HA	1:I:245:SER:HB2	1.98	0.46
1:I:397:ARG:NH1	1:I:397:ARG:CB	2.79	0.46
1:J:13:GLN:HB2	1:J:248:LYS:H	1.80	0.46
1:B:49:ASP:OD1	1:B:397:ARG:NH1	2.49	0.46
1:E:135:GLU:C	1:E:136:ILE:HD12	2.36	0.46
1:L:3:LYS:HB2	1:L:416:VAL:CG2	2.46	0.46
1:L:56:LEU:CD1	1:L:93:SER:HB2	2.45	0.46
1:D:64:VAL:HG13	1:D:72:ILE:HD13	1.98	0.45
1:I:7:GLN:NE2	1:I:386:THR:OG1	2.48	0.45
1:I:64:VAL:HG13	1:I:72:ILE:HD13	1.98	0.45
1:I:332:PHE:CZ	1:I:352:VAL:HG22	2.51	0.45
1:W:97:LEU:O	1:W:101:VAL:HG12	2.16	0.45
1:X:351:THR:CG2	4:X:548:HOH:O	2.65	0.45
1:Y:84:TYR:O	1:Y:86:LEU:N	2.50	0.45
1:Y:324:THR:HG23	1:Y:351:THR:HG22	1.98	0.45
1:Y:418:GLY:O	1:Y:419:GLU:C	2.54	0.45
1:A:34:LEU:HB3	1:A:221:LEU:HD12	1.97	0.45
1:C:299:HIS:CG	1:C:300:PRO:HA	2.51	0.45
1:F:164:GLY:HA3	3:F:1475:EDO:C2	2.46	0.45
1:H:49:ASP:OD2	1:H:397:ARG:HG2	2.16	0.45
1:H:249:ILE:HG12	1:H:250:VAL:N	2.31	0.45
1:H:290:LYS:HZ3	1:W:286:GLY:C	2.20	0.45
1:W:23:ASN:HB3	4:W:434:HOH:O	2.16	0.45
1:W:332:PHE:CZ	1:W:352:VAL:HG22	2.51	0.45
1:E:40:GLU:HG3	1:E:71:TRP:NE1	2.31	0.45
1:E:359:LYS:NZ	1:E:384:GLU:OE1	2.46	0.45
1:F:136:ILE:N	1:F:136:ILE:CD1	2.79	0.45
1:H:143:VAL:HG13	1:H:143:VAL:O	2.16	0.45
1:X:101:VAL:HG21	1:X:145:ALA:CB	2.46	0.45
1:X:249:ILE:HG12	1:X:250:VAL:N	2.31	0.45
1:Y:48:LYS:HD2	1:Y:397:ARG:NH1	2.32	0.45
1:Y:136:ILE:HG12	1:Y:145:ALA:HB2	1.98	0.45
1:Z:335:VAL:HB	1:Z:336:PRO:HD3	1.99	0.45
1:B:143:VAL:HG13	1:B:143:VAL:O	2.16	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:64:VAL:HG13	1:F:72:ILE:HD13	1.97	0.45
1:I:126:ILE:HG23	1:I:136:ILE:HD13	1.99	0.45
1:J:64:VAL:HG13	1:J:72:ILE:HD13	1.98	0.45
1:J:277:GLU:HG2	4:J:873:HOH:O	2.17	0.45
1:L:7:GLN:HB2	1:L:412:ASN:CG	2.37	0.45
1:L:77:VAL:HB	1:L:104:PHE:CZ	2.51	0.45
1:L:84:TYR:C	1:L:86:LEU:H	2.19	0.45
1:A:335:VAL:HB	1:A:336:PRO:HD3	1.99	0.45
1:D:136:ILE:N	1:D:136:ILE:HD12	2.32	0.45
1:D:143:VAL:O	1:D:143:VAL:HG13	2.16	0.45
1:E:295:ARG:NE	1:H:160:LYS:HZ2	2.15	0.45
1:G:417:LYS:HD2	1:G:417:LYS:N	2.31	0.45
1:H:299:HIS:ND1	1:H:300:PRO:HA	2.31	0.45
1:I:323:ILE:HB	1:I:352:VAL:HG23	1.99	0.45
1:X:64:VAL:HG13	1:X:72:ILE:HD13	1.97	0.45
1:X:243:ALA:HA	1:X:284:MET:HG2	1.97	0.45
1:Z:36:GLU:OE1	1:Z:220:ARG:HD2	2.17	0.45
1:Z:64:VAL:HG13	1:Z:72:ILE:HD13	1.99	0.45
1:D:400:GLU:O	1:D:401:ARG:HG2	2.17	0.45
1:G:85:ASP:HA	1:G:88:LYS:HE2	1.98	0.45
1:H:332:PHE:CZ	1:H:352:VAL:HG22	2.52	0.45
1:J:276:GLY:HA3	1:J:279:TRP:CE2	2.51	0.45
1:J:313:LEU:C	1:J:313:LEU:HD23	2.36	0.45
1:K:79:ASN:ND2	1:K:80:PHE:H	2.14	0.45
1:K:138:LEU:HD12	1:K:142:TYR:O	2.16	0.45
1:L:276:GLY:HA3	1:L:279:TRP:CE2	2.51	0.45
1:Y:56:LEU:C	1:Y:56:LEU:HD23	2.37	0.45
1:Y:84:TYR:C	1:Y:86:LEU:H	2.20	0.45
1:A:276:GLY:HA3	1:A:279:TRP:NE1	2.32	0.45
1:B:56:LEU:HD23	1:B:56:LEU:C	2.37	0.45
1:F:21:ALA:HA	1:F:231:ASP:CB	2.46	0.45
1:G:243:ALA:HA	1:G:284:MET:HG3	1.99	0.45
1:H:418:GLY:O	1:H:419:GLU:C	2.54	0.45
1:J:40:GLU:HG3	1:J:71:TRP:NE1	2.31	0.45
1:J:122:VAL:HG22	1:J:125:HIS:CG	2.52	0.45
1:L:56:LEU:C	1:L:56:LEU:HD23	2.37	0.45
1:L:81:SER:CB	1:L:108:GLN:HG3	2.47	0.45
1:L:215:ILE:N	1:L:215:ILE:HD12	2.31	0.45
1:X:3:LYS:HE2	1:X:390:ASP:OD1	2.16	0.45
1:Y:419:GLU:O	1:Y:419:GLU:HG3	2.16	0.45
1:A:329:GLU:HG3	4:A:444:HOH:O	2.16	0.45

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:117:ILE:HA	1:B:330:ASN:O	2.17	0.45
1:D:156:ILE:HG22	1:D:158:MET:CE	2.46	0.45
1:X:243:ALA:HA	1:X:284:MET:HG3	1.96	0.45
1:Z:29:LEU:HD23	1:Z:41:ILE:CD1	2.46	0.45
1:B:276:GLY:HA3	1:B:279:TRP:NE1	2.32	0.45
1:D:271:ALA:HB1	1:D:282:LEU:HG	1.99	0.45
1:D:417:LYS:O	1:D:418:GLY:C	2.55	0.45
1:F:97:LEU:O	1:F:101:VAL:HG12	2.17	0.45
1:J:323:ILE:HB	1:J:352:VAL:HG23	1.98	0.45
1:L:30:PHE:CZ	1:L:93:SER:HA	2.52	0.45
1:X:265:LYS:CE	1:X:293:THR:O	2.65	0.45
1:B:1:MET:CE	1:B:391:ARG:NH1	2.80	0.45
1:W:392:ILE:O	1:W:395:ILE:HG22	2.17	0.45
1:X:20:GLY:HA3	1:X:43:ASN:O	2.17	0.45
1:X:158:MET:HA	1:X:158:MET:CE	2.47	0.45
1:A:249:ILE:HG12	1:A:250:VAL:N	2.33	0.44
1:B:299:HIS:ND1	1:B:300:PRO:HA	2.32	0.44
1:F:265:LYS:CE	1:F:293:THR:O	2.65	0.44
1:G:150:ARG:NH1	1:G:219:GLU:HA	2.32	0.44
1:I:21:ALA:HA	1:I:231:ASP:CB	2.47	0.44
1:J:122:VAL:O	1:J:122:VAL:HG13	2.16	0.44
1:J:188:GLU:OE2	1:J:188:GLU:N	2.49	0.44
1:L:249:ILE:HG12	1:L:250:VAL:N	2.32	0.44
1:L:299:HIS:ND1	1:L:300:PRO:HA	2.32	0.44
1:W:63:LYS:HA	4:W:950:HOH:O	2.16	0.44
1:W:83:PRO:O	1:W:87:VAL:HG13	2.16	0.44
1:Y:313:LEU:C	1:Y:313:LEU:HD23	2.37	0.44
1:G:335:VAL:HB	1:G:336:PRO:HD3	1.99	0.44
1:I:130:GLU:HG3	1:I:136:ILE:HD12	1.99	0.44
1:I:336:PRO:HG3	1:J:119:ALA:HB1	1.98	0.44
1:L:265:LYS:CE	1:L:293:THR:O	2.65	0.44
1:C:37:GLU:HB3	1:C:38:PRO:CD	2.47	0.44
1:G:161:VAL:HA	4:G:697:HOH:O	2.18	0.44
1:H:64:VAL:HG13	1:H:72:ILE:HD13	1.99	0.44
1:W:13:GLN:HB2	1:W:248:LYS:H	1.82	0.44
1:Z:81:SER:HA	1:Z:108:GLN:O	2.17	0.44
1:A:323:ILE:HB	1:A:352:VAL:HG23	1.99	0.44
1:D:3:LYS:HE2	1:D:390:ASP:OD1	2.16	0.44
1:E:74:ALA:O	1:E:77:VAL:HG23	2.18	0.44
1:F:81:SER:HB3	1:F:108:GLN:HG3	1.99	0.44
1:I:122:VAL:O	1:I:122:VAL:HG13	2.16	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:248:LYS:HA	1:J:282:LEU:O	2.17	0.44
1:L:243:ALA:HA	1:L:284:MET:HG2	2.00	0.44
1:Y:249:ILE:HG12	1:Y:250:VAL:N	2.32	0.44
1:B:243:ALA:HA	1:B:284:MET:HG2	1.99	0.44
1:F:248:LYS:HA	1:F:282:LEU:O	2.18	0.44
1:J:56:LEU:C	1:J:56:LEU:HD23	2.38	0.44
1:Y:215:ILE:HD12	1:Y:215:ILE:N	2.32	0.44
1:Y:336:PRO:HG3	1:Z:119:ALA:HB1	1.99	0.44
1:H:3:LYS:HE2	1:H:390:ASP:OD1	2.17	0.44
1:I:38:PRO:O	1:I:223:GLY:HA3	2.18	0.44
1:J:353:ILE:CD1	1:L:353:ILE:HD11	2.48	0.44
1:L:21:ALA:HA	1:L:231:ASP:CB	2.47	0.44
1:X:122:VAL:HG22	1:X:125:HIS:CG	2.53	0.44
1:Y:358:GLU:HG3	1:Y:359:LYS:HG3	1.99	0.44
1:A:136:ILE:N	1:A:136:ILE:HD12	2.33	0.44
1:C:243:ALA:HA	1:C:284:MET:HG3	2.00	0.44
1:D:332:PHE:CZ	1:D:352:VAL:HG22	2.53	0.44
1:F:1:MET:H3	1:F:418:GLY:HA2	1.82	0.44
1:F:56:LEU:C	1:F:56:LEU:HD23	2.38	0.44
1:G:82:ALA:HB3	1:G:109:VAL:HG13	2.00	0.44
1:J:36:GLU:OE1	1:J:220:ARG:HD2	2.18	0.44
1:W:143:VAL:HG22	1:W:143:VAL:O	2.16	0.44
1:X:295:ARG:HH11	1:X:295:ARG:HG2	1.82	0.44
1:Y:265:LYS:CE	1:Y:293:THR:O	2.66	0.44
1:Z:265:LYS:CE	1:Z:293:THR:O	2.66	0.44
1:Z:400:GLU:HG2	1:Z:401:ARG:HG2	1.99	0.44
1:A:156:ILE:HG22	1:A:158:MET:HE2	1.99	0.44
1:B:265:LYS:CE	1:B:293:THR:O	2.66	0.44
1:C:64:VAL:HG13	1:C:72:ILE:HD13	2.00	0.44
1:C:265:LYS:CE	1:C:293:THR:O	2.66	0.44
1:E:249:ILE:HG12	1:E:250:VAL:N	2.33	0.44
1:F:160:LYS:HB2	1:F:160:LYS:NZ	2.33	0.44
1:H:392:ILE:O	1:H:395:ILE:HG22	2.18	0.44
1:I:139:GLU:O	1:I:140:GLU:CG	2.66	0.44
1:J:351:THR:HG21	1:L:348:GLU:CG	2.48	0.44
1:K:233:ILE:HA	1:K:306:MET:CE	2.46	0.44
1:K:367:ALA:HB1	1:K:373:SER:HB3	1.99	0.44
1:L:4:PHE:HE2	1:L:415:ARG:HB2	1.83	0.44
1:L:230:PRO:HB2	4:L:436:HOH:O	2.18	0.44
1:X:188:GLU:OE2	1:X:188:GLU:N	2.51	0.44
1:A:122:VAL:O	1:A:122:VAL:HG13	2.18	0.44

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:359:LYS:HZ2	1:A:384:GLU:HB2	1.83	0.44
1:A:419:GLU:HA	1:A:419:GLU:OE1	2.18	0.44
1:E:295:ARG:NH1	1:E:326:THR:HG21	2.32	0.44
1:F:117:ILE:HA	1:F:330:ASN:O	2.18	0.44
1:G:21:ALA:HA	1:G:231:ASP:CB	2.47	0.44
1:J:40:GLU:HB3	1:J:225:VAL:HG22	2.00	0.44
1:L:85:ASP:HA	1:L:88:LYS:CE	2.46	0.44
1:B:160:LYS:HZ2	1:C:295:ARG:HD2	1.81	0.43
1:E:295:ARG:CD	1:H:160:LYS:HZ2	2.30	0.43
1:F:323:ILE:HB	1:F:352:VAL:HG23	1.99	0.43
1:I:29:LEU:HD23	1:I:41:ILE:CD1	2.48	0.43
1:J:249:ILE:HG12	1:J:250:VAL:N	2.33	0.43
1:K:233:ILE:O	1:K:306:MET:HE1	2.18	0.43
1:Y:120:ARG:HA	2:Y:1464:UDA:O11	2.18	0.43
1:Y:282:LEU:C	1:Y:282:LEU:HD23	2.39	0.43
1:Z:77:VAL:HB	1:Z:104:PHE:CZ	2.53	0.43
1:A:56:LEU:HD11	1:A:93:SER:HB2	2.00	0.43
1:A:353:ILE:HD12	1:C:353:ILE:HD12	2.00	0.43
1:B:64:VAL:HG13	1:B:72:ILE:HD13	1.99	0.43
1:B:392:ILE:O	1:B:395:ILE:HG22	2.18	0.43
1:C:85:ASP:HA	1:C:88:LYS:HE2	2.00	0.43
1:E:367:ALA:HB1	1:E:373:SER:HB3	2.00	0.43
1:F:122:VAL:HG13	1:F:122:VAL:O	2.18	0.43
1:F:211:ASP:HB3	4:F:832:HOH:O	2.18	0.43
1:G:265:LYS:CE	1:G:293:THR:O	2.66	0.43
1:J:136:ILE:CG2	1:J:143:VAL:HG23	2.49	0.43
1:W:11:ARG:HA	1:W:245:SER:HB2	2.01	0.43
1:W:282:LEU:C	1:W:282:LEU:HD23	2.39	0.43
1:Y:416:VAL:HG23	1:Y:416:VAL:O	2.18	0.43
1:Z:276:GLY:HA3	1:Z:279:TRP:NE1	2.33	0.43
1:C:54:MET:HG2	1:C:64:VAL:HG11	2.00	0.43
1:D:124:LEU:HD11	1:D:160:LYS:HB3	2.01	0.43
1:E:56:LEU:C	1:E:56:LEU:HD23	2.39	0.43
1:E:136:ILE:N	1:E:136:ILE:CD1	2.81	0.43
1:J:21:ALA:HA	1:J:231:ASP:CB	2.48	0.43
1:L:370:LEU:HB2	1:L:397:ARG:NH1	2.33	0.43
1:W:75:SER:C	1:W:76:ASN:HD22	2.22	0.43
1:C:282:LEU:C	1:C:282:LEU:HD23	2.39	0.43
1:E:418:GLY:O	1:E:419:GLU:C	2.57	0.43
1:F:1:MET:HB3	1:F:419:GLU:HG2	2.01	0.43
1:F:11:ARG:HD3	1:F:247:GLY:HA2	1.99	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:299:HIS:ND1	1:F:300:PRO:HA	2.33	0.43
1:J:13:GLN:HE21	1:J:13:GLN:HB3	1.59	0.43
1:L:122:VAL:HG22	1:L:125:HIS:CG	2.53	0.43
1:L:303:PRO:HG2	1:L:306:MET:HB2	1.99	0.43
1:Z:20:GLY:HA3	1:Z:43:ASN:O	2.19	0.43
1:A:414:GLU:HG2	1:A:416:VAL:CG1	2.47	0.43
1:B:417:LYS:HE2	1:B:417:LYS:N	2.33	0.43
1:C:5:ARG:HG2	1:C:5:ARG:HH11	1.81	0.43
1:F:391:ARG:HD2	1:F:393:TYR:CE2	2.50	0.43
1:H:351:THR:CG2	4:H:852:HOH:O	2.65	0.43
1:I:59:GLN:HE22	1:I:86:LEU:HD12	1.83	0.43
1:L:124:LEU:HD11	1:L:160:LYS:HB3	2.00	0.43
1:L:324:THR:HG23	1:L:351:THR:HG22	2.01	0.43
1:X:85:ASP:CA	1:X:88:LYS:HE2	2.46	0.43
1:B:30:PHE:CZ	1:B:93:SER:HA	2.54	0.43
1:D:30:PHE:CZ	1:D:93:SER:HA	2.53	0.43
1:F:136:ILE:HG23	1:F:143:VAL:HG23	2.01	0.43
1:H:215:ILE:HD12	1:H:215:ILE:N	2.33	0.43
1:L:64:VAL:HG13	1:L:72:ILE:HD13	2.01	0.43
1:W:77:VAL:HB	1:W:104:PHE:CZ	2.54	0.43
1:X:160:LYS:HE2	1:Y:295:ARG:CZ	2.49	0.43
1:X:299:HIS:ND1	1:X:300:PRO:HA	2.33	0.43
1:Z:56:LEU:HD23	1:Z:56:LEU:C	2.39	0.43
1:C:56:LEU:C	1:C:56:LEU:HD23	2.39	0.43
1:D:249:ILE:HG12	1:D:250:VAL:N	2.33	0.43
1:E:323:ILE:HB	1:E:352:VAL:HG23	2.00	0.43
1:F:163:VAL:HG11	4:F:820:HOH:O	2.18	0.43
1:F:390:ASP:O	1:F:391:ARG:HB2	2.18	0.43
1:I:157:VAL:HG11	1:L:261:ALA:HA	2.00	0.43
1:L:36:GLU:OE1	1:L:220:ARG:HD2	2.19	0.43
1:L:136:ILE:CD1	1:L:145:ALA:HB2	2.49	0.43
1:Y:21:ALA:HA	1:Y:231:ASP:CB	2.49	0.43
1:A:233:ILE:O	1:A:306:MET:HE3	2.18	0.43
1:E:122:VAL:O	1:E:122:VAL:HG13	2.19	0.43
1:I:1:MET:O	1:I:418:GLY:HA2	2.17	0.43
1:I:101:VAL:HG11	1:I:145:ALA:HB3	2.01	0.43
1:I:311:THR:HA	1:I:323:ILE:CD1	2.49	0.43
1:J:3:LYS:HE2	1:J:390:ASP:OD1	2.18	0.43
1:J:20:GLY:HA3	1:J:43:ASN:O	2.19	0.43
1:J:233:ILE:HG21	1:J:371:ARG:CZ	2.48	0.43
1:W:249:ILE:HG12	1:W:250:VAL:N	2.33	0.43

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:W:271:ALA:HB1	1:W:282:LEU:HG	2.01	0.43
1:X:282:LEU:C	1:X:282:LEU:HD23	2.39	0.43
1:Z:7:GLN:HB2	1:Z:412:ASN:CG	2.39	0.43
1:Z:84:TYR:C	1:Z:86:LEU:N	2.71	0.43
1:A:36:GLU:OE1	1:A:220:ARG:HD2	2.19	0.43
1:B:358:GLU:HG3	1:B:359:LYS:HG3	2.00	0.43
1:C:249:ILE:HG12	1:C:250:VAL:N	2.33	0.43
1:D:103:ARG:HD3	1:D:104:PHE:CE1	2.54	0.43
1:D:122:VAL:HG22	1:D:125:HIS:CG	2.53	0.43
1:E:336:PRO:HG3	1:F:119:ALA:HB1	2.00	0.43
1:E:358:GLU:HG3	1:E:359:LYS:HG3	1.99	0.43
1:G:37:GLU:HB3	1:G:38:PRO:CD	2.49	0.43
1:G:59:GLN:HE22	1:G:83:PRO:CG	2.31	0.43
1:J:243:ALA:HA	1:J:284:MET:HG2	1.99	0.43
1:J:416:VAL:O	1:J:416:VAL:HG23	2.18	0.43
1:K:249:ILE:HG12	1:K:250:VAL:N	2.34	0.43
1:C:37:GLU:HB3	1:C:38:PRO:HD2	2.00	0.43
1:D:20:GLY:HA3	1:D:43:ASN:O	2.19	0.43
1:D:56:LEU:HD23	1:D:56:LEU:O	2.19	0.43
1:F:243:ALA:HA	1:F:284:MET:HG2	2.01	0.43
1:G:78:ASN:C	1:G:78:ASN:HD22	2.21	0.43
1:G:233:ILE:HG21	1:G:371:ARG:CZ	2.48	0.43
1:G:367:ALA:HB1	1:G:373:SER:HB3	2.01	0.43
1:I:82:ALA:HB3	1:I:109:VAL:HA	2.00	0.43
1:B:323:ILE:HB	1:B:352:VAL:HG23	1.99	0.42
1:H:265:LYS:CE	1:H:293:THR:O	2.67	0.42
1:H:401:ARG:HB3	1:H:401:ARG:CZ	2.45	0.42
1:Y:136:ILE:HG12	1:Y:145:ALA:CB	2.48	0.42
1:Z:243:ALA:HA	1:Z:284:MET:HG2	2.01	0.42
1:D:323:ILE:HB	1:D:352:VAL:HG23	2.01	0.42
1:G:139:GLU:O	1:G:140:GLU:HG3	2.18	0.42
1:G:183:GLU:OE2	1:G:212:ARG:CZ	2.67	0.42
1:K:122:VAL:HG22	1:K:125:HIS:CG	2.54	0.42
1:L:136:ILE:HD12	1:L:145:ALA:HB2	2.01	0.42
1:Y:233:ILE:HG21	1:Y:371:ARG:CZ	2.49	0.42
1:A:20:GLY:HA3	1:A:43:ASN:O	2.19	0.42
1:C:29:LEU:HD23	1:C:41:ILE:CD1	2.49	0.42
1:E:243:ALA:HA	1:E:284:MET:HG2	2.00	0.42
1:H:20:GLY:HA3	1:H:43:ASN:O	2.19	0.42
1:K:303:PRO:HG2	1:K:306:MET:HB2	2.01	0.42
1:W:157:VAL:HG11	1:Z:261:ALA:HA	2.00	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:Z:150:ARG:HG3	1:Z:150:ARG:NH1	2.33	0.42
1:A:59:GLN:NE2	1:A:81:SER:O	2.51	0.42
1:G:323:ILE:HB	1:G:352:VAL:HG23	2.01	0.42
1:G:392:ILE:O	1:G:395:ILE:HG22	2.19	0.42
1:H:40:GLU:HB3	1:H:225:VAL:HG22	2.00	0.42
1:I:40:GLU:HB3	1:I:225:VAL:HG22	2.01	0.42
1:K:21:ALA:HA	1:K:231:ASP:CB	2.50	0.42
1:K:324:THR:OG1	1:K:351:THR:HB	2.19	0.42
1:X:103:ARG:HD3	1:X:104:PHE:CE1	2.54	0.42
1:Y:122:VAL:HG22	1:Y:125:HIS:CG	2.54	0.42
1:Z:4:PHE:HZ	1:Z:403:GLU:HG2	1.75	0.42
1:Z:282:LEU:HD23	1:Z:282:LEU:C	2.39	0.42
1:A:215:ILE:HD12	1:A:215:ILE:N	2.33	0.42
1:A:265:LYS:HA	1:A:265:LYS:HD2	1.87	0.42
1:D:290:LYS:NZ	1:I:286:GLY:HA3	2.30	0.42
1:E:122:VAL:HG22	1:E:125:HIS:CG	2.54	0.42
1:E:335:VAL:HB	1:E:336:PRO:HD3	2.01	0.42
1:F:315:LEU:HD21	1:F:345:ALA:HB2	2.02	0.42
1:K:366:MET:CG	1:K:391:ARG:HD2	2.49	0.42
1:Y:30:PHE:CZ	1:Y:93:SER:HA	2.54	0.42
1:Z:295:ARG:HH11	1:Z:295:ARG:CB	2.32	0.42
1:A:79:ASN:ND2	1:A:80:PHE:H	2.17	0.42
1:A:233:ILE:HG21	1:A:371:ARG:CZ	2.49	0.42
1:A:265:LYS:CE	1:A:293:THR:O	2.67	0.42
1:B:249:ILE:HG12	1:B:250:VAL:N	2.35	0.42
1:D:233:ILE:HG21	1:D:371:ARG:CZ	2.50	0.42
1:E:3:LYS:HE2	1:E:390:ASP:OD1	2.19	0.42
1:E:56:LEU:CD1	1:E:93:SER:HB2	2.49	0.42
1:E:64:VAL:HG13	1:E:72:ILE:CD1	2.49	0.42
1:F:83:PRO:O	1:F:87:VAL:HG13	2.19	0.42
1:G:249:ILE:HG12	1:G:250:VAL:N	2.33	0.42
1:H:313:LEU:C	1:H:313:LEU:HD23	2.40	0.42
1:I:265:LYS:CE	1:I:293:THR:O	2.67	0.42
1:K:248:LYS:HA	1:K:282:LEU:O	2.19	0.42
1:Z:122:VAL:HG22	1:Z:125:HIS:CG	2.55	0.42
1:Z:299:HIS:ND1	1:Z:300:PRO:HA	2.35	0.42
1:A:243:ALA:HA	1:A:284:MET:HG2	2.01	0.42
1:B:20:GLY:HA3	1:B:43:ASN:O	2.20	0.42
1:B:81:SER:HB2	1:B:108:GLN:HE21	1.83	0.42
1:H:233:ILE:HG21	1:H:371:ARG:CZ	2.50	0.42
1:K:20:GLY:HA3	1:K:43:ASN:O	2.20	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:122:VAL:O	1:K:122:VAL:HG13	2.19	0.42
1:L:233:ILE:HG21	1:L:371:ARG:CZ	2.49	0.42
1:L:313:LEU:HD23	1:L:313:LEU:C	2.40	0.42
1:D:188:GLU:N	1:D:188:GLU:OE2	2.53	0.42
1:D:392:ILE:O	1:D:395:ILE:HG22	2.20	0.42
1:F:20:GLY:HA3	1:F:43:ASN:O	2.20	0.42
1:F:30:PHE:CZ	1:F:93:SER:HA	2.55	0.42
1:G:271:ALA:HB1	1:G:282:LEU:HG	2.02	0.42
1:H:59:GLN:HE22	1:H:83:PRO:HD3	1.85	0.42
1:I:276:GLY:HA3	1:I:279:TRP:NE1	2.34	0.42
1:J:137:LYS:N	1:J:137:LYS:CD	2.83	0.42
1:K:85:ASP:HA	1:K:88:LYS:HE2	2.02	0.42
1:K:265:LYS:CE	1:K:293:THR:O	2.68	0.42
1:K:282:LEU:HD23	1:K:282:LEU:C	2.40	0.42
1:X:91:ARG:HG3	3:X:1483:EDO:H22	2.02	0.42
1:X:215:ILE:N	1:X:215:ILE:HD12	2.35	0.42
1:A:3:LYS:HE2	1:A:390:ASP:OD1	2.19	0.42
1:A:367:ALA:HB1	1:A:373:SER:HB3	2.01	0.42
1:D:21:ALA:HA	1:D:231:ASP:CB	2.49	0.42
1:F:249:ILE:HG12	1:F:250:VAL:N	2.35	0.42
1:H:82:ALA:HB3	1:H:109:VAL:HA	2.02	0.42
1:J:11:ARG:HG2	1:J:13:GLN:NE2	2.34	0.42
1:J:392:ILE:O	1:J:395:ILE:HG22	2.19	0.42
1:W:119:ALA:HB1	1:X:336:PRO:HG3	2.02	0.42
1:X:47:LEU:HB3	1:X:397:ARG:O	2.20	0.42
1:Z:136:ILE:HD13	1:Z:145:ALA:CB	2.50	0.42
1:Z:233:ILE:HG21	1:Z:371:ARG:CZ	2.49	0.42
1:B:188:GLU:OE2	1:B:188:GLU:N	2.53	0.42
1:B:417:LYS:HA	1:B:417:LYS:CE	2.47	0.42
1:C:367:ALA:HB1	1:C:373:SER:HB3	2.02	0.42
1:D:366:MET:CG	1:D:391:ARG:HD2	2.49	0.42
1:F:215:ILE:HD12	1:F:215:ILE:N	2.35	0.42
1:F:392:ILE:O	1:F:395:ILE:HG22	2.19	0.42
1:G:2:ASP:CB	1:G:392:ILE:HD11	2.47	0.42
1:G:91:ARG:NE	4:G:573:HOH:O	2.40	0.42
1:K:29:LEU:HD23	1:K:41:ILE:CD1	2.49	0.42
1:K:323:ILE:HB	1:K:352:VAL:HG23	2.01	0.42
1:W:397:ARG:HG3	1:W:397:ARG:NH1	2.35	0.42
1:W:418:GLY:O	1:W:419:GLU:HB2	2.20	0.42
1:X:64:VAL:HG13	1:X:72:ILE:CD1	2.50	0.42
1:Z:271:ALA:HB1	1:Z:282:LEU:HG	2.02	0.42

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:22:LYS:HB2	1:A:47:LEU:CD1	2.50	0.41
1:D:313:LEU:C	1:D:313:LEU:HD23	2.40	0.41
1:F:64:VAL:HG13	1:F:72:ILE:CD1	2.50	0.41
1:H:315:LEU:HD21	1:H:345:ALA:HB2	2.01	0.41
1:I:20:GLY:HA3	1:I:43:ASN:O	2.20	0.41
1:I:295:ARG:HD2	1:L:160:LYS:HZ3	1.85	0.41
1:L:401:ARG:HG2	1:L:401:ARG:HH11	1.84	0.41
1:W:215:ILE:HD12	1:W:215:ILE:N	2.35	0.41
1:Y:2:ASP:CB	1:Y:392:ILE:HD11	2.47	0.41
1:Z:122:VAL:O	1:Z:122:VAL:HG13	2.19	0.41
1:B:82:ALA:HB3	1:B:109:VAL:HG13	2.02	0.41
1:B:85:ASP:HA	1:B:88:LYS:HE2	2.02	0.41
1:B:313:LEU:HD23	1:B:313:LEU:C	2.40	0.41
1:D:59:GLN:NE2	4:D:427:HOH:O	2.47	0.41
1:F:36:GLU:OE1	1:F:220:ARG:HD2	2.20	0.41
1:G:22:LYS:HB2	1:G:47:LEU:CD1	2.51	0.41
1:G:182:ILE:O	1:G:212:ARG:HA	2.21	0.41
1:H:56:LEU:C	1:H:56:LEU:HD23	2.41	0.41
1:I:122:VAL:HG22	1:I:125:HIS:CG	2.54	0.41
1:J:7:GLN:HB2	1:J:412:ASN:CB	2.50	0.41
1:J:81:SER:HA	1:J:108:GLN:O	2.21	0.41
1:L:276:GLY:HA3	1:L:279:TRP:NE1	2.35	0.41
1:L:315:LEU:HD21	1:L:345:ALA:HB2	2.01	0.41
1:W:2:ASP:CB	1:W:392:ILE:HD11	2.46	0.41
1:W:29:LEU:HD23	1:W:41:ILE:CD1	2.51	0.41
1:W:400:GLU:O	1:W:401:ARG:HG2	2.20	0.41
1:X:233:ILE:HG21	1:X:371:ARG:CZ	2.50	0.41
1:Y:36:GLU:OE1	1:Y:220:ARG:HD2	2.20	0.41
1:Y:243:ALA:HA	1:Y:284:MET:HG2	1.99	0.41
1:Z:3:LYS:HE2	1:Z:390:ASP:OD1	2.20	0.41
1:A:64:VAL:HG13	1:A:72:ILE:CD1	2.50	0.41
1:C:47:LEU:HB3	1:C:397:ARG:O	2.21	0.41
1:E:248:LYS:HA	1:E:282:LEU:O	2.20	0.41
1:E:282:LEU:C	1:E:282:LEU:HD23	2.40	0.41
1:F:56:LEU:HD23	1:F:56:LEU:O	2.20	0.41
1:I:56:LEU:HD23	1:I:56:LEU:C	2.39	0.41
1:J:85:ASP:HA	1:J:88:LYS:CD	2.50	0.41
1:K:1:MET:HB3	1:K:419:GLU:HB3	2.01	0.41
1:Y:122:VAL:O	1:Y:122:VAL:HG13	2.20	0.41
1:A:414:GLU:HG2	1:A:416:VAL:HG13	2.01	0.41
1:B:1:MET:HE3	1:B:391:ARG:NH1	2.35	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:271:ALA:HB1	1:B:282:LEU:HG	2.03	0.41
1:E:59:GLN:HE21	1:E:86:LEU:HD12	1.85	0.41
1:F:233:ILE:HG21	1:F:371:ARG:CZ	2.50	0.41
1:H:311:THR:HA	1:H:323:ILE:CD1	2.50	0.41
1:H:367:ALA:HB1	1:H:373:SER:HB3	2.01	0.41
1:L:29:LEU:HD23	1:L:41:ILE:CD1	2.49	0.41
1:L:39:VAL:HG12	1:L:40:GLU:N	2.35	0.41
1:W:64:VAL:HG13	1:W:72:ILE:CD1	2.50	0.41
1:W:131:LYS:HE3	1:W:131:LYS:HB3	1.96	0.41
1:Z:249:ILE:HG12	1:Z:250:VAL:N	2.35	0.41
1:A:271:ALA:HB1	1:A:282:LEU:HG	2.02	0.41
1:D:49:ASP:OD2	1:D:397:ARG:HG2	2.20	0.41
1:D:351:THR:CG2	4:D:990:HOH:O	2.68	0.41
1:E:21:ALA:HA	1:E:231:ASP:CB	2.50	0.41
1:G:276:GLY:HA3	1:G:279:TRP:NE1	2.35	0.41
1:I:3:LYS:HE2	1:I:390:ASP:OD1	2.20	0.41
1:L:271:ALA:HB1	1:L:282:LEU:HG	2.03	0.41
1:X:29:LEU:HD23	1:X:41:ILE:CD1	2.49	0.41
1:X:286:GLY:HA3	4:X:544:HOH:O	2.20	0.41
1:Y:64:VAL:HG13	1:Y:72:ILE:CD1	2.50	0.41
1:B:418:GLY:O	1:B:419:GLU:CB	2.69	0.41
1:D:344:HIS:CD2	1:D:357:VAL:CG1	3.04	0.41
1:D:400:GLU:C	1:D:401:ARG:HG2	2.41	0.41
1:F:313:LEU:C	1:F:313:LEU:HD23	2.40	0.41
1:H:271:ALA:HB1	1:H:282:LEU:HG	2.03	0.41
1:I:109:VAL:O	1:I:143:VAL:CG1	2.69	0.41
1:J:137:LYS:HD3	1:J:137:LYS:H	1.82	0.41
1:L:367:ALA:HB1	1:L:373:SER:HB3	2.02	0.41
1:W:122:VAL:HG22	1:W:125:HIS:CG	2.55	0.41
1:X:236:GLY:C	1:X:306:MET:HE1	2.41	0.41
1:Y:3:LYS:HB2	1:Y:416:VAL:CG2	2.51	0.41
1:Y:299:HIS:ND1	1:Y:300:PRO:HA	2.35	0.41
1:Z:315:LEU:HD21	1:Z:345:ALA:HB2	2.02	0.41
1:A:130:GLU:CG	1:A:136:ILE:HD13	2.51	0.41
1:C:335:VAL:HG21	1:C:352:VAL:HG11	2.03	0.41
1:D:344:HIS:CD2	1:D:357:VAL:HG11	2.56	0.41
1:K:36:GLU:OE1	1:K:220:ARG:HD2	2.20	0.41
1:K:271:ALA:HB1	1:K:282:LEU:HG	2.03	0.41
1:L:103:ARG:HD3	1:L:104:PHE:CE1	2.56	0.41
1:W:3:LYS:HE2	1:W:390:ASP:OD1	2.20	0.41
1:A:60:LEU:O	1:A:77:VAL:HG13	2.20	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:159:ASP:O	1:A:160:LYS:HB2	2.20	0.41
1:B:3:LYS:HE2	1:B:390:ASP:OD1	2.20	0.41
1:B:36:GLU:OE1	1:B:220:ARG:HD2	2.20	0.41
1:C:183:GLU:OE2	1:C:212:ARG:CZ	2.69	0.41
1:C:265:LYS:HD2	1:C:265:LYS:HA	1.88	0.41
1:C:276:GLY:HA3	1:C:279:TRP:NE1	2.36	0.41
1:G:56:LEU:C	1:G:56:LEU:HD23	2.41	0.41
1:I:64:VAL:HG13	1:I:72:ILE:CD1	2.51	0.41
1:J:359:LYS:HD3	4:J:845:HOH:O	2.20	0.41
1:K:64:VAL:HG13	1:K:72:ILE:CD1	2.51	0.41
1:K:299:HIS:ND1	1:K:300:PRO:HA	2.35	0.41
1:K:313:LEU:C	1:K:313:LEU:HD23	2.40	0.41
1:K:324:THR:HG23	1:K:351:THR:HG22	2.03	0.41
1:W:20:GLY:HA3	1:W:43:ASN:O	2.21	0.41
1:W:276:GLY:HA3	1:W:279:TRP:NE1	2.35	0.41
1:X:248:LYS:HA	1:X:282:LEU:O	2.21	0.41
1:Y:271:ALA:HB1	1:Y:282:LEU:HG	2.03	0.41
1:Z:344:HIS:ND1	1:Z:357:VAL:HG11	2.36	0.41
1:A:56:LEU:O	1:A:56:LEU:HD23	2.21	0.41
1:B:108:GLN:HB3	1:B:144:LYS:HG2	2.02	0.41
1:C:215:ILE:HD12	1:C:215:ILE:N	2.35	0.41
1:D:164:GLY:HA3	3:D:1473:EDO:C1	2.41	0.41
1:E:215:ILE:N	1:E:215:ILE:HD12	2.34	0.41
1:E:392:ILE:O	1:E:395:ILE:HG22	2.20	0.41
1:F:276:GLY:HA3	1:F:279:TRP:NE1	2.36	0.41
1:I:243:ALA:HA	1:I:284:MET:HG3	1.99	0.41
1:I:271:ALA:HB1	1:I:282:LEU:HG	2.03	0.41
1:J:56:LEU:HD23	1:J:56:LEU:O	2.21	0.41
1:J:271:ALA:HB1	1:J:282:LEU:HG	2.01	0.41
1:K:265:LYS:HA	1:K:265:LYS:HD2	1.89	0.41
1:L:60:LEU:HA	1:L:79:ASN:HB3	2.03	0.41
1:W:21:ALA:HA	1:W:231:ASP:CB	2.51	0.41
1:W:311:THR:HA	1:W:323:ILE:CD1	2.51	0.41
1:W:414:GLU:HG3	1:W:414:GLU:O	2.21	0.41
1:X:56:LEU:HD23	1:X:56:LEU:C	2.41	0.41
1:X:416:VAL:O	1:X:416:VAL:CG2	2.67	0.41
1:Y:248:LYS:HG3	1:Y:283:ASP:HB2	2.03	0.41
1:Z:367:ALA:HB1	1:Z:373:SER:HB3	2.02	0.41
1:A:91:ARG:HH11	1:A:91:ARG:HG3	1.86	0.41
1:E:56:LEU:HD23	1:E:56:LEU:O	2.21	0.41
1:E:101:VAL:HG21	1:E:145:ALA:HB3	2.03	0.41

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:271:ALA:HB1	1:F:282:LEU:HG	2.03	0.41
1:H:282:LEU:C	1:H:282:LEU:HD23	2.41	0.41
1:I:3:LYS:HE3	1:I:418:GLY:HA2	2.03	0.41
1:L:80:PHE:O	1:L:108:GLN:HG2	2.21	0.41
1:Y:48:LYS:HD2	1:Y:397:ARG:CZ	2.51	0.41
1:A:29:LEU:HD23	1:A:41:ILE:CD1	2.50	0.40
1:B:183:GLU:OE2	1:B:212:ARG:CZ	2.69	0.40
1:H:122:VAL:HG22	1:H:125:HIS:CG	2.55	0.40
1:I:36:GLU:OE1	1:I:220:ARG:HD2	2.20	0.40
1:J:15:GLU:HB3	4:J:982:HOH:O	2.21	0.40
1:J:29:LEU:HD23	1:J:41:ILE:CD1	2.50	0.40
1:K:2:ASP:CB	1:K:392:ILE:HD11	2.48	0.40
1:W:3:LYS:HG2	1:W:390:ASP:HA	2.04	0.40
1:W:7:GLN:NE2	1:W:386:THR:OG1	2.53	0.40
1:Z:59:GLN:O	1:Z:59:GLN:HG2	2.21	0.40
1:B:7:GLN:HB2	1:B:412:ASN:HB3	2.03	0.40
1:B:122:VAL:HG22	1:B:125:HIS:CG	2.55	0.40
1:B:418:GLY:O	1:B:419:GLU:HB2	2.21	0.40
1:D:164:GLY:CA	3:D:1473:EDO:H11	2.41	0.40
1:G:266:LEU:HD23	1:G:266:LEU:HA	1.97	0.40
1:H:290:LYS:NZ	1:W:286:GLY:C	2.74	0.40
1:I:3:LYS:HG2	1:I:390:ASP:HA	2.04	0.40
1:K:7:GLN:HB2	1:K:412:ASN:CB	2.51	0.40
1:Y:84:TYR:CE2	1:Y:88:LYS:HD3	2.56	0.40
1:C:2:ASP:CB	1:C:392:ILE:HD11	2.48	0.40
1:C:392:ILE:O	1:C:395:ILE:HG22	2.21	0.40
1:G:143:VAL:O	1:G:143:VAL:HG22	2.21	0.40
1:J:311:THR:HA	1:J:323:ILE:CD1	2.51	0.40
1:K:40:GLU:HB3	1:K:225:VAL:HG22	2.04	0.40
1:K:188:GLU:HA	1:K:189:PRO:HD3	1.89	0.40
1:W:36:GLU:OE1	1:W:220:ARG:HD2	2.21	0.40
1:W:56:LEU:C	1:W:56:LEU:HD23	2.40	0.40
1:W:233:ILE:HG21	1:W:371:ARG:CZ	2.51	0.40
1:X:236:GLY:HA3	1:X:306:MET:HE2	2.03	0.40
1:X:392:ILE:O	1:X:395:ILE:HG22	2.21	0.40
1:Z:120:ARG:HA	2:Z:1465:UDA:O11	2.20	0.40
1:Z:131:LYS:HE3	1:Z:131:LYS:HB3	1.97	0.40
1:B:215:ILE:HD12	1:B:215:ILE:N	2.36	0.40
1:B:367:ALA:HB1	1:B:373:SER:HB3	2.04	0.40
1:D:359:LYS:HD3	1:D:384:GLU:HB2	2.03	0.40
1:E:271:ALA:HB1	1:E:282:LEU:HG	2.03	0.40

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:313:LEU:HD23	1:E:313:LEU:C	2.42	0.40
1:G:64:VAL:HG13	1:G:72:ILE:HD13	2.04	0.40
1:G:295:ARG:NE	4:G:459:HOH:O	2.46	0.40
1:I:111:LEU:O	1:J:340:ARG:NH1	2.49	0.40
1:L:282:LEU:HD23	1:L:282:LEU:C	2.42	0.40
1:X:313:LEU:C	1:X:313:LEU:HD23	2.41	0.40
1:Y:56:LEU:CD1	1:Y:93:SER:HB2	2.52	0.40
1:Z:311:THR:HA	1:Z:323:ILE:CD1	2.52	0.40
1:A:21:ALA:HA	1:A:231:ASP:CB	2.51	0.40
1:C:397:ARG:NH2	2:C:1452:UDA:O15	2.55	0.40
1:F:3:LYS:HE2	1:F:390:ASP:OD1	2.21	0.40
1:F:351:THR:CG2	4:F:451:HOH:O	2.70	0.40
1:G:3:LYS:HE2	1:G:390:ASP:OD1	2.21	0.40
1:H:103:ARG:HD3	1:H:104:PHE:CE1	2.57	0.40
1:I:215:ILE:N	1:I:215:ILE:HD12	2.36	0.40
1:I:265:LYS:HD2	1:I:265:LYS:HA	1.89	0.40
1:L:136:ILE:HD13	1:L:145:ALA:CB	2.51	0.40
1:X:266:LEU:HD23	1:X:266:LEU:HA	1.96	0.40
1:Y:265:LYS:HA	1:Y:265:LYS:HD2	1.90	0.40
1:Z:1:MET:N	1:Z:419:GLU:HB2	2.36	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	415/419 (99%)	402 (97%)	11 (3%)	2 (0%)	29	43
1	B	415/419 (99%)	403 (97%)	12 (3%)	0	100	100
1	C	415/419 (99%)	404 (97%)	10 (2%)	1 (0%)	47	64
1	D	415/419 (99%)	400 (96%)	14 (3%)	1 (0%)	47	64

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	E	415/419 (99%)	404 (97%)	11 (3%)	0	100	100
1	F	415/419 (99%)	402 (97%)	12 (3%)	1 (0%)	47	64
1	G	415/419 (99%)	402 (97%)	13 (3%)	0	100	100
1	H	415/419 (99%)	405 (98%)	8 (2%)	2 (0%)	29	43
1	I	415/419 (99%)	402 (97%)	11 (3%)	2 (0%)	29	43
1	J	415/419 (99%)	403 (97%)	11 (3%)	1 (0%)	47	64
1	K	415/419 (99%)	401 (97%)	14 (3%)	0	100	100
1	L	415/419 (99%)	400 (96%)	13 (3%)	2 (0%)	29	43
1	W	415/419 (99%)	402 (97%)	13 (3%)	0	100	100
1	X	415/419 (99%)	403 (97%)	11 (3%)	1 (0%)	47	64
1	Y	415/419 (99%)	402 (97%)	11 (3%)	2 (0%)	29	43
1	Z	415/419 (99%)	403 (97%)	9 (2%)	3 (1%)	22	33
All	All	6640/6704 (99%)	6438 (97%)	184 (3%)	18 (0%)	41	56

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	75	SER
1	F	418	GLY
1	L	418	GLY
1	A	160	LYS
1	C	160	LYS
1	D	418	GLY
1	H	418	GLY
1	J	418	GLY
1	Y	85	ASP
1	Z	75	SER
1	Z	85	ASP
1	I	160	LYS
1	L	85	ASP
1	Z	74	ALA
1	H	417	LYS
1	I	418	GLY
1	X	38	PRO
1	Y	418	GLY

### 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	328/328 (100%)	315 (96%)	13 (4%)	31	47
1	B	328/328 (100%)	315 (96%)	13 (4%)	31	47
1	C	328/328 (100%)	315 (96%)	13 (4%)	31	47
1	D	328/328 (100%)	309 (94%)	19 (6%)	20	31
1	E	328/328 (100%)	316 (96%)	12 (4%)	34	50
1	F	328/328 (100%)	314 (96%)	14 (4%)	29	44
1	G	328/328 (100%)	317 (97%)	11 (3%)	37	53
1	H	328/328 (100%)	314 (96%)	14 (4%)	29	44
1	I	328/328 (100%)	315 (96%)	13 (4%)	31	47
1	J	328/328 (100%)	313 (95%)	15 (5%)	27	41
1	K	328/328 (100%)	316 (96%)	12 (4%)	34	50
1	L	328/328 (100%)	311 (95%)	17 (5%)	23	36
1	W	328/328 (100%)	313 (95%)	15 (5%)	27	41
1	X	328/328 (100%)	319 (97%)	9 (3%)	44	63
1	Y	328/328 (100%)	317 (97%)	11 (3%)	37	53
1	Z	328/328 (100%)	313 (95%)	15 (5%)	27	41
All	All	5248/5248 (100%)	5032 (96%)	216 (4%)	30	46

All (216) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	87	VAL
1	A	91	ARG
1	A	108	GLN
1	A	111	LEU
1	A	122	VAL
1	A	187	ARG
1	A	211	ASP

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	212	ARG
1	A	307	GLN
1	A	329	GLU
1	A	351	THR
1	A	352	VAL
1	B	76	ASN
1	B	78	ASN
1	B	86	LEU
1	B	87	VAL
1	B	111	LEU
1	B	122	VAL
1	B	137	LYS
1	B	152	LYS
1	B	212	ARG
1	B	307	GLN
1	B	351	THR
1	B	352	VAL
1	B	416	VAL
1	C	85	ASP
1	C	86	LEU
1	C	87	VAL
1	C	111	LEU
1	C	122	VAL
1	C	143	VAL
1	C	211	ASP
1	C	212	ARG
1	C	307	GLN
1	C	329	GLU
1	C	351	THR
1	C	352	VAL
1	C	419	GLU
1	D	11	ARG
1	D	76	ASN
1	D	78	ASN
1	D	85	ASP
1	D	86	LEU
1	D	87	VAL
1	D	101	VAL
1	D	108	GLN
1	D	111	LEU
1	D	122	VAL
1	D	138	LEU

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	D	148	ASN
1	D	187	ARG
1	D	211	ASP
1	D	212	ARG
1	D	307	GLN
1	D	351	THR
1	D	352	VAL
1	D	401	ARG
1	E	7	GLN
1	E	85	ASP
1	E	87	VAL
1	E	111	LEU
1	E	122	VAL
1	E	211	ASP
1	E	212	ARG
1	E	295	ARG
1	E	307	GLN
1	E	351	THR
1	E	352	VAL
1	E	419	GLU
1	F	76	ASN
1	F	87	VAL
1	F	91	ARG
1	F	111	LEU
1	F	122	VAL
1	F	143	VAL
1	F	148	ASN
1	F	160	LYS
1	F	187	ARG
1	F	211	ASP
1	F	212	ARG
1	F	307	GLN
1	F	351	THR
1	F	352	VAL
1	G	78	ASN
1	G	86	LEU
1	G	87	VAL
1	G	91	ARG
1	G	111	LEU
1	G	122	VAL
1	G	212	ARG
1	G	307	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	G	351	THR
1	G	352	VAL
1	G	419	GLU
1	H	85	ASP
1	H	86	LEU
1	H	87	VAL
1	H	111	LEU
1	H	122	VAL
1	H	148	ASN
1	H	211	ASP
1	H	212	ARG
1	H	307	GLN
1	H	324	THR
1	H	351	THR
1	H	352	VAL
1	H	401	ARG
1	H	419	GLU
1	I	13	GLN
1	I	76	ASN
1	I	86	LEU
1	I	87	VAL
1	I	91	ARG
1	I	111	LEU
1	I	122	VAL
1	I	143	VAL
1	I	212	ARG
1	I	295	ARG
1	I	307	GLN
1	I	351	THR
1	I	352	VAL
1	J	13	GLN
1	J	59	GLN
1	J	76	ASN
1	J	85	ASP
1	J	86	LEU
1	J	87	VAL
1	J	111	LEU
1	J	122	VAL
1	J	137	LYS
1	J	143	VAL
1	J	148	ASN
1	J	212	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	J	307	GLN
1	J	351	THR
1	J	352	VAL
1	K	7	GLN
1	K	59	GLN
1	K	79	ASN
1	K	87	VAL
1	K	91	ARG
1	K	111	LEU
1	K	122	VAL
1	K	137	LYS
1	K	212	ARG
1	K	307	GLN
1	K	351	THR
1	K	352	VAL
1	L	59	GLN
1	L	78	ASN
1	L	86	LEU
1	L	87	VAL
1	L	101	VAL
1	L	108	GLN
1	L	111	LEU
1	L	122	VAL
1	L	158	MET
1	L	187	ARG
1	L	211	ASP
1	L	212	ARG
1	L	274	GLU
1	L	307	GLN
1	L	351	THR
1	L	352	VAL
1	L	414	GLU
1	W	11	ARG
1	W	13	GLN
1	W	87	VAL
1	W	91	ARG
1	W	111	LEU
1	W	122	VAL
1	W	143	VAL
1	W	211	ASP
1	W	212	ARG
1	W	295	ARG

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	W	307	GLN
1	W	351	THR
1	W	352	VAL
1	W	401	ARG
1	W	419	GLU
1	X	38	PRO
1	X	86	LEU
1	X	87	VAL
1	X	111	LEU
1	X	122	VAL
1	X	212	ARG
1	X	307	GLN
1	X	351	THR
1	X	352	VAL
1	Y	85	ASP
1	Y	87	VAL
1	Y	91	ARG
1	Y	111	LEU
1	Y	122	VAL
1	Y	137	LYS
1	Y	143	VAL
1	Y	212	ARG
1	Y	307	GLN
1	Y	351	THR
1	Y	352	VAL
1	Z	78	ASN
1	Z	86	LEU
1	Z	87	VAL
1	Z	91	ARG
1	Z	111	LEU
1	Z	122	VAL
1	Z	187	ARG
1	Z	211	ASP
1	Z	212	ARG
1	Z	274	GLU
1	Z	307	GLN
1	Z	351	THR
1	Z	352	VAL
1	Z	403	GLU
1	Z	419	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	7	GLN
1	A	76	ASN
1	A	79	ASN
1	A	330	ASN
1	A	344	HIS
1	B	76	ASN
1	B	78	ASN
1	C	108	GLN
1	C	330	ASN
1	C	344	HIS
1	D	76	ASN
1	D	78	ASN
1	D	148	ASN
1	D	344	HIS
1	E	7	GLN
1	E	59	GLN
1	E	344	HIS
1	F	76	ASN
1	F	344	HIS
1	G	59	GLN
1	G	78	ASN
1	G	344	HIS
1	H	7	GLN
1	H	59	GLN
1	H	148	ASN
1	H	344	HIS
1	I	7	GLN
1	I	148	ASN
1	I	330	ASN
1	I	344	HIS
1	J	7	GLN
1	J	13	GLN
1	J	59	GLN
1	J	330	ASN
1	J	344	HIS
1	K	7	GLN
1	K	79	ASN
1	K	108	GLN
1	K	148	ASN
1	K	330	ASN
1	L	7	GLN
1	L	59	GLN
1	W	7	GLN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	W	59	GLN
1	W	76	ASN
1	W	330	ASN
1	W	344	HIS
1	X	108	GLN
1	X	344	HIS
1	X	364	GLN
1	Y	13	GLN
1	Y	108	GLN
1	Y	330	ASN
1	Y	344	HIS
1	Z	13	GLN
1	Z	108	GLN
1	Z	148	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

16 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
1	IAS	J	67	1	4,7,8	0.64	0	2,8,10	1.28	0
1	IAS	K	67	1	4,7,8	0.55	0	2,8,10	1.22	0
1	IAS	Z	67	1	4,7,8	0.59	0	2,8,10	1.31	0
1	IAS	H	67	1	4,7,8	0.64	0	2,8,10	1.18	0
1	IAS	E	67	1	4,7,8	0.59	0	2,8,10	1.29	0
1	IAS	G	67	1	4,7,8	0.63	0	2,8,10	1.43	0
1	IAS	B	67	1	4,7,8	0.59	0	2,8,10	1.21	0
1	IAS	L	67	1	4,7,8	0.53	0	2,8,10	1.39	0
1	IAS	X	67	1	4,7,8	0.64	0	2,8,10	1.26	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
1	IAS	D	67	1	4,7,8	0.49	0	2,8,10	1.31	0
1	IAS	I	67	1	4,7,8	0.76	0	2,8,10	1.14	0
1	IAS	F	67	1	4,7,8	0.54	0	2,8,10	1.21	0
1	IAS	A	67	1	4,7,8	0.54	0	2,8,10	1.33	0
1	IAS	Y	67	1	4,7,8	0.60	0	2,8,10	1.28	0
1	IAS	C	67	1	4,7,8	0.57	0	2,8,10	1.36	0
1	IAS	W	67	1	4,7,8	0.80	0	2,8,10	1.15	0

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
1	IAS	J	67	1	-	0/3/7/8	-
1	IAS	K	67	1	-	0/3/7/8	-
1	IAS	Z	67	1	-	0/3/7/8	-
1	IAS	H	67	1	-	0/3/7/8	-
1	IAS	E	67	1	-	0/3/7/8	-
1	IAS	G	67	1	-	0/3/7/8	-
1	IAS	B	67	1	-	0/3/7/8	-
1	IAS	L	67	1	-	0/3/7/8	-
1	IAS	X	67	1	-	0/3/7/8	-
1	IAS	D	67	1	-	0/3/7/8	-
1	IAS	I	67	1	-	0/3/7/8	-
1	IAS	F	67	1	-	0/3/7/8	-
1	IAS	A	67	1	-	0/3/7/8	-
1	IAS	Y	67	1	-	0/3/7/8	-
1	IAS	C	67	1	-	0/3/7/8	-
1	IAS	W	67	1	-	0/3/7/8	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

32 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	$\# Z  > 2$
3	EDO	I	1478	-	3,3,3	0.57	0	2,2,2	0.29	0
2	UDA	A	1450	-	40,51,51	2.35	16 (40%)	52,79,79	1.78	11 (21%)
3	EDO	G	1476	-	3,3,3	0.56	0	2,2,2	0.27	0
2	UDA	H	1457	-	40,51,51	2.43	15 (37%)	52,79,79	1.73	12 (23%)
3	EDO	C	1472	-	3,3,3	0.50	0	2,2,2	0.18	0
2	UDA	K	1460	-	40,51,51	2.29	16 (40%)	52,79,79	1.75	13 (25%)
2	UDA	Z	1465	-	40,51,51	2.25	17 (42%)	52,79,79	1.68	11 (21%)
3	EDO	X	1483	-	3,3,3	0.47	0	2,2,2	0.20	0
3	EDO	Y	1484	-	3,3,3	0.45	0	2,2,2	0.19	0
2	UDA	X	1463	-	40,51,51	2.34	15 (37%)	52,79,79	1.78	13 (25%)
3	EDO	F	1475	-	3,3,3	0.79	0	2,2,2	0.29	0
2	UDA	C	1452	-	40,51,51	2.22	15 (37%)	52,79,79	1.73	10 (19%)
2	UDA	D	1453	-	40,51,51	2.40	16 (40%)	52,79,79	1.71	12 (23%)
2	UDA	B	1451	-	40,51,51	2.35	18 (45%)	52,79,79	1.73	12 (23%)
2	UDA	J	1459	-	40,51,51	2.36	15 (37%)	52,79,79	1.75	10 (19%)
3	EDO	K	1480	-	3,3,3	0.41	0	2,2,2	0.05	0
2	UDA	G	1456	-	40,51,51	2.36	16 (40%)	52,79,79	1.78	11 (21%)
2	UDA	L	1461	-	40,51,51	2.36	15 (37%)	52,79,79	1.76	12 (23%)
3	EDO	W	1482	-	3,3,3	0.51	0	2,2,2	0.27	0
3	EDO	B	1471	-	3,3,3	0.48	0	2,2,2	0.16	0
3	EDO	A	1470	-	3,3,3	0.56	0	2,2,2	0.27	0
3	EDO	L	1481	-	3,3,3	0.57	0	2,2,2	0.22	0
2	UDA	Y	1464	-	40,51,51	2.36	14 (35%)	52,79,79	1.68	11 (21%)
3	EDO	H	1477	-	3,3,3	0.41	0	2,2,2	0.11	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	UDA	W	1462	-	40,51,51	2.32	15 (37%)	52,79,79	1.69	12 (23%)
3	EDO	E	1474	-	3,3,3	0.39	0	2,2,2	0.19	0
3	EDO	Z	1485	-	3,3,3	0.60	0	2,2,2	0.29	0
3	EDO	J	1479	-	3,3,3	0.60	0	2,2,2	0.32	0
2	UDA	E	1454	-	40,51,51	2.36	14 (35%)	52,79,79	1.76	12 (23%)
3	EDO	D	1473	-	3,3,3	0.83	0	2,2,2	0.62	0
2	UDA	F	1455	-	40,51,51	2.33	16 (40%)	52,79,79	1.75	12 (23%)
2	UDA	I	1458	-	40,51,51	2.23	15 (37%)	52,79,79	1.67	11 (21%)

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
3	EDO	I	1478	-	-	1/1/1/1	-
2	UDA	A	1450	-	-	9/29/80/80	0/3/3/3
3	EDO	G	1476	-	-	1/1/1/1	-
2	UDA	H	1457	-	-	8/29/80/80	0/3/3/3
3	EDO	C	1472	-	-	1/1/1/1	-
2	UDA	K	1460	-	-	8/29/80/80	0/3/3/3
2	UDA	Z	1465	-	-	9/29/80/80	0/3/3/3
3	EDO	X	1483	-	-	1/1/1/1	-
3	EDO	Y	1484	-	-	1/1/1/1	-
2	UDA	X	1463	-	-	7/29/80/80	0/3/3/3
3	EDO	F	1475	-	-	1/1/1/1	-
2	UDA	C	1452	-	-	7/29/80/80	0/3/3/3
2	UDA	D	1453	-	-	8/29/80/80	0/3/3/3
2	UDA	B	1451	-	-	8/29/80/80	0/3/3/3
2	UDA	J	1459	-	-	7/29/80/80	0/3/3/3
3	EDO	K	1480	-	-	1/1/1/1	-
2	UDA	G	1456	-	-	9/29/80/80	0/3/3/3
2	UDA	L	1461	-	-	8/29/80/80	0/3/3/3
3	EDO	W	1482	-	-	1/1/1/1	-
3	EDO	B	1471	-	-	1/1/1/1	-
3	EDO	A	1470	-	-	1/1/1/1	-
3	EDO	L	1481	-	-	1/1/1/1	-
2	UDA	Y	1464	-	-	8/29/80/80	0/3/3/3
3	EDO	H	1477	-	-	1/1/1/1	-

Continued on next page...

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UDA	W	1462	-	-	8/29/80/80	0/3/3/3
3	EDO	E	1474	-	-	1/1/1/1	-
3	EDO	Z	1485	-	-	1/1/1/1	-
3	EDO	J	1479	-	-	1/1/1/1	-
2	UDA	E	1454	-	-	7/29/80/80	0/3/3/3
3	EDO	D	1473	-	-	1/1/1/1	-
2	UDA	F	1455	-	-	9/29/80/80	0/3/3/3
2	UDA	I	1458	-	-	8/29/80/80	0/3/3/3

All (248) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1457	UDA	C5-N2	6.99	1.44	1.35
2	D	1453	UDA	C5-N2	6.91	1.44	1.35
2	X	1463	UDA	C5-N2	6.88	1.44	1.35
2	G	1456	UDA	O21-C13	6.74	1.50	1.42
2	A	1450	UDA	C5-N2	6.67	1.44	1.35
2	L	1461	UDA	C5-N2	6.60	1.44	1.35
2	B	1451	UDA	O21-C13	6.58	1.50	1.42
2	J	1459	UDA	C5-N2	6.55	1.43	1.35
2	K	1460	UDA	C5-N2	6.51	1.43	1.35
2	Y	1464	UDA	C5-N2	6.48	1.43	1.35
2	X	1463	UDA	O21-C13	6.45	1.50	1.42
2	I	1458	UDA	C5-N2	6.45	1.43	1.35
2	H	1457	UDA	O21-C13	6.41	1.50	1.42
2	E	1454	UDA	C5-N2	6.38	1.43	1.35
2	B	1451	UDA	C5-N2	6.34	1.43	1.35
2	L	1461	UDA	O21-C13	6.30	1.50	1.42
2	W	1462	UDA	C5-N2	6.30	1.43	1.35
2	A	1450	UDA	O21-C13	6.26	1.50	1.42
2	F	1455	UDA	C5-N2	6.25	1.43	1.35
2	D	1453	UDA	O21-C13	6.20	1.49	1.42
2	J	1459	UDA	O21-C13	6.14	1.49	1.42
2	E	1454	UDA	O21-C13	6.12	1.49	1.42
2	F	1455	UDA	O21-C13	6.02	1.49	1.42
2	Z	1465	UDA	C5-N2	5.81	1.43	1.35
2	G	1456	UDA	C5-N2	5.80	1.43	1.35
2	W	1462	UDA	O21-C13	5.77	1.49	1.42
2	C	1452	UDA	O21-C13	5.62	1.49	1.42
2	Z	1465	UDA	O21-C13	5.58	1.49	1.42
2	K	1460	UDA	O21-C13	5.51	1.49	1.42

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	1464	UDA	O21-C13	5.20	1.48	1.42
2	C	1452	UDA	C5-N2	5.19	1.42	1.35
2	I	1458	UDA	O21-C13	4.82	1.48	1.42
2	J	1459	UDA	O11-C9	4.28	1.53	1.43
2	F	1455	UDA	O11-C9	4.26	1.53	1.43
2	Z	1465	UDA	O11-C9	4.23	1.52	1.43
2	Y	1464	UDA	O11-C9	4.20	1.52	1.43
2	C	1452	UDA	O11-C9	4.17	1.52	1.43
2	E	1454	UDA	O11-C9	4.09	1.52	1.43
2	E	1454	UDA	C1-N1	4.08	1.40	1.33
2	Y	1464	UDA	C10-C18	4.03	1.59	1.53
2	W	1462	UDA	O11-C9	4.00	1.52	1.43
2	I	1458	UDA	O11-C9	4.00	1.52	1.43
2	A	1450	UDA	O11-C9	3.99	1.52	1.43
2	L	1461	UDA	O11-C9	3.96	1.52	1.43
2	X	1463	UDA	O11-C9	3.91	1.52	1.43
2	D	1453	UDA	O13-C11	3.89	1.51	1.43
2	B	1451	UDA	O11-C9	3.88	1.52	1.43
2	K	1460	UDA	O11-C9	3.84	1.52	1.43
2	E	1454	UDA	O13-C11	3.67	1.51	1.43
2	H	1457	UDA	O11-C9	3.66	1.51	1.43
2	Y	1464	UDA	O13-C11	3.61	1.50	1.43
2	B	1451	UDA	C1-N1	3.60	1.39	1.33
2	H	1457	UDA	C1-N1	3.58	1.39	1.33
2	K	1460	UDA	C1-N1	3.48	1.39	1.33
2	F	1455	UDA	O14-C15	3.46	1.51	1.43
2	D	1453	UDA	O11-C9	3.45	1.51	1.43
2	Y	1464	UDA	O14-C15	3.42	1.51	1.43
2	D	1453	UDA	C1-N1	3.40	1.39	1.33
2	H	1457	UDA	O14-C15	3.39	1.50	1.43
2	A	1450	UDA	C1-N1	3.37	1.38	1.33
2	D	1453	UDA	O14-C15	3.33	1.50	1.43
2	J	1459	UDA	O14-C15	3.31	1.50	1.43
2	A	1450	UDA	O13-C11	3.29	1.50	1.43
2	G	1456	UDA	O11-C9	3.28	1.50	1.43
2	C	1452	UDA	O14-C15	3.27	1.50	1.43
2	I	1458	UDA	C1-N1	3.27	1.38	1.33
2	B	1451	UDA	O14-C15	3.25	1.50	1.43
2	L	1461	UDA	C1-N1	3.24	1.38	1.33
2	L	1461	UDA	P3-O15	-3.20	1.42	1.54
2	I	1458	UDA	O14-C15	3.20	1.50	1.43
2	Z	1465	UDA	C1-N1	3.17	1.38	1.33

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1457	UDA	C10-C18	3.16	1.58	1.53
2	K	1460	UDA	P3-O15	-3.15	1.42	1.54
2	G	1456	UDA	P3-O15	-3.14	1.42	1.54
2	H	1457	UDA	O13-C11	3.12	1.49	1.43
2	X	1463	UDA	O14-C15	3.10	1.50	1.43
2	F	1455	UDA	C1-N1	3.10	1.38	1.33
2	E	1454	UDA	P3-O15	-3.08	1.43	1.54
2	W	1462	UDA	O14-C15	3.08	1.50	1.43
2	A	1450	UDA	P2-O9	-3.08	1.40	1.50
2	C	1452	UDA	P3-O15	-3.08	1.43	1.54
2	G	1456	UDA	P2-O9	-3.08	1.40	1.50
2	W	1462	UDA	C1-N1	3.07	1.38	1.33
2	X	1463	UDA	C1-N1	3.06	1.38	1.33
2	Z	1465	UDA	O13-C11	3.06	1.49	1.43
2	Z	1465	UDA	P3-O15	-3.05	1.43	1.54
2	Y	1464	UDA	C13-C18	3.05	1.58	1.53
2	D	1453	UDA	P2-O9	-3.04	1.40	1.50
2	L	1461	UDA	O14-C15	3.04	1.50	1.43
2	A	1450	UDA	P3-O15	-3.04	1.43	1.54
2	I	1458	UDA	P3-O15	-3.03	1.43	1.54
2	Z	1465	UDA	O14-C15	3.03	1.50	1.43
2	K	1460	UDA	O14-C15	3.03	1.50	1.43
2	X	1463	UDA	P2-O9	-3.02	1.40	1.50
2	J	1459	UDA	O13-C11	3.02	1.49	1.43
2	J	1459	UDA	P3-O15	-3.02	1.43	1.54
2	K	1460	UDA	O13-C11	3.01	1.49	1.43
2	J	1459	UDA	P2-O9	-3.01	1.40	1.50
2	G	1456	UDA	O14-C15	3.00	1.50	1.43
2	C	1452	UDA	P2-O9	-2.99	1.40	1.50
2	W	1462	UDA	O13-C11	2.99	1.49	1.43
2	F	1455	UDA	C13-C18	2.97	1.57	1.53
2	H	1457	UDA	C13-C18	2.97	1.57	1.53
2	J	1459	UDA	C1-N1	2.97	1.38	1.33
2	D	1453	UDA	P3-O15	-2.97	1.43	1.54
2	E	1454	UDA	C9-C2	-2.97	1.49	1.53
2	A	1450	UDA	C9-C2	-2.96	1.49	1.53
2	I	1458	UDA	C20-C16	2.96	1.59	1.53
2	Y	1464	UDA	C1-N1	2.94	1.38	1.33
2	X	1463	UDA	P3-O15	-2.94	1.43	1.54
2	G	1456	UDA	O13-C11	2.94	1.49	1.43
2	L	1461	UDA	O13-C11	2.94	1.49	1.43
2	H	1457	UDA	C20-C16	2.93	1.59	1.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	1457	UDA	P2-O9	-2.93	1.40	1.50
2	F	1455	UDA	P2-O9	-2.92	1.40	1.50
2	H	1457	UDA	P3-O15	-2.92	1.43	1.54
2	Y	1464	UDA	P3-O15	-2.91	1.43	1.54
2	W	1462	UDA	C20-C16	2.90	1.59	1.53
2	A	1450	UDA	O14-C15	2.89	1.49	1.43
2	J	1459	UDA	C13-C18	2.88	1.57	1.53
2	Z	1465	UDA	P2-O9	-2.88	1.40	1.50
2	F	1455	UDA	P3-O15	-2.86	1.43	1.54
2	E	1454	UDA	P2-O9	-2.86	1.40	1.50
2	G	1456	UDA	C20-C13	2.83	1.59	1.52
2	F	1455	UDA	O13-C11	2.82	1.49	1.43
2	X	1463	UDA	O13-C11	2.82	1.49	1.43
2	W	1462	UDA	P3-O15	-2.82	1.44	1.54
2	L	1461	UDA	P2-O9	-2.81	1.40	1.50
2	D	1453	UDA	C9-C2	-2.81	1.49	1.53
2	D	1453	UDA	C20-C16	2.81	1.58	1.53
2	G	1456	UDA	C20-C16	2.81	1.58	1.53
2	E	1454	UDA	C20-C16	2.81	1.58	1.53
2	K	1460	UDA	C10-C18	2.81	1.57	1.53
2	G	1456	UDA	C10-C18	2.80	1.57	1.53
2	F	1455	UDA	C10-C18	2.80	1.57	1.53
2	W	1462	UDA	C9-C2	-2.79	1.49	1.53
2	B	1451	UDA	P3-O15	-2.73	1.44	1.54
2	G	1456	UDA	C1-N1	2.73	1.37	1.33
2	W	1462	UDA	C10-C18	2.72	1.57	1.53
2	L	1461	UDA	C20-C13	2.71	1.59	1.52
2	Y	1464	UDA	C15-C4	2.70	1.59	1.53
2	I	1458	UDA	P2-O9	-2.68	1.41	1.50
2	B	1451	UDA	P2-O9	-2.66	1.41	1.50
2	Z	1465	UDA	C13-C18	2.65	1.57	1.53
2	I	1458	UDA	C13-C18	2.64	1.57	1.53
2	C	1452	UDA	C20-C16	2.64	1.58	1.53
2	C	1452	UDA	C1-N1	2.64	1.37	1.33
2	E	1454	UDA	C20-C13	2.64	1.59	1.52
2	W	1462	UDA	P2-O9	-2.63	1.41	1.50
2	E	1454	UDA	C10-C18	2.62	1.57	1.53
2	C	1452	UDA	C13-C18	2.62	1.57	1.53
2	E	1454	UDA	O14-C15	2.62	1.49	1.43
2	Y	1464	UDA	P2-O9	-2.61	1.41	1.50
2	L	1461	UDA	C13-C18	2.60	1.57	1.53
2	C	1452	UDA	O13-C11	2.60	1.48	1.43

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	L	1461	UDA	C15-C4	2.59	1.59	1.53
2	Z	1465	UDA	C10-C18	2.59	1.57	1.53
2	W	1462	UDA	C20-C13	2.59	1.59	1.52
2	B	1451	UDA	C15-C4	2.58	1.59	1.53
2	G	1456	UDA	C9-C2	-2.58	1.49	1.53
2	K	1460	UDA	P2-O9	-2.58	1.41	1.50
2	W	1462	UDA	C15-C4	2.58	1.59	1.53
2	A	1450	UDA	C13-C18	2.58	1.57	1.53
2	J	1459	UDA	C20-C16	2.57	1.58	1.53
2	D	1453	UDA	C20-C13	2.55	1.59	1.52
2	F	1455	UDA	C20-C16	2.55	1.58	1.53
2	L	1461	UDA	C20-C16	2.55	1.58	1.53
2	B	1451	UDA	C10-C18	2.54	1.57	1.53
2	X	1463	UDA	C20-C16	2.54	1.58	1.53
2	B	1451	UDA	C20-C13	2.52	1.59	1.52
2	Z	1465	UDA	C20-C16	2.51	1.58	1.53
2	G	1456	UDA	O22-C20	2.50	1.48	1.43
2	C	1452	UDA	C20-C13	2.49	1.59	1.52
2	I	1458	UDA	O13-C11	2.49	1.48	1.43
2	H	1457	UDA	C9-C2	-2.49	1.50	1.53
2	C	1452	UDA	O22-C20	2.48	1.48	1.43
2	H	1457	UDA	C20-C13	2.46	1.58	1.52
2	G	1456	UDA	C15-C4	2.46	1.59	1.53
2	I	1458	UDA	C9-C2	-2.46	1.50	1.53
2	J	1459	UDA	C10-C18	2.44	1.57	1.53
2	H	1457	UDA	C15-C4	2.43	1.59	1.53
2	X	1463	UDA	C15-C4	2.43	1.59	1.53
2	X	1463	UDA	C20-C13	2.42	1.58	1.52
2	E	1454	UDA	O22-C20	2.41	1.48	1.43
2	Y	1464	UDA	C20-C13	2.41	1.58	1.52
2	B	1451	UDA	C9-C2	-2.40	1.50	1.53
2	K	1460	UDA	C15-C4	2.39	1.59	1.53
2	C	1452	UDA	C15-C4	2.39	1.59	1.53
2	A	1450	UDA	O22-C20	2.38	1.48	1.43
2	J	1459	UDA	C20-C13	2.38	1.58	1.52
2	F	1455	UDA	O22-C20	2.38	1.48	1.43
2	D	1453	UDA	C10-C18	2.37	1.57	1.53
2	W	1462	UDA	C13-C18	2.36	1.56	1.53
2	B	1451	UDA	C13-C18	2.35	1.56	1.53
2	D	1453	UDA	C13-C18	2.35	1.56	1.53
2	Y	1464	UDA	O22-C20	2.34	1.48	1.43
2	D	1453	UDA	C15-C4	2.34	1.59	1.53

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1452	UDA	C10-C18	2.34	1.56	1.53
2	K	1460	UDA	C13-C18	2.33	1.56	1.53
2	Z	1465	UDA	P2-O10	-2.33	1.44	1.55
2	L	1461	UDA	O22-C20	2.32	1.48	1.43
2	F	1455	UDA	C20-C13	2.31	1.58	1.52
2	A	1450	UDA	C10-C18	2.31	1.56	1.53
2	Z	1465	UDA	C9-C2	-2.31	1.50	1.53
2	J	1459	UDA	C15-C4	2.30	1.58	1.53
2	K	1460	UDA	C20-C13	2.30	1.58	1.52
2	A	1450	UDA	C20-C16	2.29	1.57	1.53
2	B	1451	UDA	O13-C11	2.29	1.48	1.43
2	W	1462	UDA	O22-C20	2.29	1.48	1.43
2	I	1458	UDA	C15-C4	2.29	1.58	1.53
2	L	1461	UDA	C10-C18	2.28	1.56	1.53
2	A	1450	UDA	C15-C4	2.27	1.58	1.53
2	B	1451	UDA	C20-C16	2.26	1.57	1.53
2	H	1457	UDA	O22-C20	2.26	1.48	1.43
2	K	1460	UDA	C9-C2	-2.24	1.50	1.53
2	J	1459	UDA	C9-C2	-2.24	1.50	1.53
2	E	1454	UDA	P2-O10	-2.24	1.44	1.55
2	G	1456	UDA	O23-C16	2.24	1.49	1.44
2	K	1460	UDA	O22-C20	2.23	1.48	1.43
2	K	1460	UDA	P2-O10	-2.23	1.44	1.55
2	A	1450	UDA	C20-C13	2.22	1.58	1.52
2	I	1458	UDA	O22-C20	2.21	1.48	1.43
2	I	1458	UDA	P3-O13	-2.21	1.55	1.59
2	B	1451	UDA	O22-C20	2.21	1.48	1.43
2	Z	1465	UDA	O22-C20	2.21	1.48	1.43
2	A	1450	UDA	P2-O10	-2.19	1.45	1.55
2	J	1459	UDA	O22-C20	2.18	1.48	1.43
2	Y	1464	UDA	C20-C16	2.18	1.57	1.53
2	I	1458	UDA	C20-C13	2.16	1.58	1.52
2	Z	1465	UDA	C20-C13	2.15	1.58	1.52
2	B	1451	UDA	P3-O13	-2.12	1.55	1.59
2	X	1463	UDA	C13-C18	2.12	1.56	1.53
2	B	1451	UDA	P2-O10	-2.12	1.45	1.55
2	Z	1465	UDA	O24-C17	2.12	1.51	1.42
2	L	1461	UDA	O24-C17	2.11	1.51	1.42
2	D	1453	UDA	P2-O10	-2.09	1.45	1.55
2	K	1460	UDA	C20-C16	2.08	1.57	1.53
2	F	1455	UDA	O24-C17	2.08	1.51	1.42
2	F	1455	UDA	P2-O10	-2.08	1.45	1.55

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	F	1455	UDA	C3-N1	-2.07	1.34	1.38
2	X	1463	UDA	O22-C20	2.06	1.47	1.43
2	X	1463	UDA	O24-C17	2.06	1.51	1.42
2	D	1453	UDA	O24-C17	2.05	1.51	1.42
2	G	1456	UDA	C13-C18	2.05	1.56	1.53
2	C	1452	UDA	C9-C2	-2.01	1.50	1.53
2	B	1451	UDA	O24-C17	2.01	1.50	1.42
2	Z	1465	UDA	C15-C4	2.00	1.58	1.53
2	X	1463	UDA	P2-O10	-2.00	1.45	1.55

All (185) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	X	1463	UDA	O7-P2-O8	4.66	111.88	102.48
2	J	1459	UDA	O7-P2-O8	4.58	111.73	102.48
2	A	1450	UDA	O7-P2-O8	4.28	111.12	102.48
2	E	1454	UDA	O7-P2-O8	4.21	110.97	102.48
2	G	1456	UDA	O7-P2-O8	4.18	110.91	102.48
2	F	1455	UDA	O7-P2-O8	4.12	110.79	102.48
2	L	1461	UDA	O7-P2-O8	4.09	110.74	102.48
2	W	1462	UDA	O7-P2-O8	4.08	110.72	102.48
2	I	1458	UDA	O14-C15-C4	4.04	122.72	111.05
2	H	1457	UDA	O14-C15-C4	4.01	122.64	111.05
2	D	1453	UDA	O14-C15-C4	3.97	122.53	111.05
2	D	1453	UDA	O7-P2-O8	3.90	110.34	102.48
2	G	1456	UDA	O14-C15-C4	3.87	122.24	111.05
2	B	1451	UDA	O7-P2-O8	3.87	110.28	102.48
2	W	1462	UDA	O14-C15-C4	3.81	122.07	111.05
2	X	1463	UDA	O14-C15-C4	3.79	122.01	111.05
2	Y	1464	UDA	O14-C15-C4	3.79	122.01	111.05
2	C	1452	UDA	O7-P2-O8	3.78	110.11	102.48
2	C	1452	UDA	O14-C15-C4	3.75	121.90	111.05
2	L	1461	UDA	O14-C15-C4	3.71	121.77	111.05
2	K	1460	UDA	O14-C15-C4	3.67	121.67	111.05
2	I	1458	UDA	O7-P2-O8	3.67	109.88	102.48
2	J	1459	UDA	O14-C15-C4	3.66	121.62	111.05
2	K	1460	UDA	O7-P2-O8	3.65	109.84	102.48
2	E	1454	UDA	C6-C1-N1	-3.63	115.33	123.31
2	B	1451	UDA	O14-C15-C4	3.62	121.52	111.05
2	Y	1464	UDA	O7-P2-O8	3.62	109.79	102.48
2	A	1450	UDA	O14-C15-C4	3.61	121.49	111.05
2	K	1460	UDA	C6-C1-N1	-3.61	115.37	123.31

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Z	1465	UDA	O14-C15-C4	3.57	121.38	111.05
2	H	1457	UDA	C6-C1-N1	-3.56	115.47	123.31
2	C	1452	UDA	C6-C1-N1	-3.56	115.47	123.31
2	H	1457	UDA	O7-P2-O8	3.56	109.66	102.48
2	Z	1465	UDA	O21-C11-C19	3.55	131.30	105.57
2	Z	1465	UDA	C6-C1-N1	-3.53	115.53	123.31
2	B	1451	UDA	O21-C11-C19	3.53	131.16	105.57
2	F	1455	UDA	O14-C15-C4	3.53	121.25	111.05
2	W	1462	UDA	O21-C11-C19	3.53	131.13	105.57
2	L	1461	UDA	O21-C11-C19	3.52	131.08	105.57
2	A	1450	UDA	C6-C1-N1	-3.51	115.58	123.31
2	D	1453	UDA	C6-C1-N1	-3.51	115.58	123.31
2	A	1450	UDA	O21-C11-C19	3.51	131.02	105.57
2	F	1455	UDA	C6-C1-N1	-3.50	115.60	123.31
2	Y	1464	UDA	C6-C1-N1	-3.50	115.60	123.31
2	X	1463	UDA	O21-C11-C19	3.50	130.95	105.57
2	F	1455	UDA	O21-C11-C19	3.50	130.94	105.57
2	J	1459	UDA	O21-C11-C19	3.50	130.91	105.57
2	J	1459	UDA	C6-C1-N1	-3.48	115.64	123.31
2	E	1454	UDA	O21-C11-C19	3.47	130.74	105.57
2	K	1460	UDA	O21-C11-C19	3.46	130.66	105.57
2	B	1451	UDA	C6-C1-N1	-3.46	115.70	123.31
2	X	1463	UDA	C6-C1-N1	-3.45	115.71	123.31
2	I	1458	UDA	O21-C11-C19	3.45	130.58	105.57
2	G	1456	UDA	O21-C11-C19	3.45	130.58	105.57
2	C	1452	UDA	O21-C11-C19	3.43	130.42	105.57
2	E	1454	UDA	O11-C9-C15	3.42	122.88	111.82
2	H	1457	UDA	O21-C11-C19	3.41	130.29	105.57
2	W	1462	UDA	C6-C1-N1	-3.41	115.82	123.31
2	C	1452	UDA	O15-P3-O13	-3.40	90.75	105.99
2	L	1461	UDA	C6-C1-N1	-3.40	115.83	123.31
2	H	1457	UDA	O15-P3-O13	-3.39	90.81	105.99
2	G	1456	UDA	C6-C1-N1	-3.38	115.87	123.31
2	Z	1465	UDA	O7-P2-O8	3.37	109.29	102.48
2	E	1454	UDA	O14-C15-C4	3.37	120.80	111.05
2	I	1458	UDA	O15-P3-O13	-3.36	90.93	105.99
2	X	1463	UDA	O15-P3-O13	-3.36	90.95	105.99
2	I	1458	UDA	C6-C1-N1	-3.34	115.97	123.31
2	A	1450	UDA	O11-C9-C15	3.33	122.61	111.82
2	L	1461	UDA	O15-P3-O13	-3.33	91.09	105.99
2	Y	1464	UDA	O21-C11-C19	3.32	129.65	105.57
2	G	1456	UDA	O15-P3-O13	-3.30	91.19	105.99

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	J	1459	UDA	O15-P3-O13	-3.28	91.28	105.99
2	A	1450	UDA	O15-P3-O13	-3.27	91.34	105.99
2	D	1453	UDA	O15-P3-O13	-3.24	91.47	105.99
2	D	1453	UDA	O21-C11-C19	3.22	128.92	105.57
2	B	1451	UDA	O15-P3-O13	-3.21	91.62	105.99
2	F	1455	UDA	O15-P3-O13	-3.18	91.74	105.99
2	K	1460	UDA	O15-P3-O13	-3.16	91.85	105.99
2	Z	1465	UDA	O15-P3-O13	-3.15	91.88	105.99
2	W	1462	UDA	O15-P3-O13	-3.11	92.08	105.99
2	F	1455	UDA	O11-C9-C15	3.08	121.77	111.82
2	B	1451	UDA	O11-C9-C15	3.07	121.77	111.82
2	K	1460	UDA	O11-C9-C15	3.07	121.74	111.82
2	Z	1465	UDA	O11-C9-C15	3.05	121.70	111.82
2	W	1462	UDA	O11-C9-C15	3.05	121.69	111.82
2	G	1456	UDA	O11-C9-C15	3.05	121.67	111.82
2	C	1452	UDA	O11-C9-C15	3.03	121.64	111.82
2	E	1454	UDA	O15-P3-O13	-2.96	92.71	105.99
2	Y	1464	UDA	O11-C9-C15	2.96	121.39	111.82
2	I	1458	UDA	O11-C9-C15	2.94	121.33	111.82
2	Y	1464	UDA	O15-P3-O13	-2.94	92.84	105.99
2	L	1461	UDA	O11-C9-C15	2.93	121.29	111.82
2	J	1459	UDA	O11-C9-C15	2.91	121.25	111.82
2	H	1457	UDA	O11-C9-C15	2.90	121.21	111.82
2	X	1463	UDA	O11-C9-C15	2.88	121.14	111.82
2	D	1453	UDA	O11-C9-C15	2.86	121.06	111.82
2	E	1454	UDA	O15-P3-O17	-2.73	99.99	110.68
2	J	1459	UDA	O15-P3-O17	-2.52	100.82	110.68
2	Y	1464	UDA	O22-C20-C13	2.52	116.61	109.94
2	A	1450	UDA	O15-P3-O17	-2.50	100.89	110.68
2	Z	1465	UDA	O15-P3-O17	-2.50	100.91	110.68
2	G	1456	UDA	O22-C20-C13	2.46	116.46	109.94
2	G	1456	UDA	O15-P3-O17	-2.44	101.13	110.68
2	K	1460	UDA	O22-C20-C13	2.44	116.41	109.94
2	K	1460	UDA	O15-P3-O17	-2.44	101.15	110.68
2	Y	1464	UDA	O15-P3-O17	-2.43	101.16	110.68
2	L	1461	UDA	O15-P3-O17	-2.42	101.23	110.68
2	E	1454	UDA	O24-C17-C16	2.40	119.54	111.29
2	L	1461	UDA	O22-C20-C13	2.39	116.27	109.94
2	A	1450	UDA	C9-C15-C4	-2.38	98.02	102.64
2	W	1462	UDA	O15-P3-O17	-2.37	101.41	110.68
2	F	1455	UDA	O15-P3-O17	-2.36	101.44	110.68
2	X	1463	UDA	O15-P3-O17	-2.36	101.44	110.68

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1452	UDA	O15-P3-O17	-2.36	101.45	110.68
2	B	1451	UDA	O22-C20-C13	2.35	116.17	109.94
2	B	1451	UDA	C9-C15-C4	-2.32	98.14	102.64
2	I	1458	UDA	O15-P3-O17	-2.31	101.63	110.68
2	H	1457	UDA	O15-P3-O17	-2.31	101.63	110.68
2	D	1453	UDA	O15-P3-O17	-2.31	101.64	110.68
2	E	1454	UDA	O22-C20-C13	2.31	116.05	109.94
2	X	1463	UDA	O22-C20-C13	2.30	116.04	109.94
2	F	1455	UDA	O22-C20-C13	2.30	116.04	109.94
2	F	1455	UDA	C9-C15-C4	-2.29	98.20	102.64
2	G	1456	UDA	O13-P3-O17	2.28	118.21	109.39
2	C	1452	UDA	O22-C20-C13	2.28	115.98	109.94
2	A	1450	UDA	O22-C20-C13	2.28	115.98	109.94
2	J	1459	UDA	O11-C9-C2	2.27	119.23	110.85
2	A	1450	UDA	O12-C7-C8	2.27	126.27	122.06
2	Y	1464	UDA	O11-C9-C2	2.27	119.22	110.85
2	W	1462	UDA	O13-P3-O17	2.26	118.13	109.39
2	H	1457	UDA	O22-C20-C13	2.26	115.93	109.94
2	C	1452	UDA	O13-P3-O17	2.25	118.09	109.39
2	H	1457	UDA	O13-P3-O17	2.24	118.05	109.39
2	B	1451	UDA	O15-P3-O17	-2.24	101.93	110.68
2	D	1453	UDA	O22-C20-C13	2.23	115.86	109.94
2	X	1463	UDA	O11-C9-C2	2.22	119.07	110.85
2	E	1454	UDA	C9-C15-C4	-2.22	98.34	102.64
2	D	1453	UDA	O13-P3-O17	2.20	117.89	109.39
2	J	1459	UDA	O22-C20-C13	2.20	115.78	109.94
2	E	1454	UDA	O4-C12-C4	2.20	116.56	108.99
2	F	1455	UDA	O11-C9-C2	2.20	118.97	110.85
2	G	1456	UDA	C9-C15-C4	-2.19	98.38	102.64
2	Z	1465	UDA	O22-C20-C13	2.19	115.74	109.94
2	B	1451	UDA	O24-C17-C16	2.19	118.80	111.29
2	H	1457	UDA	C9-C15-C4	-2.17	98.43	102.64
2	Z	1465	UDA	O13-P3-O17	2.17	117.76	109.39
2	A	1450	UDA	O13-P3-O17	2.17	117.75	109.39
2	L	1461	UDA	O11-C9-C2	2.16	118.84	110.85
2	G	1456	UDA	O24-C17-C16	2.16	118.70	111.29
2	Y	1464	UDA	C9-C15-C4	-2.16	98.44	102.64
2	H	1457	UDA	O12-C7-C8	2.15	126.06	122.06
2	I	1458	UDA	O13-P3-O17	2.15	117.69	109.39
2	E	1454	UDA	O13-P3-O17	2.14	117.65	109.39
2	J	1459	UDA	O13-P3-O17	2.13	117.63	109.39
2	X	1463	UDA	O12-C7-C8	2.13	126.02	122.06

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1453	UDA	O12-C7-C8	2.13	126.02	122.06
2	C	1452	UDA	O11-C9-C2	2.12	118.70	110.85
2	Y	1464	UDA	O22-C20-C16	-2.11	104.05	109.30
2	W	1462	UDA	O12-C7-C8	2.11	125.98	122.06
2	X	1463	UDA	O13-P3-O17	2.11	117.53	109.39
2	X	1463	UDA	O14-C15-C9	-2.11	105.01	111.82
2	D	1453	UDA	O11-C9-C2	2.11	118.63	110.85
2	L	1461	UDA	C9-C15-C4	-2.10	98.55	102.64
2	I	1458	UDA	C9-C15-C4	-2.10	98.56	102.64
2	W	1462	UDA	O22-C20-C13	2.10	115.50	109.94
2	B	1451	UDA	O22-C20-C16	-2.08	104.14	109.30
2	K	1460	UDA	O22-C20-C16	-2.08	104.14	109.30
2	D	1453	UDA	C9-C15-C4	-2.07	98.61	102.64
2	F	1455	UDA	C10-O23-C16	2.06	117.73	113.69
2	K	1460	UDA	C9-C15-C4	-2.05	98.66	102.64
2	W	1462	UDA	O11-C9-C2	2.05	118.41	110.85
2	H	1457	UDA	O11-C9-C2	2.04	118.40	110.85
2	Z	1465	UDA	O12-C7-C8	2.03	125.83	122.06
2	L	1461	UDA	O13-P3-O17	2.03	117.22	109.39
2	X	1463	UDA	O4-C12-C4	2.03	115.97	108.99
2	I	1458	UDA	O12-C7-C8	2.03	125.82	122.06
2	F	1455	UDA	O13-P3-O17	2.02	117.19	109.39
2	W	1462	UDA	O14-C15-C9	-2.02	105.29	111.82
2	I	1458	UDA	O11-C9-C2	2.02	118.30	110.85
2	B	1451	UDA	O11-C9-C2	2.02	118.30	110.85
2	K	1460	UDA	O24-C17-C16	2.01	118.19	111.29
2	Z	1465	UDA	O11-C9-C2	2.01	118.28	110.85
2	K	1460	UDA	O11-C9-C2	2.01	118.27	110.85
2	L	1461	UDA	O22-C20-C16	-2.01	104.31	109.30
2	K	1460	UDA	O13-P3-O17	2.01	117.13	109.39

There are no chirality outliers.

All (144) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1450	UDA	C9-C2-N2-C5
2	A	1450	UDA	O3-C2-N2-C5
2	A	1450	UDA	C12-O4-P1-O5
2	A	1450	UDA	C12-O4-P1-O6
2	B	1451	UDA	C9-C2-N2-C5
2	B	1451	UDA	O3-C2-N2-C5
2	B	1451	UDA	C12-O4-P1-O5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	B	1451	UDA	C12-O4-P1-O6
2	C	1452	UDA	O3-C2-N2-C5
2	C	1452	UDA	C12-O4-P1-O5
2	C	1452	UDA	C12-O4-P1-O6
2	D	1453	UDA	C9-C2-N2-C5
2	D	1453	UDA	O3-C2-N2-C5
2	D	1453	UDA	C12-O4-P1-O5
2	D	1453	UDA	C12-O4-P1-O6
2	E	1454	UDA	C9-C2-N2-C5
2	E	1454	UDA	O3-C2-N2-C5
2	E	1454	UDA	C12-O4-P1-O5
2	E	1454	UDA	C12-O4-P1-O6
2	F	1455	UDA	C9-C2-N2-C5
2	F	1455	UDA	O3-C2-N2-C5
2	F	1455	UDA	C12-O4-P1-O5
2	F	1455	UDA	C12-O4-P1-O6
2	G	1456	UDA	C9-C2-N2-C5
2	G	1456	UDA	O3-C2-N2-C5
2	G	1456	UDA	C12-O4-P1-O5
2	G	1456	UDA	C12-O4-P1-O6
2	H	1457	UDA	C9-C2-N2-C5
2	H	1457	UDA	O3-C2-N2-C5
2	H	1457	UDA	C12-O4-P1-O5
2	H	1457	UDA	C12-O4-P1-O6
2	I	1458	UDA	C9-C2-N2-C5
2	I	1458	UDA	O3-C2-N2-C5
2	I	1458	UDA	C12-O4-P1-O5
2	I	1458	UDA	C12-O4-P1-O6
2	J	1459	UDA	C9-C2-N2-C5
2	J	1459	UDA	O3-C2-N2-C5
2	J	1459	UDA	C12-O4-P1-O5
2	J	1459	UDA	C12-O4-P1-O6
2	K	1460	UDA	C9-C2-N2-C5
2	K	1460	UDA	O3-C2-N2-C5
2	K	1460	UDA	C12-O4-P1-O5
2	K	1460	UDA	C12-O4-P1-O6
2	L	1461	UDA	C9-C2-N2-C5
2	L	1461	UDA	O3-C2-N2-C5
2	L	1461	UDA	C12-O4-P1-O5
2	L	1461	UDA	C12-O4-P1-O6
2	W	1462	UDA	C9-C2-N2-C5
2	W	1462	UDA	O3-C2-N2-C5

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	W	1462	UDA	C12-O4-P1-O5
2	W	1462	UDA	C12-O4-P1-O6
2	X	1463	UDA	C9-C2-N2-C5
2	X	1463	UDA	O3-C2-N2-C5
2	X	1463	UDA	C12-O4-P1-O5
2	X	1463	UDA	C12-O4-P1-O6
2	Y	1464	UDA	C9-C2-N2-C5
2	Y	1464	UDA	O3-C2-N2-C5
2	Y	1464	UDA	C12-O4-P1-O5
2	Y	1464	UDA	C12-O4-P1-O6
2	Z	1465	UDA	C9-C2-N2-C5
2	Z	1465	UDA	O3-C2-N2-C5
2	Z	1465	UDA	C12-O4-P1-O5
2	Z	1465	UDA	C12-O4-P1-O6
2	A	1450	UDA	C13-C18-N3-C7
2	F	1455	UDA	C13-C18-N3-C7
2	K	1460	UDA	C13-C18-N3-C7
2	G	1456	UDA	C13-C18-N3-C7
2	A	1450	UDA	P2-O7-P1-O5
2	B	1451	UDA	P2-O7-P1-O5
2	E	1454	UDA	P2-O7-P1-O5
2	F	1455	UDA	P2-O7-P1-O5
2	I	1458	UDA	P2-O7-P1-O5
2	J	1459	UDA	P2-O7-P1-O5
2	L	1461	UDA	P2-O7-P1-O5
2	W	1462	UDA	P2-O7-P1-O5
2	X	1463	UDA	P2-O7-P1-O5
2	Z	1465	UDA	P2-O7-P1-O5
2	H	1457	UDA	C13-C18-N3-C7
2	Y	1464	UDA	C13-C18-N3-C7
2	A	1450	UDA	C12-O4-P1-O7
2	B	1451	UDA	C12-O4-P1-O7
2	C	1452	UDA	C12-O4-P1-O7
2	D	1453	UDA	C12-O4-P1-O7
2	E	1454	UDA	C12-O4-P1-O7
2	F	1455	UDA	C12-O4-P1-O7
2	G	1456	UDA	C12-O4-P1-O7
2	H	1457	UDA	C12-O4-P1-O7
2	I	1458	UDA	C12-O4-P1-O7
2	J	1459	UDA	C12-O4-P1-O7
2	K	1460	UDA	C12-O4-P1-O7
2	L	1461	UDA	C12-O4-P1-O7

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
2	W	1462	UDA	C12-O4-P1-O7
2	X	1463	UDA	C12-O4-P1-O7
2	Y	1464	UDA	C12-O4-P1-O7
2	Z	1465	UDA	C12-O4-P1-O7
2	D	1453	UDA	P2-O7-P1-O5
2	H	1457	UDA	P2-O7-P1-O5
2	Y	1464	UDA	P2-O7-P1-O5
2	A	1450	UDA	C11-O13-P3-O16
2	B	1451	UDA	C11-O13-P3-O16
2	C	1452	UDA	C11-O13-P3-O16
2	D	1453	UDA	C11-O13-P3-O16
2	E	1454	UDA	C11-O13-P3-O16
2	F	1455	UDA	C11-O13-P3-O16
2	G	1456	UDA	C11-O13-P3-O16
2	H	1457	UDA	C11-O13-P3-O16
2	I	1458	UDA	C11-O13-P3-O16
2	J	1459	UDA	C11-O13-P3-O16
2	K	1460	UDA	C11-O13-P3-O16
2	L	1461	UDA	C11-O13-P3-O16
2	W	1462	UDA	C11-O13-P3-O16
2	X	1463	UDA	C11-O13-P3-O16
2	Y	1464	UDA	C11-O13-P3-O16
2	Z	1465	UDA	C11-O13-P3-O16
2	B	1451	UDA	C13-C18-N3-C7
2	I	1458	UDA	C13-C18-N3-C7
2	G	1456	UDA	P2-O7-P1-O5
2	K	1460	UDA	P2-O7-P1-O5
2	L	1461	UDA	C13-C18-N3-C7
2	W	1462	UDA	C13-C18-N3-C7
2	Z	1465	UDA	C13-C18-N3-C7
2	D	1453	UDA	C13-C18-N3-C7
3	A	1470	EDO	O1-C1-C2-O2
3	B	1471	EDO	O1-C1-C2-O2
3	C	1472	EDO	O1-C1-C2-O2
3	D	1473	EDO	O1-C1-C2-O2
3	E	1474	EDO	O1-C1-C2-O2
3	F	1475	EDO	O1-C1-C2-O2
3	G	1476	EDO	O1-C1-C2-O2
3	H	1477	EDO	O1-C1-C2-O2
3	I	1478	EDO	O1-C1-C2-O2
3	K	1480	EDO	O1-C1-C2-O2
3	W	1482	EDO	O1-C1-C2-O2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms
3	X	1483	EDO	O1-C1-C2-O2
3	Y	1484	EDO	O1-C1-C2-O2
3	Z	1485	EDO	O1-C1-C2-O2
2	Z	1465	UDA	C20-C13-O21-C11
2	C	1452	UDA	P2-O7-P1-O6
2	G	1456	UDA	P2-O7-P1-O6
2	C	1452	UDA	C13-C18-N3-C7
3	J	1479	EDO	O1-C1-C2-O2
3	L	1481	EDO	O1-C1-C2-O2
2	A	1450	UDA	C10-C18-N3-C7
2	F	1455	UDA	C10-C18-N3-C7

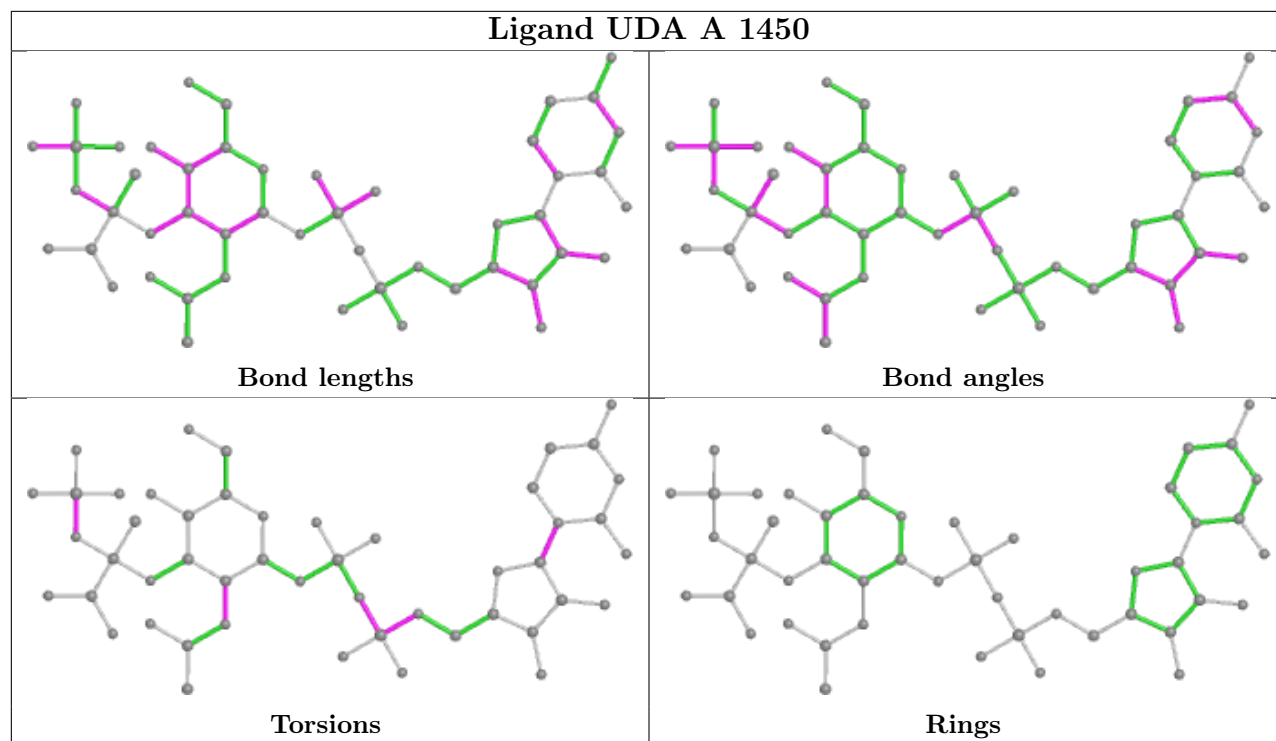
There are no ring outliers.

10 monomers are involved in 14 short contacts:

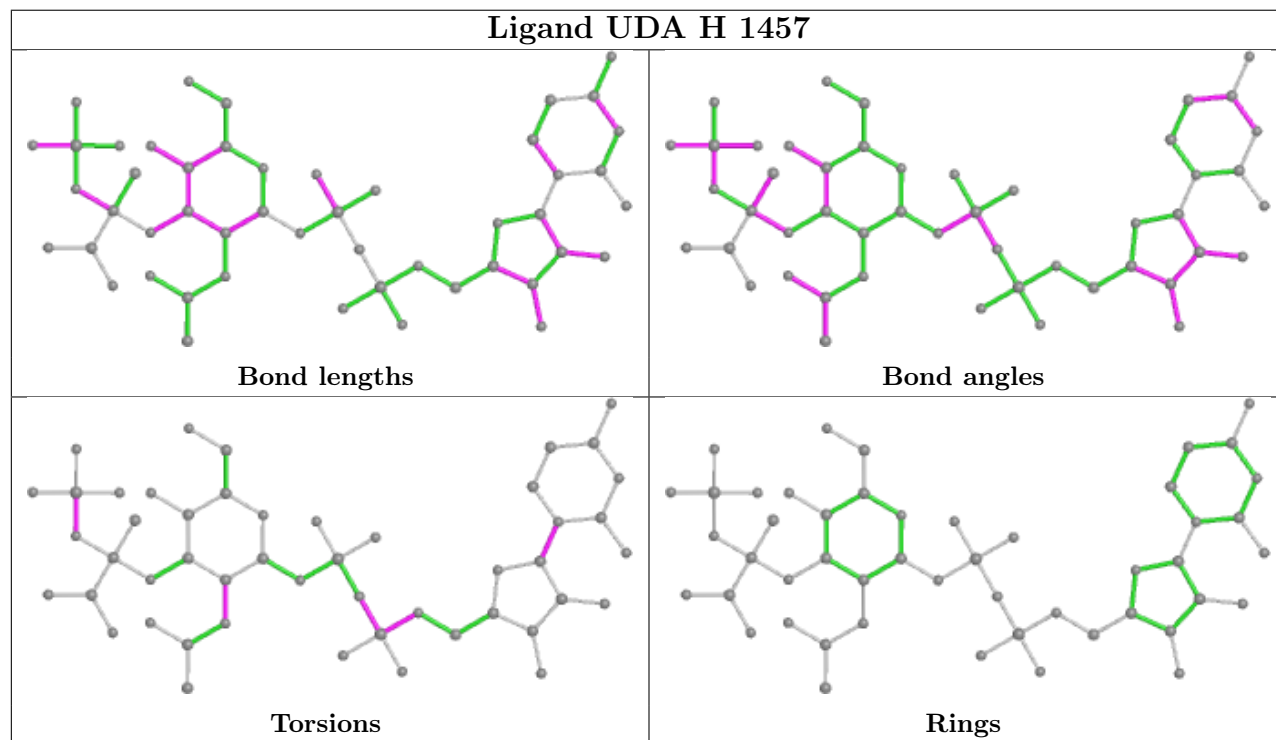
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1450	UDA	1	0
2	Z	1465	UDA	1	0
3	X	1483	EDO	1	0
3	F	1475	EDO	2	0
2	C	1452	UDA	1	0
3	B	1471	EDO	1	0
2	Y	1464	UDA	1	0
2	W	1462	UDA	1	0
3	D	1473	EDO	3	0
2	I	1458	UDA	2	0

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.

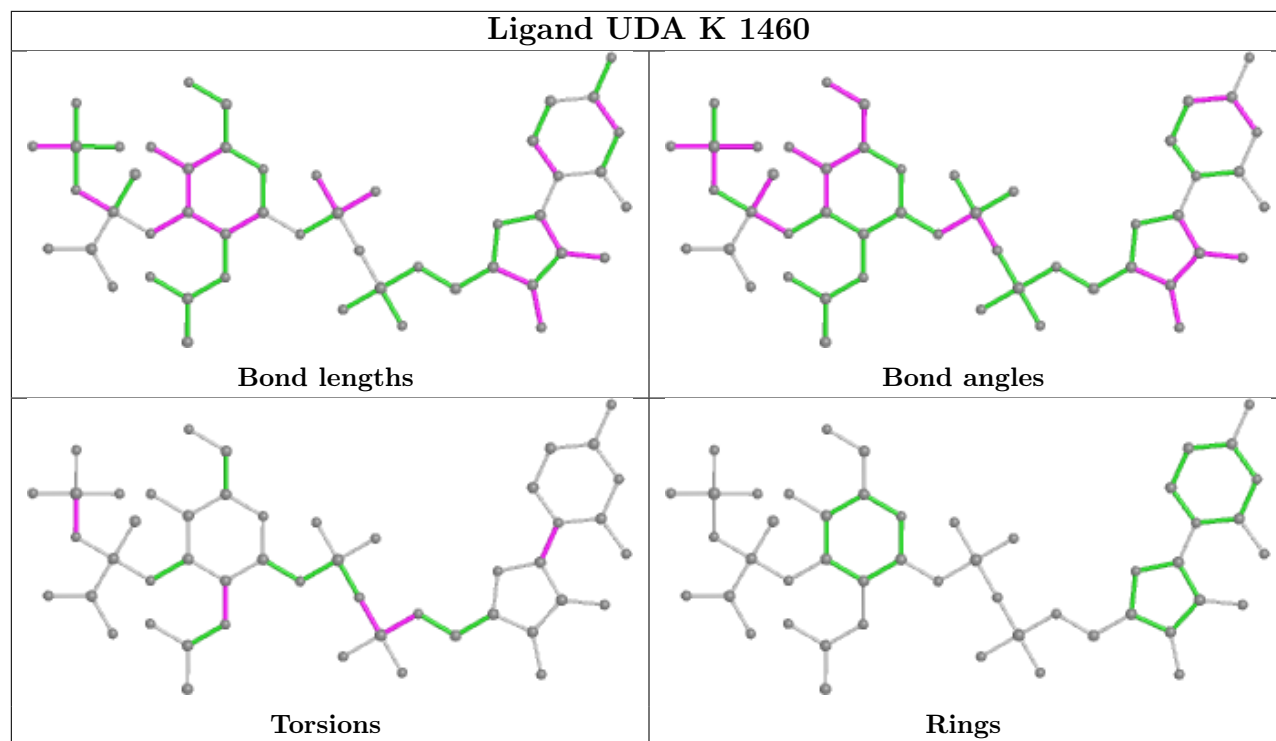
## Ligand UDA A 1450



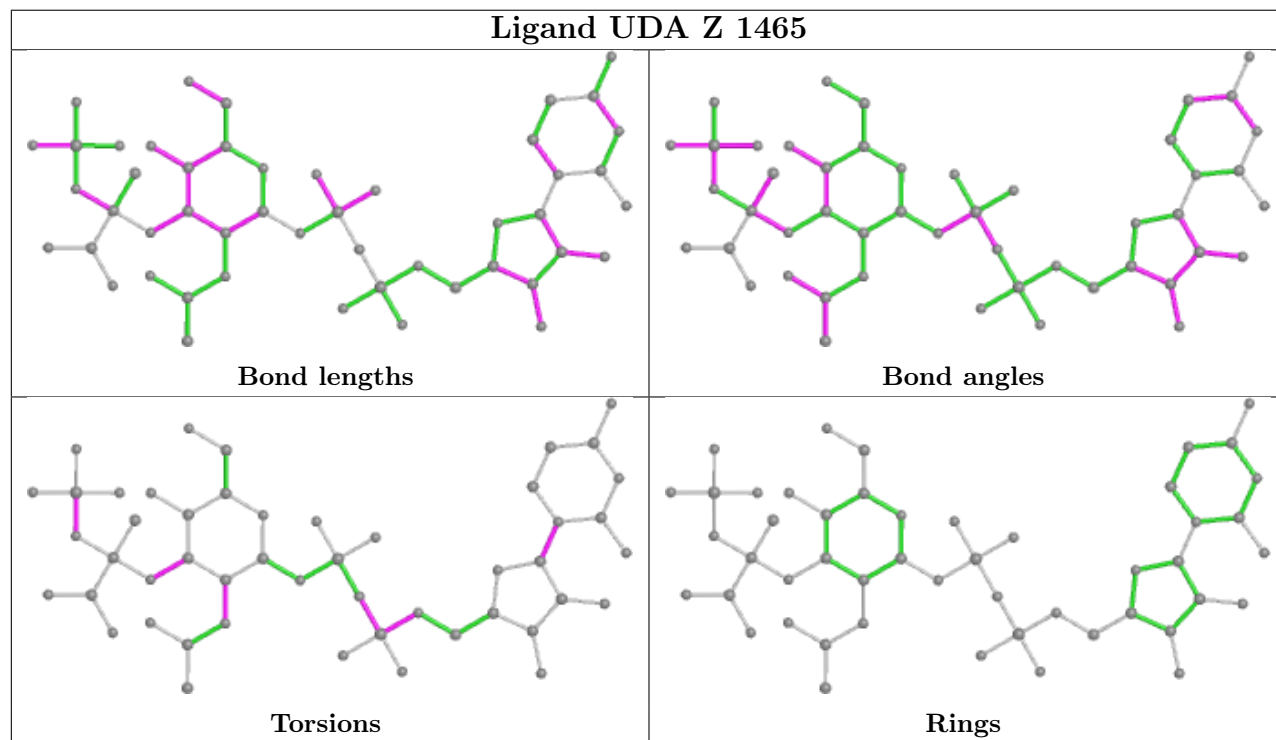
## Ligand UDA H 1457



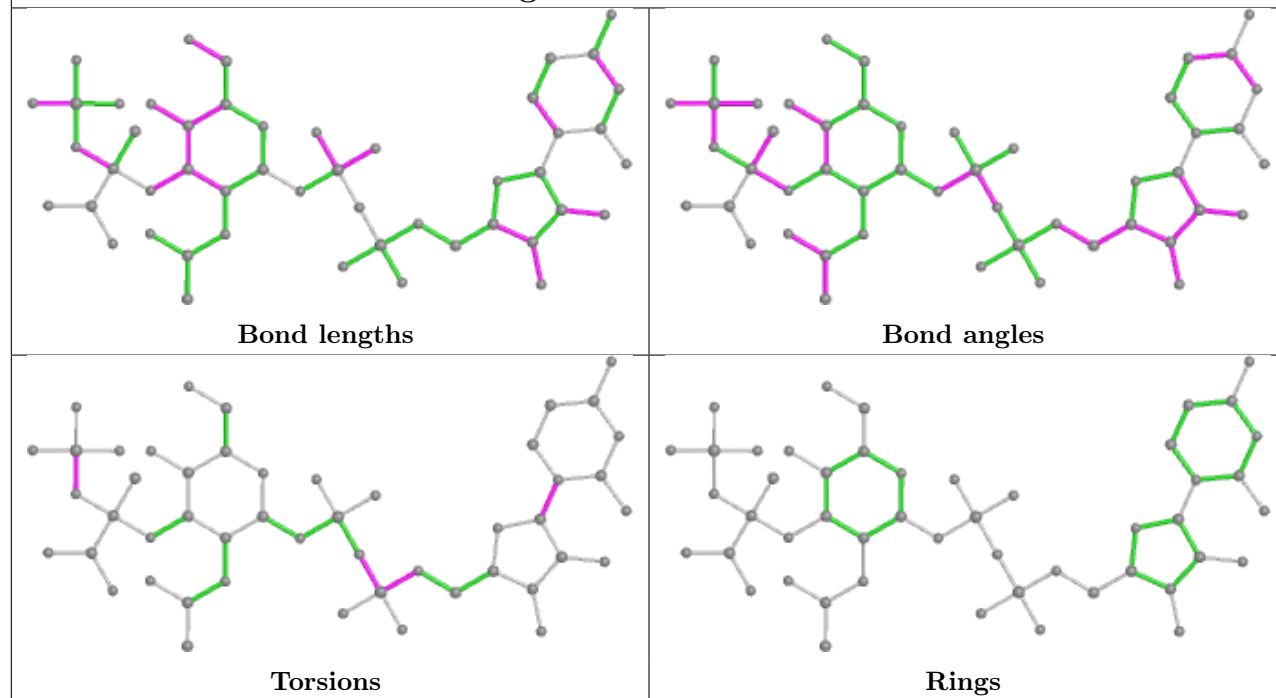
## Ligand UDA K 1460



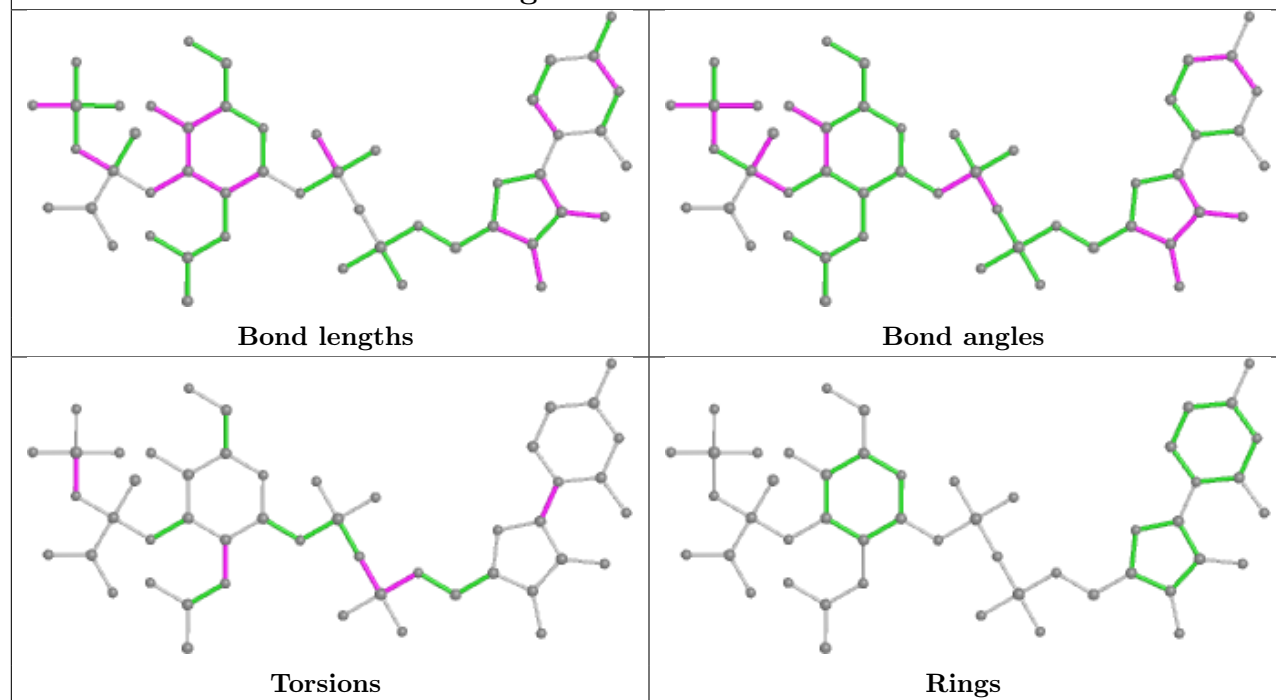
## Ligand UDA Z 1465



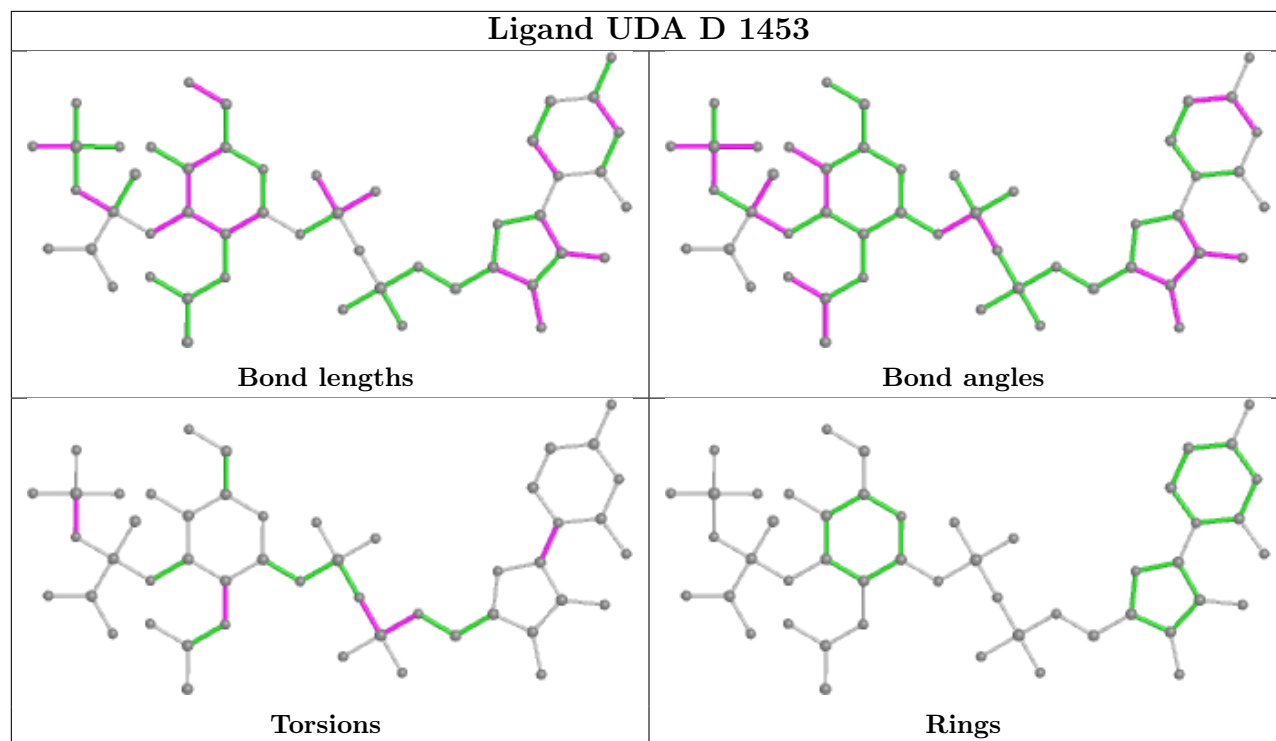
## Ligand UDA X 1463



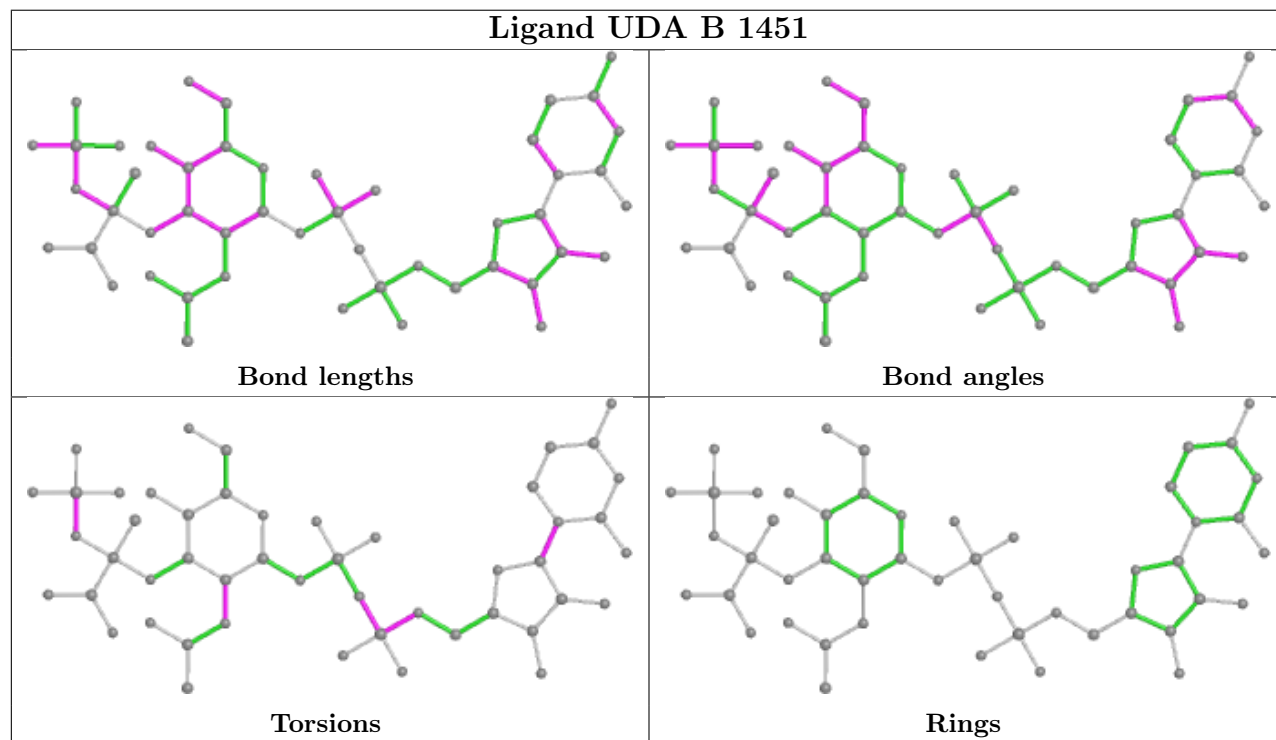
## Ligand UDA C 1452



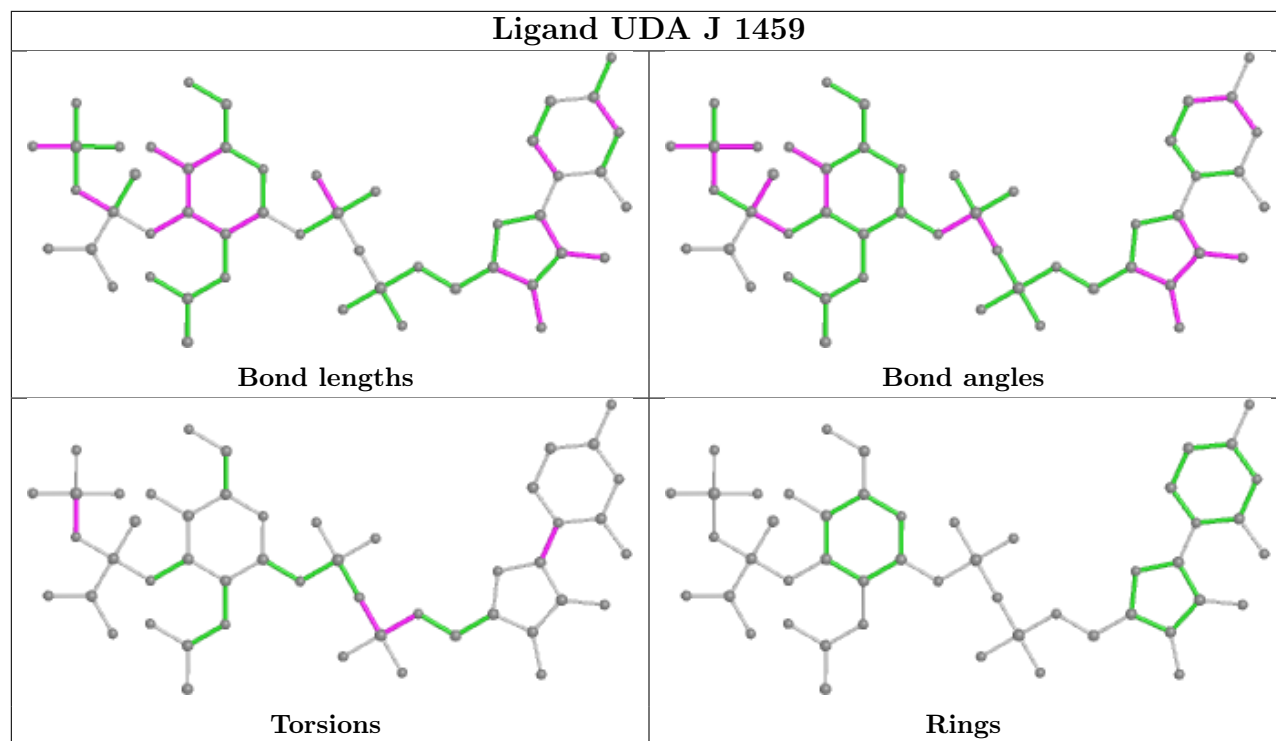
## Ligand UDA D 1453



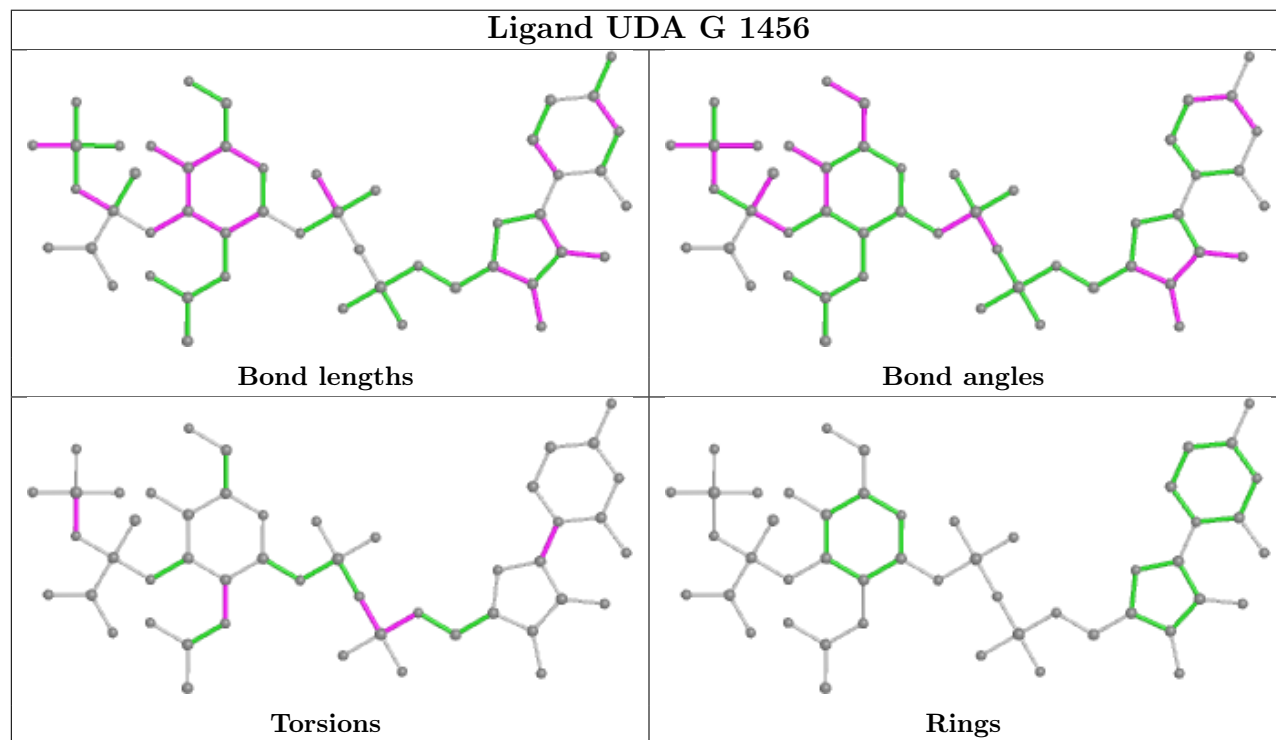
## Ligand UDA B 1451



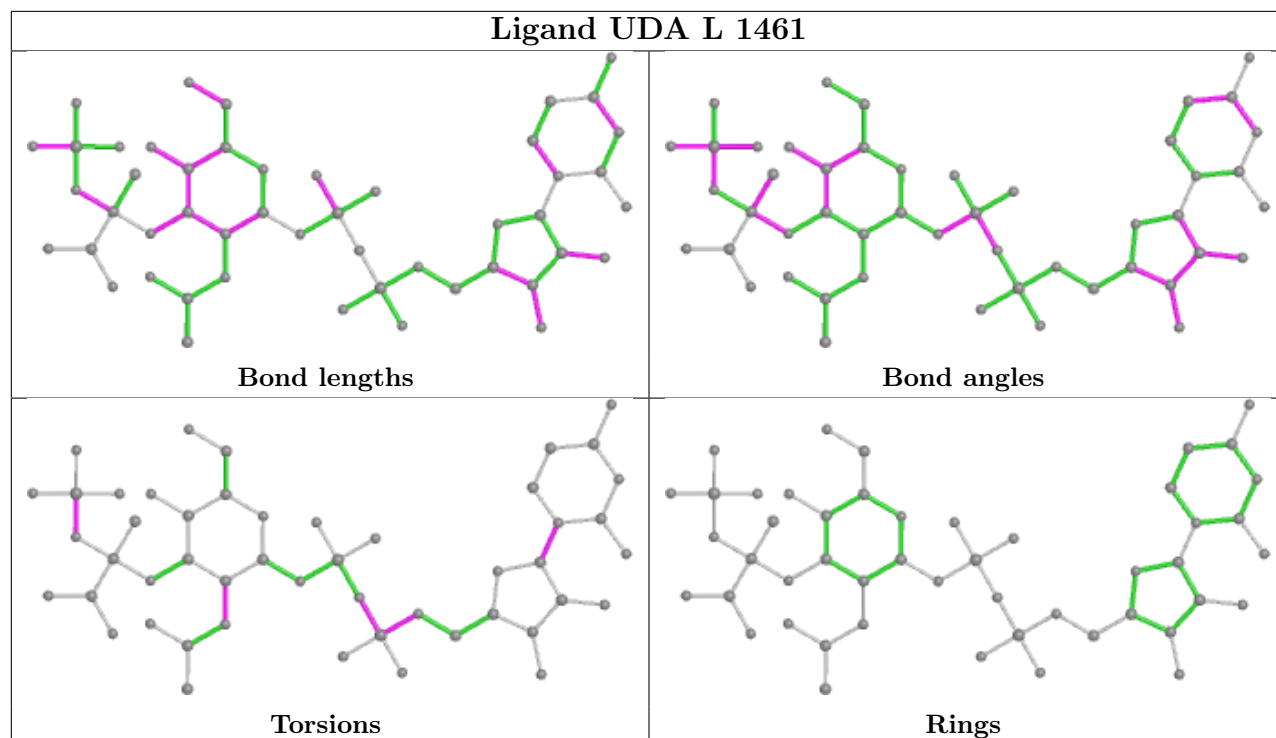
## Ligand UDA J 1459



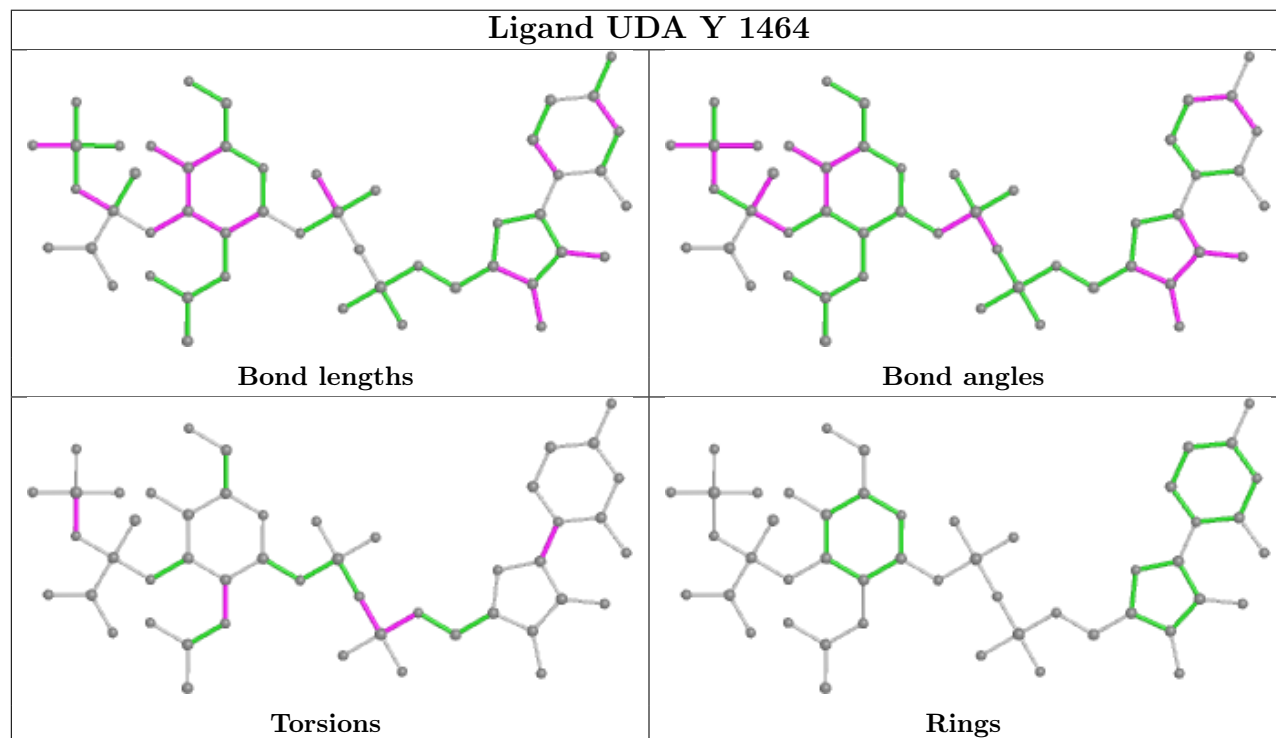
## Ligand UDA G 1456



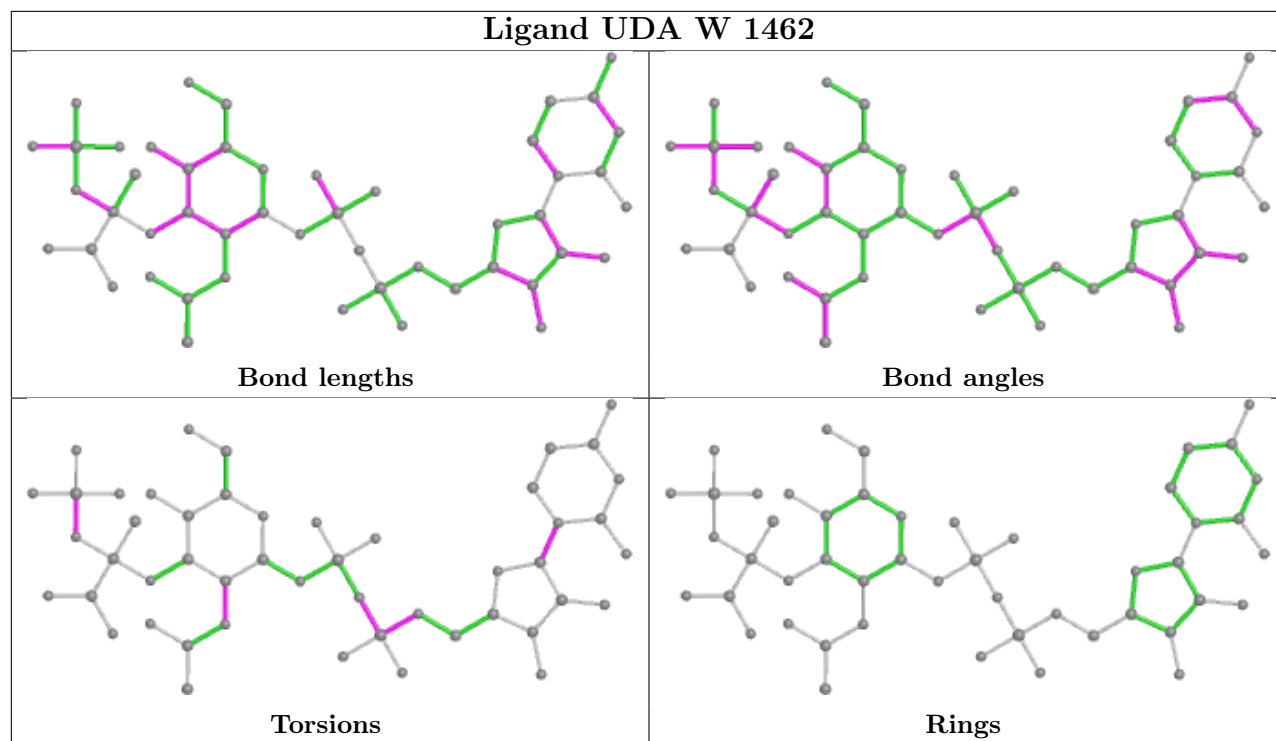
## Ligand UDA L 1461



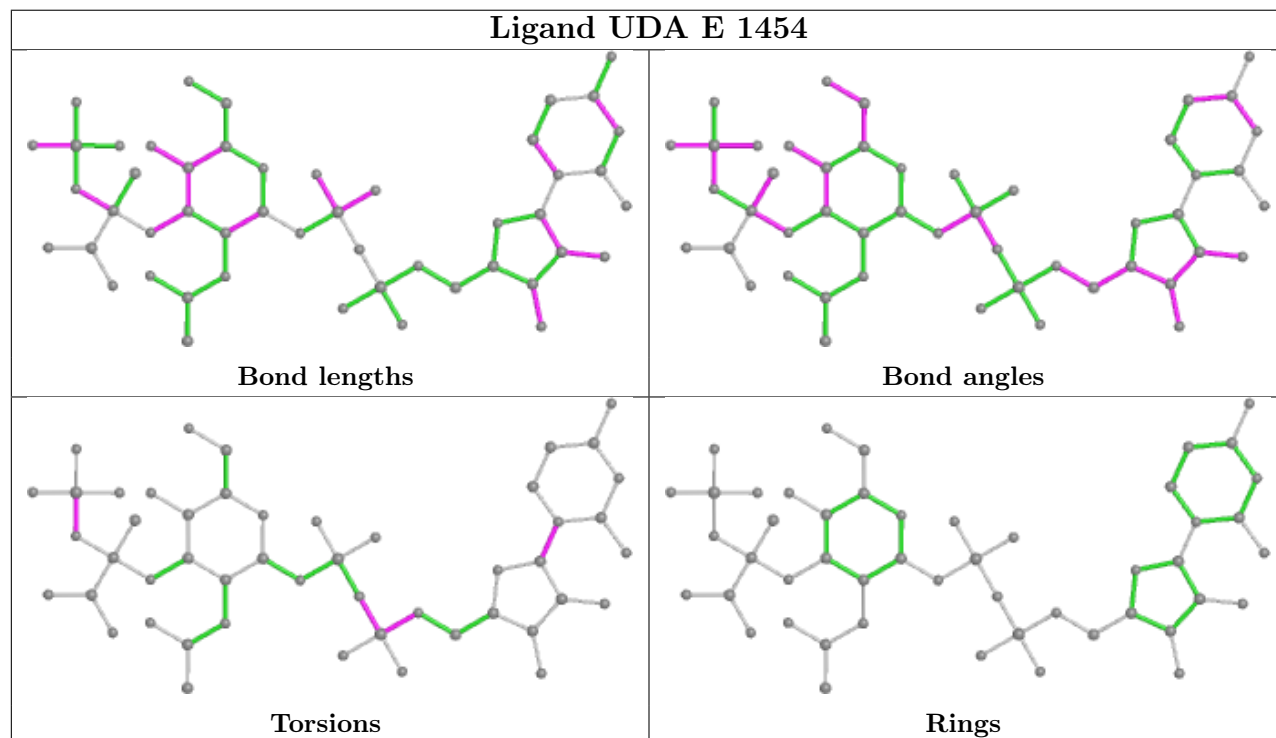
## Ligand UDA Y 1464

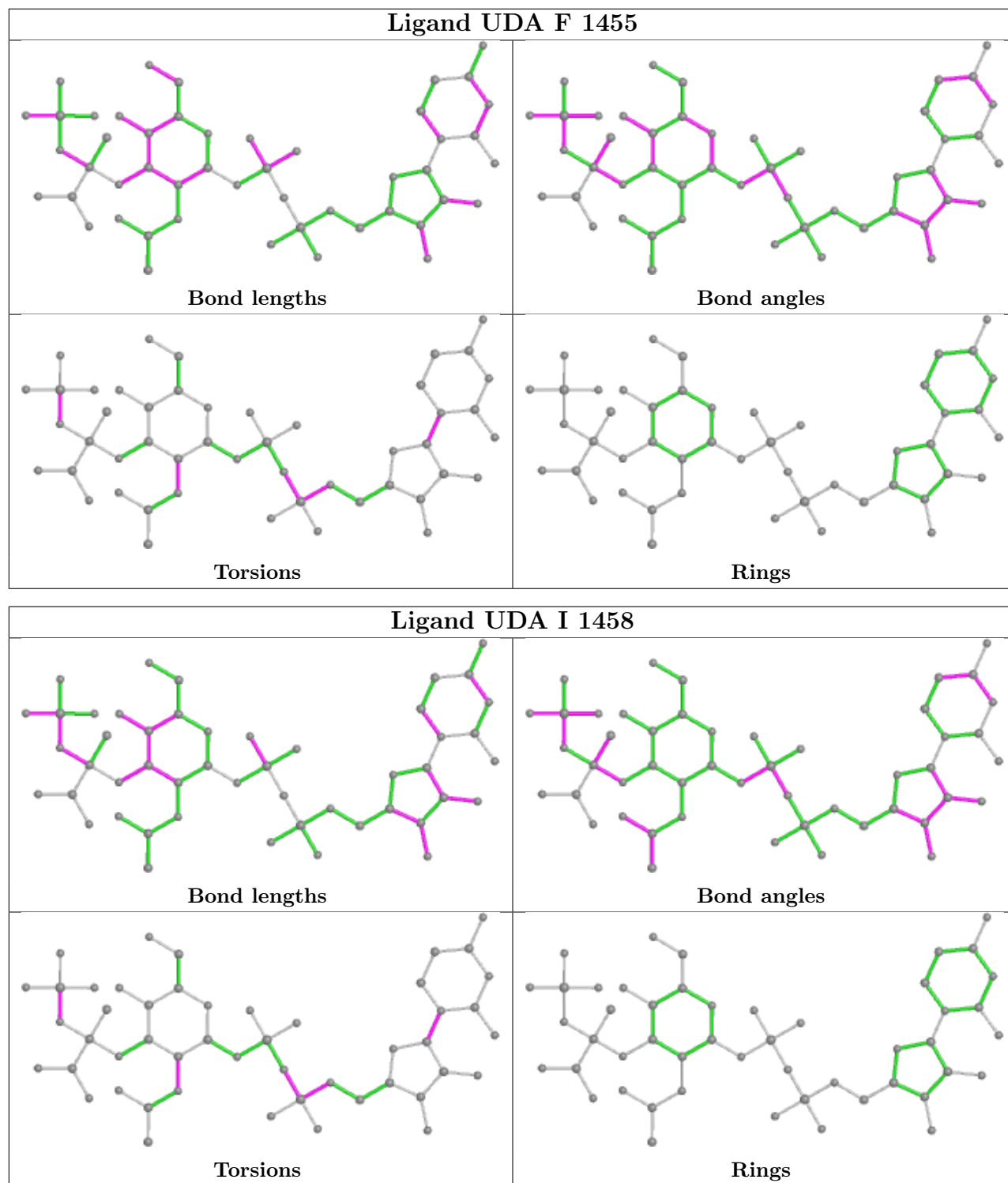


## Ligand UDA W 1462



## Ligand UDA E 1454





## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<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	418/419 (99%)	-0.28	3 (0%) 87 87	18, 35, 58, 99	0
1	B	418/419 (99%)	-0.37	4 (0%) 82 81	20, 34, 52, 107	0
1	C	418/419 (99%)	-0.52	2 (0%) 91 91	19, 31, 47, 93	0
1	D	418/419 (99%)	-0.45	4 (0%) 82 81	18, 32, 50, 109	0
1	E	418/419 (99%)	-0.41	2 (0%) 91 91	18, 32, 50, 93	0
1	F	418/419 (99%)	-0.37	3 (0%) 87 87	20, 34, 50, 93	0
1	G	418/419 (99%)	-0.49	1 (0%) 95 96	18, 31, 47, 86	0
1	H	418/419 (99%)	-0.41	4 (0%) 82 81	18, 34, 53, 104	0
1	I	418/419 (99%)	-0.40	2 (0%) 91 91	20, 34, 52, 105	0
1	J	418/419 (99%)	-0.29	4 (0%) 82 81	22, 37, 56, 103	0
1	K	418/419 (99%)	-0.27	6 (1%) 75 73	20, 36, 53, 102	0
1	L	418/419 (99%)	-0.25	3 (0%) 87 87	22, 37, 58, 92	0
1	W	418/419 (99%)	-0.34	1 (0%) 95 96	22, 35, 54, 96	0
1	X	418/419 (99%)	-0.11	9 (2%) 62 57	22, 38, 61, 99	0
1	Y	418/419 (99%)	-0.22	6 (1%) 75 73	23, 37, 54, 99	0
1	Z	418/419 (99%)	-0.21	3 (0%) 87 87	22, 39, 61, 89	0
All	All	6688/6704 (99%)	-0.34	57 (0%) 84 83	18, 35, 54, 109	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	418	GLY	5.8
1	D	419	GLU	5.6
1	K	418	GLY	5.5
1	Y	418	GLY	5.5
1	F	418	GLY	5.4

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	418	GLY	5.1
1	J	419	GLU	4.7
1	L	418	GLY	4.4
1	E	419	GLU	4.2
1	H	419	GLU	4.1
1	X	419	GLU	4.1
1	Z	419	GLU	4.0
1	C	419	GLU	3.9
1	A	419	GLU	3.9
1	W	419	GLU	3.8
1	H	418	GLY	3.8
1	K	419	GLU	3.5
1	C	418	GLY	3.5
1	J	418	GLY	3.4
1	I	418	GLY	3.2
1	B	419	GLU	3.1
1	L	419	GLU	2.9
1	F	419	GLU	2.9
1	X	177	GLU	2.9
1	X	1	MET	2.8
1	X	63	LYS	2.8
1	J	1	MET	2.8
1	Y	252	ARG	2.8
1	G	419	GLU	2.8
1	E	1	MET	2.7
1	I	419	GLU	2.7
1	Y	275	THR	2.7
1	B	63	LYS	2.7
1	B	1	MET	2.7
1	Y	279	TRP	2.6
1	Y	417	LYS	2.5
1	Z	417	LYS	2.5
1	Y	419	GLU	2.5
1	D	417	LYS	2.5
1	K	417	LYS	2.5
1	X	68	GLY	2.5
1	H	219	GLU	2.5
1	F	1	MET	2.4
1	X	77	VAL	2.4
1	X	65	GLU	2.4
1	K	277	GLU	2.3
1	X	148	ASN	2.3

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	D	1	MET	2.3
1	X	219	GLU	2.3
1	J	148	ASN	2.2
1	H	277	GLU	2.2
1	L	1	MET	2.1
1	Z	1	MET	2.1
1	K	252	ARG	2.1
1	A	418	GLY	2.0
1	A	65	GLU	2.0
1	K	73	ASP	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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
1	IAS	E	67	8/9	0.86	0.25	40,44,47,49	0
1	IAS	A	67	8/9	0.88	0.22	45,47,49,51	0
1	IAS	I	67	8/9	0.88	0.23	37,40,41,44	0
1	IAS	J	67	8/9	0.88	0.26	43,46,48,50	0
1	IAS	W	67	8/9	0.88	0.18	33,38,42,42	0
1	IAS	Y	67	8/9	0.88	0.17	45,46,50,55	0
1	IAS	Z	67	8/9	0.91	0.24	47,48,51,53	0
1	IAS	L	67	8/9	0.92	0.23	44,46,48,52	0
1	IAS	K	67	8/9	0.92	0.19	43,48,51,56	0
1	IAS	H	67	8/9	0.93	0.20	30,41,46,51	0
1	IAS	B	67	8/9	0.93	0.20	40,43,47,50	0
1	IAS	F	67	8/9	0.94	0.20	37,41,44,46	0
1	IAS	X	67	8/9	0.94	0.23	45,46,50,52	0
1	IAS	G	67	8/9	0.95	0.11	30,33,39,39	0
1	IAS	C	67	8/9	0.95	0.10	31,35,37,37	0
1	IAS	D	67	8/9	0.97	0.19	32,40,44,45	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands ⓘ

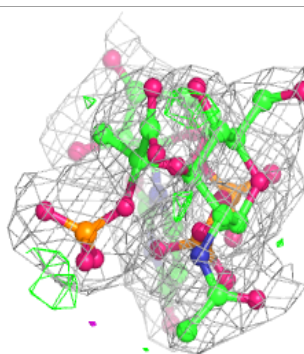
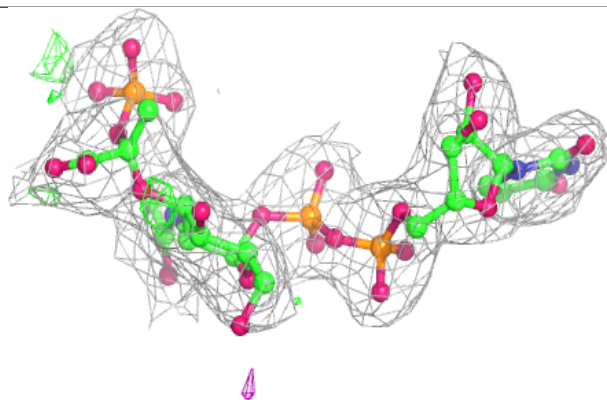
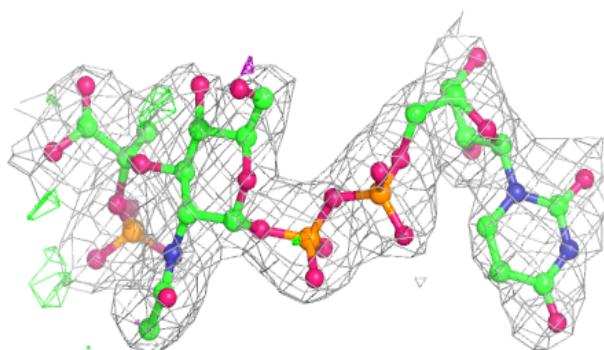
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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
3	EDO	D	1473	4/4	0.71	0.39	31,32,38,41	0
3	EDO	F	1475	4/4	0.73	0.33	32,35,37,38	0
3	EDO	A	1470	4/4	0.86	0.48	36,36,42,42	0
3	EDO	L	1481	4/4	0.88	0.34	42,42,50,53	0
3	EDO	Z	1485	4/4	0.89	0.27	39,40,43,46	0
3	EDO	B	1471	4/4	0.92	0.26	25,32,37,44	0
3	EDO	C	1472	4/4	0.93	0.24	23,28,32,38	0
3	EDO	K	1480	4/4	0.93	0.24	28,30,33,38	0
3	EDO	X	1483	4/4	0.94	0.22	41,45,45,47	0
3	EDO	G	1476	4/4	0.95	0.27	23,26,30,38	0
3	EDO	Y	1484	4/4	0.95	0.21	29,29,32,39	0
3	EDO	W	1482	4/4	0.95	0.29	28,30,34,38	0
2	UDA	W	1462	49/49	0.96	0.14	19,40,51,56	0
2	UDA	X	1463	49/49	0.96	0.14	30,41,57,60	0
3	EDO	H	1477	4/4	0.96	0.23	26,28,29,31	0
2	UDA	Z	1465	49/49	0.96	0.14	25,38,61,66	0
2	UDA	A	1450	49/49	0.96	0.15	20,32,56,63	0
2	UDA	J	1459	49/49	0.96	0.14	27,36,57,61	0
2	UDA	K	1460	49/49	0.96	0.14	24,30,54,58	0
2	UDA	L	1461	49/49	0.96	0.15	24,38,57,58	0
3	EDO	E	1474	4/4	0.96	0.27	33,36,39,41	0
2	UDA	E	1454	49/49	0.97	0.15	17,27,53,57	0
2	UDA	F	1455	49/49	0.97	0.12	26,32,49,52	0
2	UDA	Y	1464	49/49	0.97	0.13	22,30,53,55	0
3	EDO	J	1479	4/4	0.97	0.17	28,30,31,32	0
2	UDA	G	1456	49/49	0.97	0.16	11,30,59,65	0
2	UDA	H	1457	49/49	0.97	0.15	16,33,53,57	0
2	UDA	I	1458	49/49	0.97	0.13	16,35,51,55	0
2	UDA	B	1451	49/49	0.97	0.13	23,34,54,57	0
2	UDA	C	1452	49/49	0.97	0.16	22,32,56,61	0
2	UDA	D	1453	49/49	0.97	0.15	24,32,45,50	0
3	EDO	I	1478	4/4	0.98	0.17	30,31,34,40	0

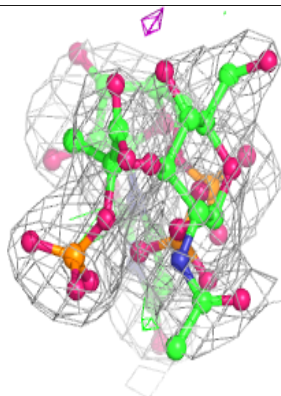
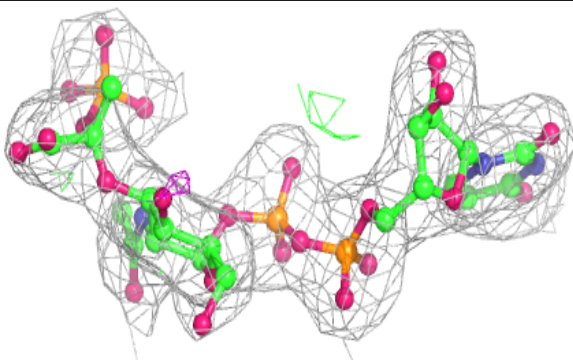
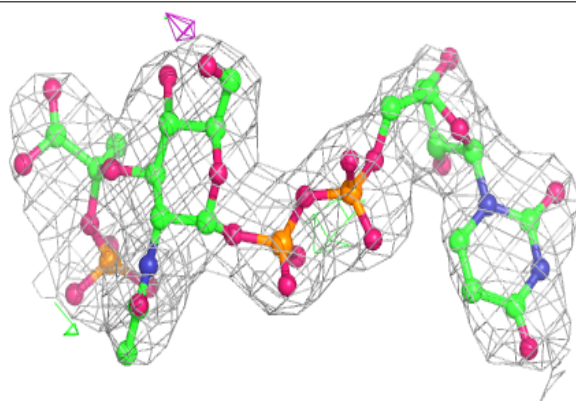
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

**Electron density around UDA W 1462:**

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

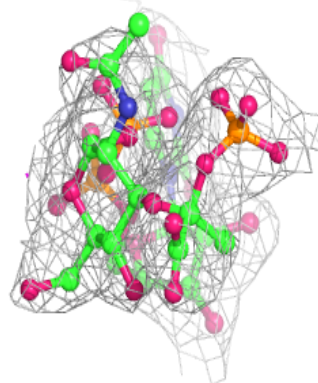
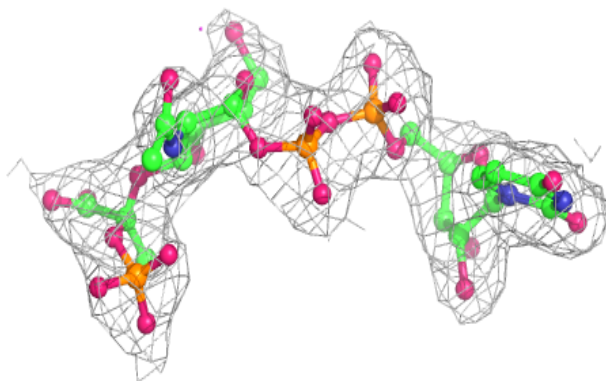
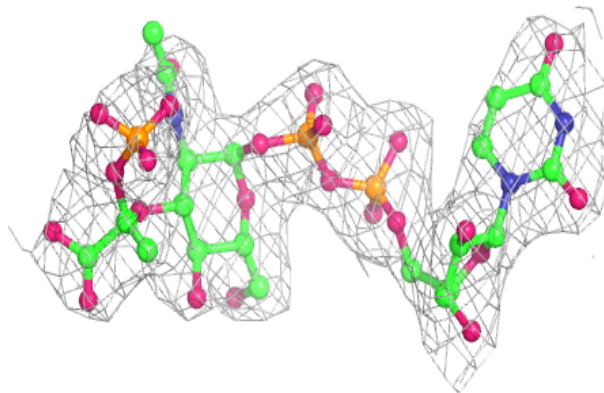
**Electron density around UDA X 1463:**

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

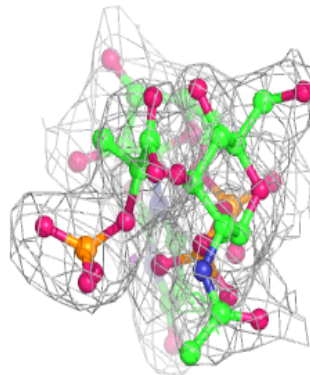
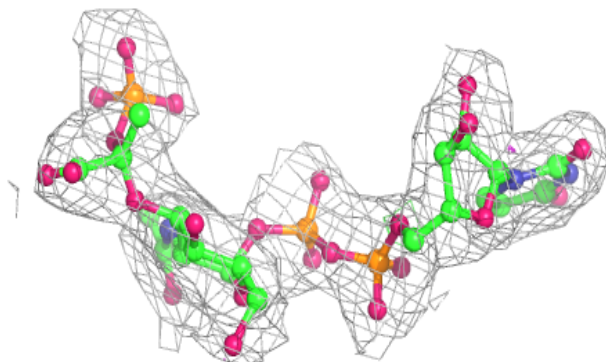
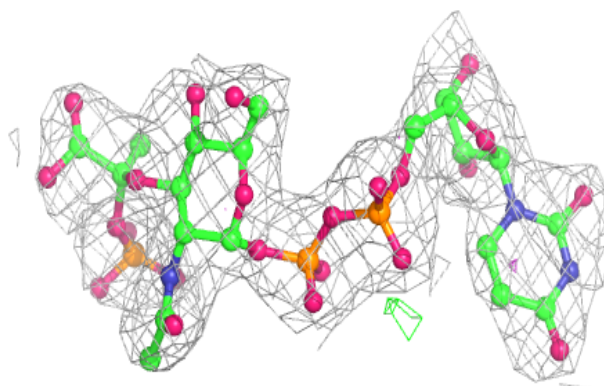


**Electron density around UDA Z 1465:**

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

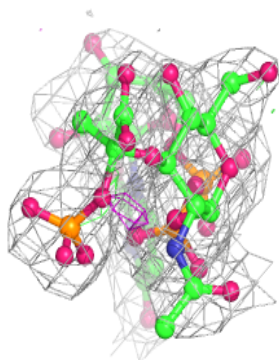
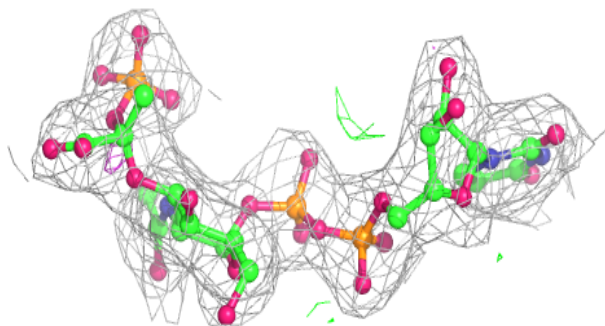
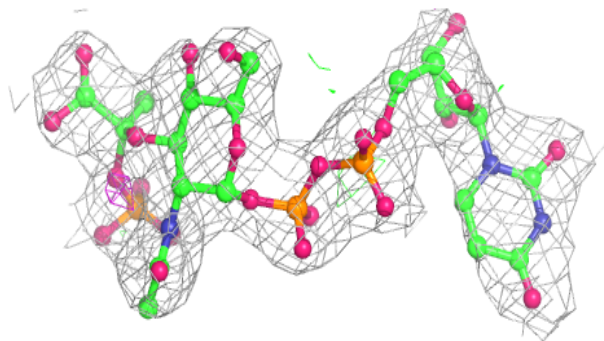
**Electron density around UDA A 1450:**

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

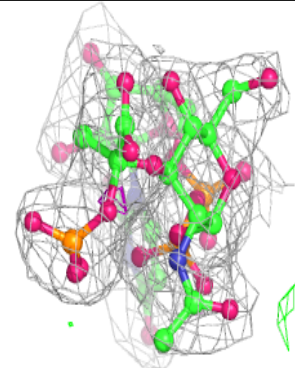
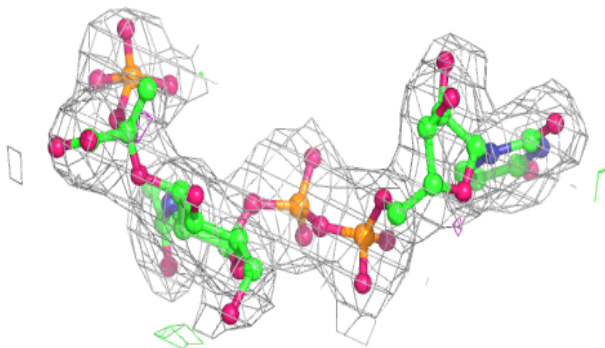
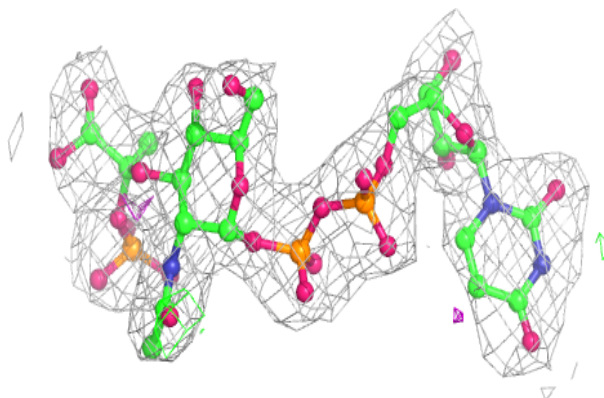


**Electron density around UDA J 1459:**

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

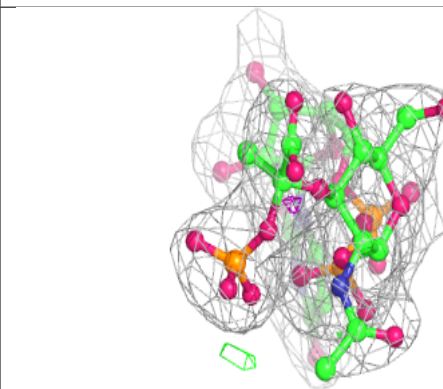
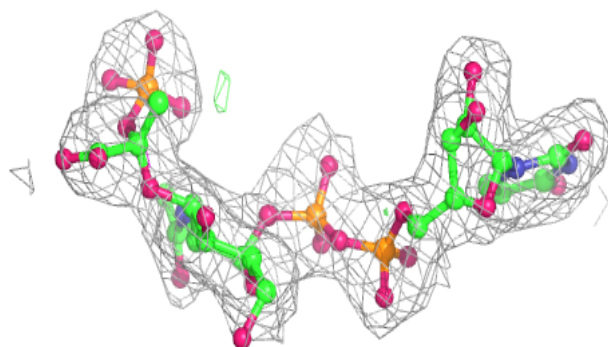
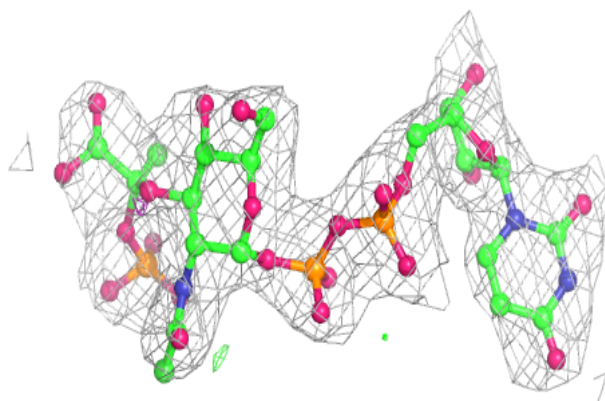
**Electron density around UDA K 1460:**

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

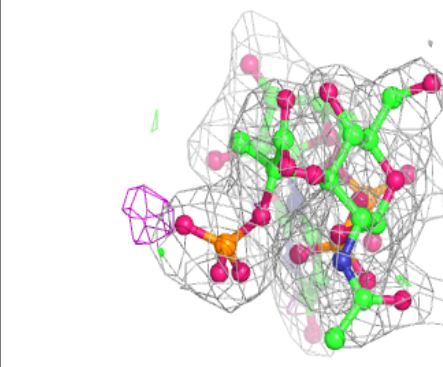
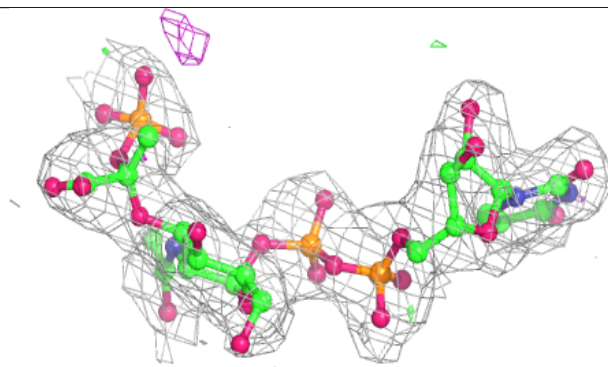
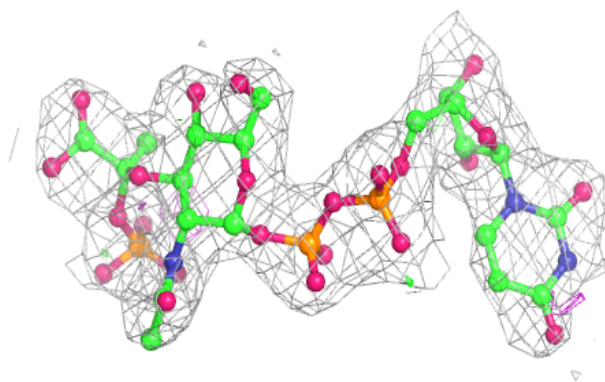


**Electron density around UDA L 1461:**

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

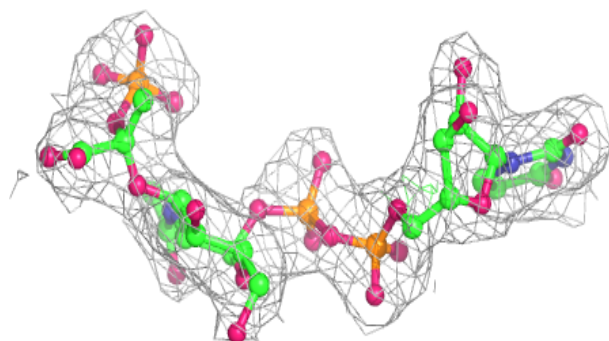
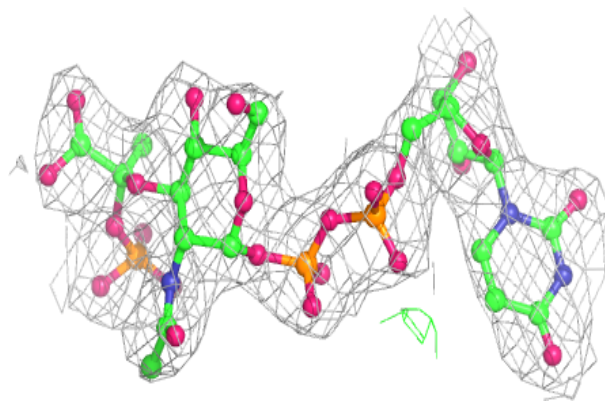
**Electron density around UDA E 1454:**

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

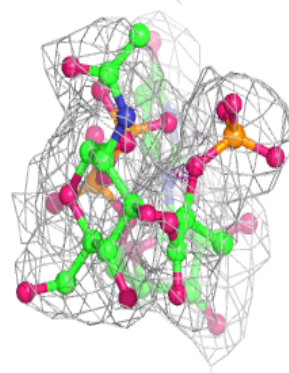
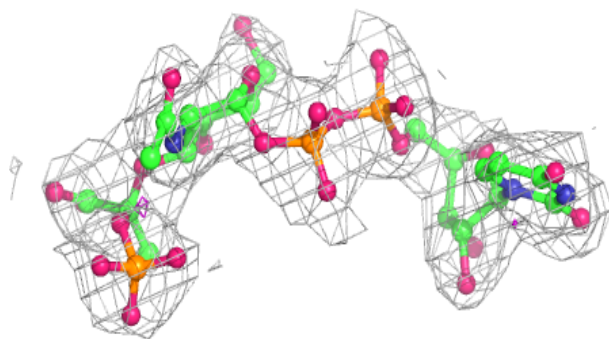
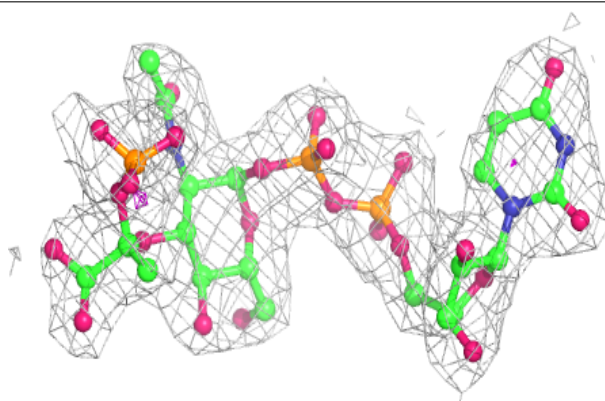


**Electron density around UDA F 1455:**

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

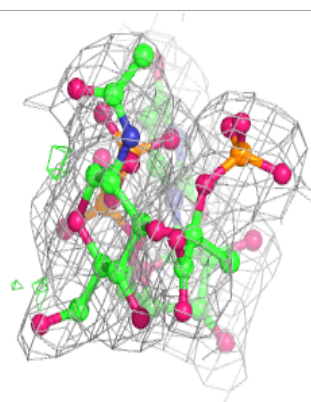
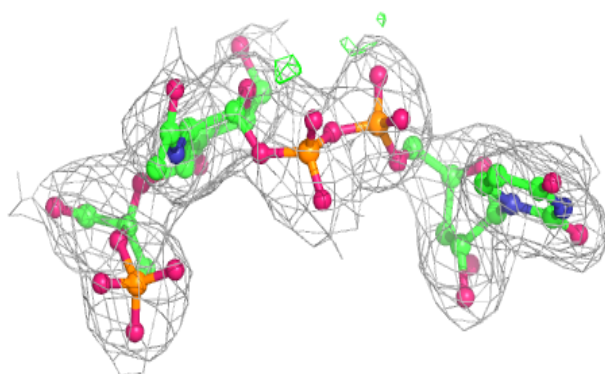
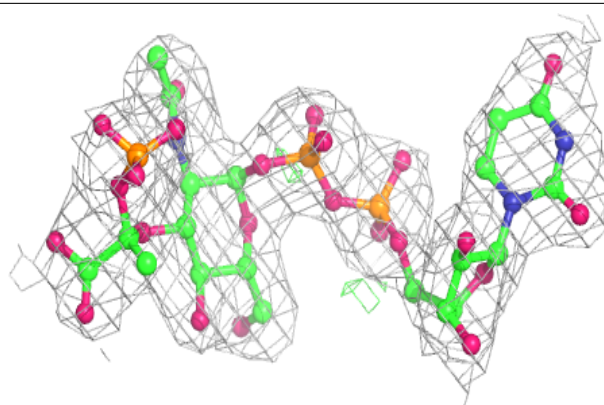
**Electron density around UDA Y 1464:**

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

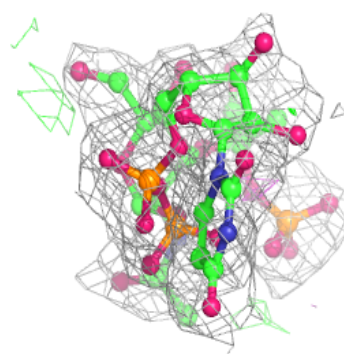
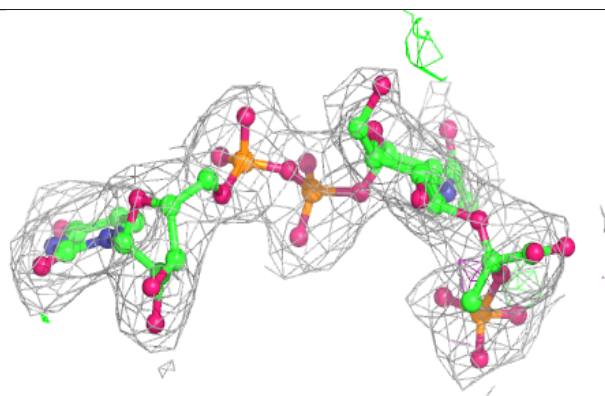
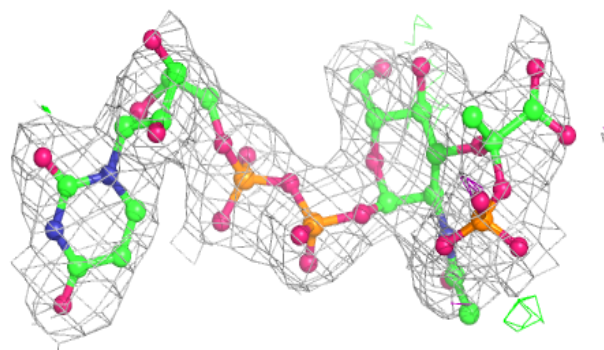


**Electron density around UDA G 1456:**

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

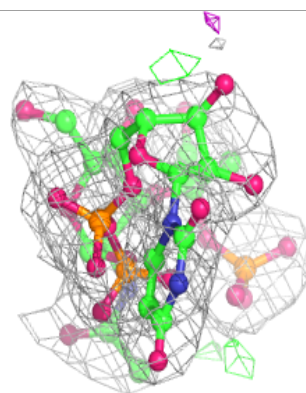
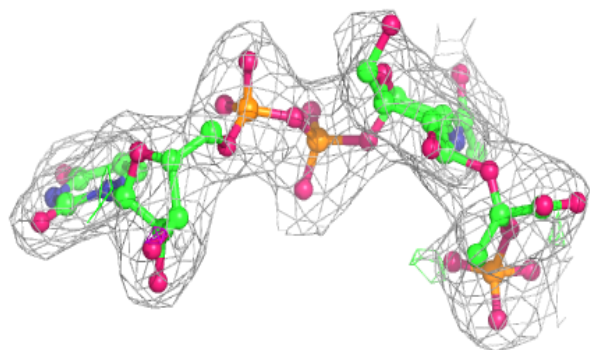
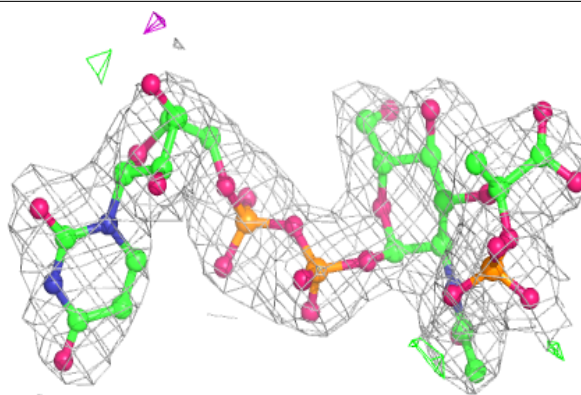
**Electron density around UDA H 1457:**

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

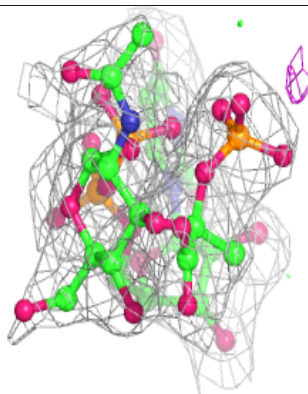
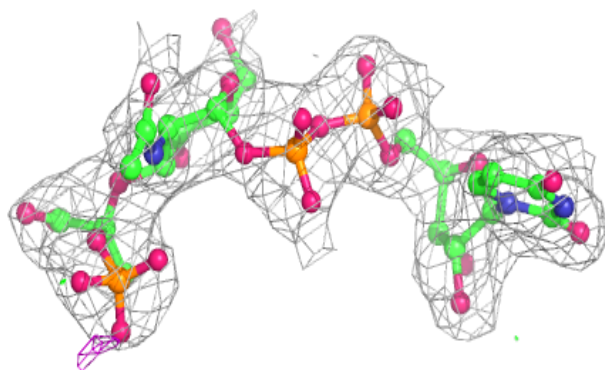
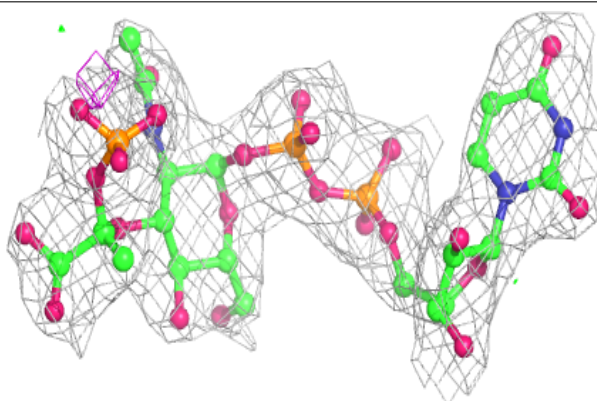


**Electron density around UDA I 1458:**

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

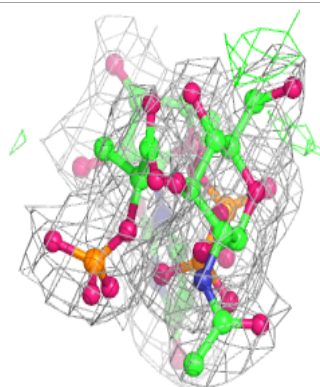
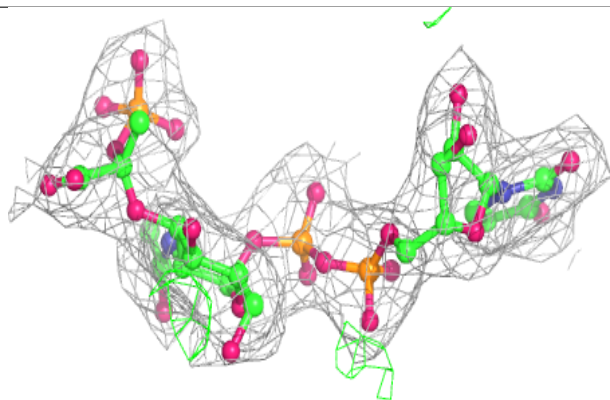
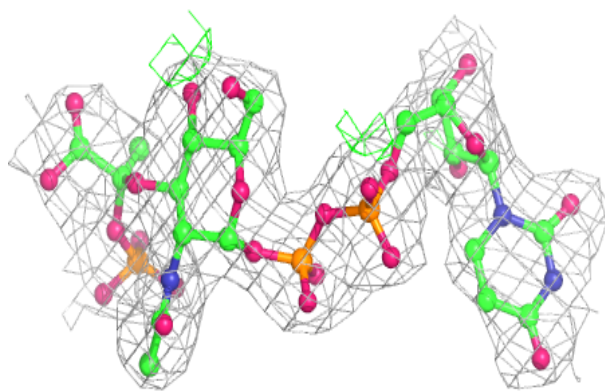
**Electron density around UDA B 1451:**

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

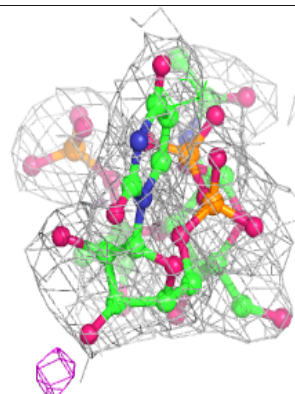
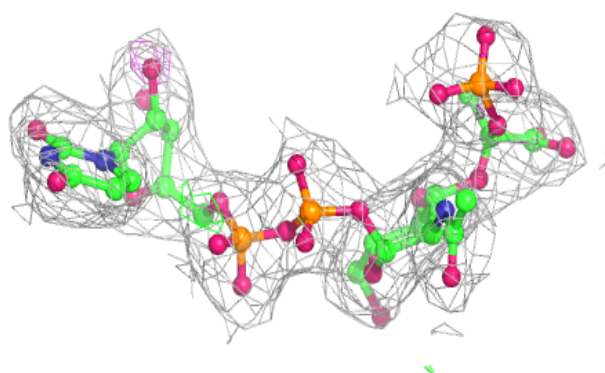
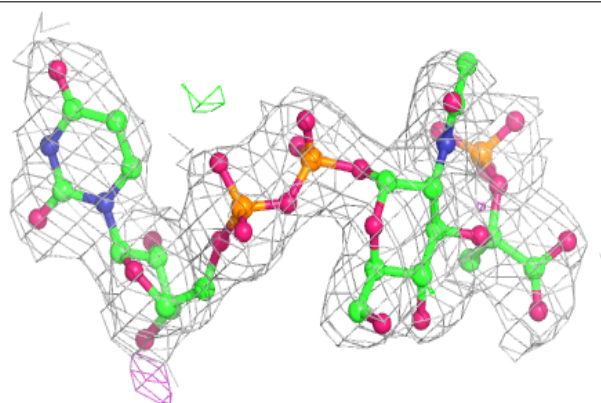


**Electron density around UDA C 1452:**

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

**Electron density around UDA D 1453:**

$2mF_o-DF_c$  (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.