



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 02:55 am BST

PDB ID : 2WTZ  
Title : MurE ligase of Mycobacterium Tuberculosis  
Authors : Basavannacharya, C.; Robertson, G.; Munshi, T.; Keep, N.H.; Bhakta, S.  
Deposited on : 2009-09-25  
Resolution : 3.00 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
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) : 2.11

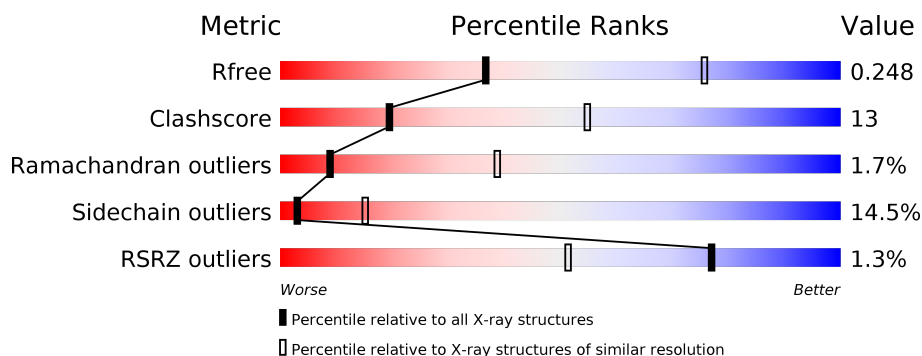
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 3.00 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	2092 (3.00-3.00)
Clashscore	141614	2416 (3.00-3.00)
Ramachandran outliers	138981	2333 (3.00-3.00)
Sidechain outliers	138945	2336 (3.00-3.00)
RSRZ outliers	127900	1990 (3.00-3.00)

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

Mol	Chain	Length	Quality of chain
1	A	535	<div> <div>69%</div> <div>20%</div> <div>5%</div> <div>6%</div> </div>
1	B	535	<div> <div>2%</div> <div>67%</div> <div>23%</div> <div>5%</div> </div>
1	C	535	<div> <div>2%</div> <div>61%</div> <div>18%</div> <div>18%</div> </div>
1	D	535	<div> <div>2%</div> <div>65%</div> <div>20%</div> <div>13%</div> </div>

## 2 Entry composition [i](#)

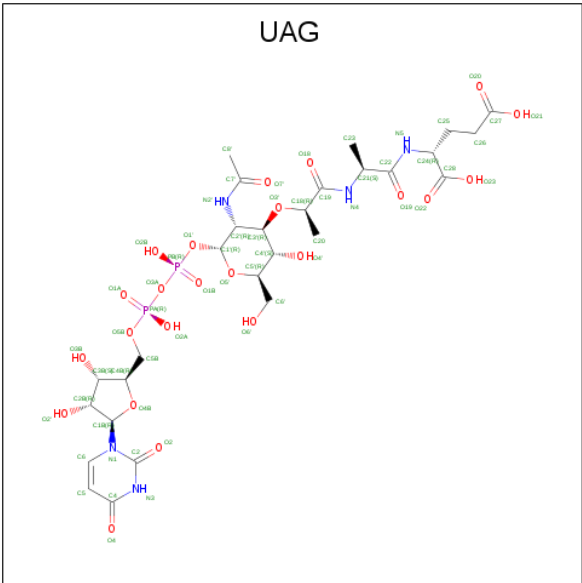
There are 3 unique types of molecules in this entry. The entry contains 14008 atoms, of which 0 are hydrogens and 0 are deuteriums.

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-ACETYLMURAMOYL-L-ALANYL-D-GLUTAMATE--2,6-DIAMINOPIMELATE LIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	504	Total	C	N	O	S	0	0	0
			3634	2256	681	689	8			
1	B	508	Total	C	N	O	S	0	0	0
			3663	2271	686	698	8			
1	C	439	Total	C	N	O	S	0	0	0
			3109	1949	563	590	7			
1	D	468	Total	C	N	O	S	0	0	0
			3366	2091	622	645	8			

- Molecule 2 is URIDINE-5'-DIPHOSPHATE-N-ACETYLMURAMOYL-L-ALANINE-D-GLUTAMATE (three-letter code: UAG) (formula: C<sub>28</sub>H<sub>43</sub>N<sub>5</sub>O<sub>23</sub>P<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			58	28	5	23	2		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			58	28	5	23	2		
2	C	1	Total	C	N	O	P	0	0
			58	28	5	23	2		
2	D	1	Total	C	N	O	P	0	0
			58	28	5	23	2		

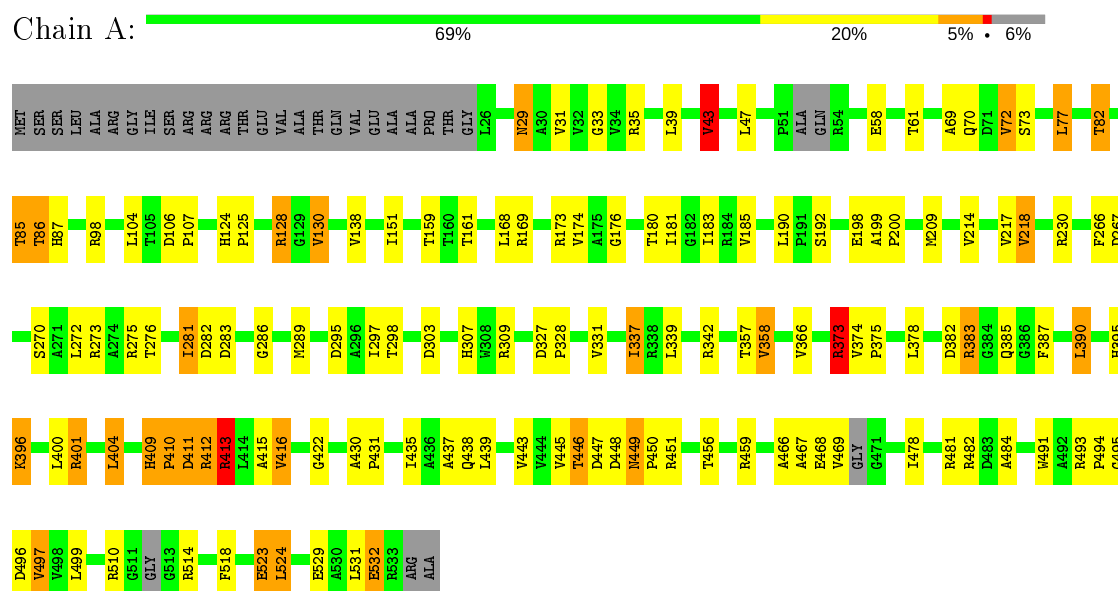
- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total	Mg	0	0
			1	1		
3	A	1	Total	Mg	0	0
			1	1		
3	D	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

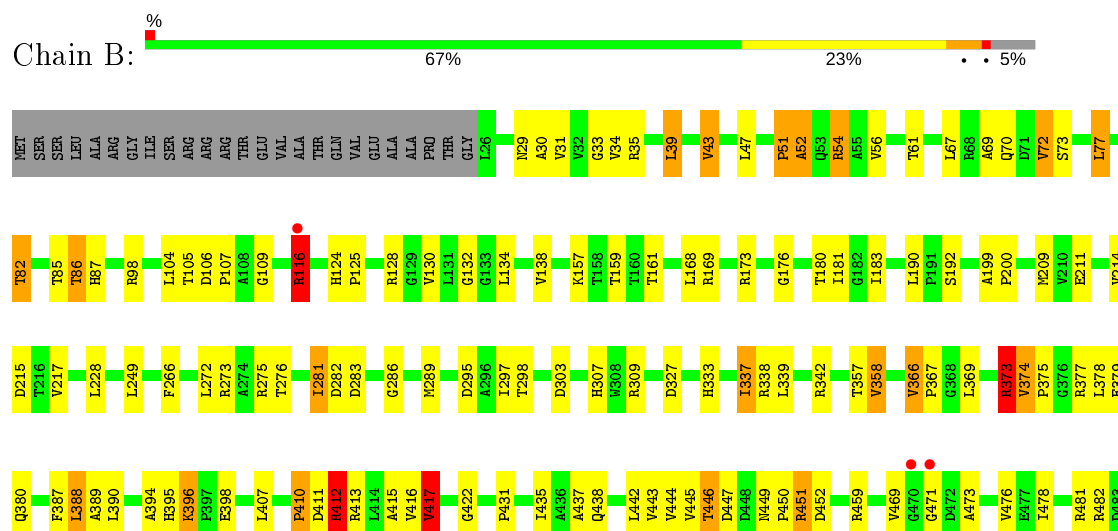
### 3 Residue-property plots

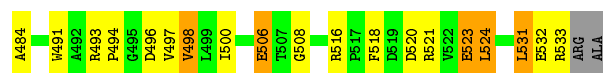
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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-ACETYLMURAMOYL-L-ALANYL-D-GLUTAMATE--2,6-DIAMINOPI MELATE LIGASE

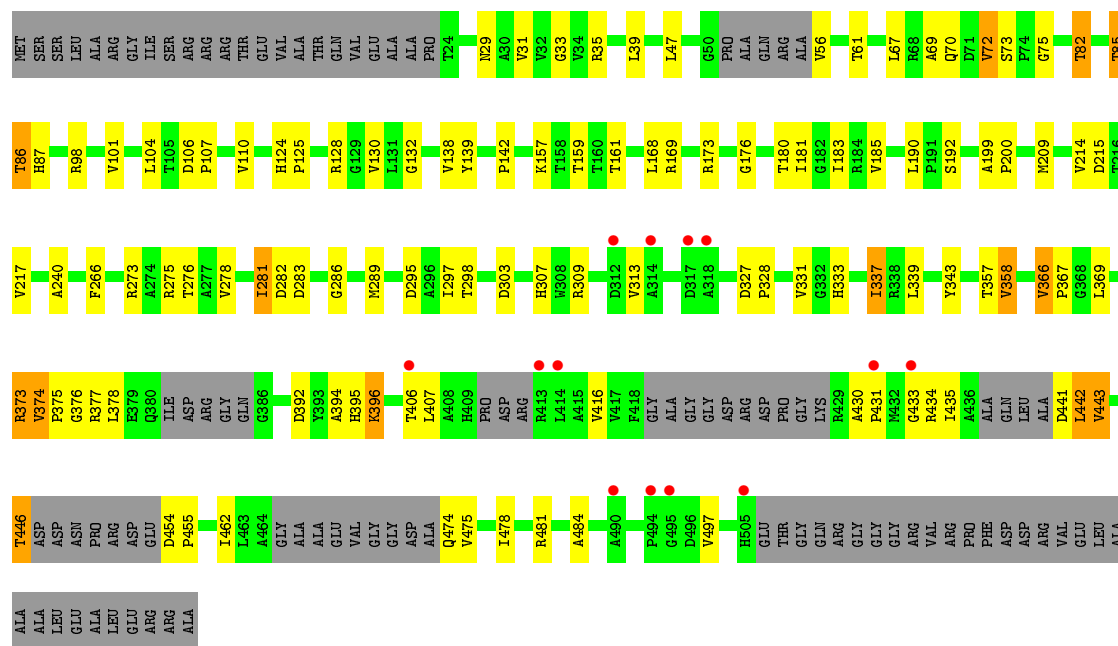


- Molecule 1: UDP-N-ACETYLMURAMOYL-L-ALANYL-D-GLUTAMATE--2,6-DIAMINOPI MELATE LIGASE

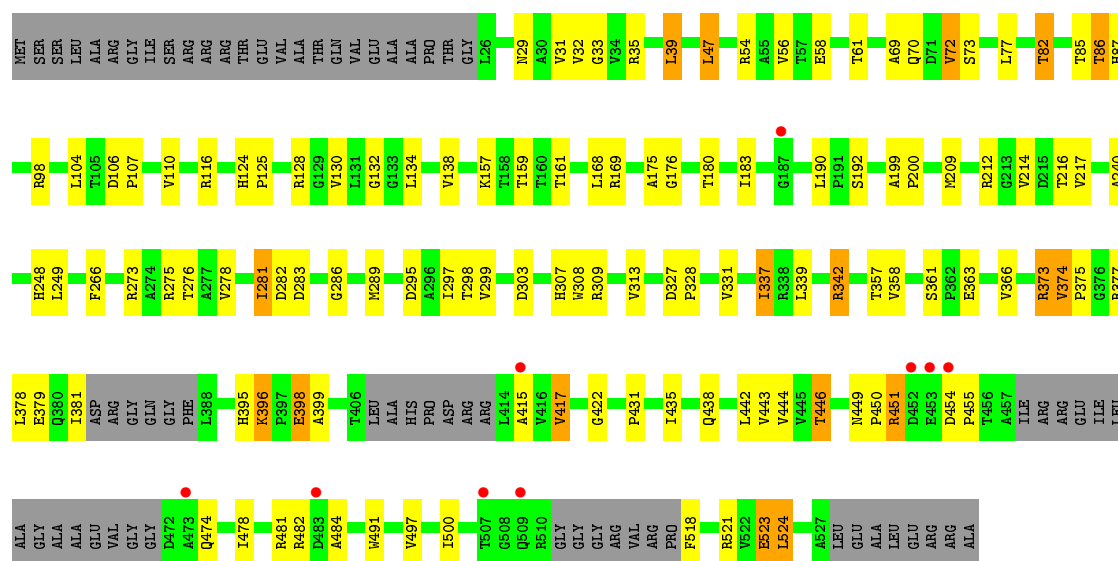




• Molecule 1: UDP-N-ACETYLMURAMOYL-L-ALANYL-D-GLUTAMATE--2,6-DIAMINOPI  
MELATE LIGASE



• Molecule 1: UDP-N-ACETYLMURAMOYL-L-ALANYL-D-GLUTAMATE--2,6-DIAMINOPI  
MELATE LIGASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	76.92Å 79.80Å 82.92Å 111.09° 92.16° 93.98°	Depositor
Resolution (Å)	74.16 – 3.00 56.29 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.4 (74.16-3.00) 79.2 (56.29-3.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.68 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, $R_{free}$	0.193 , 0.251 0.196 , 0.248	Depositor DCC
$R_{free}$ test set	1661 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	43.2	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 17.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.106 for -h,-l,-k	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	14008	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.76% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: MG, KCX, UAG

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	0.61	0/3678	0.85	8/5017 (0.2%)
1	B	0.62	0/3710	0.83	9/5064 (0.2%)
1	C	0.58	0/3142	0.75	2/4296 (0.0%)
1	D	0.57	0/3405	0.81	3/4649 (0.1%)
All	All	0.59	0/13935	0.81	22/19026 (0.1%)

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	309	ARG	NE-CZ-NH1	-11.70	114.45	120.30
1	D	309	ARG	NE-CZ-NH2	9.89	125.25	120.30
1	C	309	ARG	NE-CZ-NH1	8.03	124.31	120.30
1	A	390	LEU	CA-CB-CG	7.34	132.18	115.30
1	C	309	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	B	309	ARG	NE-CZ-NH2	-6.56	117.02	120.30
1	A	43	VAL	CG1-CB-CG2	6.51	121.32	110.90
1	B	309	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	A	309	ARG	NE-CZ-NH1	6.01	123.31	120.30
1	B	77	LEU	CA-CB-CG	5.90	128.87	115.30
1	A	218	VAL	CB-CA-C	-5.79	100.40	111.40
1	D	309	ARG	CD-NE-CZ	5.65	131.51	123.60
1	B	77	LEU	CB-CG-CD2	5.46	120.28	111.00
1	A	77	LEU	CA-CB-CG	5.37	127.66	115.30
1	A	309	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	B	417	VAL	CG1-CB-CG2	5.31	119.40	110.90
1	A	390	LEU	CB-CG-CD2	5.28	119.97	111.00
1	B	43	VAL	CG1-CB-CG2	5.28	119.34	110.90
1	B	498	VAL	CG1-CB-CG2	5.11	119.07	110.90
1	A	373	ARG	NE-CZ-NH2	5.09	122.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	416	VAL	CB-CA-C	-5.09	101.73	111.40
1	B	373	ARG	NE-CZ-NH2	5.06	122.83	120.30

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	3634	0	3629	103	0
1	B	3663	0	3657	96	0
1	C	3109	0	3092	80	0
1	D	3366	0	3357	80	0
2	A	58	0	39	2	0
2	B	58	0	39	0	0
2	C	58	0	39	1	0
2	D	58	0	39	1	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
All	All	14008	0	13891	358	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 (358) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:281:ILE:HG22	1:B:282:ASP:H	1.22	1.03
1:C:209:MET:HE2	1:C:217:VAL:HG22	1.38	1.03
1:D:281:ILE:HG22	1:D:282:ASP:H	1.15	1.03
1:D:209:MET:HE2	1:D:217:VAL:HG22	1.42	1.00
1:B:124:HIS:ND1	1:B:125:PRO:O	1.98	0.97
1:A:281:ILE:HG22	1:A:282:ASP:H	1.31	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:THR:H	1:A:307:HIS:HD2	1.07	0.95
1:D:298:THR:H	1:D:307:HIS:HD2	1.11	0.95
1:C:298:THR:H	1:C:307:HIS:HD2	1.08	0.95
1:C:209:MET:CE	1:C:217:VAL:HG22	1.98	0.94
1:A:412:ARG:HG3	1:A:495:GLY:O	1.68	0.94
1:C:281:ILE:HG22	1:C:282:ASP:H	1.30	0.93
1:B:298:THR:H	1:B:307:HIS:HD2	1.09	0.93
1:A:209:MET:HE2	1:A:217:VAL:HG22	1.49	0.92
1:B:176:GLY:HA3	1:B:209:MET:HE3	1.51	0.92
1:B:209:MET:HE2	1:B:217:VAL:HG22	1.52	0.92
1:C:373:ARG:HG3	1:C:373:ARG:HH21	1.31	0.92
1:D:209:MET:CE	1:D:217:VAL:HG22	2.01	0.91
1:B:446:THR:HG22	1:B:478:ILE:O	1.69	0.91
1:C:124:HIS:ND1	1:C:125:PRO:O	2.02	0.90
1:B:446:THR:CG2	1:B:478:ILE:O	2.19	0.90
1:A:446:THR:HG22	1:A:478:ILE:O	1.72	0.90
1:D:398:GLU:HG2	1:D:399:ALA:N	1.83	0.90
1:A:373:ARG:HG3	1:A:373:ARG:HH21	1.37	0.90
1:A:124:HIS:ND1	1:A:125:PRO:O	2.05	0.88
1:D:281:ILE:HG22	1:D:282:ASP:N	1.88	0.88
1:A:446:THR:CG2	1:A:478:ILE:O	2.22	0.88
1:A:176:GLY:HA3	1:A:209:MET:HE3	1.56	0.86
1:B:281:ILE:HG22	1:B:282:ASP:N	1.89	0.86
1:C:298:THR:H	1:C:307:HIS:CD2	1.93	0.86
1:D:373:ARG:HG3	1:D:373:ARG:HH21	1.40	0.85
1:D:124:HIS:ND1	1:D:125:PRO:O	2.08	0.85
1:A:209:MET:CE	1:A:217:VAL:HG22	2.06	0.84
1:B:373:ARG:HH21	1:B:373:ARG:HG3	1.41	0.84
1:B:298:THR:H	1:B:307:HIS:CD2	1.95	0.84
1:D:446:THR:HG22	1:D:478:ILE:O	1.77	0.84
1:B:209:MET:CE	1:B:217:VAL:HG22	2.08	0.84
1:D:446:THR:CG2	1:D:478:ILE:O	2.25	0.84
1:A:298:THR:H	1:A:307:HIS:CD2	1.95	0.83
1:C:446:THR:HG22	1:C:478:ILE:O	1.79	0.83
1:B:411:ASP:O	1:B:412:ARG:HB3	1.81	0.81
1:C:209:MET:HE2	1:C:217:VAL:CG2	2.11	0.79
1:C:281:ILE:HG22	1:C:282:ASP:N	1.98	0.79
1:C:373:ARG:CG	1:C:373:ARG:HH21	1.95	0.79
1:C:446:THR:CG2	1:C:478:ILE:O	2.30	0.79
1:C:176:GLY:HA3	1:C:209:MET:HE3	1.64	0.78
1:A:281:ILE:HG22	1:A:282:ASP:N	1.99	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:PHE:HB2	1:A:289:MET:HE1	1.66	0.77
1:D:298:THR:H	1:D:307:HIS:CD2	1.99	0.77
1:A:445:VAL:HG12	1:A:459:ARG:HG2	1.67	0.76
1:B:388:LEU:HG	1:B:390:LEU:HD11	1.68	0.76
1:A:159:THR:HG23	1:A:374:VAL:HG21	1.68	0.76
1:A:401:ARG:HH11	1:A:401:ARG:CB	1.99	0.74
1:A:412:ARG:O	1:A:413:ARG:HB2	1.85	0.74
1:C:159:THR:HG23	1:C:374:VAL:HG11	1.67	0.74
1:B:469:VAL:HG21	1:B:473:ALA:HB3	1.68	0.74
1:C:266:PHE:HB2	1:C:289:MET:HE1	1.69	0.74
1:A:86:THR:OG1	1:A:87:HIS:N	2.21	0.73
1:C:446:THR:CG2	1:C:484:ALA:HB2	2.18	0.73
1:C:298:THR:N	1:C:307:HIS:HD2	1.86	0.73
1:D:72:VAL:HG22	1:D:98:ARG:HB2	1.71	0.73
1:B:51:PRO:HD3	1:B:54:ARG:HH21	1.53	0.72
1:C:72:VAL:HG22	1:C:98:ARG:HB2	1.71	0.72
1:B:446:THR:HG21	1:B:484:ALA:HB2	1.72	0.72
1:D:373:ARG:CG	1:D:373:ARG:HH21	2.02	0.72
1:D:176:GLY:HA3	1:D:209:MET:HE3	1.71	0.71
1:A:467:ALA:O	1:A:468:GLU:HB2	1.91	0.71
1:B:176:GLY:HA3	1:B:209:MET:CE	2.20	0.71
1:A:176:GLY:HA3	1:A:209:MET:CE	2.20	0.70
1:C:373:ARG:HG3	1:C:373:ARG:NH2	2.00	0.70
1:A:410:PRO:O	1:A:411:ASP:HB2	1.91	0.70
1:B:159:THR:HG23	1:B:374:VAL:HG11	1.73	0.70
1:A:72:VAL:HG22	1:A:98:ARG:HB2	1.73	0.70
1:D:209:MET:HE2	1:D:217:VAL:CG2	2.19	0.70
1:A:446:THR:CG2	1:A:484:ALA:HB2	2.21	0.70
1:A:481:ARG:HG2	1:A:518:PHE:CZ	2.27	0.69
1:B:446:THR:CG2	1:B:484:ALA:HB2	2.22	0.69
1:B:281:ILE:CG2	1:B:282:ASP:H	1.96	0.69
1:C:446:THR:HG21	1:C:484:ALA:HB2	1.74	0.69
1:C:86:THR:OG1	1:C:87:HIS:N	2.24	0.69
1:B:446:THR:HG23	1:B:478:ILE:O	1.93	0.68
1:C:446:THR:HG21	1:C:484:ALA:CB	2.23	0.68
1:A:446:THR:HG21	1:A:484:ALA:HB2	1.74	0.68
1:B:289:MET:HA	1:B:289:MET:HE3	1.77	0.67
1:B:72:VAL:HG22	1:B:98:ARG:HB2	1.74	0.67
1:B:373:ARG:HH21	1:B:373:ARG:CG	2.07	0.67
1:A:373:ARG:HH21	1:A:373:ARG:CG	2.05	0.67
1:B:481:ARG:HG2	1:B:518:PHE:CZ	2.30	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:266:PHE:HB2	1:D:289:MET:HE1	1.76	0.66
1:D:446:THR:CG2	1:D:484:ALA:HB2	2.25	0.66
1:D:289:MET:HE3	1:D:289:MET:HA	1.78	0.65
1:A:412:ARG:CD	1:A:497:VAL:HG12	2.26	0.65
1:A:446:THR:HG21	1:A:484:ALA:CB	2.27	0.65
1:D:446:THR:HG23	1:D:478:ILE:O	1.97	0.65
1:D:373:ARG:NH2	1:D:373:ARG:HG3	2.08	0.65
1:B:373:ARG:HG3	1:B:373:ARG:NH2	2.11	0.64
1:B:446:THR:HG21	1:B:484:ALA:CB	2.27	0.64
1:D:446:THR:HG21	1:D:484:ALA:HB2	1.80	0.64
1:D:342:ARG:HH11	1:D:342:ARG:HA	1.62	0.63
1:A:529:GLU:HG2	1:B:338:ARG:HH21	1.64	0.63
1:A:446:THR:HG23	1:A:478:ILE:O	1.96	0.63
1:D:281:ILE:CG2	1:D:282:ASP:H	1.94	0.63
1:D:481:ARG:HG2	1:D:518:PHE:CZ	2.34	0.63
1:B:298:THR:N	1:B:307:HIS:HD2	1.89	0.63
1:D:446:THR:HG21	1:D:484:ALA:CB	2.29	0.63
1:A:401:ARG:HH11	1:A:401:ARG:HB2	1.63	0.62
1:B:266:PHE:HB2	1:B:289:MET:HE1	1.81	0.62
1:D:176:GLY:HA3	1:D:209:MET:CE	2.29	0.62
1:A:373:ARG:NH2	1:A:373:ARG:HG3	2.07	0.62
1:A:209:MET:HE2	1:A:217:VAL:CG2	2.25	0.62
1:C:176:GLY:HA3	1:C:209:MET:CE	2.30	0.62
1:D:337:ILE:HG12	1:D:339:LEU:H	1.64	0.61
1:A:298:THR:N	1:A:307:HIS:HD2	1.89	0.61
1:C:343:TYR:HD2	1:C:406:THR:HG21	1.64	0.61
1:B:469:VAL:O	1:B:469:VAL:HG13	2.01	0.60
1:A:431:PRO:O	1:A:435:ILE:HD12	2.02	0.60
1:D:86:THR:OG1	1:D:87:HIS:N	2.34	0.60
1:D:431:PRO:O	1:D:435:ILE:HD12	2.00	0.60
1:B:116:ARG:NE	1:B:116:ARG:O	2.34	0.60
1:B:395:HIS:O	1:B:396:LYS:HB2	2.02	0.60
1:C:376:GLY:O	1:C:392:ASP:HA	2.02	0.60
1:D:183:ILE:CD1	1:D:192:SER:HB3	2.32	0.59
1:A:69:ALA:O	1:A:72:VAL:HG13	2.02	0.59
1:B:431:PRO:O	1:B:435:ILE:HD12	2.02	0.59
1:B:132:GLY:HA2	1:B:199:ALA:HB1	1.83	0.59
1:B:86:THR:OG1	1:B:87:HIS:N	2.34	0.59
1:B:69:ALA:O	1:B:72:VAL:HG13	2.03	0.58
1:A:437:ALA:HB1	1:A:469:VAL:HG13	1.84	0.58
1:B:437:ALA:HB1	1:B:469:VAL:HB	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:379:GLU:OE2	1:B:521:ARG:HD3	2.03	0.58
1:C:273:ARG:NH2	1:C:295:ASP:OD2	2.36	0.58
1:D:363:GLU:H	1:D:363:GLU:CD	2.07	0.58
1:C:343:TYR:CD2	1:C:406:THR:HG21	2.39	0.58
1:B:209:MET:HE2	1:B:217:VAL:CG2	2.33	0.57
1:B:199:ALA:HB3	1:B:200:PRO:HD3	1.86	0.57
1:C:441:ASP:O	1:C:474:GLN:N	2.38	0.57
1:D:199:ALA:HB3	1:D:200:PRO:HD3	1.86	0.57
1:C:446:THR:HG23	1:C:478:ILE:O	2.04	0.57
1:C:69:ALA:O	1:C:72:VAL:HG13	2.04	0.57
1:A:337:ILE:HG12	1:A:339:LEU:H	1.69	0.56
1:B:531:LEU:C	1:B:533:ARG:H	2.08	0.56
1:C:289:MET:HE3	1:C:289:MET:HA	1.87	0.56
1:D:159:THR:HG23	1:D:374:VAL:HG11	1.86	0.56
1:A:173:ARG:HH22	1:A:358:VAL:HG13	1.70	0.56
1:A:183:ILE:CD1	1:A:192:SER:HB3	2.36	0.56
1:B:273:ARG:NH2	1:B:295:ASP:OD2	2.38	0.56
1:B:337:ILE:HG12	1:B:339:LEU:H	1.70	0.56
1:A:85:THR:HG23	2:A:1498:UAG:PA	2.45	0.56
1:C:337:ILE:HG12	1:C:339:LEU:H	1.70	0.56
1:D:69:ALA:O	1:D:72:VAL:HG13	2.07	0.55
1:D:313:VAL:HG11	1:D:342:ARG:NH1	2.22	0.55
1:A:404:LEU:HD11	1:A:416:VAL:HG11	1.88	0.55
1:A:173:ARG:NH2	1:A:358:VAL:HG13	2.21	0.55
1:B:388:LEU:HG	1:B:390:LEU:CD1	2.37	0.54
1:D:298:THR:N	1:D:307:HIS:HD2	1.91	0.54
1:A:395:HIS:O	1:A:396:LYS:HB2	2.06	0.54
1:B:523:GLU:O	1:B:524:LEU:CB	2.54	0.54
1:C:183:ILE:CD1	1:C:192:SER:HB3	2.38	0.54
1:A:400:LEU:HG	1:A:404:LEU:HD22	1.90	0.54
1:C:157:LYS:O	1:C:161:THR:HG23	2.08	0.54
1:D:33:GLY:HA3	1:D:61:THR:CG2	2.38	0.53
1:C:209:MET:CE	1:C:217:VAL:CG2	2.79	0.53
1:D:415:ALA:HB2	1:D:491:TRP:CZ3	2.44	0.53
1:A:33:GLY:HA3	1:A:61:THR:CG2	2.39	0.53
1:D:327:ASP:HB2	1:D:328:PRO:HD2	1.91	0.53
1:C:395:HIS:O	1:C:396:LYS:HB2	2.09	0.53
1:A:387:PHE:HB2	1:A:496:ASP:O	2.09	0.52
1:D:523:GLU:O	1:D:524:LEU:HB3	2.09	0.52
1:A:43:VAL:HG22	1:A:130:VAL:HG21	1.90	0.52
1:B:289:MET:HE3	1:B:289:MET:CA	2.40	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:PHE:HB2	1:A:289:MET:CE	2.37	0.52
1:B:183:ILE:CD1	1:B:192:SER:HB3	2.39	0.52
1:D:82:THR:CG2	1:D:106:ASP:OD2	2.58	0.52
1:C:82:THR:HG22	1:C:87:HIS:NE2	2.24	0.52
1:D:283:ASP:HB3	1:D:286:GLY:H	1.75	0.52
1:A:401:ARG:HH11	1:A:401:ARG:HB3	1.74	0.52
1:B:506:GLU:HA	1:B:506:GLU:OE2	2.09	0.52
1:D:374:VAL:HG22	1:D:377:ARG:HB2	1.92	0.52
1:A:412:ARG:HD2	1:A:497:VAL:HG12	1.91	0.51
1:B:266:PHE:HB2	1:B:289:MET:CE	2.40	0.51
1:C:173:ARG:HH22	1:C:358:VAL:HG13	1.76	0.51
1:B:523:GLU:O	1:B:524:LEU:HB3	2.10	0.51
1:D:451:ARG:N	1:D:451:ARG:HD3	2.26	0.51
1:B:417:VAL:HG13	1:B:500:ILE:HD13	1.92	0.51
1:D:209:MET:HE1	1:D:217:VAL:HG22	1.91	0.51
1:D:361:SER:OG	1:D:363:GLU:HG2	2.11	0.51
1:D:523:GLU:O	1:D:524:LEU:CB	2.59	0.50
1:B:209:MET:HG2	1:B:214:VAL:HG21	1.92	0.50
1:D:395:HIS:O	1:D:396:LYS:HB2	2.12	0.50
1:D:82:THR:HG22	1:D:87:HIS:NE2	2.27	0.50
1:C:132:GLY:HA2	1:C:199:ALA:HB1	1.94	0.50
1:A:82:THR:CG2	1:A:106:ASP:OD2	2.59	0.50
1:B:209:MET:HE1	1:B:217:VAL:HG13	1.93	0.50
1:A:523:GLU:O	1:A:524:LEU:CB	2.60	0.49
1:B:82:THR:CG2	1:B:106:ASP:OD2	2.60	0.49
1:C:446:THR:HG21	1:C:481:ARG:HA	1.93	0.49
1:A:281:ILE:CG2	1:A:282:ASP:H	2.07	0.49
1:A:412:ARG:O	1:A:413:ARG:CB	2.56	0.49
1:D:313:VAL:HG11	1:D:342:ARG:CZ	2.43	0.49
1:C:209:MET:HE1	1:C:217:VAL:HG13	1.94	0.49
1:C:377:ARG:HA	1:C:392:ASP:OD1	2.12	0.49
1:B:33:GLY:HA3	1:B:61:THR:CG2	2.42	0.49
1:C:446:THR:CG2	1:C:484:ALA:CB	2.85	0.49
1:A:456:THR:HA	1:A:459:ARG:NH1	2.28	0.48
1:A:523:GLU:O	1:A:524:LEU:HB3	2.12	0.48
1:B:366:VAL:HG12	1:B:367:PRO:HD3	1.95	0.48
1:A:181:ILE:HD13	1:A:375:PRO:HD2	1.94	0.48
1:C:283:ASP:HB3	1:C:286:GLY:H	1.79	0.48
1:B:412:ARG:O	1:B:496:ASP:HA	2.12	0.48
1:B:387:PHE:HB2	1:B:496:ASP:O	2.14	0.48
1:C:281:ILE:CG2	1:C:282:ASP:N	2.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:417:VAL:HG13	1:D:500:ILE:HD13	1.94	0.48
1:B:327:ASP:OD1	1:B:333:HIS:HE1	1.97	0.47
1:C:431:PRO:O	1:C:435:ILE:HD12	2.14	0.47
1:D:183:ILE:HD12	1:D:192:SER:HB3	1.96	0.47
1:B:422:GLY:HA3	1:B:450:PRO:O	2.14	0.47
1:B:116:ARG:N	1:B:116:ARG:HD3	2.29	0.47
1:C:446:THR:HG23	1:C:484:ALA:HB2	1.94	0.47
1:D:183:ILE:HD11	1:D:192:SER:HB3	1.95	0.47
1:C:33:GLY:HA3	1:C:61:THR:CG2	2.44	0.47
1:C:433:GLY:HA3	1:C:462:ILE:HG12	1.97	0.47
1:A:199:ALA:HB3	1:A:200:PRO:HD3	1.95	0.47
1:B:82:THR:HG22	1:B:87:HIS:NE2	2.28	0.47
1:C:442:LEU:HA	1:C:474:GLN:O	2.15	0.47
1:D:106:ASP:HB2	1:D:107:PRO:HD2	1.97	0.47
1:A:283:ASP:HB3	1:A:286:GLY:H	1.79	0.47
1:B:410:PRO:O	1:B:411:ASP:HB3	2.15	0.47
1:B:411:ASP:O	1:B:412:ARG:CB	2.58	0.47
1:A:82:THR:HG22	1:A:87:HIS:NE2	2.30	0.47
1:A:467:ALA:O	1:A:468:GLU:CB	2.63	0.47
1:A:481:ARG:HG2	1:A:518:PHE:CE2	2.49	0.47
1:B:451:ARG:HB3	1:B:452:ASP:H	1.49	0.47
1:D:281:ILE:O	1:D:282:ASP:HB2	2.15	0.47
1:D:446:THR:CG2	1:D:484:ALA:CB	2.91	0.47
1:A:209:MET:HE1	1:A:217:VAL:HG13	1.97	0.46
1:D:273:ARG:NH2	1:D:295:ASP:OD2	2.47	0.46
1:B:209:MET:HE1	1:B:217:VAL:HG22	1.94	0.46
1:C:181:ILE:HD13	1:C:375:PRO:HD2	1.97	0.46
1:D:132:GLY:HA2	1:D:199:ALA:HB1	1.97	0.46
1:A:401:ARG:CB	1:A:401:ARG:NH1	2.75	0.46
1:A:422:GLY:HA3	1:A:450:PRO:O	2.15	0.46
1:D:209:MET:CE	1:D:217:VAL:CG2	2.84	0.46
1:D:39:LEU:HG	1:D:134:LEU:HD22	1.97	0.46
1:C:374:VAL:HG22	1:C:377:ARG:HB2	1.97	0.46
1:A:531:LEU:O	1:A:532:GLU:HB2	2.16	0.46
1:B:51:PRO:HA	1:B:54:ARG:HE	1.80	0.46
1:A:183:ILE:HD11	1:A:192:SER:HB3	1.98	0.46
1:C:209:MET:HE1	1:C:217:VAL:HG22	1.93	0.46
1:B:157:LYS:O	1:B:161:THR:HG23	2.16	0.45
1:B:183:ILE:HD12	1:B:192:SER:HB3	1.98	0.45
1:C:327:ASP:HB2	1:C:328:PRO:HD2	1.98	0.45
1:A:382:ASP:O	1:A:383:ARG:HD3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:183:ILE:HD12	1:A:192:SER:HB3	1.98	0.45
1:C:281:ILE:CG2	1:C:282:ASP:H	2.03	0.45
1:A:415:ALA:HB2	1:A:491:TRP:CZ3	2.52	0.45
1:B:106:ASP:HB2	1:B:107:PRO:HD2	1.99	0.45
1:A:411:ASP:OD2	1:A:412:ARG:N	2.43	0.45
1:A:70:GLN:OE1	1:A:70:GLN:N	2.48	0.45
1:B:415:ALA:HB2	1:B:491:TRP:CZ3	2.52	0.45
1:D:374:VAL:HA	1:D:375:PRO:HD3	1.86	0.45
1:B:297:ILE:CD1	1:B:357:THR:HG21	2.47	0.45
1:B:51:PRO:O	1:B:52:ALA:HB2	2.17	0.45
1:C:183:ILE:HD12	1:C:192:SER:HB3	1.99	0.45
1:D:417:VAL:HB	1:D:444:VAL:HB	1.97	0.45
1:A:281:ILE:O	1:A:282:ASP:HB2	2.18	0.44
1:C:199:ALA:HB3	1:C:200:PRO:HD3	1.98	0.44
1:D:422:GLY:HA3	1:D:450:PRO:O	2.17	0.44
1:A:128:ARG:NH2	1:A:198:GLU:OE2	2.51	0.44
1:C:183:ILE:HD11	1:C:192:SER:HB3	2.00	0.44
1:C:297:ILE:HA	1:C:307:HIS:CD2	2.52	0.44
1:D:446:THR:HG23	1:D:484:ALA:HB2	2.00	0.44
1:D:47:LEU:HD22	1:D:54:ARG:NH1	2.32	0.44
1:B:446:THR:CG2	1:B:484:ALA:CB	2.92	0.44
1:C:327:ASP:OD1	1:C:333:HIS:HE1	2.01	0.44
1:C:70:GLN:N	1:C:70:GLN:OE1	2.50	0.44
1:A:327:ASP:HB2	1:A:328:PRO:HD2	2.00	0.44
1:A:446:THR:HG23	1:A:484:ALA:HB2	1.98	0.44
1:A:198:GLU:HA	1:A:230:ARG:HG2	1.99	0.44
1:A:209:MET:CE	1:A:217:VAL:CG2	2.87	0.44
1:B:493:ARG:O	1:B:494:PRO:C	2.56	0.44
1:C:82:THR:CG2	1:C:106:ASP:OD2	2.66	0.44
1:D:82:THR:HG23	1:D:106:ASP:OD2	2.18	0.44
1:D:209:MET:HE1	1:D:217:VAL:HG13	2.00	0.44
1:B:281:ILE:CG2	1:B:282:ASP:N	2.59	0.43
1:C:173:ARG:NH2	1:C:358:VAL:HG13	2.33	0.43
1:C:374:VAL:HA	1:C:375:PRO:HD3	1.82	0.43
1:A:43:VAL:HG22	1:A:130:VAL:CG2	2.48	0.43
1:A:273:ARG:NH2	1:A:295:ASP:OD2	2.51	0.43
1:A:413:ARG:NH1	1:A:496:ASP:OD1	2.51	0.43
1:D:266:PHE:HB2	1:D:289:MET:CE	2.45	0.43
1:D:281:ILE:CG2	1:D:282:ASP:N	2.59	0.43
1:D:379:GLU:OE2	1:D:521:ARG:HD3	2.18	0.43
1:A:410:PRO:O	1:A:411:ASP:CB	2.65	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:174:VAL:HG12	1:A:214:VAL:HA	2.00	0.43
1:A:267:ASP:O	1:A:270:SER:HB3	2.18	0.43
1:B:105:THR:OG1	1:B:109:GLY:HA3	2.18	0.43
1:A:446:THR:CG2	1:A:484:ALA:CB	2.90	0.43
1:B:374:VAL:HG22	1:B:377:ARG:HB2	2.01	0.43
1:B:70:GLN:N	1:B:70:GLN:OE1	2.52	0.43
1:A:151:ILE:HD12	1:A:161:THR:HG22	2.01	0.43
1:B:380:GLN:HA	1:B:389:ALA:O	2.19	0.42
1:C:209:MET:HG2	1:C:214:VAL:HG21	2.01	0.42
1:C:266:PHE:HB2	1:C:289:MET:CE	2.41	0.42
1:C:337:ILE:HD11	1:C:339:LEU:HD12	2.01	0.42
1:C:443:VAL:HG13	1:C:475:VAL:HB	2.02	0.42
1:D:297:ILE:CD1	1:D:357:THR:HG21	2.49	0.42
1:A:297:ILE:CD1	1:A:357:THR:HG21	2.48	0.42
1:A:437:ALA:HB2	1:A:466:ALA:HA	2.01	0.42
1:A:412:ARG:HD2	1:A:497:VAL:CG1	2.49	0.42
1:B:39:LEU:HG	1:B:134:LEU:HD22	2.01	0.42
1:C:75:GLY:HA2	1:C:101:VAL:HG13	2.01	0.42
1:C:240:ALA:HA	1:C:278:VAL:O	2.19	0.42
1:D:107:PRO:HA	1:D:110:VAL:HG22	2.01	0.42
1:D:70:GLN:N	1:D:70:GLN:OE1	2.49	0.42
1:A:446:THR:HB	1:A:447:ASP:H	1.64	0.42
1:B:446:THR:HG23	1:B:484:ALA:HB2	2.00	0.42
1:B:446:THR:HB	1:B:447:ASP:H	1.62	0.42
1:A:448:ASP:O	1:A:449:ASN:C	2.58	0.42
1:C:297:ILE:CD1	1:C:357:THR:HG21	2.50	0.42
1:D:209:MET:HG2	1:D:214:VAL:HG21	2.00	0.42
1:A:493:ARG:O	1:A:494:PRO:C	2.58	0.42
1:B:508:GLY:HA2	1:B:516:ARG:O	2.20	0.42
1:A:209:MET:HE1	1:A:217:VAL:HG22	1.95	0.42
1:A:430:ALA:HB3	1:A:431:PRO:HD3	2.01	0.42
1:B:417:VAL:HB	1:B:444:VAL:HB	2.02	0.41
1:B:445:VAL:HG12	1:B:459:ARG:HG2	2.02	0.41
1:B:173:ARG:HH22	1:B:358:VAL:HG13	1.84	0.41
1:B:374:VAL:HA	1:B:375:PRO:HD3	1.82	0.41
1:C:430:ALA:HB3	1:C:431:PRO:HD3	2.02	0.41
1:D:175:ALA:HA	1:D:216:THR:O	2.20	0.41
1:B:181:ILE:HD13	1:B:375:PRO:HD2	2.02	0.41
1:C:366:VAL:HG12	1:C:367:PRO:HD3	2.01	0.41
1:D:454:ASP:HA	1:D:455:PRO:HD3	1.96	0.41
1:B:30:ALA:HB3	1:B:211:GLU:OE1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:481:ARG:NH2	1:B:520:ASP:OD1	2.51	0.41
1:C:106:ASP:HB2	1:C:107:PRO:HD2	2.02	0.41
1:A:230:ARG:HH12	2:A:1498:UAG:C28	2.34	0.41
1:A:342:ARG:HD2	1:A:342:ARG:HA	1.94	0.41
1:C:139:TYR:O	1:C:142:PRO:HD3	2.21	0.41
1:C:446:THR:HG21	1:C:484:ALA:HB3	2.03	0.41
1:A:409:HIS:O	1:A:411:ASP:O	2.39	0.41
1:C:107:PRO:O	1:C:110:VAL:HG22	2.20	0.41
1:C:433:GLY:HA3	1:C:462:ILE:CG2	2.51	0.41
1:C:454:ASP:HA	1:C:455:PRO:HD3	1.99	0.41
1:A:289:MET:HE3	1:A:289:MET:HA	2.02	0.41
1:A:307:HIS:HB3	1:A:328:PRO:HG3	2.02	0.41
1:A:29:ASN:C	1:A:29:ASN:HD22	2.25	0.41
1:B:283:ASP:HB3	1:B:286:GLY:H	1.85	0.41
1:D:248:HIS:HE1	2:D:1498:UAG:H262	1.86	0.41
1:B:34:VAL:HG11	1:B:39:LEU:HD13	2.03	0.40
1:D:299:VAL:HG22	1:D:308:TRP:HB2	2.02	0.40
1:A:106:ASP:HB2	1:A:107:PRO:HD2	2.03	0.40
1:D:240:ALA:HA	1:D:278:VAL:O	2.20	0.40
1:A:412:ARG:HE	1:A:412:ARG:HB2	1.64	0.40
1:B:531:LEU:C	1:B:533:ARG:N	2.74	0.40
1:C:85:THR:HG23	2:C:1498:UAG:PA	2.61	0.40
1:B:82:THR:HG23	1:B:106:ASP:OD2	2.21	0.40
1:D:157:LYS:O	1:D:161:THR:HG23	2.21	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	495/535 (92%)	458 (92%)	26 (5%)	11 (2%)	<b>6</b> 31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	505/535 (94%)	469 (93%)	22 (4%)	14 (3%)	5	25
1	C	422/535 (79%)	407 (96%)	12 (3%)	3 (1%)	22	60
1	D	457/535 (85%)	436 (95%)	17 (4%)	4 (1%)	17	55
All	All	1879/2140 (88%)	1770 (94%)	77 (4%)	32 (2%)	9	39

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	281	ILE
1	A	411	ASP
1	A	413	ARG
1	A	524	LEU
1	A	532	GLU
1	B	52	ALA
1	B	281	ILE
1	B	412	ARG
1	B	524	LEU
1	C	281	ILE
1	D	281	ILE
1	D	524	LEU
1	A	385	GLN
1	B	532	GLU
1	A	412	ARG
1	A	514	ARG
1	B	394	ALA
1	B	410	PRO
1	B	531	LEU
1	C	394	ALA
1	B	413	ARG
1	B	449	ASN
1	B	471	GLY
1	A	449	ASN
1	B	116	ARG
1	D	449	ASN
1	A	410	PRO
1	B	51	PRO
1	B	396	LYS
1	D	396	LYS
1	A	396	LYS
1	C	396	LYS

### 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	353/382 (92%)	303 (86%)	50 (14%)	3	16
1	B	356/382 (93%)	301 (85%)	55 (15%)	2	13
1	C	301/382 (79%)	260 (86%)	41 (14%)	3	17
1	D	330/382 (86%)	282 (86%)	48 (14%)	3	15
All	All	1340/1528 (88%)	1146 (86%)	194 (14%)	3	15

All (194) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	31	VAL
1	A	35	ARG
1	A	39	LEU
1	A	43	VAL
1	A	47	LEU
1	A	58	GLU
1	A	72	VAL
1	A	73	SER
1	A	77	LEU
1	A	82	THR
1	A	85	THR
1	A	86	THR
1	A	104	LEU
1	A	128	ARG
1	A	130	VAL
1	A	138	VAL
1	A	168	LEU
1	A	169	ARG
1	A	180	THR
1	A	185	VAL
1	A	190	LEU
1	A	218	VAL
1	A	272	LEU

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Mol	Chain	Res	Type
1	A	275	ARG
1	A	276	THR
1	A	303	ASP
1	A	331	VAL
1	A	337	ILE
1	A	358	VAL
1	A	366	VAL
1	A	373	ARG
1	A	378	LEU
1	A	383	ARG
1	A	390	LEU
1	A	401	ARG
1	A	404	LEU
1	A	409	HIS
1	A	413	ARG
1	A	416	VAL
1	A	438	GLN
1	A	439	LEU
1	A	443	VAL
1	A	446	THR
1	A	451	ARG
1	A	482	ARG
1	A	497	VAL
1	A	499	LEU
1	A	510	ARG
1	A	523	GLU
1	B	29	ASN
1	B	31	VAL
1	B	35	ARG
1	B	39	LEU
1	B	43	VAL
1	B	47	LEU
1	B	54	ARG
1	B	56	VAL
1	B	67	LEU
1	B	72	VAL
1	B	73	SER
1	B	77	LEU
1	B	82	THR
1	B	85	THR
1	B	86	THR
1	B	104	LEU

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Mol	Chain	Res	Type
1	B	116	ARG
1	B	128	ARG
1	B	130	VAL
1	B	138	VAL
1	B	168	LEU
1	B	169	ARG
1	B	180	THR
1	B	190	LEU
1	B	215	ASP
1	B	228	LEU
1	B	249	LEU
1	B	272	LEU
1	B	275	ARG
1	B	276	THR
1	B	303	ASP
1	B	337	ILE
1	B	342	ARG
1	B	358	VAL
1	B	366	VAL
1	B	369	LEU
1	B	373	ARG
1	B	374	VAL
1	B	378	LEU
1	B	388	LEU
1	B	398	GLU
1	B	407	LEU
1	B	412	ARG
1	B	417	VAL
1	B	438	GLN
1	B	442	LEU
1	B	443	VAL
1	B	446	THR
1	B	451	ARG
1	B	476	VAL
1	B	482	ARG
1	B	497	VAL
1	B	498	VAL
1	B	506	GLU
1	B	523	GLU
1	C	29	ASN
1	C	31	VAL
1	C	35	ARG

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Mol	Chain	Res	Type
1	C	39	LEU
1	C	47	LEU
1	C	56	VAL
1	C	67	LEU
1	C	72	VAL
1	C	73	SER
1	C	82	THR
1	C	85	THR
1	C	86	THR
1	C	104	LEU
1	C	128	ARG
1	C	130	VAL
1	C	138	VAL
1	C	168	LEU
1	C	169	ARG
1	C	180	THR
1	C	185	VAL
1	C	190	LEU
1	C	215	ASP
1	C	275	ARG
1	C	276	THR
1	C	303	ASP
1	C	313	VAL
1	C	331	VAL
1	C	337	ILE
1	C	358	VAL
1	C	366	VAL
1	C	369	LEU
1	C	373	ARG
1	C	374	VAL
1	C	378	LEU
1	C	407	LEU
1	C	416	VAL
1	C	434	ARG
1	C	442	LEU
1	C	443	VAL
1	C	446	THR
1	C	497	VAL
1	D	29	ASN
1	D	31	VAL
1	D	32	VAL
1	D	35	ARG

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Mol	Chain	Res	Type
1	D	39	LEU
1	D	47	LEU
1	D	56	VAL
1	D	58	GLU
1	D	72	VAL
1	D	73	SER
1	D	77	LEU
1	D	82	THR
1	D	85	THR
1	D	86	THR
1	D	104	LEU
1	D	116	ARG
1	D	128	ARG
1	D	130	VAL
1	D	138	VAL
1	D	168	LEU
1	D	169	ARG
1	D	180	THR
1	D	190	LEU
1	D	212	ARG
1	D	249	LEU
1	D	275	ARG
1	D	276	THR
1	D	303	ASP
1	D	331	VAL
1	D	337	ILE
1	D	342	ARG
1	D	358	VAL
1	D	366	VAL
1	D	373	ARG
1	D	374	VAL
1	D	378	LEU
1	D	381	ILE
1	D	398	GLU
1	D	417	VAL
1	D	438	GLN
1	D	442	LEU
1	D	443	VAL
1	D	446	THR
1	D	451	ARG
1	D	474	GLN
1	D	482	ARG

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Mol	Chain	Res	Type
1	D	497	VAL
1	D	523	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	307	HIS
1	A	333	HIS
1	B	29	ASN
1	B	307	HIS
1	B	333	HIS
1	C	29	ASN
1	C	307	HIS
1	C	333	HIS
1	D	29	ASN
1	D	307	HIS
1	D	333	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	KCX	C	262	1	7,11,12	0.85	0	4,12,14	0.33	0
1	KCX	A	262	1	7,11,12	0.52	0	4,12,14	0.32	0
1	KCX	D	262	1	7,11,12	0.83	0	4,12,14	0.27	0
1	KCX	B	262	1	7,11,12	1.13	1 (14%)	4,12,14	0.73	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	KCX	C	262	1	-	1/7/10/12	-
1	KCX	A	262	1	-	0/7/10/12	-
1	KCX	D	262	1	-	0/7/10/12	-
1	KCX	B	262	1	-	1/7/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	262	KCX	CE-NZ	2.55	1.51	1.45

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	C	262	KCX	O-C-CA-CB
1	B	262	KCX	O-C-CA-CB

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	UAG	D	1498	3	47,60,60	1.38	6 (12%)	60,88,88	1.81	9 (15%)
2	UAG	C	1498	3	47,60,60	1.49	6 (12%)	60,88,88	1.78	10 (16%)
2	UAG	B	1498	3	47,60,60	1.42	5 (10%)	60,88,88	1.66	9 (15%)
2	UAG	A	1498	3	47,60,60	1.36	4 (8%)	60,88,88	1.80	10 (16%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	UAG	D	1498	3	-	10/47/92/92	0/3/3/3
2	UAG	C	1498	3	-	13/47/92/92	0/3/3/3
2	UAG	B	1498	3	-	9/47/92/92	0/3/3/3
2	UAG	A	1498	3	-	9/47/92/92	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1498	UAG	C6-N1	5.23	1.42	1.35
2	C	1498	UAG	C6-N1	5.22	1.42	1.35
2	B	1498	UAG	C6-N1	5.18	1.42	1.35
2	D	1498	UAG	C4-N3	4.27	1.40	1.33
2	B	1498	UAG	C4-N3	4.25	1.40	1.33
2	A	1498	UAG	PA-O1A	4.25	1.66	1.50
2	A	1498	UAG	C4-N3	4.18	1.40	1.33
2	A	1498	UAG	C6-N1	4.03	1.40	1.35
2	C	1498	UAG	C4-N3	4.00	1.40	1.33
2	C	1498	UAG	O4B-C1B	3.60	1.46	1.41
2	C	1498	UAG	PA-O1A	3.19	1.62	1.50
2	C	1498	UAG	PB-O1B	3.12	1.62	1.50
2	A	1498	UAG	PB-O1B	2.94	1.61	1.50
2	B	1498	UAG	PB-O1B	2.71	1.60	1.50
2	D	1498	UAG	PB-O1B	2.56	1.60	1.50
2	D	1498	UAG	O4B-C1B	2.44	1.44	1.41
2	B	1498	UAG	C2B-C1B	-2.39	1.50	1.53
2	C	1498	UAG	C24-N5	2.31	1.49	1.46
2	B	1498	UAG	C25-C24	-2.23	1.50	1.53
2	D	1498	UAG	PA-O5B	2.09	1.67	1.59
2	D	1498	UAG	PA-O1A	2.00	1.58	1.50

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1498	UAG	O5B-PA-O1A	-8.84	74.51	109.07
2	A	1498	UAG	O5B-PA-O1A	-8.61	75.42	109.07
2	C	1498	UAG	O5B-PA-O1A	-8.32	76.57	109.07
2	B	1498	UAG	O5B-PA-O1A	-6.69	82.94	109.07
2	C	1498	UAG	O2A-PA-O5B	-4.43	87.16	107.75
2	A	1498	UAG	O2A-PA-O5B	-4.33	87.63	107.75
2	D	1498	UAG	O2A-PA-O5B	-4.24	88.06	107.75
2	B	1498	UAG	PB-O3A-PA	-4.19	118.44	132.83
2	A	1498	UAG	C25-C24-N5	-4.17	104.12	110.19
2	B	1498	UAG	O2A-PA-O5B	-4.11	88.65	107.75
2	D	1498	UAG	C25-C24-N5	-3.60	104.95	110.19
2	C	1498	UAG	PB-O3A-PA	-3.54	120.68	132.83
2	D	1498	UAG	PB-O3A-PA	-3.50	120.82	132.83
2	B	1498	UAG	C25-C26-C27	-3.42	106.24	113.59
2	B	1498	UAG	C24-N5-C22	3.14	127.89	123.19
2	C	1498	UAG	C25-C26-C27	-3.12	106.89	113.59
2	A	1498	UAG	PB-O3A-PA	-3.08	122.25	132.83
2	C	1498	UAG	C3'-C2'-N2'	-3.08	105.80	110.91
2	D	1498	UAG	C25-C26-C27	-2.93	107.29	113.59
2	C	1498	UAG	C25-C24-N5	-2.80	106.12	110.19
2	C	1498	UAG	C8'-C7'-N2'	-2.76	111.42	116.10
2	C	1498	UAG	C24-N5-C22	2.64	127.15	123.19
2	D	1498	UAG	O7'-C7'-N2'	2.61	126.75	121.95
2	A	1498	UAG	C24-N5-C22	2.59	127.07	123.19
2	D	1498	UAG	O5'-C1'-O1'	2.56	114.71	111.36
2	B	1498	UAG	C25-C24-N5	-2.55	106.47	110.19
2	A	1498	UAG	C6'-C5'-C4'	-2.55	107.03	113.00
2	B	1498	UAG	C3'-C2'-N2'	-2.53	106.72	110.91
2	A	1498	UAG	C25-C26-C27	-2.42	108.39	113.59
2	D	1498	UAG	C1'-C2'-N2'	-2.32	107.01	111.00
2	D	1498	UAG	C24-N5-C22	2.16	126.42	123.19
2	A	1498	UAG	O7'-C7'-N2'	2.12	125.84	121.95
2	A	1498	UAG	C3'-C2'-N2'	-2.10	107.43	110.91
2	C	1498	UAG	C20-C18-C19	-2.07	106.00	111.11
2	A	1498	UAG	C8'-C7'-N2'	-2.06	112.61	116.10
2	B	1498	UAG	O4B-C1B-C2B	-2.05	103.93	106.93
2	B	1498	UAG	O7'-C7'-N2'	2.04	125.70	121.95
2	C	1498	UAG	O7'-C7'-N2'	2.01	125.65	121.95

There are no chirality outliers.

All (41) torsion outliers are listed below:

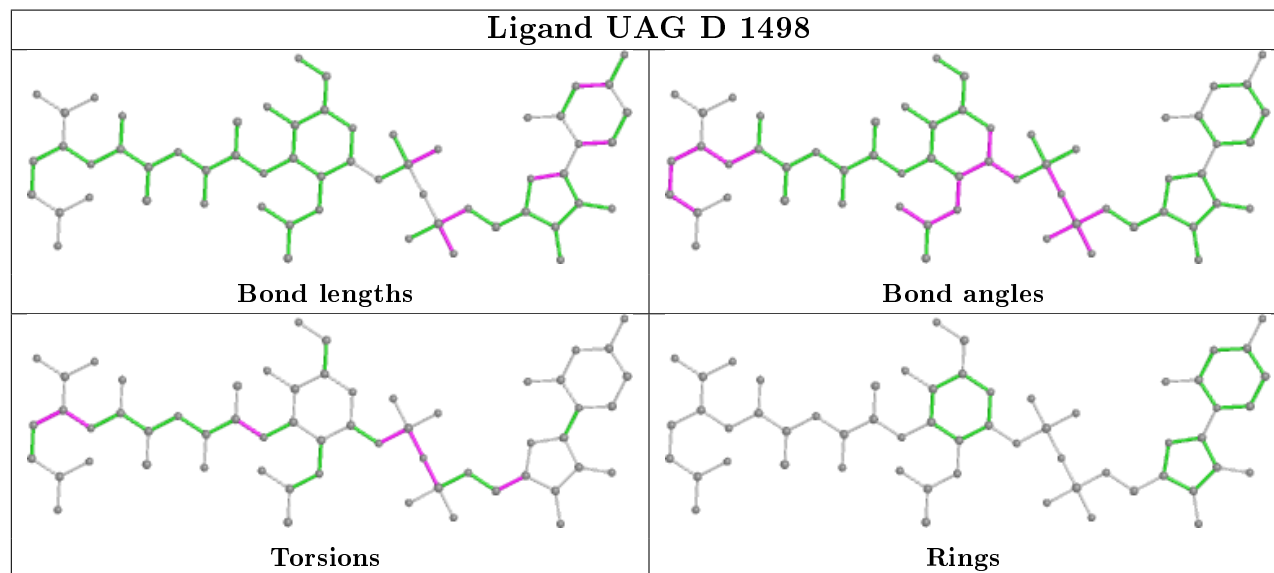
Mol	Chain	Res	Type	Atoms
2	B	1498	UAG	C2B-C1B-N1-C6
2	B	1498	UAG	C28-C24-N5-C22
2	D	1498	UAG	C28-C24-N5-C22
2	D	1498	UAG	N5-C24-C25-C26
2	D	1498	UAG	C28-C24-C25-C26
2	A	1498	UAG	C1'-O1'-PB-O2B
2	A	1498	UAG	C28-C24-N5-C22
2	A	1498	UAG	N5-C24-C25-C26
2	A	1498	UAG	C28-C24-C25-C26
2	C	1498	UAG	C2B-C1B-N1-C6
2	C	1498	UAG	C1'-O1'-PB-O2B
2	C	1498	UAG	C20-C18-O3'-C3'
2	C	1498	UAG	C28-C24-N5-C22
2	C	1498	UAG	C28-C24-C25-C26
2	C	1498	UAG	N5-C24-C25-C26
2	B	1498	UAG	N5-C24-C25-C26
2	B	1498	UAG	C20-C18-O3'-C3'
2	D	1498	UAG	C20-C18-O3'-C3'
2	A	1498	UAG	C20-C18-O3'-C3'
2	D	1498	UAG	C1'-O1'-PB-O3A
2	A	1498	UAG	C1'-O1'-PB-O3A
2	C	1498	UAG	C1'-O1'-PB-O3A
2	D	1498	UAG	C1'-O1'-PB-O2B
2	B	1498	UAG	C1'-O1'-PB-O3A
2	D	1498	UAG	C19-C18-O3'-C3'
2	D	1498	UAG	PB-O3A-PA-O1A
2	D	1498	UAG	PA-O3A-PB-O1B
2	C	1498	UAG	PB-O3A-PA-O1A
2	B	1498	UAG	C5B-O5B-PA-O1A
2	D	1498	UAG	O4B-C4B-C5B-O5B
2	C	1498	UAG	O4B-C4B-C5B-O5B
2	B	1498	UAG	C28-C24-C25-C26
2	A	1498	UAG	PB-O3A-PA-O1A
2	C	1498	UAG	PA-O3A-PB-O1B
2	B	1498	UAG	C1'-O1'-PB-O2B
2	A	1498	UAG	PA-O3A-PB-O1B
2	B	1498	UAG	C19-C18-O3'-C3'
2	A	1498	UAG	C19-C18-O3'-C3'
2	C	1498	UAG	C19-C18-O3'-C3'
2	C	1498	UAG	C5B-O5B-PA-O1A
2	C	1498	UAG	C3B-C4B-C5B-O5B

There are no ring outliers.

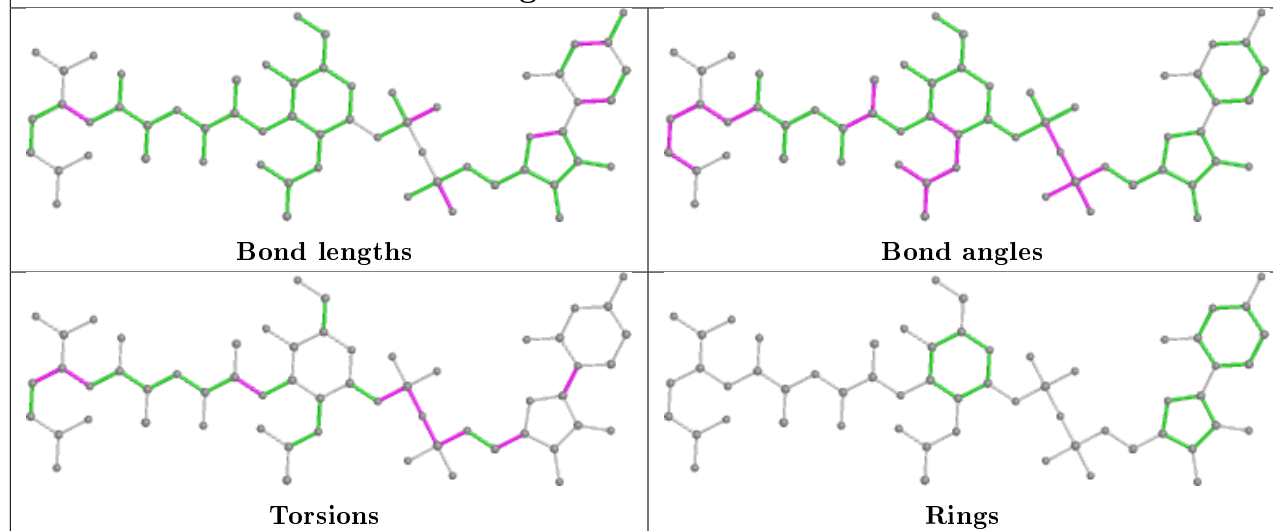
3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1498	UAG	1	0
2	C	1498	UAG	1	0
2	A	1498	UAG	2	0

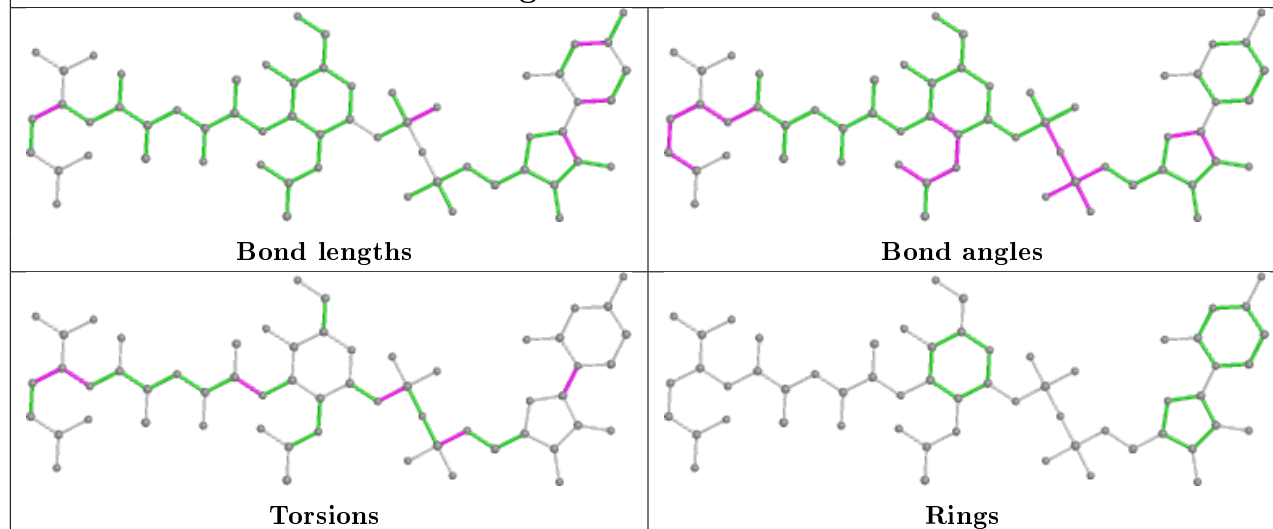
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



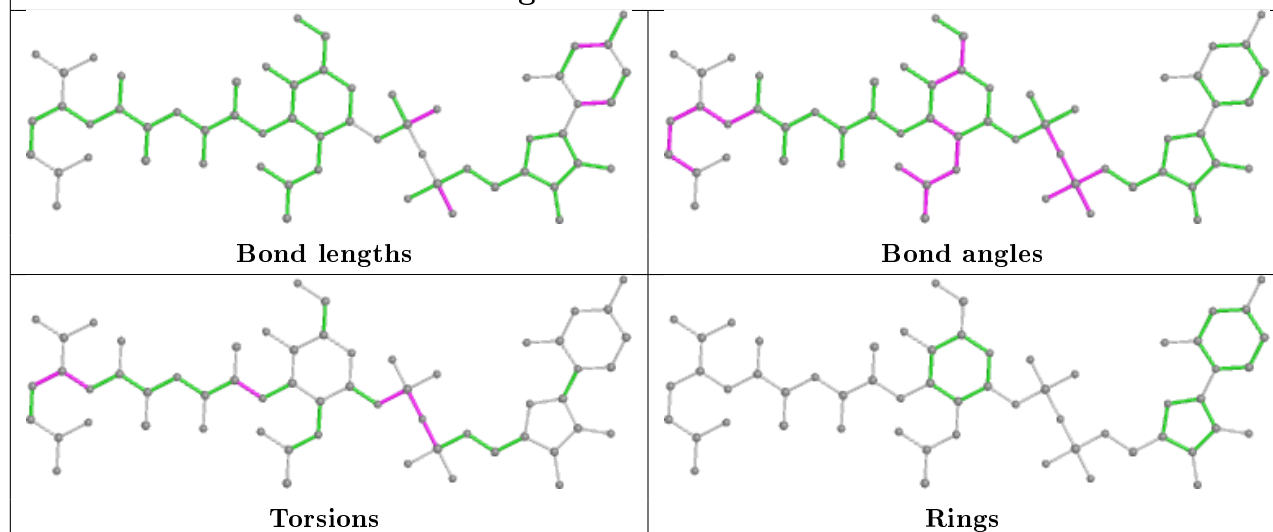
## Ligand UAG C 1498



## Ligand UAG B 1498



## Ligand UAG A 1498



## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	503/535 (94%)	-0.44	0 100 100	3, 15, 25, 42	0
1	B	507/535 (94%)	-0.43	3 (0%) 89 72	3, 14, 27, 37	0
1	C	438/535 (81%)	-0.17	13 (2%) 50 22	2, 13, 32, 37	0
1	D	467/535 (87%)	-0.24	9 (1%) 66 37	3, 16, 28, 43	0
All	All	1915/2140 (89%)	-0.33	25 (1%) 77 51	2, 14, 29, 43	0

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	494	PRO	4.6
1	D	454	ASP	4.6
1	C	317	ASP	4.5
1	C	318	ALA	4.4
1	D	187	GLY	4.0
1	C	431	PRO	4.0
1	D	473	ALA	3.8
1	C	490	ALA	3.0
1	B	116	ARG	2.9
1	C	314	ALA	2.7
1	C	505	HIS	2.7
1	C	312	ASP	2.6
1	D	483	ASP	2.4
1	B	471	GLY	2.4
1	D	452	ASP	2.4
1	C	413	ARG	2.3
1	D	509	GLN	2.3
1	B	470	GLY	2.2
1	C	495	GLY	2.2
1	C	414	LEU	2.2
1	D	415	ALA	2.2

*Continued on next page...*

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Mol	Chain	Res	Type	RSRZ
1	C	433	GLY	2.1
1	D	453	GLU	2.1
1	D	507	THR	2.0
1	C	406	THR	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( $\text{\AA}^2$ )	Q<0.9
1	KCX	B	262	12/13	0.96	0.15	10,11,17,18	0
1	KCX	A	262	12/13	0.97	0.17	13,14,20,21	0
1	KCX	C	262	12/13	0.97	0.13	9,11,20,21	0
1	KCX	D	262	12/13	0.98	0.15	11,13,22,22	0

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

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

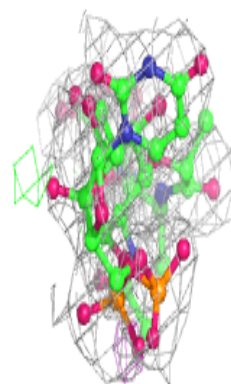
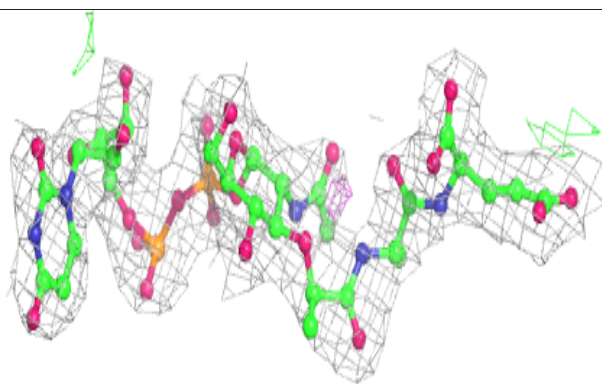
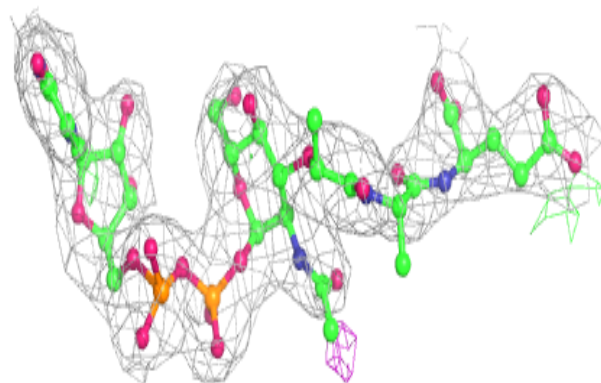
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	MG	B	1499	1/1	0.86	0.18	33,33,33,33	0
3	MG	A	1499	1/1	0.92	0.14	37,37,37,37	0
2	UAG	C	1498	58/58	0.94	0.18	36,43,46,49	0
2	UAG	A	1498	58/58	0.95	0.18	26,36,42,45	0
3	MG	D	1499	1/1	0.95	0.09	38,38,38,38	0
2	UAG	B	1498	58/58	0.95	0.16	31,34,42,45	0
2	UAG	D	1498	58/58	0.96	0.16	30,35,42,47	0
3	MG	C	1499	1/1	0.98	0.14	35,35,35,35	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.

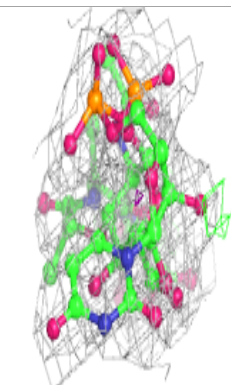
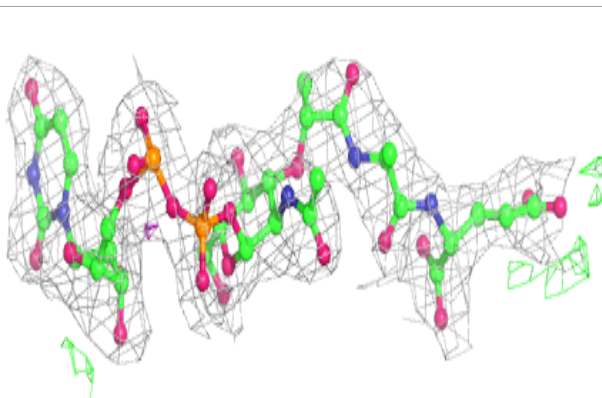
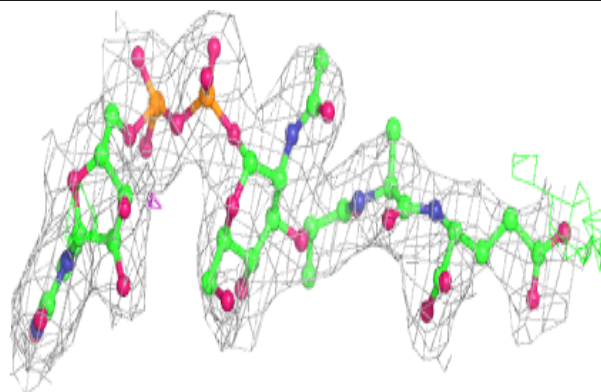
**Electron density around UAG C 1498:**

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



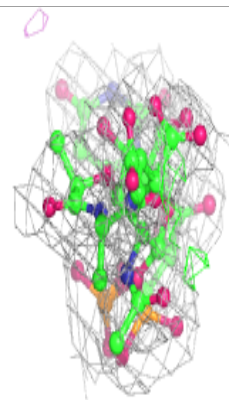
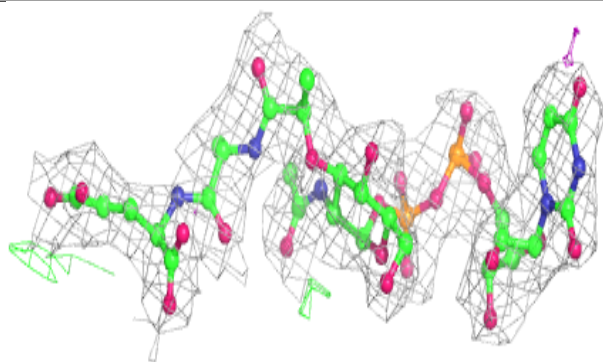
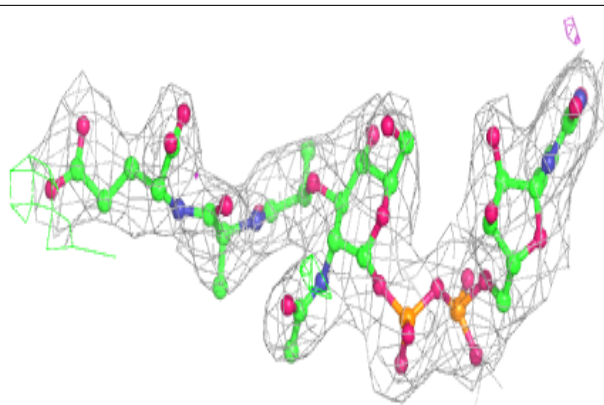
**Electron density around UAG A 1498:**

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

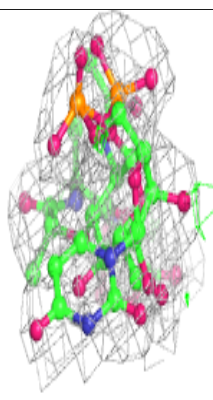
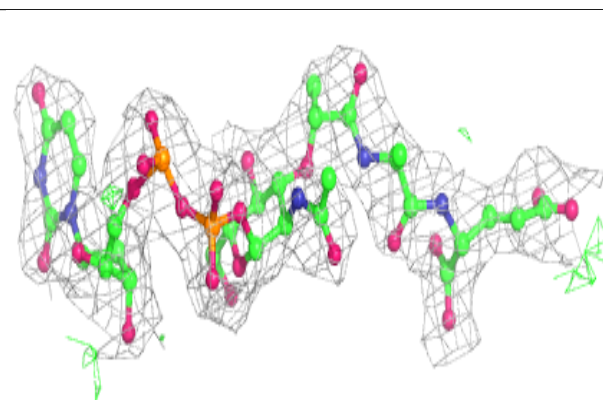
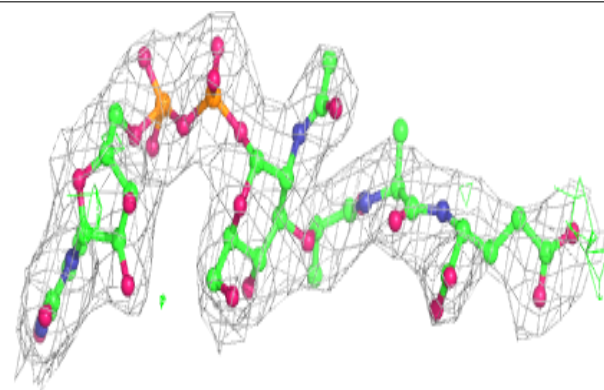


**Electron density around UAG B 1498:**

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

**Electron density around UAG D 1498:**

$2mF_o-DF_c$  (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.