



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 02:06 PM UTC

PDB ID : 2WTZ / pdb_00002wtz
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

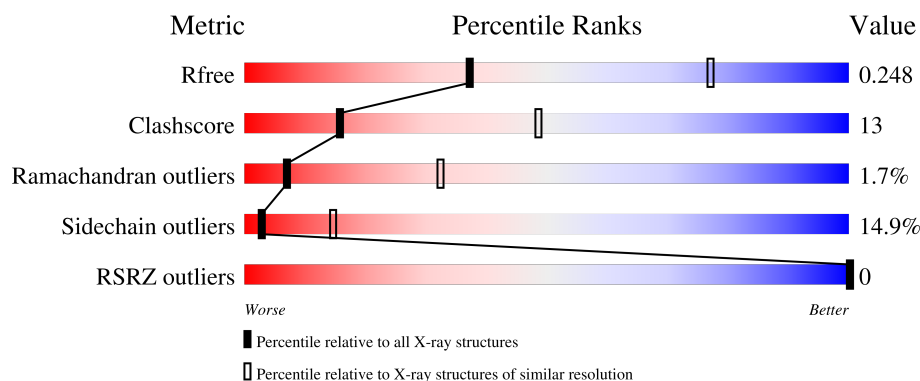
1 Overall quality at a glance

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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	 67% 20% 6% • 6%
1	B	535	 67% 22% 5% • 5%
1	C	535	 60% 19% • 18%
1	D	535	 63% 20% • • 13%

2 Entry composition [i](#)

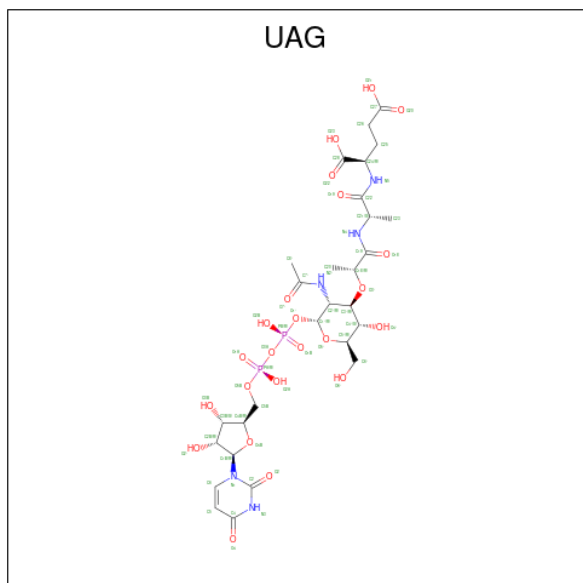
There are 3 unique types of molecules in this entry. The entry contains 14008 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 (CCD ID: UAG) (formula: $C_{28}H_{43}N_5O_{23}P_2$).



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

Continued on next page...

Continued from previous page...

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		

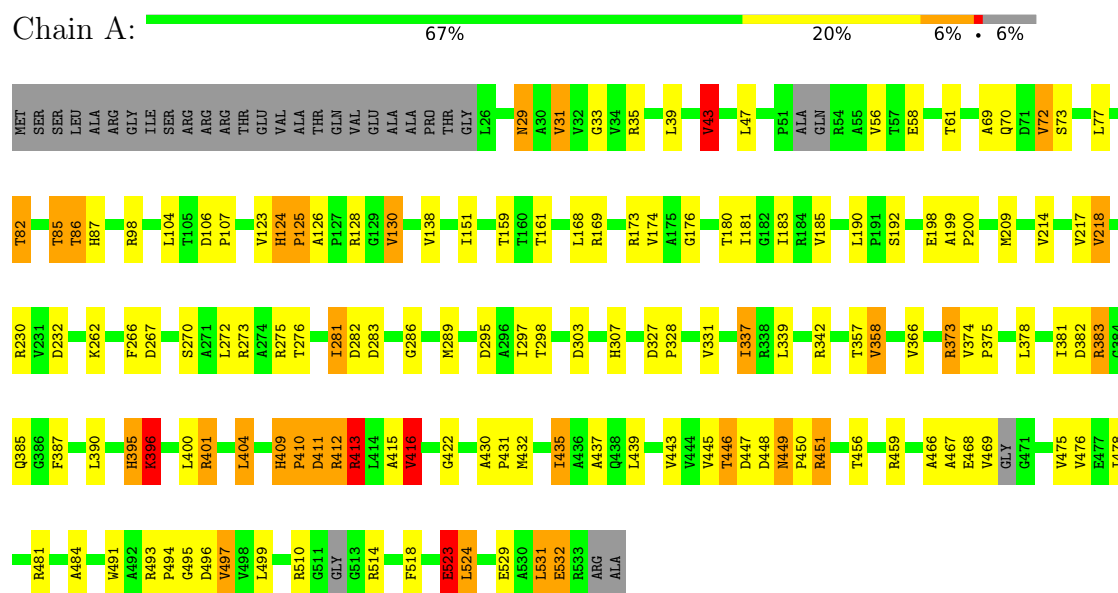
- Molecule 3 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

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

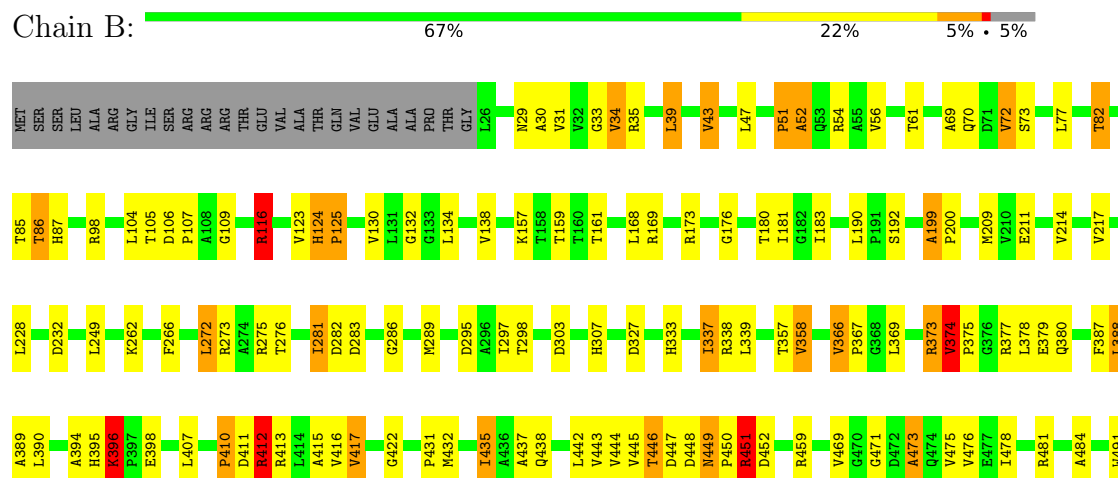
3 Residue-property plots

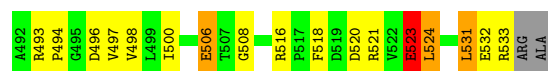
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density.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

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

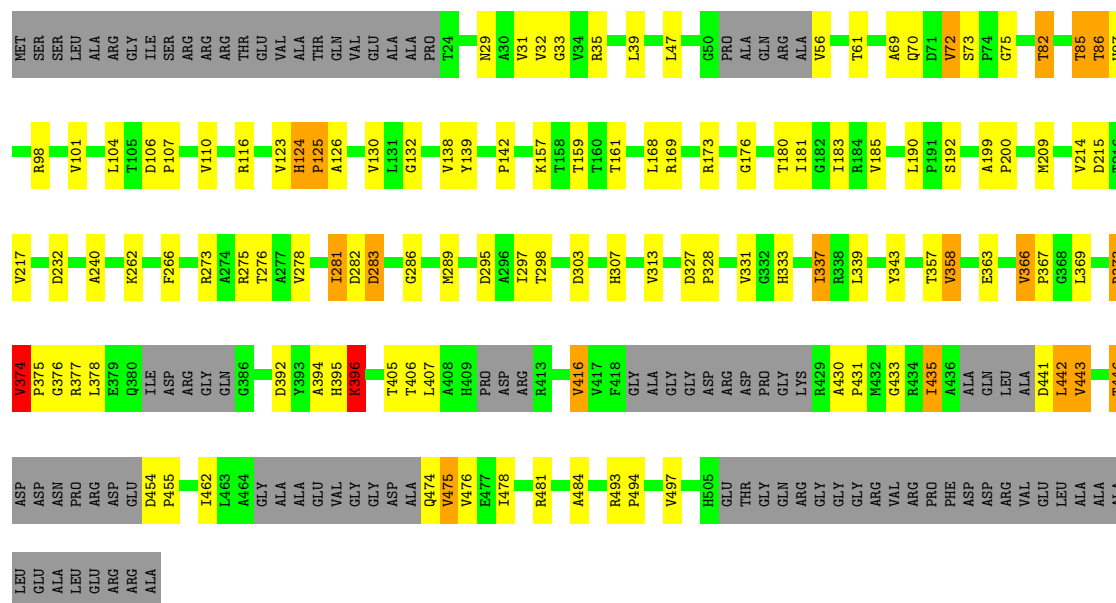


- Molecule 1: UDP-N-ACETYLMURAMOYL-L-ALANYL-D-GLUTAMATE--2,6-DIAMINOPI MELATE LIGASE

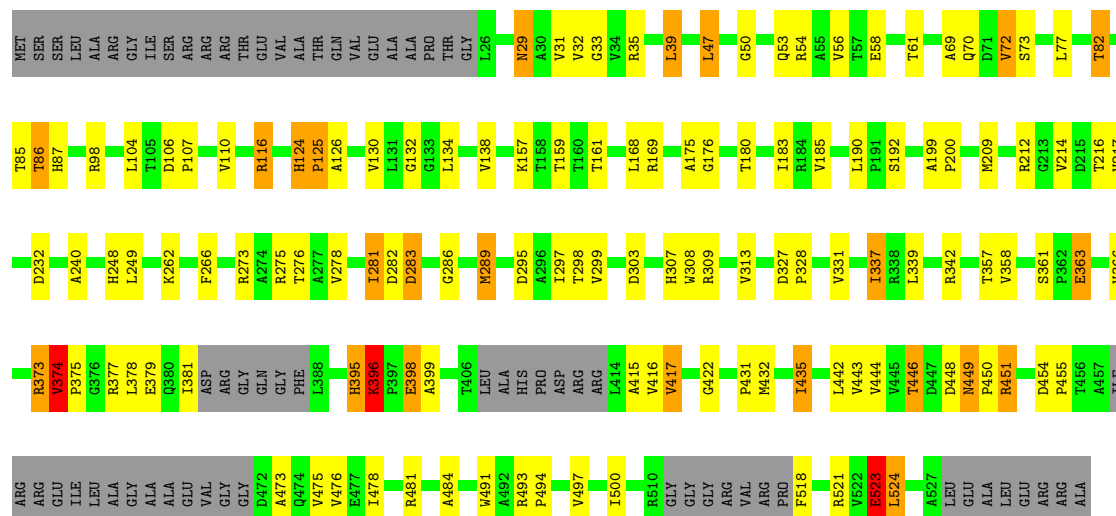




• Molecule 1: UDP-N-ACETYL MURAMOYL-L-ALANYL-D-GLUTAMATE--2,6-DIAMINOPI MELATE LIGASE



• Molecule 1: UDP-N-ACETYL MURAMOYL-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, α , β , γ	76.92Å 79.80Å 82.92Å 111.09° 92.16° 93.98°	Depositor
Resolution (Å)	74.16 – 3.00 74.16 – 3.00	Depositor EDS
% Data completeness (in resolution range)	91.4 (74.16-3.00) 79.2 (74.16-3.00)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (4.69%)	wwPDB-VP
Wilson B-factor (Å ²)	43.2	Xtriage
Anisotropy	0.163	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 33.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.106 for -h,-l,-k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14008	wwPDB-VP
Average B, all atoms (Å ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: KCX, UAG, MG

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	0.84	3/3678 (0.1%)	1.11	15/5017 (0.3%)
1	B	0.83	1/3710 (0.0%)	1.09	13/5064 (0.3%)
1	C	0.82	1/3142 (0.0%)	1.03	12/4296 (0.3%)
1	D	0.79	1/3405 (0.0%)	1.08	21/4649 (0.5%)
All	All	0.82	6/13935 (0.0%)	1.08	61/19026 (0.3%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	126	ALA	CA-C	7.07	1.58	1.53
1	A	126	ALA	N-CA	6.58	1.51	1.46
1	A	31	VAL	CA-CB	5.83	1.60	1.54
1	B	199	ALA	CA-CB	-5.65	1.49	1.54
1	C	126	ALA	CA-C	5.56	1.57	1.53
1	A	126	ALA	CA-C	5.06	1.58	1.53

All (61) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	232	ASP	N-CA-C	7.96	119.96	111.28
1	A	523	GLU	N-CA-C	-7.58	99.07	110.28
1	A	43	VAL	N-CA-CB	-7.54	102.53	112.26
1	A	218	VAL	CB-CA-C	-7.50	100.40	110.98
1	B	43	VAL	N-CA-CB	-7.20	102.98	112.26
1	B	451	ARG	CB-CA-C	-7.14	108.32	116.54
1	D	396	LYS	CA-C-N	7.13	126.66	119.24
1	D	396	LYS	C-N-CA	7.13	126.66	119.24
1	D	309	ARG	NE-CZ-NH1	-7.05	114.45	121.50
1	D	125	PRO	N-CA-C	-7.02	100.88	111.41
1	B	523	GLU	N-CA-C	-6.76	100.27	110.28

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	309	ARG	NE-CZ-NH2	6.72	125.25	119.20
1	A	451	ARG	CB-CA-C	-6.67	108.86	116.54
1	A	125	PRO	N-CA-C	-6.63	101.47	111.41
1	A	396	LYS	CA-C-N	6.60	126.11	119.24
1	A	396	LYS	C-N-CA	6.60	126.11	119.24
1	D	125	PRO	CA-C-N	-6.57	116.80	123.10
1	D	125	PRO	C-N-CA	-6.57	116.80	123.10
1	C	125	PRO	CA-C-N	-6.34	117.02	123.10
1	C	125	PRO	C-N-CA	-6.34	117.02	123.10
1	B	125	PRO	N-CA-C	-6.33	101.92	111.41
1	C	232	ASP	N-CA-C	6.32	118.17	111.28
1	D	395	HIS	N-CA-C	-6.31	100.86	110.14
1	D	232	ASP	N-CA-C	6.24	118.08	111.28
1	D	523	GLU	N-CA-C	-6.24	101.04	110.28
1	C	124	HIS	CA-C-N	-6.21	113.88	120.03
1	C	124	HIS	C-N-CA	-6.21	113.88	120.03
1	B	416	VAL	CB-CA-C	-6.17	101.73	110.12
1	A	124	HIS	CA-C-N	-6.08	114.01	120.03
1	A	124	HIS	C-N-CA	-6.08	114.01	120.03
1	B	396	LYS	CA-C-N	5.95	125.43	119.24
1	B	396	LYS	C-N-CA	5.95	125.43	119.24
1	A	125	PRO	CA-C-N	-5.94	117.02	124.21
1	A	125	PRO	C-N-CA	-5.94	117.02	124.21
1	C	125	PRO	N-CA-C	-5.91	102.54	111.41
1	C	116	ARG	N-CA-C	5.90	119.37	110.64
1	C	396	LYS	CA-C-N	5.85	125.05	118.97
1	C	396	LYS	C-N-CA	5.85	125.05	118.97
1	D	374	VAL	CB-CA-C	5.85	116.62	110.37
1	B	34	VAL	N-CA-C	-5.67	100.50	108.27
1	C	283	ASP	N-CA-C	-5.66	99.80	109.24
1	A	232	ASP	N-CA-C	5.61	117.40	111.28
1	A	416	VAL	N-CA-C	5.53	116.01	107.78
1	D	283	ASP	N-CA-C	-5.48	100.73	109.23
1	B	374	VAL	CB-CA-C	5.47	116.22	110.37
1	D	116	ARG	N-CA-C	5.41	118.65	110.64
1	C	374	VAL	CB-CA-C	5.40	116.25	110.53
1	D	124	HIS	CA-C-N	-5.35	114.73	120.03
1	D	124	HIS	C-N-CA	-5.35	114.73	120.03
1	D	50	GLY	CA-C-N	5.29	126.45	119.84
1	D	50	GLY	C-N-CA	5.29	126.45	119.84
1	D	185	VAL	CB-CA-C	-5.29	102.93	110.12
1	D	473	ALA	N-CA-C	5.22	117.55	110.35

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	416	VAL	N-CA-C	5.20	115.53	107.78
1	B	473	ALA	N-CA-C	5.14	117.44	110.35
1	B	124	HIS	CA-C-N	-5.09	114.99	120.03
1	B	124	HIS	C-N-CA	-5.09	114.99	120.03
1	A	395	HIS	N-CA-C	-5.08	102.66	110.14
1	D	309	ARG	CD-NE-CZ	5.08	131.51	124.40
1	D	416	VAL	CB-CA-C	-5.06	103.24	110.12
1	A	56	VAL	CB-CA-C	-5.04	105.33	112.14

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	105	0
1	B	3663	0	3657	99	0
1	C	3109	0	3092	82	0
1	D	3366	0	3357	85	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	370	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 (370) 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:D:281:ILE:HG22	1:D:282:ASP:H	1.15	1.03
1:C:209:MET:HE2	1:C:217:VAL:HG22	1.40	1.01
1:B:209:MET:HE2	1:B:217:VAL:HG22	1.46	0.98
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
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:D:209:MET:HE2	1:D:217:VAL:HG22	1.47	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	1.50	0.92
1:C:373:ARG:HH21	1:C:373:ARG:HG3	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:HH21	1:A:373:ARG:HG3	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	1.55	0.87
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:HH21	1:D:373:ARG:HG3	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:HG3	1:B:373:ARG:HH21	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:176:GLY:HA3	1:B:209:MET:HE3	1.60	0.82
1:C:176:GLY:HA3	1:C:209:MET:HE3	1.61	0.81
1:B:411:ASP:O	1:B:412:ARG:HB3	1.81	0.81

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:373:ARG:HH21	1:C:373:ARG:CG	1.95	0.79
1:C:446:THR:CG2	1:C:478:ILE:O	2.30	0.79
1:D:176:GLY:HA3	1:D:209:MET:HE3	1.65	0.78
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:C:209:MET:HE2	1:C:217:VAL:CG2	2.13	0.76
1:A:159:THR:HG23	1:A:374:VAL:HG21	1.68	0.76
1:A:401:ARG:CB	1:A:401:ARG:HH11	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: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:HH21	1:D:373:ARG:CG	2.02	0.72
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:C:281:ILE:HG22	1:C:282:ASP:N	1.98	0.70
1:A:72:VAL:HG22	1:A:98:ARG:HB2	1.73	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:289:MET:HE3	1:B:289:MET:HA	1.75	0.69
1:A:281:ILE:HG22	1:A:282:ASP:N	1.99	0.68
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:481:ARG:HG2	1:B:518:PHE:CZ	2.30	0.67
1:D:289:MET:HE3	1:D:289:MET:HA	1.76	0.67
1:A:86:THR:OG1	1:A:87:HIS:N	2.21	0.67
1:D:446:THR:CG2	1:D:484:ALA:HB2	2.25	0.66
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:A:266:PHE:HB2	1:A:289:MET:HE1	1.78	0.65
1:D:373:ARG:HG3	1:D:373:ARG:NH2	2.08	0.65
1:B:209:MET:HE2	1:B:217:VAL:CG2	2.24	0.65
1:D:209:MET:HE2	1:D:217:VAL:CG2	2.26	0.65
1:B:373:ARG:HG3	1:B:373:ARG:NH2	2.11	0.64
1:D:266:PHE:HB2	1:D:289:MET:HE1	1.79	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:C:289:MET:HA	1:C:289:MET:HE3	1.80	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:D:363:GLU:CD	1:D:363:GLU:H	2.07	0.62
1:D:176:GLY:HA3	1:D:209:MET:CE	2.29	0.62
1:A:373:ARG:HG3	1:A:373:ARG:NH2	2.07	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:A:209:MET:HE2	1:A:217:VAL:CG2	2.27	0.61
1:B:469:VAL:HG13	1:B:469:VAL:O	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:O	1:B:116:ARG:NE	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:C:266:PHE:HB2	1:C:289:MET:HE1	1.83	0.60
1:B:531:LEU:C	1:B:533:ARG:H	2.08	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:86:THR:OG1	1:B:87:HIS:N	2.34	0.59
1:B:132:GLY:HA2	1:B:199:ALA:HB1	1.83	0.59
1:B:266:PHE:HB2	1:B:289:MET:HE1	1.85	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:379:GLU:OE2	1:B:521:ARG:HD3	2.03	0.58
1:B:437:ALA:HB1	1:B:469:VAL:HB	1.84	0.58
1:C:273:ARG:NH2	1:C:295:ASP:OD2	2.36	0.58
1:C:343:TYR:CD2	1:C:406:THR:HG21	2.39	0.58
1:D:209:MET:HE1	1:D:217:VAL:HG22	1.85	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:D:395:HIS:HA	1:D:432:MET:HE1	1.87	0.57
1:A:337:ILE:HG12	1:A:339:LEU:H	1.69	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:B:289:MET:HE3	1:B:289:MET:CA	2.37	0.55
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:A:266:PHE:HB2	1:A:289:MET:CE	2.37	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:289:MET:HE3	1:C:289:MET:CA	2.39	0.52
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: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: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:A:209:MET:CE	1:A:217:VAL:CG2	2.87	0.51
1:B:506:GLU:OE2	1:B:506:GLU:HA	2.09	0.51
1:D:451:ARG:HD3	1:D:451:ARG:N	2.26	0.51
1:B:417:VAL:HG13	1:B:500:ILE:HD13	1.92	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:C:266:PHE:HB2	1:C:289:MET:CE	2.41	0.50
1:D:209:MET:CE	1:D:217:VAL:CG2	2.84	0.50
1:B:209:MET:HG2	1:B:214:VAL:HG21	1.92	0.50
1:D:82:THR:HG22	1:D:87:HIS:NE2	2.27	0.50
1:D:395:HIS:O	1:D:396:LYS:HB2	2.12	0.50
1:C:209:MET:HE1	1:C:217:VAL:HG13	1.93	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: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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:493:ARG:O	1:B:494:PRO:C	2.56	0.48
1:C:209:MET:HE1	1:C:217:VAL:HG22	1.90	0.48
1:B:395:HIS:HA	1:B:432:MET:HE1	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
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:HD3	1:B:116:ARG:N	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:A:209:MET:HE1	1:A:217:VAL:HG13	1.96	0.47
1:A:283:ASP:HB3	1:A:286:GLY:H	1.79	0.47
1:A:289:MET:HE3	1:A:289:MET:HA	1.96	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: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:448:ASP:O	1:A:449:ASN:C	2.58	0.47
1:B:209:MET:HE1	1:B:217:VAL:HG13	1.96	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:493:ARG:O	1:A:494:PRO:C	2.58	0.46
1:D:273:ARG:NH2	1:D:295:ASP:OD2	2.47	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:209:MET:HE1	1:D:217:VAL:HG13	1.97	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:39:LEU:HG	1:D:134:LEU:HD22	1.97	0.46
1:A:395:HIS:HA	1:A:432:MET:HE1	1.98	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:B:531:LEU:C	1:B:533:ARG:N	2.74	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
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:70:GLN:N	1:A:70:GLN:OE1	2.48	0.45
1:A:411:ASP:OD2	1:A:412:ARG:N	2.43	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:51:PRO:O	1:B:52:ALA:HB2	2.17	0.45
1:B:297:ILE:CD1	1:B:357:THR:HG21	2.47	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:B:272:LEU:O	1:B:273:ARG:C	2.58	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:47:LEU:HD22	1:D:54:ARG:NH1	2.32	0.44
1:D:446:THR:HG23	1:D:484:ALA:HB2	2.00	0.44
1:B:446:THR:CG2	1:B:484:ALA:CB	2.92	0.44
1:C:70:GLN:N	1:C:70:GLN:OE1	2.50	0.44
1:C:327:ASP:OD1	1:C:333:HIS:HE1	2.01	0.44
1:A:327:ASP:HB2	1:A:328:PRO:HD2	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:29:ASN:C	1:A:29:ASN:HD22	2.25	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: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:C:493:ARG:O	1:C:494:PRO:C	2.61	0.43
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:448:ASP:O	1:D:449:ASN:C	2.61	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
1:A:174:VAL:HG12	1:A:214:VAL:HA	2.00	0.43
1:A:209:MET:HE1	1:A:217:VAL:HG22	1.94	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:70:GLN:OE1	1:B:70:GLN:N	2.52	0.43
1:B:374:VAL:HG22	1:B:377:ARG:HB2	2.01	0.43
1:D:493:ARG:O	1:D:494:PRO:C	2.61	0.43
1:A:151:ILE:HD12	1:A:161:THR:HG22	2.01	0.43
1:A:281:ILE:C	1:A:283:ASP:H	2.27	0.42
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: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:412:ARG:HD2	1:A:497:VAL:CG1	2.49	0.42
1:A:437:ALA:HB2	1:A:466:ALA:HA	2.01	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:70:GLN:OE1	1:D:70:GLN:N	2.49	0.42
1:D:107:PRO:HA	1:D:110:VAL:HG22	2.01	0.42
1:A:446:THR:HB	1:A:447:ASP:H	1.64	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:B:508:GLY:HA2	1:B:516:ARG:O	2.20	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
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:D:289:MET:HE3	1:D:289:MET:CA	2.46	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:B:481:ARG:HH21	1:B:520:ASP:CG	2.29	0.41
1:C:139:TYR:O	1:C:142:PRO:HD3	2.21	0.41
1:B:448:ASP:O	1:B:449:ASN:C	2.63	0.41
1:C:446:THR:HG21	1:C:484:ALA:HB3	2.03	0.41
1:A:307:HIS:HB3	1:A:328:PRO:HG3	2.02	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:B:283:ASP:HB3	1:B:286:GLY:H	1.85	0.41
1:D:29:ASN:HD22	1:D:29:ASN:C	2.29	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: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%)	5	26
1	B	505/535 (94%)	469 (93%)	22 (4%)	14 (3%)	4	21
1	C	422/535 (79%)	407 (96%)	12 (3%)	3 (1%)	18	53
1	D	457/535 (85%)	436 (95%)	17 (4%)	4 (1%)	14	48
All	All	1879/2140 (88%)	1770 (94%)	77 (4%)	32 (2%)	7	32

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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%)	300 (85%)	53 (15%)	3	14
1	B	356/382 (93%)	304 (85%)	52 (15%)	3	15
1	C	301/382 (79%)	256 (85%)	45 (15%)	3	14
1	D	330/382 (86%)	281 (85%)	49 (15%)	3	15
All	All	1340/1528 (88%)	1141 (85%)	199 (15%)	3	15

All (199) 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	77	LEU
1	A	82	THR
1	A	85	THR
1	A	86	THR
1	A	104	LEU
1	A	123	VAL
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
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	381	ILE
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	435	ILE
1	A	439	LEU
1	A	443	VAL
1	A	446	THR
1	A	451	ARG
1	A	475	VAL
1	A	476	VAL
1	A	497	VAL
1	A	499	LEU
1	A	510	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	523	GLU
1	A	531	LEU
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	56	VAL
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
1	B	116	ARG
1	B	123	VAL
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	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	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	435	ILE
1	B	438	GLN
1	B	442	LEU
1	B	443	VAL
1	B	446	THR
1	B	451	ARG
1	B	475	VAL
1	B	476	VAL
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	32	VAL
1	C	35	ARG
1	C	39	LEU
1	C	47	LEU
1	C	56	VAL
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	123	VAL
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	363	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	366	VAL
1	C	369	LEU
1	C	373	ARG
1	C	374	VAL
1	C	378	LEU
1	C	405	THR
1	C	407	LEU
1	C	416	VAL
1	C	435	ILE
1	C	442	LEU
1	C	443	VAL
1	C	446	THR
1	C	475	VAL
1	C	476	VAL
1	C	497	VAL
1	D	29	ASN
1	D	31	VAL
1	D	32	VAL
1	D	35	ARG
1	D	39	LEU
1	D	47	LEU
1	D	53	GLN
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	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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	289	MET
1	D	303	ASP
1	D	331	VAL
1	D	337	ILE
1	D	358	VAL
1	D	363	GLU
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	435	ILE
1	D	442	LEU
1	D	443	VAL
1	D	446	THR
1	D	451	ARG
1	D	475	VAL
1	D	476	VAL
1	D	497	VAL
1	D	523	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	29	ASN
1	A	203	GLN
1	A	224	HIS
1	A	307	HIS
1	A	333	HIS
1	A	380	GLN
1	B	29	ASN
1	B	91	HIS
1	B	203	GLN
1	B	224	HIS
1	B	307	HIS
1	B	333	HIS
1	C	29	ASN
1	C	203	GLN
1	C	307	HIS
1	C	333	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	380	GLN
1	D	29	ASN
1	D	91	HIS
1	D	203	GLN
1	D	224	HIS
1	D	307	HIS
1	D	333	HIS
1	D	380	GLN

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	A	262	1	10,11,12	0.84	1 (10%)	6,12,14	1.13	1 (16%)
1	KCX	D	262	1	10,11,12	1.09	1 (10%)	6,12,14	0.70	0
1	KCX	B	262	1	10,11,12	1.24	2 (20%)	6,12,14	0.77	0
1	KCX	C	262	1	10,11,12	1.14	1 (10%)	6,12,14	0.61	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	A	262	1	-	0/9/10/12	-
1	KCX	D	262	1	-	0/9/10/12	-
1	KCX	B	262	1	-	1/9/10/12	-

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	KCX	C	262	1	-	1/9/10/12	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	262	KCX	OQ1-CX	2.65	1.26	1.21
1	D	262	KCX	OQ1-CX	2.53	1.26	1.21
1	B	262	KCX	OQ1-CX	2.34	1.26	1.21
1	B	262	KCX	CE-NZ	2.23	1.51	1.46
1	A	262	KCX	OQ1-CX	2.03	1.25	1.21

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	262	KCX	OQ1-CX-NZ	-2.64	120.92	124.92

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	262	KCX	O-C-CA-CB
1	C	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 oligosaccharides 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	B	1498	3	59,60,60	1.33	4 (6%)	82,88,88	2.02	19 (23%)
2	UAG	D	1498	3	59,60,60	1.24	5 (8%)	82,88,88	1.97	16 (19%)
2	UAG	C	1498	3	59,60,60	1.45	5 (8%)	82,88,88	1.99	19 (23%)
2	UAG	A	1498	3	59,60,60	1.31	5 (8%)	82,88,88	1.92	18 (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
2	UAG	B	1498	3	-	10/55/92/92	0/3/3/3
2	UAG	D	1498	3	-	11/55/92/92	0/3/3/3
2	UAG	C	1498	3	-	12/55/92/92	0/3/3/3
2	UAG	A	1498	3	-	10/55/92/92	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1498	UAG	PA-O3A	6.56	1.66	1.59
2	B	1498	UAG	PB-O3A	5.58	1.65	1.59
2	D	1498	UAG	PA-O3A	4.91	1.64	1.59
2	A	1498	UAG	PA-O1A	4.37	1.66	1.50
2	A	1498	UAG	PA-O3A	4.32	1.64	1.59
2	C	1498	UAG	PA-O1A	3.29	1.62	1.50
2	C	1498	UAG	PB-O1B	3.22	1.62	1.50
2	C	1498	UAG	C2-N1	3.04	1.43	1.38
2	A	1498	UAG	PB-O1B	3.03	1.61	1.50
2	B	1498	UAG	C2-N1	2.98	1.43	1.38
2	B	1498	UAG	PB-O1B	2.80	1.60	1.50
2	D	1498	UAG	PB-O1B	2.65	1.60	1.50
2	A	1498	UAG	C5-C4	-2.64	1.38	1.43
2	C	1498	UAG	C5-C4	-2.30	1.38	1.43
2	B	1498	UAG	PA-O3A	2.28	1.62	1.59
2	D	1498	UAG	PA-O5B	2.13	1.67	1.59
2	D	1498	UAG	C5-C4	-2.08	1.39	1.43
2	D	1498	UAG	PA-O1A	2.08	1.58	1.50
2	A	1498	UAG	PB-O3A	2.07	1.61	1.59

All (72) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1498	UAG	O5B-PA-O1A	-8.69	74.51	108.94
2	A	1498	UAG	O5B-PA-O1A	-8.46	75.42	108.94
2	C	1498	UAG	O5B-PA-O1A	-8.16	76.57	108.94
2	B	1498	UAG	O5B-PA-O1A	-6.56	82.94	108.94
2	B	1498	UAG	C4-N3-C2	-6.46	118.60	126.61
2	B	1498	UAG	C5-C4-N3	5.86	123.01	114.80
2	C	1498	UAG	C5-C4-N3	5.71	122.80	114.80
2	C	1498	UAG	C4-N3-C2	-5.60	119.66	126.61
2	D	1498	UAG	C4-N3-C2	-5.42	119.88	126.61
2	B	1498	UAG	O2A-PA-O3A	4.99	120.75	107.27
2	D	1498	UAG	C5-C4-N3	4.86	121.61	114.80
2	A	1498	UAG	C4-N3-C2	-4.81	120.64	126.61
2	C	1498	UAG	O2A-PA-O5B	-4.50	87.16	107.57
2	C	1498	UAG	O2A-PA-O3A	4.44	119.27	107.27
2	A	1498	UAG	O2A-PA-O5B	-4.40	87.63	107.57
2	A	1498	UAG	C5-C4-N3	4.36	120.90	114.80
2	D	1498	UAG	O2A-PA-O3A	4.33	118.99	107.27
2	D	1498	UAG	O2A-PA-O5B	-4.30	88.06	107.57
2	B	1498	UAG	O2A-PA-O5B	-4.17	88.65	107.57
2	B	1498	UAG	O3A-PA-O1A	4.08	122.97	110.70
2	A	1498	UAG	O2A-PA-O3A	4.01	118.12	107.27
2	B	1498	UAG	C2B-C1B-N1	-3.80	102.68	113.25
2	C	1498	UAG	O4-C4-C5	-3.73	118.74	125.16
2	B	1498	UAG	O4-C4-C5	-3.68	118.82	125.16
2	D	1498	UAG	C2B-C1B-N1	-3.61	103.19	113.25
2	C	1498	UAG	C2B-C1B-N1	-3.55	103.38	113.25
2	B	1498	UAG	N3-C2-N1	3.48	119.42	114.89
2	B	1498	UAG	C25-C24-C28	-3.47	102.11	110.35
2	A	1498	UAG	C25-C24-N5	-3.43	104.12	110.91
2	A	1498	UAG	C2B-C1B-N1	-3.40	103.78	113.25
2	D	1498	UAG	O2B-PB-O3A	3.35	116.33	107.27
2	A	1498	UAG	O2B-PB-O3A	3.30	116.19	107.27
2	C	1498	UAG	C3'-C2'-N2'	-3.20	105.80	110.91
2	D	1498	UAG	N3-C2-N1	3.06	118.87	114.89
2	D	1498	UAG	C25-C24-N5	-3.01	104.95	110.91
2	D	1498	UAG	O4-C4-C5	-3.00	119.99	125.16
2	C	1498	UAG	O2B-PB-O3A	2.96	115.27	107.27
2	B	1498	UAG	C24-N5-C22	2.91	127.89	121.65
2	A	1498	UAG	N3-C2-N1	2.90	118.67	114.89
2	A	1498	UAG	O4-C4-C5	-2.87	120.22	125.16
2	C	1498	UAG	C8'-C7'-N2'	-2.83	111.42	116.12
2	B	1498	UAG	O2B-PB-O3A	2.73	114.65	107.27

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1498	UAG	O20-C27-C26	-2.73	114.43	123.09
2	D	1498	UAG	O7'-C7'-N2'	2.70	126.75	121.98
2	B	1498	UAG	C3'-C2'-N2'	-2.63	106.72	110.91
2	C	1498	UAG	N3-C2-N1	2.60	118.27	114.89
2	C	1498	UAG	C24-N5-C22	2.56	127.15	121.65
2	D	1498	UAG	O5'-C1'-O1'	2.56	114.71	111.36
2	A	1498	UAG	C24-N5-C22	2.52	127.07	121.65
2	B	1498	UAG	O20-C27-C26	-2.49	115.20	123.09
2	A	1498	UAG	C6'-C5'-C4'	-2.44	107.03	113.02
2	C	1498	UAG	C25-C24-N5	-2.42	106.12	110.91
2	B	1498	UAG	O1'-PB-O1B	-2.40	102.14	109.81
2	A	1498	UAG	O20-C27-C26	-2.40	115.49	123.09
2	C	1498	UAG	O20-C27-C26	-2.39	115.50	123.09
2	C	1498	UAG	C25-C24-C28	-2.39	104.69	110.35
2	B	1498	UAG	C25-C26-C27	-2.34	106.24	112.49
2	A	1498	UAG	O1'-PB-O1B	-2.34	102.33	109.81
2	D	1498	UAG	C1'-C2'-N2'	-2.33	107.01	110.92
2	B	1498	UAG	C25-C24-N5	-2.24	106.47	110.91
2	D	1498	UAG	C24-N5-C22	2.22	126.42	121.65
2	C	1498	UAG	C1B-N1-C2	2.20	121.54	117.59
2	A	1498	UAG	O7'-C7'-N2'	2.19	125.84	121.98
2	A	1498	UAG	C3'-C2'-N2'	-2.18	107.43	110.91
2	A	1498	UAG	C8'-C7'-N2'	-2.12	112.61	116.12
2	B	1498	UAG	O7'-C7'-N2'	2.11	125.70	121.98
2	C	1498	UAG	C25-C26-C27	-2.10	106.89	112.49
2	C	1498	UAG	O7'-C7'-N2'	2.08	125.65	121.98
2	C	1498	UAG	C20-C18-C19	-2.05	106.00	111.11
2	A	1498	UAG	C1B-N1-C2	2.02	121.23	117.59
2	B	1498	UAG	C8'-C7'-N2'	-2.02	112.77	116.12
2	D	1498	UAG	C25-C24-C28	-2.02	105.57	110.35

There are no chirality outliers.

All (43) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1498	UAG	N5-C24-C25-C26
2	C	1498	UAG	C20-C18-O3'-C3'
2	D	1498	UAG	N5-C24-C25-C26
2	C	1498	UAG	N5-C24-C25-C26
2	A	1498	UAG	C28-C24-N5-C22
2	D	1498	UAG	C28-C24-N5-C22
2	A	1498	UAG	C28-C24-C25-C26

Continued on next page...

Continued from previous page...

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

There are no ring outliers.

3 monomers are involved in 4 short contacts:

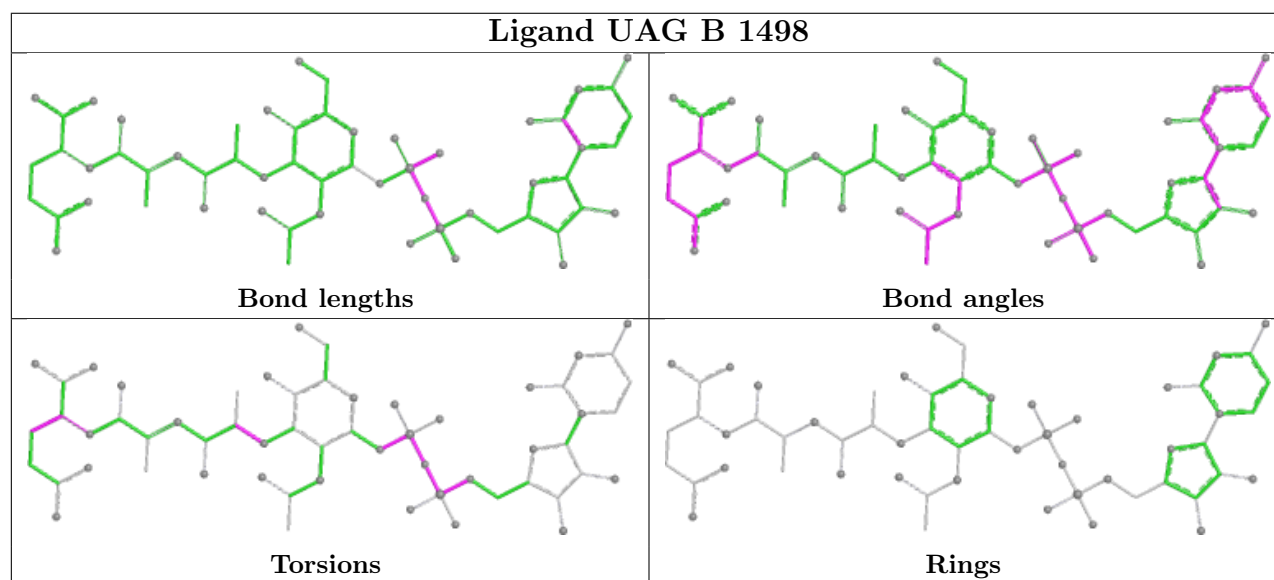
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	1498	UAG	1	0

Continued on next page...

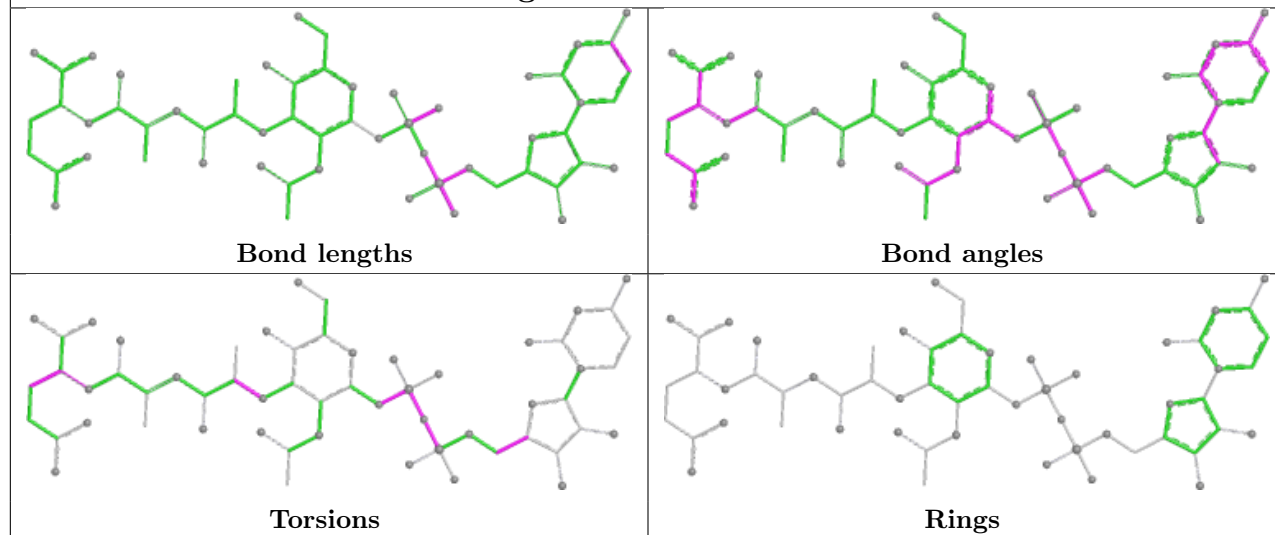
Continued from previous page...

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

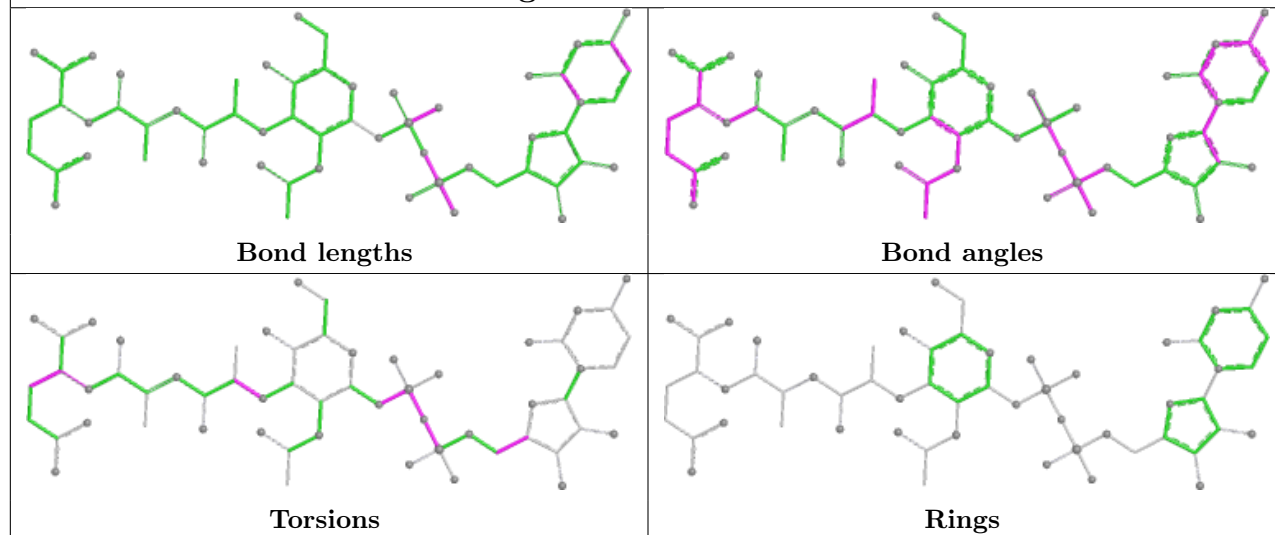
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



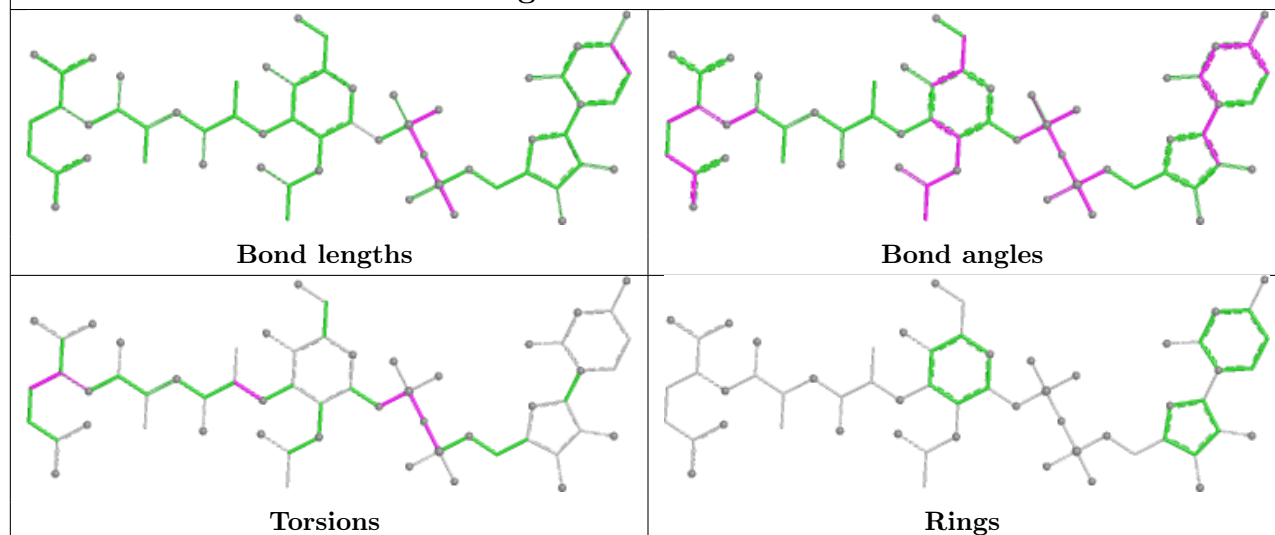
Ligand UAG D 1498



Ligand UAG C 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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	503/535 (94%)	-1.55	0 100 100	3, 15, 25, 42	0
1	B	507/535 (94%)	-1.54	0 100 100	3, 14, 27, 37	0
1	C	438/535 (81%)	-1.30	0 100 100	2, 13, 32, 37	0
1	D	467/535 (87%)	-1.40	0 100 100	3, 16, 28, 43	0
All	All	1915/2140 (89%)	-1.45	0 100 100	2, 14, 29, 43	0

There are no RSRZ outliers to report.

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	KCX	A	262	12/13	0.99	0.03	13,14,20,21	0
1	KCX	B	262	12/13	0.99	0.04	10,11,17,18	0
1	KCX	C	262	12/13	1.00	0.03	9,11,20,21	0
1	KCX	D	262	12/13	1.00	0.02	11,13,22,22	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands ⓘ

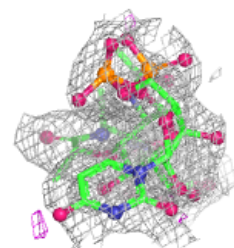
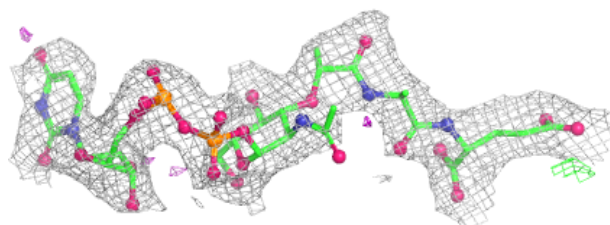
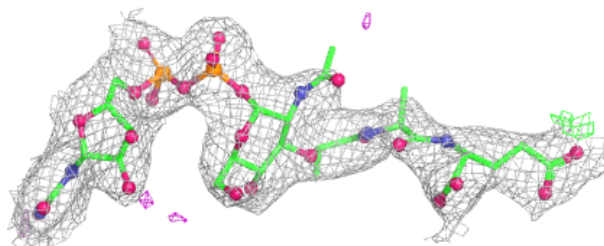
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	MG	C	1499	1/1	0.97	0.06	35,35,35,35	0
3	MG	A	1499	1/1	0.98	0.08	37,37,37,37	0
2	UAG	C	1498	58/58	0.99	0.04	36,43,46,49	0
2	UAG	D	1498	58/58	0.99	0.03	30,35,42,47	0
2	UAG	A	1498	58/58	0.99	0.03	26,36,42,45	0
3	MG	B	1499	1/1	0.99	0.06	33,33,33,33	0
2	UAG	B	1498	58/58	0.99	0.03	31,34,42,45	0
3	MG	D	1499	1/1	0.99	0.03	38,38,38,38	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.

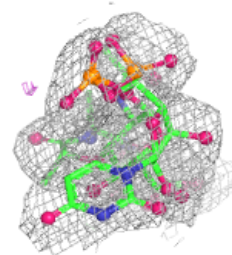
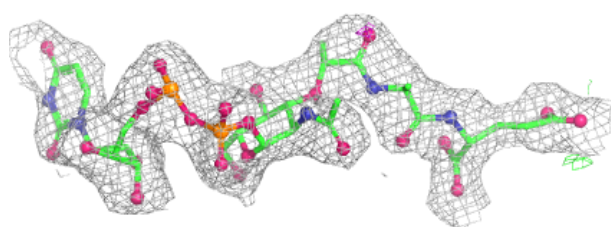
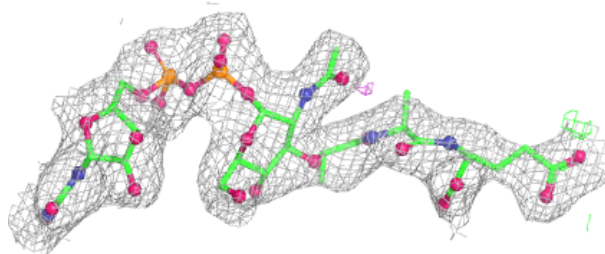
Electron density around UAG C 1498:

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

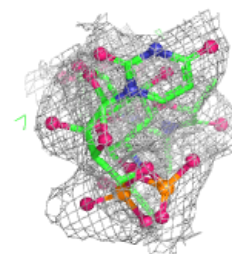
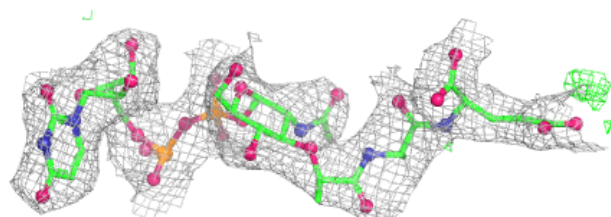
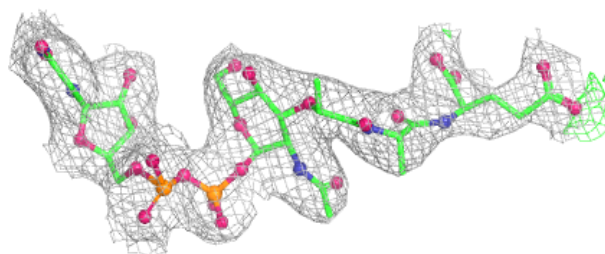


Electron density around UAG D 1498:

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

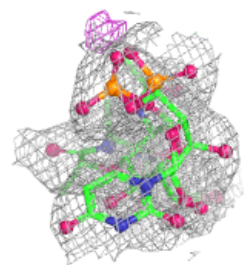
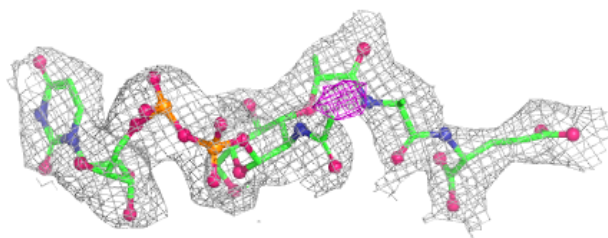
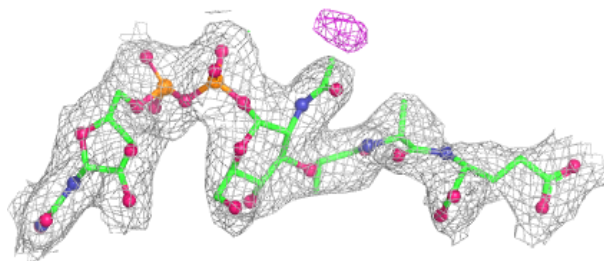
**Electron density around UAG A 1498:**

$2mF_o-DF_c$ (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)



6.5 Other polymers [i](#)

There are no such residues in this entry.