



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:13 PM UTC

PDB ID : 4CQN / pdb_00004cqn
Title : Crystal structure of the E.coli LeuRS-tRNA complex with the non- cognate
isoleucyl adenylate analogue
Authors : Palencia, A.; Cusack, S.; Cvetic, N.; Haslaz, I.; Gruic-Sovulj, I.
Deposited on : 2014-02-20
Resolution : 2.50 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

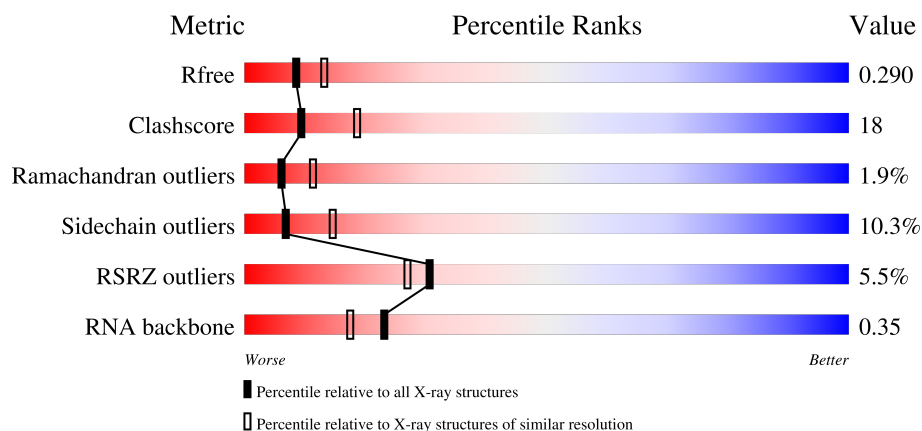
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

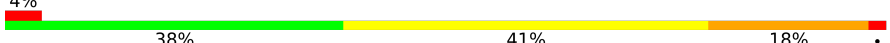
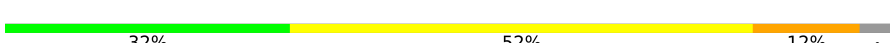
The reported resolution of this entry is 2.50 Å.

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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)
RNA backbone	3983	1003 (2.78-2.22)

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	880	 53% 39% 5% .
1	D	880	 11% 58% 35% 5% .
2	B	82	 4% 38% 41% 18% .
2	E	82	 32% 52% 12% .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	ILA	A	1863	X	-	X	-
4	ILA	D	1863	X	-	-	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 17558 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 LEUCINE-TRNA LIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	860	Total	C	N	O	S	0	2	0
			6844	4345	1161	1293	45			
1	D	860	Total	C	N	O	S	0	0	0
			6834	4339	1158	1292	45			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	expression tag	UNP P07813
A	-18	GLY	-	expression tag	UNP P07813
A	-17	SER	-	expression tag	UNP P07813
A	-16	SER	-	expression tag	UNP P07813
A	-15	HIS	-	expression tag	UNP P07813
A	-14	HIS	-	expression tag	UNP P07813
A	-13	HIS	-	expression tag	UNP P07813
A	-12	HIS	-	expression tag	UNP P07813
A	-11	HIS	-	expression tag	UNP P07813
A	-10	HIS	-	expression tag	UNP P07813
A	-9	SER	-	expression tag	UNP P07813
A	-8	SER	-	expression tag	UNP P07813
A	-7	GLY	-	expression tag	UNP P07813
A	-6	LEU	-	expression tag	UNP P07813
A	-5	VAL	-	expression tag	UNP P07813
A	-4	PRO	-	expression tag	UNP P07813
A	-3	ARG	-	expression tag	UNP P07813
A	-2	GLY	-	expression tag	UNP P07813
A	-1	SER	-	expression tag	UNP P07813
A	0	HIS	-	expression tag	UNP P07813
D	-19	MET	-	expression tag	UNP P07813
D	-18	GLY	-	expression tag	UNP P07813
D	-17	SER	-	expression tag	UNP P07813
D	-16	SER	-	expression tag	UNP P07813
D	-15	HIS	-	expression tag	UNP P07813

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	-14	HIS	-	expression tag	UNP P07813
D	-13	HIS	-	expression tag	UNP P07813
D	-12	HIS	-	expression tag	UNP P07813
D	-11	HIS	-	expression tag	UNP P07813
D	-10	HIS	-	expression tag	UNP P07813
D	-9	SER	-	expression tag	UNP P07813
D	-8	SER	-	expression tag	UNP P07813
D	-7	GLY	-	expression tag	UNP P07813
D	-6	LEU	-	expression tag	UNP P07813
D	-5	VAL	-	expression tag	UNP P07813
D	-4	PRO	-	expression tag	UNP P07813
D	-3	ARG	-	expression tag	UNP P07813
D	-2	GLY	-	expression tag	UNP P07813
D	-1	SER	-	expression tag	UNP P07813
D	0	HIS	-	expression tag	UNP P07813

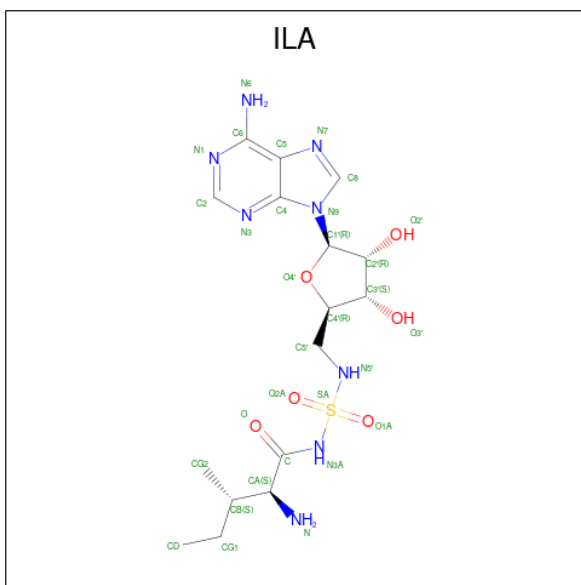
- Molecule 2 is a RNA chain called ESCHERICHIA COLI TRNA-LEU UAA ISOACCEPTOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	82	Total	C	N	O	P	0	0	0
			1755	781	317	575	82			
2	E	79	Total	C	N	O	P	0	0	0
			1691	752	305	555	79			

- Molecule 3 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Zn	0	0
			1	1		
3	D	1	Total	Zn	0	0
			1	1		

- Molecule 4 is N-[ISOLEUCINYL]-N'-[ADENOSYL]-DIAMINOSUFONE (CCD ID: ILA) (formula: C₁₆H₂₆N₈O₆S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 31	C 16	N 8	O 6	S 1	0	0
4	A	1	Total 31	C 16	N 8	O 6	S 1	0	0
4	D	1	Total 31	C 16	N 8	O 6	S 1	0	0
4	D	1	Total 31	C 16	N 8	O 6	S 1	0	0

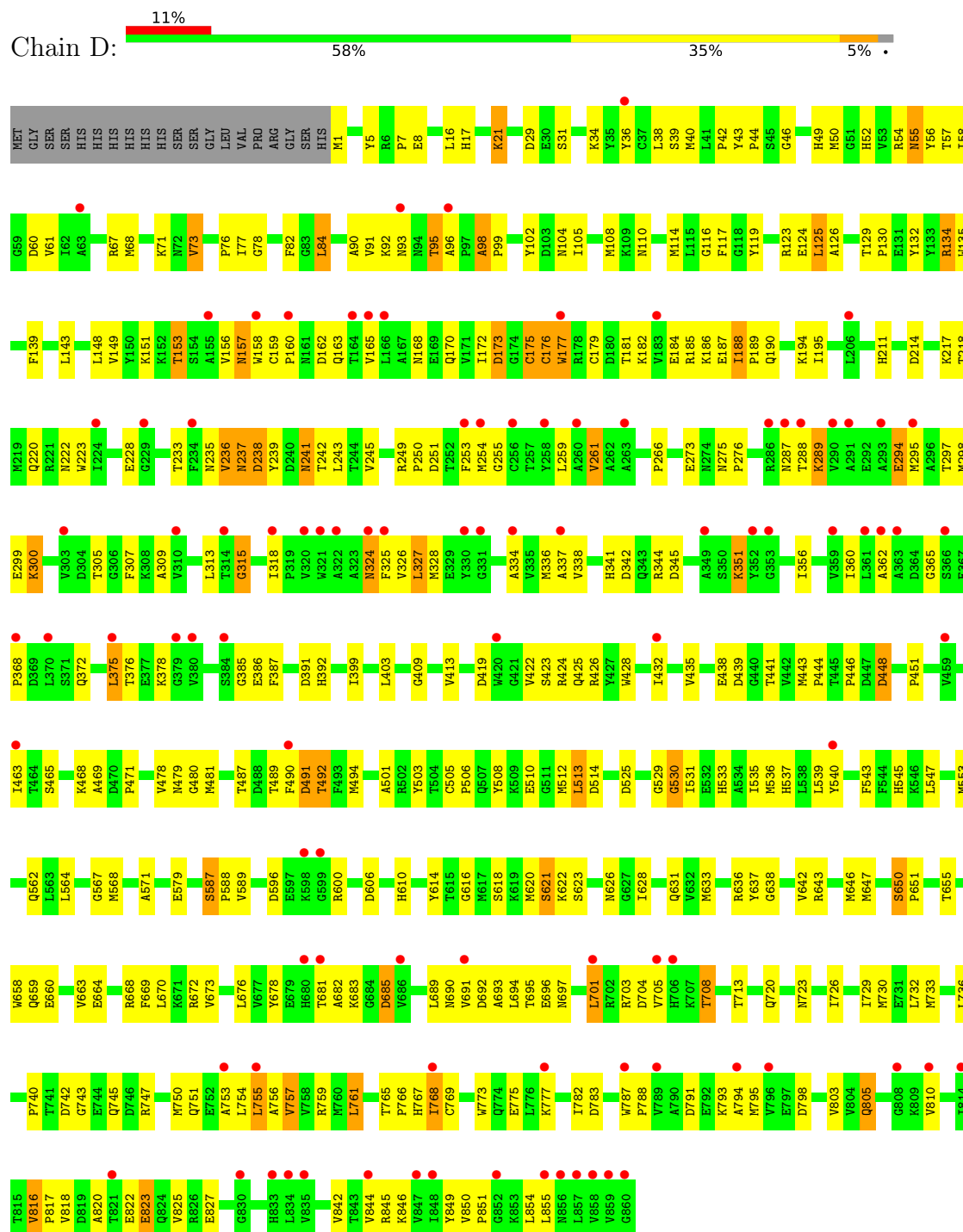
- Molecule 5 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	B	1	Total Mg 1 1	0	0
5	E	1	Total Mg 1 1	0	0

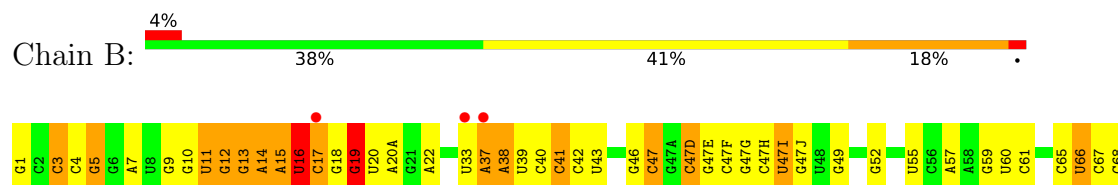
- Molecule 6 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	233	Total O 233 233	0	0
6	B	57	Total O 57 57	0	0
6	D	16	Total O 16 16	0	0

- Molecule 1: LEUCINE-TRNA LIGASE

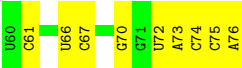
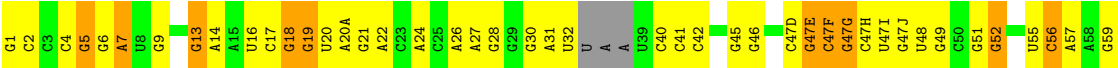


- Molecule 2: ESCHERICHIA COLI TRNA-LEU UAA ISOACCEPTOR.





● Molecule 2: ESCHERICHIA COLI TRNA-LEU UAA ISOACCEPTOR



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	155.62Å 67.58Å 224.59Å 90.00° 105.00° 90.00°	Depositor
Resolution (Å)	46.49 – 2.50 46.49 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.1 (46.49-2.50) 97.1 (46.49-2.50)	Depositor EDS
R_{merge}	0.17	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.7.0029	Depositor
R, R_{free}	0.214 , 0.290 0.214 , 0.290	Depositor DCC
R_{free} test set	3828 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	28.2	Xtriage
Anisotropy	0.592	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 44.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	17558	wwPDB-VP
Average B, all atoms (Å ²)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.32% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.93	1/7014 (0.0%)	1.19	37/9520 (0.4%)
1	D	0.50	0/6995	0.92	8/9495 (0.1%)
2	B	0.55	1/1959 (0.1%)	1.06	18/3047 (0.6%)
2	E	0.41	0/1887	0.75	0/2935
All	All	0.70	2/17855 (0.0%)	1.03	63/24997 (0.3%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	544	PHE	N-CA	-6.80	1.38	1.46
2	B	12	G	O3'-P	-5.18	1.53	1.61

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	20(A)	A	C4'-C3'-O3'	-7.86	101.20	113.00
2	B	75	C	C2'-C3'-O3'	-7.40	102.60	113.70
1	A	717	GLY	N-CA-C	7.30	123.72	114.66
2	B	5	G	C3'-C2'-O2'	6.83	120.94	110.70
2	B	5	G	C1'-C2'-O2'	6.59	118.28	108.40
1	D	73	VAL	N-CA-C	6.56	117.31	107.80
2	B	22	A	C2'-C3'-O3'	-6.50	103.95	113.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	47(I)	U	C3'-C2'-O2'	6.48	120.43	110.70
1	A	644	LEU	N-CA-C	-6.46	104.32	111.36
1	D	241	ASN	N-CA-C	6.46	117.97	108.86
1	A	253	PHE	N-CA-C	6.42	118.28	111.28
1	A	742	ASP	N-CA-C	-6.40	105.48	113.55
1	A	741	THR	N-CA-C	6.30	117.85	110.41
1	A	756	ALA	N-CA-C	-6.30	103.94	111.69
1	A	373	GLN	N-CA-C	6.22	117.68	108.60
1	A	212	TRP	CA-C-N	-6.19	113.30	119.92
1	A	212	TRP	C-N-CA	-6.19	113.30	119.92
1	D	92	LYS	N-CA-C	-6.18	104.23	110.97
1	A	491	ASP	N-CA-C	-6.09	101.29	110.24
1	A	850	VAL	CA-C-N	6.06	126.42	119.93
1	A	850	VAL	C-N-CA	6.06	126.42	119.93
1	A	760	MET	N-CA-C	-6.02	104.83	111.82
1	A	666	ALA	N-CA-C	-6.01	104.81	111.36
1	A	806	VAL	N-CA-C	-5.99	99.73	108.11
2	B	3	C	C1'-C2'-O2'	-5.95	99.47	108.40
2	B	61	C	C4'-C3'-O3'	-5.86	104.21	113.00
1	A	440	GLY	N-CA-C	-5.77	106.56	114.64
2	B	52	G	C1'-C2'-O2'	5.77	117.06	108.40
2	B	13	G	C1'-C2'-O2'	-5.75	99.78	108.40
1	A	319	PRO	CA-C-N	-5.72	115.58	122.90
1	A	319	PRO	C-N-CA	-5.72	115.58	122.90
1	A	709	ILE	N-CA-C	-5.69	104.95	110.42
1	D	324	ASN	N-CA-C	5.66	117.14	110.97
1	A	665	GLY	N-CA-C	-5.61	105.99	112.50
2	B	16	U	C4'-C3'-O3'	5.47	117.60	109.40
2	B	65	C	C2'-C3'-O3'	5.46	121.89	113.70
1	D	631	GLN	N-CA-C	5.46	117.23	111.28
1	A	109	LYS	N-CA-C	-5.44	104.59	111.11
1	A	452	VAL	N-CA-C	-5.42	99.35	107.37
1	A	204	ASN	N-CA-C	5.38	117.14	111.28
2	B	14	A	C3'-C2'-O2'	5.37	118.76	110.70
1	A	73	VAL	N-CA-C	5.32	115.25	107.37
2	B	19	G	O4'-C4'-C3'	-5.30	100.80	106.10
1	A	427	TYR	N-CA-C	5.29	116.85	111.14
1	A	305	THR	N-CA-C	-5.29	107.00	113.50
1	A	250	PRO	N-CA-C	-5.25	107.01	113.84
1	A	706	HIS	N-CA-C	5.22	117.88	111.82
2	B	19	G	C4'-C3'-O3'	-5.22	101.56	109.40
1	A	355	ASN	N-CA-C	5.22	118.05	109.76

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	297	THR	CB-CA-C	-5.21	99.75	110.38
2	B	13	G	C4'-C3'-O3'	-5.20	105.20	113.00
1	D	587	SER	CA-C-N	5.18	126.32	119.84
1	D	587	SER	C-N-CA	5.18	126.32	119.84
1	A	785	ALA	CA-C-N	-5.17	114.66	120.14
1	A	785	ALA	C-N-CA	-5.17	114.66	120.14
1	A	663	VAL	CB-CA-C	-5.16	105.28	111.88
1	D	798	ASP	N-CA-C	-5.12	107.20	113.50
2	B	5	G	C4'-C3'-O3'	-5.12	105.33	113.00
1	A	827	GLU	N-CA-C	-5.11	105.79	111.36
1	A	770	PHE	N-CA-C	-5.09	105.38	111.03
2	B	68	C	C4'-C3'-O3'	5.08	120.62	113.00
1	A	778	GLY	N-CA-C	-5.06	106.77	112.33
1	A	10	ILE	N-CA-C	5.02	119.78	109.34

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	592	ILE	Peptide
1	A	80	ASP	Peptide

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	6844	0	6696	279	0
1	D	6834	0	6683	238	0
2	B	1755	0	890	38	0
2	E	1691	0	858	38	0
3	A	1	0	0	0	0
3	D	1	0	0	0	0
4	A	62	0	52	12	0
4	D	62	0	52	7	0
5	B	1	0	0	0	0
5	E	1	0	0	0	0
6	A	233	0	0	15	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	B	57	0	0	1	0
6	D	16	0	0	2	0
All	All	17558	0	15231	581	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 18.

All (581) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:VAL:HG11	1:A:494:MET:HE1	1.36	1.06
1:A:267:LEU:HD21	1:A:305:THR:HG21	1.40	1.00
1:A:553:MET:HE2	6:A:2052:HOH:O	1.59	0.98
1:A:801:LEU:C	1:A:801:LEU:HD23	1.90	0.97
1:A:342:ASP:HB2	4:A:1863:ILA:CG2	1.96	0.95
2:B:41:C:H5''	2:B:41:C:H6	1.32	0.95
1:A:553:MET:CE	6:A:2052:HOH:O	2.10	0.94
2:B:40:C:H2'	2:B:41:C:H5''	1.51	0.93
1:A:342:ASP:OD2	4:A:1863:ILA:HG22	1.72	0.89
1:A:676:LEU:HD23	1:A:733:MET:HE1	1.54	0.88
1:D:261:VAL:HG23	1:D:334:ALA:HB2	1.57	0.86
1:A:22:ARG:HB3	1:A:25:GLU:HG3	1.58	0.85
1:D:179:CYS:HG	1:D:181:THR:HG1	1.15	0.85
1:A:295:MET:HE1	1:A:325:PHE:HA	1.55	0.85
1:A:34:LYS:O	1:A:34:LYS:HD3	1.75	0.85
1:A:342:ASP:HB2	4:A:1863:ILA:HG21	1.57	0.85
1:A:267:LEU:CD2	1:A:305:THR:HG21	2.07	0.83
1:A:165:VAL:HG21	1:A:425:GLN:HG3	1.61	0.83
1:D:214:ASP:HA	1:D:217:LYS:HE2	1.60	0.81
1:A:139:PHE:CE1	1:A:553:MET:HE1	2.17	0.80
2:B:41:C:H6	2:B:41:C:C5'	1.93	0.80
1:A:512:MET:O	1:A:513:LEU:HD23	1.81	0.80
1:A:532:GLU:H	1:A:568:MET:HE3	1.46	0.80
1:D:438:GLU:HB3	1:D:481:MET:HE2	1.65	0.78
1:A:67:ARG:NH1	1:A:784:ASN:OD1	2.16	0.78
1:D:289:LYS:HB3	1:D:294:GLU:HB3	1.65	0.78
2:B:59:G:H2'	2:B:60:U:H5'	1.67	0.77
1:A:422:VAL:HG11	1:A:494:MET:CE	2.13	0.77
1:A:507:GLN:HA	1:A:507:GLN:OE1	1.86	0.75
2:E:20(A):A:N7	2:E:47(J):G:C2	2.53	0.75
1:D:223:TRP:HH2	2:E:72:U:H4'	1.49	0.75

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:136:GLU:OE1	1:A:495:GLU:HG3	1.87	0.74
1:A:305:THR:HG22	1:A:307:PHE:HD2	1.52	0.74
1:A:617:MET:O	2:B:69:G:H5'	1.86	0.74
1:A:606:ASP:OD1	1:A:610:HIS:HB2	1.87	0.74
1:A:633:MET:HE3	1:A:663:VAL:CG1	2.18	0.74
2:E:41:C:H2'	2:E:42:C:H6	1.53	0.74
1:D:614:TYR:CZ	1:D:616:GLY:HA2	2.23	0.73
1:D:195:ILE:HG22	1:D:419:ASP:HA	1.70	0.73
1:D:223:TRP:CH2	2:E:72:U:H4'	2.22	0.73
1:D:673:VAL:HG22	1:D:733:MET:HE2	1.70	0.73
1:A:336:MET:O	4:A:1863:ILA:N	2.22	0.73
1:A:716:ILE:HG23	1:A:722:PHE:HE1	1.52	0.73
1:D:360:ILE:O	1:D:368:PRO:HG3	1.89	0.73
1:A:617:MET:CE	1:A:657:GLU:HB3	2.19	0.73
1:D:753:ALA:O	1:D:757:VAL:HG23	1.88	0.72
1:D:139:PHE:CD2	1:D:143:LEU:HD11	2.24	0.72
1:D:664:GLU:HG3	1:D:668:ARG:HE	1.53	0.72
1:D:123:ARG:HA	1:D:506:PRO:HG3	1.72	0.71
1:A:429:GLY:O	1:A:454:LEU:HD22	1.90	0.71
1:A:617:MET:HE3	1:A:657:GLU:HB3	1.72	0.71
1:D:40:MET:SD	1:D:529:GLY:HA3	2.30	0.71
1:D:729:ILE:HG21	1:D:761:LEU:HD21	1.73	0.71
1:A:633:MET:HE3	1:A:663:VAL:HG11	1.72	0.70
1:D:805:GLN:OE1	1:D:854:LEU:HD21	1.91	0.70
1:A:536:MET:HG3	6:A:2179:HOH:O	1.90	0.70
1:A:34:LYS:HD3	1:A:34:LYS:C	2.15	0.70
1:A:660:GLU:O	1:A:663:VAL:HG22	1.91	0.70
1:A:305:THR:CG2	1:A:307:PHE:HD2	2.05	0.70
2:B:59:G:C2'	2:B:60:U:H5'	2.22	0.69
1:A:43:TYR:CD1	1:A:44:PRO:HD2	2.27	0.69
1:D:84:LEU:HD23	1:D:426:ARG:HD3	1.75	0.69
1:A:606:ASP:CG	1:A:610:HIS:HB2	2.17	0.69
1:A:139:PHE:HE1	1:A:553:MET:CE	2.05	0.69
1:A:801:LEU:C	1:A:801:LEU:CD2	2.66	0.69
1:A:532:GLU:H	1:A:568:MET:CE	2.06	0.68
1:A:698:GLN:NE2	1:A:746:ASP:OD1	2.23	0.68
2:B:41:C:C5'	2:B:41:C:C6	2.75	0.68
1:D:57:THR:O	1:D:61:VAL:HG23	1.93	0.68
1:D:134:ARG:HH11	1:D:451:PRO:HD3	1.57	0.68
1:D:17:HIS:O	1:D:21:LYS:HB2	1.94	0.68
1:D:651:PRO:HG3	2:E:14:A:OP1	1.94	0.68

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:GLN:OE1	2:B:74:C:N4	2.26	0.68
1:D:46:GLY:HA2	1:D:104:ASN:OD1	1.94	0.68
1:A:1:MET:SD	1:A:775:GLU:HG3	2.35	0.67
1:D:791:ASP:HB3	1:D:794:ALA:HB3	1.77	0.66
1:A:821:THR:HB	1:A:823:GLU:OE1	1.96	0.66
1:D:76:PRO:HG2	1:D:503:TYR:CD2	2.30	0.66
1:D:703:ARG:HG3	1:D:795:MET:HA	1.78	0.66
1:D:44:PRO:HA	1:D:108:MET:SD	2.36	0.65
1:A:271:ALA:CB	1:A:305:THR:HG23	2.26	0.65
2:B:37:A:N3	2:B:37:A:H2'	2.12	0.64
1:D:116:GLY:HA3	1:D:767:HIS:CE1	2.32	0.64
1:D:236:VAL:HG12	1:D:237:ASN:H	1.62	0.64
1:D:251:ASP:HA	1:D:399:ILE:HD12	1.79	0.64
1:D:854:LEU:HD13	2:E:19:G:H1'	1.78	0.64
1:D:822:GLU:HG3	1:D:849:TYR:CD2	2.33	0.64
1:D:143:LEU:HB3	1:D:149:VAL:HG23	1.79	0.64
1:A:568:MET:H	1:A:655:THR:HG22	1.63	0.63
1:A:42:PRO:HD2	1:A:78:GLY:O	1.98	0.63
1:A:82:PHE:CG	1:A:429:GLY:HA2	2.33	0.63
1:A:650:SER:HB2	1:A:651:PRO:CD	2.28	0.63
1:A:647:MET:HA	1:A:647:MET:HE2	1.81	0.63
1:D:469:ALA:O	1:D:471:PRO:HD3	1.98	0.63
2:E:55:U:C2	2:E:57:A:OP2	2.52	0.63
1:A:179:CYS:SG	1:A:181:THR:HG22	2.38	0.63
1:A:392:HIS:NE2	6:A:2137:HOH:O	2.30	0.63
1:D:478:VAL:C	1:D:480:GLY:H	2.05	0.63
1:A:304:ASP:OD1	1:A:305:THR:N	2.31	0.63
1:A:654:MET:HG3	6:A:2198:HOH:O	1.99	0.62
1:D:77:ILE:HB	1:D:119:TYR:CD2	2.34	0.62
1:D:151:LYS:HE3	1:D:189:PRO:HB2	1.81	0.62
1:A:54:ARG:HG2	1:A:566:GLN:OE1	2.00	0.62
1:A:139:PHE:CE1	1:A:553:MET:CE	2.82	0.62
1:D:446:PRO:HB2	1:D:448:ASP:OD1	1.99	0.62
1:A:551:ALA:CB	1:A:553:MET:HE3	2.30	0.62
1:D:236:VAL:HB	1:D:239:TYR:HB3	1.80	0.62
1:A:709:ILE:HA	1:A:760:MET:SD	2.40	0.61
1:D:817:PRO:HB2	1:D:820:ALA:HB2	1.81	0.61
1:A:328:MET:HE2	1:A:333:GLY:HA3	1.82	0.61
1:D:703:ARG:CG	1:D:795:MET:HA	2.30	0.61
1:A:680:HIS:O	1:A:747:ARG:NH2	2.33	0.61
1:D:596:ASP:HB2	1:D:600:ARG:O	1.99	0.61

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:852:GLY:C	1:A:853:LYS:HE3	2.26	0.61
1:A:139:PHE:HE1	1:A:553:MET:HE1	1.61	0.60
1:A:270:LYS:O	1:A:273:GLU:HB2	2.00	0.60
1:A:342:ASP:CB	4:A:1863:ILA:CG2	2.77	0.60
1:D:153:THR:HG23	1:D:187:GLU:HB3	1.83	0.60
2:B:41:C:H5''	2:B:41:C:C6	2.24	0.60
1:A:587:SER:OG	1:A:589:VAL:HG23	2.02	0.60
1:D:57:THR:HB	1:D:647:MET:HE3	1.82	0.60
1:A:284:GLU:HB2	6:A:2107:HOH:O	2.01	0.60
1:D:67:ARG:HG2	1:D:783:ASP:O	2.02	0.60
1:D:60:ASP:OD2	1:D:117:PHE:HA	2.02	0.60
1:D:378:LYS:HB3	1:D:392:HIS:CG	2.37	0.60
1:A:716:ILE:HG23	1:A:722:PHE:CE1	2.36	0.59
1:D:40:MET:HB2	4:D:1862:ILA:O3'	2.02	0.59
1:D:664:GLU:HG3	1:D:668:ARG:NE	2.17	0.59
1:A:801:LEU:HD23	1:A:802:VAL:N	2.17	0.59
1:A:741:THR:HA	1:A:746:ASP:HB3	1.82	0.59
2:E:41:C:H2'	2:E:42:C:C6	2.37	0.59
1:D:439:ASP:HB3	1:D:441:THR:HG23	1.85	0.59
2:E:75:C:H2'	2:E:76:A:O4'	2.02	0.59
1:A:676:LEU:CD2	1:A:733:MET:HE1	2.30	0.59
2:E:6:G:H2'	2:E:7:A:C8	2.38	0.59
1:A:305:THR:HG22	1:A:307:PHE:CD2	2.36	0.58
2:B:17:C:H2'	2:B:17:C:O2	2.03	0.58
1:A:258:TYR:OH	1:A:348:PHE:HB3	2.02	0.58
2:B:39:U:C2'	2:B:40:C:H5'	2.32	0.58
1:A:115:LEU:O	1:A:643:ARG:NH1	2.36	0.58
1:D:170:GLN:O	1:D:177:TRP:HB3	2.03	0.58
1:D:368:PRO:HB2	1:D:375:LEU:HD13	1.85	0.58
1:D:160:PRO:HD3	1:D:184:GLU:HG2	1.86	0.58
1:A:342:ASP:HB2	4:A:1863:ILA:HG22	1.81	0.58
1:D:58:ILE:HG13	1:D:647:MET:HE1	1.86	0.58
1:D:126:ALA:HB3	1:D:129:THR:HG23	1.86	0.58
1:D:158:TRP:HB2	1:D:186:LYS:HB3	1.85	0.57
1:A:22:ARG:NH1	1:A:25:GLU:OE2	2.37	0.57
1:A:136:GLU:OE2	1:A:495:GLU:OE2	2.21	0.57
1:A:435:VAL:HG11	1:A:478:VAL:HG21	1.86	0.57
1:D:621:SER:OG	1:D:623:SER:N	2.34	0.57
1:A:300:LYS:HD2	6:A:2114:HOH:O	2.04	0.57
1:A:593:VAL:HG13	1:A:601:ILE:HG23	1.86	0.57
1:D:253:PHE:C	1:D:255:GLY:H	2.11	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:342:ASP:CG	4:A:1863:ILA:HG22	2.28	0.57
2:E:56:C:H2'	2:E:57:A:C8	2.39	0.57
1:A:673:VAL:HA	1:A:733:MET:HE2	1.86	0.57
1:A:711:LYS:NZ	2:B:16:U:O4	2.34	0.57
1:A:343:GLN:NE2	1:A:347:GLU:OE2	2.36	0.57
1:D:162:ASP:O	1:D:163:GLN:HB2	2.04	0.57
1:D:305:THR:C	1:D:307:PHE:H	2.13	0.56
1:A:630:PRO:O	1:A:634:VAL:HG23	2.05	0.56
1:A:351:LYS:HD3	1:A:352:TYR:CE2	2.41	0.56
1:A:402:LYS:O	1:A:406:MET:HG3	2.04	0.56
1:A:686:VAL:HG21	1:A:751:GLN:HG2	1.88	0.56
1:D:236:VAL:HG21	1:D:239:TYR:HD2	1.70	0.56
1:D:695:THR:C	1:D:697:ASN:H	2.13	0.56
1:D:685:ASP:O	1:D:747:ARG:NH2	2.39	0.56
1:A:165:VAL:HG21	1:A:425:GLN:CG	2.32	0.56
1:A:845:ARG:HG3	1:A:845:ARG:HH11	1.70	0.56
1:A:426:ARG:CB	1:A:426:ARG:HH11	2.19	0.56
1:D:701:LEU:O	1:D:705:VAL:HG23	2.05	0.55
1:D:1:MET:HG3	1:D:775:GLU:HG3	1.89	0.55
1:D:769:CYS:HB3	1:D:782:ILE:CD1	2.37	0.55
1:D:769:CYS:HB3	1:D:782:ILE:HD13	1.87	0.55
1:D:82:PHE:HB2	1:D:492:THR:HG22	1.88	0.55
1:D:468:LYS:HG2	1:D:487:THR:HB	1.88	0.55
1:A:761:LEU:HB3	1:A:769:CYS:SG	2.45	0.55
1:D:96:ALA:HB3	1:D:99:PRO:HD2	1.86	0.55
1:D:77:ILE:O	1:D:503:TYR:CE1	2.59	0.55
2:B:4:C:H2'	2:B:5:G:O4'	2.07	0.55
1:D:289:LYS:HB2	1:D:298:MET:HE3	1.88	0.55
1:A:532:GLU:N	1:A:568:MET:HE3	2.18	0.55
1:A:823:GLU:H	1:A:823:GLU:CD	2.14	0.55
1:D:505:CYS:HB2	1:D:508:TYR:HB2	1.87	0.55
1:A:664:GLU:O	1:A:668:ARG:HG3	2.06	0.55
1:A:676:LEU:HD11	1:A:750:MET:HE3	1.89	0.55
1:D:134:ARG:CB	1:D:451:PRO:HB3	2.37	0.55
1:A:50:MET:HE2	1:A:658:TRP:CH2	2.42	0.55
1:A:195:ILE:HG22	1:A:419:ASP:HA	1.89	0.54
1:D:77:ILE:HD13	1:D:119:TYR:CE2	2.41	0.54
1:D:214:ASP:HA	1:D:217:LYS:CE	2.33	0.54
1:A:25:GLU:HA	1:A:120:ASP:OD1	2.08	0.54
1:A:213:PRO:HD2	1:A:563:LEU:HD23	1.89	0.54
4:D:1863:ILA:H8	4:D:1863:ILA:HN5	1.73	0.54

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:40:C:H2'	2:E:40:C:O2	2.08	0.54
2:E:4:C:H2'	2:E:5:G:O4'	2.07	0.54
1:A:59:GLY:HA2	1:A:528:ILE:HD13	1.90	0.54
1:D:50:MET:HE2	1:D:658:TRP:CH2	2.43	0.54
1:A:186:LYS:HG2	1:A:188:ILE:CD1	2.38	0.54
1:A:640:ASP:HB3	1:A:765:THR:HB	1.89	0.54
1:A:775:GLU:C	1:A:777:LYS:H	2.15	0.54
4:A:1863:ILA:HNA	4:A:1863:ILA:HG23	1.73	0.54
2:B:10:G:C2'	2:B:11:U:H5'	2.38	0.54
1:A:544:PHE:O	1:A:545:HIS:C	2.51	0.54
2:E:5:G:H2'	2:E:6:G:H8	1.72	0.54
1:D:681:THR:C	1:D:683:LYS:H	2.16	0.53
1:A:211:HIS:HB3	1:A:562:GLN:HG3	1.90	0.53
1:D:403:LEU:HB3	1:D:409:GLY:HA3	1.89	0.53
1:D:606:ASP:CG	1:D:610:HIS:HD1	2.16	0.53
1:A:620:MET:HG2	1:A:627:GLY:HA2	1.90	0.53
1:A:805:GLN:HB2	1:A:856:ASN:OD1	2.08	0.53
1:D:68:MET:HE1	1:D:759:ARG:HB3	1.90	0.53
1:A:606:ASP:HB3	1:A:612:LEU:HD21	1.90	0.53
1:A:5:TYR:HB2	1:A:674:TRP:CG	2.44	0.53
1:A:422:VAL:CG1	1:A:494:MET:CE	2.87	0.53
1:D:98:ALA:HB3	1:D:99:PRO:CD	2.39	0.53
1:A:564:LEU:HD22	1:A:720:GLN:HG2	1.91	0.53
1:D:443:MET:HB2	1:D:444:PRO:CD	2.39	0.53
1:D:587:SER:OG	1:D:589:VAL:HG23	2.09	0.53
1:A:828:ARG:NH1	1:A:832:GLU:OE2	2.38	0.52
1:D:426:ARG:NH2	2:E:74:C:O2	2.42	0.52
1:D:151:LYS:HG3	1:D:190:GLN:O	2.09	0.52
1:A:91:VAL:O	1:A:92:LYS:C	2.53	0.52
1:A:192:PHE:HA	1:A:420:TRP:O	2.08	0.52
1:D:300:LYS:HB3	1:D:325:PHE:HE2	1.75	0.52
1:A:342:ASP:CB	4:A:1863:ILA:HG22	2.37	0.52
1:D:289:LYS:HG3	1:D:294:GLU:HG3	1.91	0.52
1:D:638:GLY:O	1:D:642:VAL:HG23	2.10	0.52
1:A:25:GLU:HA	1:A:120:ASP:CG	2.34	0.52
1:A:712:VAL:O	1:A:716:ILE:HG13	2.10	0.52
1:A:200:ASP:OD1	1:A:415:TYR:OH	2.12	0.52
1:A:240:ASP:N	1:A:240:ASP:OD1	2.43	0.52
1:A:422:VAL:CG1	1:A:494:MET:HE1	2.25	0.52
1:A:437:LEU:HB2	1:A:439:ASP:HB2	1.92	0.52
1:D:777:LYS:HA	6:D:2015:HOH:O	2.09	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:GLY:CA	1:A:568:MET:HE1	2.40	0.52
2:E:13:G:N2	2:E:21:G:O2'	2.39	0.52
1:D:513:LEU:HD11	1:D:553:MET:HB3	1.92	0.52
1:A:426:ARG:HH11	1:A:426:ARG:HB2	1.75	0.51
2:B:12:G:H2'	2:B:13:G:O4'	2.10	0.51
1:D:424:ARG:CZ	1:D:491:ASP:HB2	2.40	0.51
1:D:514:ASP:C	1:D:514:ASP:OD1	2.52	0.51
2:B:47(D):C:O2	2:B:47(D):C:O4'	2.28	0.51
1:D:233:THR:HG22	1:D:242:THR:HB	1.92	0.51
1:A:224:ILE:HD11	1:A:539:LEU:HD11	1.93	0.51
1:A:570:LEU:HD12	1:A:657:GLU:HG2	1.92	0.51
1:A:10:ILE:O	1:A:14:VAL:HG23	2.10	0.51
1:A:157:ASN:ND2	1:A:168:ASN:OD1	2.42	0.51
1:A:333:GLY:HA2	6:A:2119:HOH:O	2.10	0.51
2:B:39:U:O2'	2:B:40:C:H5'	2.11	0.51
1:D:176:CYS:SG	1:D:177:TRP:N	2.83	0.51
1:D:139:PHE:CE2	1:D:143:LEU:HD11	2.45	0.51
1:D:849:TYR:HD1	1:D:855:LEU:HD13	1.76	0.51
1:A:368:PRO:HB3	1:A:375:LEU:HD22	1.93	0.51
1:D:98:ALA:HA	1:D:428:TRP:CH2	2.45	0.51
1:D:157:ASN:H	1:D:157:ASN:ND2	2.09	0.51
4:A:1862:ILA:H8	4:A:1862:ILA:HN5	1.76	0.51
1:D:670:LEU:HD21	1:D:765:THR:HG21	1.93	0.51
1:D:689:LEU:HD11	1:D:694:LEU:HD21	1.92	0.51
1:D:313:LEU:C	1:D:315:GLY:H	2.18	0.50
1:A:212:TRP:CH2	1:A:538:LEU:HD22	2.46	0.50
1:A:531:ILE:HG22	1:A:568:MET:HE2	1.94	0.50
1:A:828:ARG:O	1:A:829:ALA:C	2.54	0.50
1:A:131:GLU:CD	1:A:131:GLU:H	2.19	0.50
1:D:543:PHE:CZ	1:D:547:LEU:HD11	2.47	0.50
1:D:42:PRO:HD2	1:D:78:GLY:O	2.11	0.50
1:D:424:ARG:NH2	2:E:74:C:OP2	2.44	0.50
2:E:14:A:O4'	2:E:22:A:C6	2.64	0.50
1:A:262:ALA:HB3	1:A:328:MET:HG2	1.94	0.50
1:D:211:HIS:HB3	1:D:562:GLN:HG3	1.93	0.50
1:A:155:ALA:HA	1:A:186:LYS:O	2.12	0.49
2:B:14:A:H2'	2:B:15:A:O5'	2.13	0.49
1:D:43:TYR:HE2	1:D:82:PHE:O	1.95	0.49
1:D:102:TYR:HA	1:D:105:ILE:HD12	1.94	0.49
1:A:367:GLU:HG2	1:A:382:PHE:CZ	2.47	0.49
1:A:588:PRO:HD2	1:A:626:ASN:HA	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:553:MET:HE1	6:A:2052:HOH:O	1.89	0.49
1:A:614:TYR:CZ	1:A:616:GLY:HA2	2.48	0.49
1:A:692:ASP:O	1:A:693:ALA:HB2	2.12	0.49
2:B:10:G:H2'	2:B:11:U:H5'	1.95	0.49
1:A:854:LEU:HD13	2:B:19:G:H1'	1.95	0.49
1:A:258:TYR:HH	1:A:348:PHE:HB3	1.77	0.48
1:D:143:LEU:HB3	1:D:149:VAL:CG2	2.44	0.48
1:A:675:LYS:HE3	1:A:679:GLU:OE2	2.13	0.48
1:A:842:VAL:HB	1:A:859:VAL:HG13	1.95	0.48
1:D:299:GLU:HA	1:D:299:GLU:OE1	2.14	0.48
1:D:385:GLY:C	1:D:387:PHE:H	2.20	0.48
1:D:190:GLN:HE22	2:E:74:C:H41	1.61	0.48
1:D:40:MET:HE2	1:D:537:HIS:CD2	2.48	0.48
2:E:66:U:H2'	2:E:67:C:O4'	2.13	0.48
1:A:25:GLU:HB3	6:A:2006:HOH:O	2.14	0.48
1:D:681:THR:O	1:D:683:LYS:N	2.47	0.48
2:E:26:A:H2'	2:E:27:A:O4'	2.13	0.48
1:D:337:ALA:HA	1:D:345:ASP:OD2	2.14	0.48
1:A:139:PHE:CD1	1:A:553:MET:HE1	2.48	0.48
1:D:148:LEU:O	1:D:194:LYS:HB2	2.14	0.48
2:E:4:C:C2	2:E:5:G:C8	3.01	0.47
1:A:300:LYS:HE2	6:A:2123:HOH:O	2.14	0.47
2:B:66:U:H2'	2:B:67:C:O4'	2.14	0.47
1:D:77:ILE:HG13	1:D:78:GLY:H	1.79	0.47
1:D:130:PRO:C	1:D:132:TYR:H	2.22	0.47
1:D:478:VAL:O	1:D:480:GLY:N	2.47	0.47
1:D:636:ARG:HD3	1:D:637:TYR:CE2	2.48	0.47
1:A:835:VAL:O	1:A:839:LEU:HG	2.14	0.47
1:D:1:MET:HE1	1:D:678:TYR:HA	1.97	0.47
1:D:139:PHE:CD2	1:D:143:LEU:CD1	2.95	0.47
1:D:344:ARG:HD2	4:D:1863:ILA:C2	2.44	0.47
1:A:255:GLY:C	1:A:338:VAL:HG22	2.40	0.47
1:D:536:MET:O	1:D:540:TYR:CD2	2.67	0.47
1:D:606:ASP:OD2	1:D:610:HIS:ND1	2.37	0.47
1:A:47:ARG:NH1	1:D:579:GLU:OE1	2.47	0.47
1:A:342:ASP:OD1	1:A:345:ASP:N	2.31	0.47
1:D:90:ALA:HB1	1:D:95:THR:O	2.15	0.47
1:D:135:TRP:CD2	1:D:512:MET:HA	2.49	0.47
1:D:237:ASN:HB2	1:D:307:PHE:HD1	1.80	0.47
1:A:139:PHE:HE1	1:A:553:MET:HE3	1.78	0.47
1:A:533:HIS:HB3	1:A:537:HIS:HB3	1.97	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47(G):G:C2	2:B:47(H):C:C2	3.03	0.47
1:A:206:LEU:HD23	1:A:209:LEU:HD12	1.97	0.47
4:A:1863:ILA:HG23	4:A:1863:ILA:N3A	2.30	0.47
1:A:148:LEU:HA	1:A:194:LYS:HD2	1.97	0.47
1:A:258:TYR:CE1	1:A:354:LEU:HD12	2.50	0.47
1:D:245:VAL:HG11	1:D:259:LEU:HD22	1.97	0.47
2:E:47(D):C:O4'	2:E:47(D):C:O2	2.32	0.47
2:B:39:U:H2'	2:B:40:C:H5'	1.97	0.46
1:D:190:GLN:HB3	1:D:423:SER:HB2	1.97	0.46
1:A:271:ALA:HB2	1:A:305:THR:HG23	1.95	0.46
1:A:520:TYR:CD1	1:A:520:TYR:C	2.92	0.46
1:A:364:ASP:OD1	1:A:366:SER:N	2.48	0.46
1:A:800:THR:HG22	1:A:818:VAL:HA	1.97	0.46
1:D:249:ARG:HD3	1:D:378:LYS:HE2	1.97	0.46
1:A:57:THR:O	1:A:58:ILE:C	2.58	0.46
1:A:450:LEU:HA	1:A:451:PRO:C	2.40	0.46
1:D:220:GLN:HE22	1:D:539:LEU:HB2	1.80	0.46
1:D:567:GLY:CA	1:D:655:THR:HG22	2.46	0.46
1:D:823:GLU:O	1:D:827:GLU:HG2	2.15	0.46
1:A:740:PRO:HB2	1:A:746:ASP:OD2	2.15	0.46
1:D:123:ARG:O	1:D:125:LEU:HD23	2.15	0.46
1:D:750:MET:HG3	1:D:754:LEU:HD12	1.96	0.46
1:A:190:GLN:OE1	2:B:74:C:N4	2.48	0.46
1:D:40:MET:HE2	1:D:537:HIS:HD2	1.81	0.46
1:D:588:PRO:HD2	1:D:626:ASN:HA	1.96	0.46
1:D:729:ILE:HG21	1:D:761:LEU:CD2	2.44	0.46
1:A:330:TYR:N	1:A:330:TYR:CD1	2.84	0.46
2:B:37:A:H3'	2:B:38:A:H8	1.79	0.46
1:D:704:ASP:O	1:D:708:THR:OG1	2.29	0.46
1:A:364:ASP:OD1	1:A:364:ASP:C	2.57	0.46
1:D:36:TYR:CE1	1:D:38:LEU:HB2	2.51	0.46
1:D:116:GLY:HA3	1:D:767:HIS:HE1	1.80	0.46
1:D:336:MET:SD	1:D:338:VAL:HG23	2.56	0.46
1:A:135:TRP:HB2	1:A:498:TRP:CH2	2.50	0.46
1:A:137:GLN:O	1:A:141:THR:HG23	2.16	0.46
1:A:836:ALA:O	1:A:837:LYS:C	2.57	0.46
1:D:344:ARG:HH12	4:D:1863:ILA:H2'	1.81	0.46
1:D:362:ALA:HB2	1:D:368:PRO:HB3	1.98	0.46
1:D:773:TRP:HB2	1:D:782:ILE:HD12	1.97	0.46
1:A:823:GLU:CD	1:A:823:GLU:N	2.74	0.46
1:D:175:CYS:HB3	1:D:182:LYS:HA	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:5:G:H2'	2:E:6:G:C8	2.51	0.46
1:A:250:PRO:O	1:A:253:PHE:HB2	2.15	0.45
1:A:339:PRO:CG	1:A:355:ASN:O	2.64	0.45
2:B:1:G:OP1	6:B:2003:HOH:O	2.21	0.45
1:D:218:THR:HG22	1:D:222:ASN:HD21	1.81	0.45
1:D:501:ALA:HB1	1:D:513:LEU:HD22	1.97	0.45
1:D:756:ALA:O	1:D:757:VAL:C	2.58	0.45
1:A:60:ASP:OD1	1:A:118:GLY:N	2.35	0.45
1:D:76:PRO:HG2	1:D:503:TYR:CE2	2.51	0.45
1:D:235:ASN:O	1:D:309:ALA:HA	2.15	0.45
1:A:845:ARG:HG3	1:A:845:ARG:NH1	2.31	0.45
4:A:1863:ILA:HN5	4:A:1863:ILA:H8	1.79	0.45
1:D:84:LEU:HD21	1:D:170:GLN:NE2	2.31	0.45
1:A:193:ILE:O	1:A:195:ILE:N	2.43	0.45
1:A:439:ASP:HB3	1:A:441:THR:HG23	1.97	0.45
1:A:551:ALA:HB3	1:A:553:MET:HE3	1.98	0.45
1:A:618:SER:O	1:A:619:LYS:C	2.59	0.45
1:D:55:ASN:OD1	1:D:529:GLY:HA2	2.15	0.45
1:D:58:ILE:HG13	1:D:647:MET:SD	2.56	0.45
1:A:141:THR:HB	1:A:444:PRO:HB3	1.98	0.45
1:D:77:ILE:O	1:D:503:TYR:HE1	2.00	0.45
1:D:690:ASN:HB3	1:D:693:ALA:HB3	1.98	0.45
1:D:705:VAL:HG22	1:D:732:LEU:HD11	1.97	0.45
1:A:150:TYR:HE2	1:A:152:LYS:HD3	1.81	0.45
1:A:231:GLU:HA	1:A:245:VAL:O	2.15	0.45
1:D:300:LYS:HB3	1:D:325:PHE:CE2	2.51	0.45
1:A:4:GLN:HB3	1:A:6:ARG:HD2	1.99	0.45
1:A:692:ASP:OD1	1:A:692:ASP:N	2.45	0.45
1:D:250:PRO:O	1:D:253:PHE:HB2	2.17	0.45
1:D:681:THR:C	1:D:683:LYS:N	2.74	0.45
1:D:733:MET:HA	1:D:736:LEU:HD12	1.99	0.45
1:A:249:ARG:C	1:A:251:ASP:N	2.75	0.45
1:A:474:ALA:O	1:A:484:LEU:HA	2.17	0.45
2:B:46:G:H2'	2:B:47:C:O4'	2.16	0.45
1:A:47:ARG:NE	1:A:107:TYR:CE1	2.85	0.45
1:A:223:TRP:CD2	1:A:535:ILE:HG21	2.51	0.45
1:D:39:SER:HB3	1:D:55:ASN:ND2	2.32	0.45
1:D:422:VAL:HG11	1:D:494:MET:HE1	1.99	0.45
1:D:676:LEU:HG	1:D:754:LEU:HD11	1.99	0.45
1:A:172:ILE:HG13	1:A:172:ILE:O	2.16	0.45
1:A:650:SER:HB2	1:A:651:PRO:HD3	1.97	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:530:GLY:HA3	1:D:568:MET:HE1	1.99	0.45
1:D:695:THR:C	1:D:697:ASN:N	2.75	0.45
1:D:726:ILE:HG22	1:D:730:MET:HE3	1.99	0.45
1:D:845:ARG:O	1:D:846:LYS:HB3	2.17	0.45
2:B:7:A:O2'	2:B:49:G:OP2	2.27	0.44
1:D:34:LYS:NZ	1:D:525:ASP:OD1	2.40	0.44
1:D:723:ASN:OD1	1:D:723:ASN:N	2.50	0.44
1:A:2:GLN:HG3	1:A:6:ARG:HH11	1.83	0.44
1:A:130:PRO:C	1:A:132:TYR:N	2.75	0.44
1:A:543:PHE:CE2	1:A:547:LEU:HD11	2.53	0.44
1:A:219:MET:HB3	1:A:535:ILE:HD11	1.98	0.44
2:B:3:C:H2'	2:B:4:C:H5'	1.99	0.44
1:D:165:VAL:HG21	1:D:425:GLN:HG3	2.00	0.44
1:A:272:ALA:N	1:A:278:LEU:HD23	2.33	0.44
1:D:341:HIS:HA	1:D:375:LEU:O	2.18	0.44
2:B:42:C:H2'	2:B:43:U:H6	1.83	0.44
1:D:159:CYS:HA	1:D:160:PRO:HD2	1.86	0.44
1:D:663:VAL:HG23	1:D:664:GLU:N	2.33	0.44
1:A:36:TYR:CE2	1:A:524:VAL:HG22	2.53	0.44
1:A:313:LEU:HD13	1:A:387:PHE:HE2	1.83	0.44
1:D:40:MET:HB3	4:D:1862:ILA:CG1	2.48	0.44
2:E:14:A:H1'	2:E:22:A:C5	2.52	0.44
1:A:253:PHE:C	1:A:255:GLY:H	2.24	0.43
1:A:575:TYR:HA	1:A:584:ASN:O	2.18	0.43
1:A:1:MET:HE2	1:A:775:GLU:OE1	2.18	0.43
1:D:327:LEU:HD23	1:D:328:MET:HE2	2.00	0.43
2:E:40:C:O2	2:E:40:C:C2'	2.65	0.43
1:A:300:LYS:CD	6:A:2114:HOH:O	2.63	0.43
1:A:505:CYS:N	1:A:506:PRO:CD	2.81	0.43
1:D:693:ALA:O	1:D:694:LEU:HG	2.18	0.43
1:A:67:ARG:NH2	6:A:2025:HOH:O	2.48	0.43
1:A:358:PRO:HB3	1:A:370:LEU:HD11	2.00	0.43
1:D:52:HIS:O	1:D:56:TYR:CD2	2.71	0.43
1:D:571:ALA:HB2	1:D:620:MET:HE2	2.00	0.43
1:D:751:GLN:O	1:D:755:LEU:HB2	2.19	0.43
1:A:186:LYS:HG2	1:A:188:ILE:HD12	2.00	0.43
1:A:186:LYS:HG2	1:A:188:ILE:HD11	2.01	0.43
1:A:381:LEU:HD12	1:A:387:PHE:HB2	2.01	0.43
1:A:426:ARG:HB2	1:A:426:ARG:NH1	2.33	0.43
1:A:566:GLN:HG3	1:A:567:GLY:O	2.18	0.43
1:A:619:LYS:HE2	2:B:71:G:OP1	2.19	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47(G):G:H2'	2:B:47(H):C:O4'	2.19	0.43
1:A:54:ARG:HH11	1:A:54:ARG:HD3	1.71	0.43
1:A:123:ARG:HD3	1:A:503:TYR:O	2.18	0.43
1:A:303:VAL:HG12	1:A:304:ASP:O	2.19	0.43
1:A:321:TRP:CZ2	1:A:354:LEU:HD21	2.53	0.43
1:A:339:PRO:HG3	1:A:355:ASN:O	2.19	0.43
1:A:375:LEU:HD12	1:A:375:LEU:HA	1.91	0.43
1:A:531:ILE:N	1:A:568:MET:CE	2.82	0.43
1:A:761:LEU:HD12	1:A:761:LEU:HA	1.72	0.43
1:A:22:ARG:CB	1:A:25:GLU:HG3	2.39	0.43
1:D:190:GLN:HE22	2:E:74:C:N4	2.17	0.43
1:A:295:MET:HE3	1:A:295:MET:HA	2.01	0.43
1:A:272:ALA:O	1:A:273:GLU:C	2.62	0.42
1:A:683:LYS:HB2	1:A:747:ARG:NH2	2.33	0.42
1:D:733:MET:HE3	1:D:733:MET:HB3	1.95	0.42
1:A:787:TRP:CD2	1:A:788:PRO:HD2	2.55	0.42
1:D:188:ILE:O	1:D:190:GLN:HG3	2.19	0.42
2:E:47(G):G:H2'	2:E:47(H):C:O4'	2.19	0.42
1:A:153:THR:HA	1:A:189:PRO:HA	2.00	0.42
1:A:529:GLY:O	1:A:565:CYS:HA	2.19	0.42
1:A:701:LEU:O	1:A:702:ARG:C	2.62	0.42
1:A:705:VAL:HG11	1:A:753:ALA:HA	2.02	0.42
1:D:564:LEU:HD22	1:D:720:GLN:HG2	2.01	0.42
1:D:424:ARG:HB2	1:D:489:THR:O	2.19	0.42
1:D:787:TRP:CD2	1:D:788:PRO:HD2	2.54	0.42
1:A:443:MET:HB2	1:A:444:PRO:HD2	2.01	0.42
1:A:620:MET:HE2	1:A:628:ILE:HG12	2.02	0.42
1:D:185:ARG:NH1	1:D:289:LYS:O	2.52	0.42
1:D:289:LYS:HA	1:D:289:LYS:HD2	1.64	0.42
1:D:432:ILE:HG12	1:D:490:PHE:CE1	2.54	0.42
1:D:567:GLY:HA2	1:D:655:THR:HG22	2.00	0.42
1:A:84:LEU:HD21	1:A:170:GLN:NE2	2.35	0.42
1:A:703:ARG:HG3	1:A:795:MET:HA	2.02	0.42
1:D:385:GLY:O	1:D:387:PHE:N	2.50	0.42
1:A:151:LYS:HA	1:A:190:GLN:O	2.20	0.42
1:A:323:ALA:HB1	1:A:325:PHE:CE2	2.55	0.42
1:A:650:SER:CB	1:A:651:PRO:CD	2.97	0.42
1:D:40:MET:HB3	4:D:1862:ILA:HD1	2.01	0.42
1:D:84:LEU:HD22	1:D:84:LEU:O	2.20	0.42
1:A:294:GLU:C	1:A:296:ALA:N	2.77	0.42
1:D:253:PHE:C	1:D:255:GLY:N	2.78	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:328:MET:SD	1:D:328:MET:N	2.93	0.42
1:A:17:HIS:NE2	1:A:781:ASP:OD2	2.44	0.42
1:A:647:MET:HE2	1:A:647:MET:CA	2.48	0.42
1:A:729:ILE:HD13	1:A:761:LEU:HD13	2.02	0.42
1:A:773:TRP:CE2	1:A:778:GLY:HA3	2.55	0.42
2:B:47(H):C:O2'	2:B:47(I):U:H5'	2.20	0.42
1:D:68:MET:HE2	1:D:68:MET:HB3	1.81	0.42
1:A:201:GLU:OE2	1:A:546:LYS:HD3	2.19	0.42
1:D:743:GLY:C	1:D:745:GLN:H	2.27	0.42
2:E:30:G:H2'	2:E:31:A:H8	1.84	0.42
1:A:549:ARG:HH11	1:A:557:ASP:HA	1.85	0.41
2:B:55:U:O2'	2:B:57:A:N7	2.53	0.41
1:D:490:PHE:CD1	1:D:494:MET:HE3	2.55	0.41
1:A:300:LYS:HD3	6:A:2123:HOH:O	2.19	0.41
1:A:433:PRO:C	1:A:445:THR:OG1	2.63	0.41
1:A:606:ASP:OD1	1:A:606:ASP:C	2.63	0.41
1:D:49:HIS:CD2	1:D:52:HIS:CE1	3.08	0.41
1:D:54:ARG:NH2	1:D:650:SER:HB3	2.34	0.41
1:D:130:PRO:C	1:D:132:TYR:N	2.77	0.41
1:D:276:PRO:HA	6:D:2008:HOH:O	2.20	0.41
1:D:508:TYR:CE1	1:D:510:GLU:HG2	2.55	0.41
1:D:533:HIS:HB3	1:D:537:HIS:HB3	2.02	0.41
1:A:438:GLU:O	1:A:439:ASP:C	2.64	0.41
1:A:538:LEU:HA	1:A:538:LEU:HD23	1.79	0.41
1:D:545:HIS:CD2	1:D:545:HIS:C	2.98	0.41
2:E:72:U:H5''	2:E:73:A:H5'	2.01	0.41
1:A:295:MET:CE	1:A:325:PHE:HA	2.40	0.41
1:A:313:LEU:HD11	1:A:399:ILE:HG23	2.01	0.41
1:D:71:LYS:O	1:D:73:VAL:HG23	2.20	0.41
1:D:77:ILE:HD13	1:D:119:TYR:HE2	1.83	0.41
1:D:237:ASN:HB3	1:D:238:ASP:H	1.51	0.41
1:D:251:ASP:C	1:D:253:PHE:H	2.28	0.41
1:D:643:ARG:NH2	1:D:766:PRO:HD3	2.34	0.41
1:A:34:LYS:HB3	1:A:520:TYR:CE1	2.55	0.41
1:A:91:VAL:C	1:A:93:ASN:N	2.75	0.41
1:A:629:ASP:HA	1:A:630:PRO:HD2	1.87	0.41
1:D:77:ILE:HG13	1:D:78:GLY:N	2.36	0.41
1:D:351:LYS:HA	1:D:351:LYS:HD3	1.90	0.41
2:E:47(H):C:H2'	2:E:47(I):U:O4'	2.21	0.41
1:A:640:ASP:CB	1:A:765:THR:HB	2.51	0.41
1:D:110:ASN:ND2	1:D:114:MET:HE2	2.36	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:587:SER:HA	1:D:588:PRO:HD2	1.76	0.41
2:E:18:G:H1	2:E:55:U:H1'	1.85	0.41
1:A:158:TRP:CE3	1:A:186:LYS:NZ	2.88	0.41
1:A:200:ASP:CG	1:A:415:TYR:HH	2.18	0.41
2:E:27:A:H2'	2:E:28:G:C8	2.55	0.41
1:A:14:VAL:O	1:A:17:HIS:HB3	2.21	0.41
1:A:84:LEU:HB3	1:A:85:PRO:HD3	2.03	0.41
1:A:203:LEU:CD1	1:A:221:ARG:HG3	2.51	0.41
1:A:233:THR:HG22	6:A:2083:HOH:O	2.20	0.41
2:B:47(I):U:H2'	2:B:47(J):G:O5'	2.20	0.41
1:D:478:VAL:C	1:D:480:GLY:N	2.74	0.41
1:D:729:ILE:HD13	1:D:761:LEU:HD22	2.03	0.41
1:D:816:VAL:HG21	1:D:825:VAL:HG22	2.02	0.41
1:A:5:TYR:CE1	1:A:768:ILE:HD12	2.56	0.41
1:A:243:LEU:CD1	1:A:265:HIS:CE1	3.04	0.41
1:A:383:ASN:N	1:A:388:ASN:OD1	2.53	0.41
1:A:530:GLY:HA3	1:A:568:MET:HE1	2.01	0.41
1:A:634:VAL:O	1:A:638:GLY:N	2.51	0.41
1:A:723:ASN:OD1	1:A:723:ASN:N	2.52	0.41
2:B:3:C:C2'	2:B:4:C:H5'	2.51	0.41
2:B:14:A:C2'	2:B:15:A:O5'	2.68	0.41
1:D:76:PRO:CG	1:D:503:TYR:CD2	3.01	0.41
1:D:90:ALA:HB1	1:D:95:THR:C	2.45	0.41
1:D:633:MET:HE2	1:D:642:VAL:HG13	2.03	0.41
1:D:669:PHE:HA	1:D:672:ARG:CZ	2.50	0.41
2:E:1:G:C2	2:E:2:C:C2	3.09	0.41
1:A:364:ASP:OD1	1:A:366:SER:OG	2.38	0.41
1:D:214:ASP:CA	1:D:217:LYS:HE2	2.41	0.41
1:D:342:ASP:HB3	1:D:345:ASP:CG	2.46	0.41
2:E:47(E):G:H4'	2:E:47(F):C:OP2	2.20	0.41
1:D:249:ARG:HD2	1:D:249:ARG:HA	1.96	0.40
1:D:261:VAL:HG23	1:D:334:ALA:CB	2.39	0.40
1:D:850:VAL:HA	1:D:851:PRO:HD3	1.91	0.40
1:A:35:TYR:CE2	1:A:526:ILE:HG22	2.57	0.40
1:A:134:ARG:HG3	1:A:135:TRP:N	2.36	0.40
1:A:136:GLU:HB3	1:A:498:TRP:NE1	2.36	0.40
1:A:342:ASP:OD1	1:A:342:ASP:C	2.64	0.40
1:D:58:ILE:HG13	1:D:647:MET:CE	2.51	0.40
1:D:172:ILE:HG22	1:D:173:ASP:N	2.35	0.40
1:D:765:THR:O	1:D:768:ILE:HG22	2.21	0.40
2:E:51:G:H2'	2:E:52:G:O4'	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:155:ALA:HB3	1:A:329:GLU:OE2	2.21	0.40
1:A:313:LEU:HD13	1:A:387:PHE:CE2	2.57	0.40
1:A:340:GLY:C	1:A:341:HIS:CG	2.99	0.40
1:A:367:GLU:HG2	1:A:382:PHE:CE2	2.56	0.40
1:A:787:TRP:CG	1:A:788:PRO:HD2	2.56	0.40
1:D:5:TYR:CE2	1:D:7:PRO:HG3	2.56	0.40
1:D:223:TRP:CD2	1:D:535:ILE:HG21	2.56	0.40
1:A:131:GLU:CD	1:A:131:GLU:N	2.78	0.40
1:A:731:GLU:O	1:A:735:LYS:HG3	2.22	0.40
1:A:732:LEU:HD23	1:A:757:VAL:HG22	2.03	0.40
1:A:775:GLU:C	1:A:777:LYS:N	2.79	0.40
1:D:618:SER:HB2	2:E:70:G:OP1	2.21	0.40
1:D:810:VAL:HG21	2:E:20:U:H4'	2.02	0.40
1:A:220:GLN:O	1:A:224:ILE:HG13	2.20	0.40
1:A:284:GLU:O	1:A:287:ASN:HB2	2.21	0.40
1:D:345:ASP:OD1	4:D:1863:ILA:N6	2.54	0.40
1:D:822:GLU:HG3	1:D:849:TYR:CG	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	860/880 (98%)	797 (93%)	54 (6%)	9 (1%)	12	24
1	D	858/880 (98%)	716 (83%)	119 (14%)	23 (3%)	4	6
All	All	1718/1760 (98%)	1513 (88%)	173 (10%)	32 (2%)	6	11

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	439	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	693	ALA
1	D	237	ASN
1	D	463	ILE
1	A	161	ASN
1	A	162	ASP
1	A	596	ASP
1	D	93	ASN
1	D	98	ALA
1	D	173	ASP
1	D	386	GLU
1	D	530	GLY
1	D	682	ALA
1	A	290	VAL
1	D	29	ASP
1	D	176	CYS
1	D	168	ASN
1	D	254	MET
1	D	315	GLY
1	D	492	THR
1	D	685	ASP
1	A	331	GLY
1	D	740	PRO
1	D	757	VAL
1	D	295	MET
1	D	696	GLU
1	D	844	VAL
1	A	359	VAL
1	D	365	GLY
1	A	581	GLY
1	D	266	PRO
1	D	818	VAL

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.

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	726/741 (98%)	648 (89%)	78 (11%)	6	13
1	D	723/741 (98%)	652 (90%)	71 (10%)	7	16
All	All	1449/1482 (98%)	1300 (90%)	149 (10%)	7	14

All (149) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	10	ILE
1	A	12	SER
1	A	25	GLU
1	A	32	LYS
1	A	34	LYS
1	A	55	ASN
1	A	84	LEU
1	A	91	VAL
1	A	95	THR
1	A	131	GLU
1	A	142	GLU
1	A	143	LEU
1	A	156	VAL
1	A	164	THR
1	A	173	ASP
1	A	183	VAL
1	A	184	GLU
1	A	186	LYS
1	A	188	ILE
1	A	193	ILE
1	A	210	ASP
1	A	240	ASP
1	A	243	LEU
1	A	245	VAL
1	A	261	VAL
1	A	286	ARG
1	A	295	MET
1	A	297	THR
1	A	298	MET
1	A	327	LEU
1	A	330	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	336	MET
1	A	342	ASP
1	A	347	GLU
1	A	369	ASP
1	A	381	LEU
1	A	393	GLU
1	A	425	GLN
1	A	432	ILE
1	A	435	VAL
1	A	437	LEU
1	A	459	VAL
1	A	463	ILE
1	A	464	THR
1	A	466	PRO
1	A	477	THR
1	A	516	GLU
1	A	570	LEU
1	A	579	GLU
1	A	589	VAL
1	A	594	GLU
1	A	598	LYS
1	A	606	ASP
1	A	610	HIS
1	A	625	ASN
1	A	636	ARG
1	A	641	THR
1	A	646	MET
1	A	656	LEU
1	A	659	GLN
1	A	661	SER
1	A	663	VAL
1	A	664	GLU
1	A	691	VAL
1	A	692	ASP
1	A	694	LEU
1	A	695	THR
1	A	741	THR
1	A	742	ASP
1	A	761	LEU
1	A	796	VAL
1	A	798	ASP
1	A	814	ILE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	816	VAL
1	A	840	ASP
1	A	853	LYS
1	A	859	VAL
1	D	8	GLU
1	D	16	LEU
1	D	21	LYS
1	D	31	SER
1	D	55	ASN
1	D	84	LEU
1	D	91	VAL
1	D	95	THR
1	D	124	GLU
1	D	125	LEU
1	D	134	ARG
1	D	153	THR
1	D	156	VAL
1	D	157	ASN
1	D	175	CYS
1	D	177	TRP
1	D	188	ILE
1	D	228	GLU
1	D	236	VAL
1	D	238	ASP
1	D	241	ASN
1	D	243	LEU
1	D	261	VAL
1	D	273	GLU
1	D	275	ASN
1	D	287	ASN
1	D	288	THR
1	D	289	LYS
1	D	294	GLU
1	D	297	THR
1	D	300	LYS
1	D	318	ILE
1	D	324	ASN
1	D	326	VAL
1	D	327	LEU
1	D	351	LYS
1	D	356	ILE
1	D	372	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	375	LEU
1	D	376	THR
1	D	391	ASP
1	D	413	VAL
1	D	435	VAL
1	D	448	ASP
1	D	465	SER
1	D	479	ASN
1	D	491	ASP
1	D	513	LEU
1	D	531	ILE
1	D	621	SER
1	D	622	LYS
1	D	628	ILE
1	D	646	MET
1	D	650	SER
1	D	659	GLN
1	D	660	GLU
1	D	691	VAL
1	D	692	ASP
1	D	701	LEU
1	D	708	THR
1	D	713	THR
1	D	742	ASP
1	D	755	LEU
1	D	761	LEU
1	D	768	ILE
1	D	793	LYS
1	D	803	VAL
1	D	805	GLN
1	D	816	VAL
1	D	823	GLU
1	D	842	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	94	ASN
1	A	235	ASN
1	A	555	ASN
1	A	584	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	774	GLN
1	A	831	GLN
1	D	110	ASN
1	D	157	ASN
1	D	170	GLN
1	D	190	GLN
1	D	222	ASN
1	D	287	ASN
1	D	355	ASN
1	D	372	GLN
1	D	425	GLN
1	D	507	GLN
1	D	533	HIS
1	D	562	GLN
1	D	667	ASN
1	D	680	HIS
1	D	734	ASN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	81/82 (98%)	15 (18%)	6 (7%)
2	E	76/82 (92%)	21 (27%)	3 (3%)
All	All	157/164 (95%)	36 (22%)	9 (5%)

All (36) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	9	G
2	B	11	U
2	B	15	A
2	B	16	U
2	B	17	C
2	B	18	G
2	B	19	G
2	B	20	U
2	B	33	U
2	B	38	A
2	B	41	C
2	B	47	C
2	B	47(E)	G

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	47(F)	C
2	B	66	U
2	E	5	G
2	E	7	A
2	E	9	G
2	E	13	G
2	E	16	U
2	E	17	C
2	E	18	G
2	E	19	G
2	E	24	A
2	E	32	U
2	E	45	G
2	E	46	G
2	E	47(E)	G
2	E	47(F)	C
2	E	47(G)	G
2	E	48	U
2	E	49	G
2	E	52	G
2	E	56	C
2	E	59	G
2	E	61	C

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	16	U
2	B	17	C
2	B	19	G
2	B	37	A
2	B	47(D)	C
2	B	47(E)	G
2	E	19	G
2	E	47(E)	G
2	E	48	U

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

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

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
4	ILA	D	1863	-	33,33,33	2.08	8 (24%)	44,49,49	2.12	11 (25%)
4	ILA	D	1862	-	33,33,33	2.03	6 (18%)	44,49,49	2.18	11 (25%)
4	ILA	A	1863	-	33,33,33	2.18	6 (18%)	44,49,49	2.92	21 (47%)
4	ILA	A	1862	-	33,33,33	2.45	8 (24%)	44,49,49	3.00	19 (43%)

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
4	ILA	D	1863	-	1/1/8/10	7/25/41/41	0/3/3/3
4	ILA	D	1862	-	-	10/25/41/41	0/3/3/3
4	ILA	A	1863	-	1/1/8/10	1/25/41/41	0/3/3/3
4	ILA	A	1862	-	-	6/25/41/41	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1862	ILA	SA-N5'	-8.58	1.51	1.61
4	D	1862	ILA	SA-N5'	-7.13	1.52	1.61
4	D	1863	ILA	SA-N5'	-6.77	1.53	1.61
4	A	1863	ILA	SA-N5'	-6.72	1.53	1.61
4	A	1862	ILA	SA-N3A	-6.15	1.52	1.63
4	D	1863	ILA	SA-N3A	-5.85	1.52	1.63

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1863	ILA	O1A-SA	5.73	1.51	1.43
4	D	1862	ILA	SA-N3A	-5.57	1.53	1.63
4	A	1863	ILA	SA-N3A	-5.53	1.53	1.63
4	A	1862	ILA	O2A-SA	5.11	1.50	1.43
4	A	1863	ILA	O2A-SA	4.19	1.49	1.43
4	D	1863	ILA	O2A-SA	4.00	1.48	1.43
4	D	1862	ILA	O1A-SA	3.97	1.48	1.43
4	A	1862	ILA	O1A-SA	3.89	1.48	1.43
4	D	1863	ILA	O1A-SA	3.78	1.48	1.43
4	D	1862	ILA	O2A-SA	3.64	1.48	1.43
4	A	1862	ILA	C8-N9	-3.38	1.31	1.37
4	A	1863	ILA	CA-C	-3.27	1.50	1.53
4	A	1862	ILA	CA-C	-2.90	1.50	1.53
4	D	1863	ILA	CA-C	-2.51	1.50	1.53
4	A	1862	ILA	C5-N7	-2.39	1.34	1.39
4	A	1863	ILA	C8-N7	2.29	1.36	1.31
4	D	1863	ILA	C-N3A	-2.27	1.33	1.37
4	D	1862	ILA	C8-N7	2.26	1.36	1.31
4	A	1862	ILA	C5'-N5'	-2.24	1.43	1.47
4	D	1863	ILA	C5-N7	-2.19	1.35	1.39
4	D	1862	ILA	C5-N7	-2.06	1.35	1.39
4	D	1863	ILA	C8-N7	2.00	1.35	1.31

All (62) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1862	ILA	O2A-SA-O1A	-11.18	103.88	120.34
4	D	1862	ILA	O2A-SA-O1A	-7.31	109.57	120.34
4	D	1863	ILA	O2A-SA-O1A	-7.06	109.95	120.34
4	A	1863	ILA	N1-C2-N3	-6.96	118.05	128.58
4	A	1863	ILA	O2A-SA-O1A	-6.83	110.28	120.34
4	A	1862	ILA	C4'-C5'-N5'	-5.95	101.17	112.53
4	A	1862	ILA	C5-C4-N3	-5.59	119.02	126.72
4	D	1863	ILA	C5-C4-N3	-5.51	119.12	126.72
4	A	1863	ILA	N9-C8-N7	-5.25	106.48	113.94
4	A	1863	ILA	C5-C4-N3	-5.24	119.50	126.72
4	A	1862	ILA	N1-C2-N3	-5.13	120.82	128.58
4	D	1862	ILA	C5-C4-N3	-5.04	119.78	126.72
4	D	1863	ILA	N1-C2-N3	-4.96	121.07	128.58
4	A	1862	ILA	C4-C5-N7	-4.81	105.09	110.58
4	A	1863	ILA	O-C-CA	-4.62	117.01	120.66
4	A	1863	ILA	C2-N3-C4	4.45	122.71	111.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1862	ILA	N1-C2-N3	-4.27	122.11	128.58
4	A	1862	ILA	N9-C8-N7	-4.23	107.94	113.94
4	A	1863	ILA	C5-N7-C8	4.14	109.96	103.45
4	A	1862	ILA	O2A-SA-N5'	4.08	113.88	106.77
4	A	1863	ILA	C4-N9-C8	4.07	110.02	105.74
4	D	1862	ILA	N9-C8-N7	-4.00	108.26	113.94
4	A	1862	ILA	C2-N3-C4	3.95	121.48	111.83
4	A	1862	ILA	C5-N7-C8	3.91	109.60	103.45
4	A	1863	ILA	C4-C5-N7	-3.88	106.14	110.58
4	A	1863	ILA	O1A-SA-N5'	3.85	113.48	106.77
4	A	1863	ILA	C4'-C5'-N5'	-3.71	105.45	112.53
4	D	1863	ILA	C2-N3-C4	3.63	120.70	111.83
4	D	1862	ILA	N3-C4-N9	3.61	133.31	127.17
4	D	1863	ILA	N3-C4-N9	3.58	133.25	127.17
4	A	1863	ILA	O3'-C3'-C2'	-3.50	100.60	111.82
4	A	1863	ILA	N3-C4-N9	3.49	133.11	127.17
4	A	1862	ILA	O-C-CA	-3.40	117.98	120.66
4	D	1862	ILA	C4-N9-C8	3.40	109.30	105.74
4	A	1862	ILA	O3'-C3'-C4'	-3.28	101.67	111.08
4	A	1863	ILA	C3'-C2'-C1'	3.12	107.36	101.46
4	D	1862	ILA	C2-N3-C4	3.11	119.43	111.83
4	D	1863	ILA	N9-C8-N7	-2.94	109.76	113.94
4	A	1862	ILA	N3-C4-N9	2.92	132.13	127.17
4	A	1863	ILA	C2'-C1'-N9	-2.79	106.37	113.30
4	A	1863	ILA	N3A-SA-N5'	-2.79	103.78	110.59
4	D	1862	ILA	C5-N7-C8	2.72	107.73	103.45
4	A	1862	ILA	C5-C4-N9	2.69	108.75	105.81
4	A	1862	ILA	C4-N9-C8	2.69	108.56	105.74
4	D	1862	ILA	C4'-C5'-N5'	-2.68	107.41	112.53
4	A	1863	ILA	O2A-SA-N3A	2.62	114.80	106.80
4	D	1863	ILA	C4-C5-N7	-2.55	107.66	110.58
4	A	1863	ILA	O4'-C1'-N9	2.51	112.91	108.09
4	A	1862	ILA	C2'-C1'-N9	-2.50	107.08	113.30
4	A	1863	ILA	C2-N1-C6	2.50	122.84	118.73
4	A	1862	ILA	O3'-C3'-C2'	-2.48	103.88	111.82
4	D	1862	ILA	C4-C5-N7	-2.44	107.79	110.58
4	D	1863	ILA	C5-N7-C8	2.43	107.27	103.45
4	A	1862	ILA	O-C-N3A	2.38	127.30	122.98
4	D	1862	ILA	C2'-C1'-N9	-2.38	107.39	113.30
4	A	1863	ILA	CG1-CB-CA	2.30	117.03	111.18
4	D	1863	ILA	CB-CA-C	2.25	113.06	110.27
4	A	1862	ILA	C6-C5-N7	2.17	136.28	132.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1863	ILA	C3'-C2'-C1'	2.12	105.48	101.46
4	A	1863	ILA	C6-C5-N7	2.09	136.12	132.09
4	D	1863	ILA	C4'-C5'-N5'	-2.07	108.59	112.53
4	A	1862	ILA	O2'-C2'-C1'	2.04	117.12	110.10

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	1863	ILA	CB
4	D	1863	ILA	CB

All (24) torsion outliers are listed below:

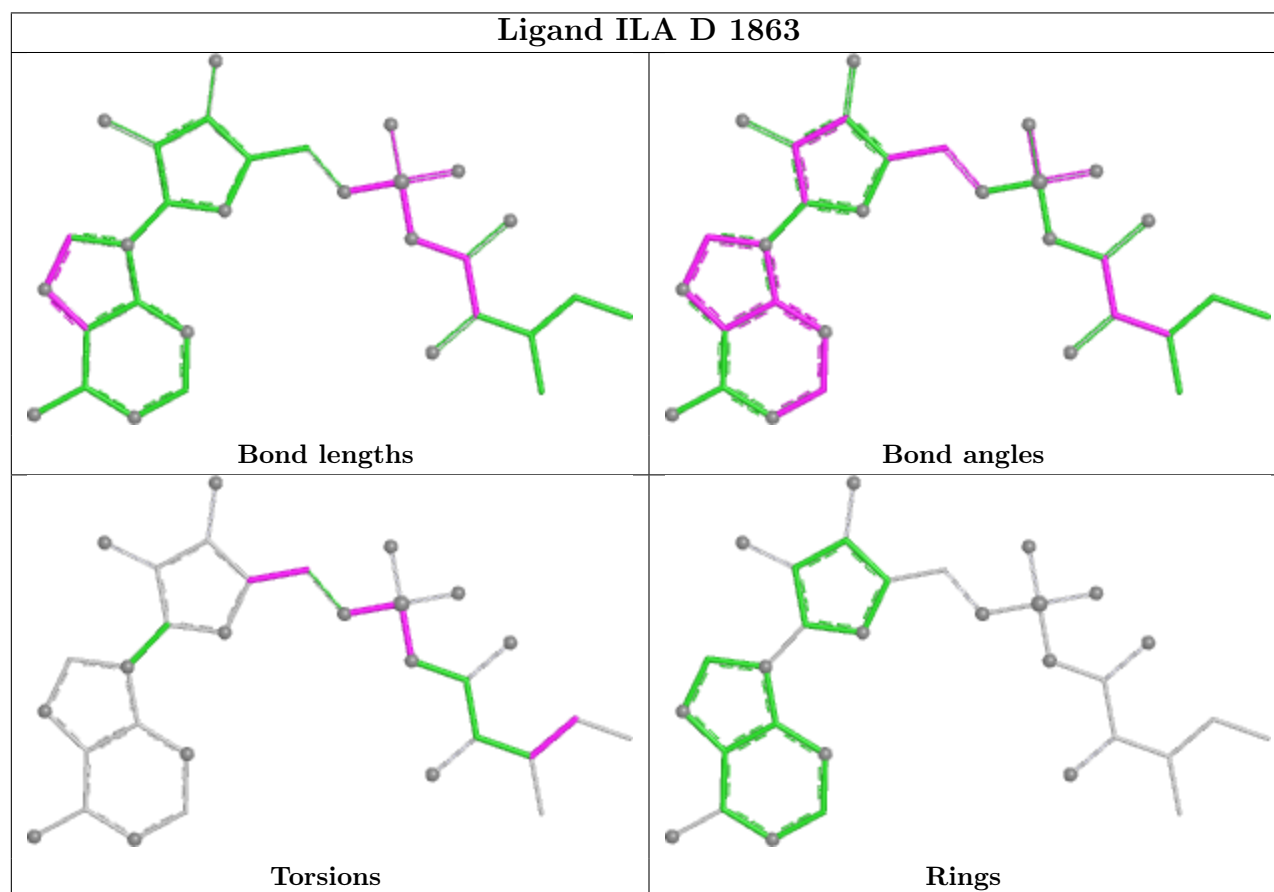
Mol	Chain	Res	Type	Atoms
4	A	1862	ILA	O-C-CA-CB
4	A	1862	ILA	N3A-C-CA-CB
4	A	1863	ILA	C5'-N5'-SA-N3A
4	D	1862	ILA	CG2-CB-CG1-CD
4	D	1862	ILA	C-N3A-SA-O2A
4	D	1862	ILA	C5'-N5'-SA-O1A
4	D	1862	ILA	C5'-N5'-SA-O2A
4	D	1862	ILA	C5'-N5'-SA-N3A
4	D	1862	ILA	O4'-C4'-C5'-N5'
4	D	1863	ILA	C-N3A-SA-N5'
4	D	1863	ILA	C5'-N5'-SA-O2A
4	D	1863	ILA	C5'-N5'-SA-N3A
4	D	1863	ILA	O4'-C4'-C5'-N5'
4	A	1862	ILA	CG2-CB-CG1-CD
4	D	1863	ILA	CG2-CB-CG1-CD
4	A	1862	ILA	CA-CB-CG1-CD
4	D	1863	ILA	CA-CB-CG1-CD
4	D	1862	ILA	CA-CB-CG1-CD
4	A	1862	ILA	C5'-N5'-SA-O2A
4	A	1862	ILA	C-CA-CB-CG2
4	D	1862	ILA	C-CA-CB-CG2
4	D	1863	ILA	C3'-C4'-C5'-N5'
4	D	1862	ILA	C-N3A-SA-N5'
4	D	1862	ILA	C3'-C4'-C5'-N5'

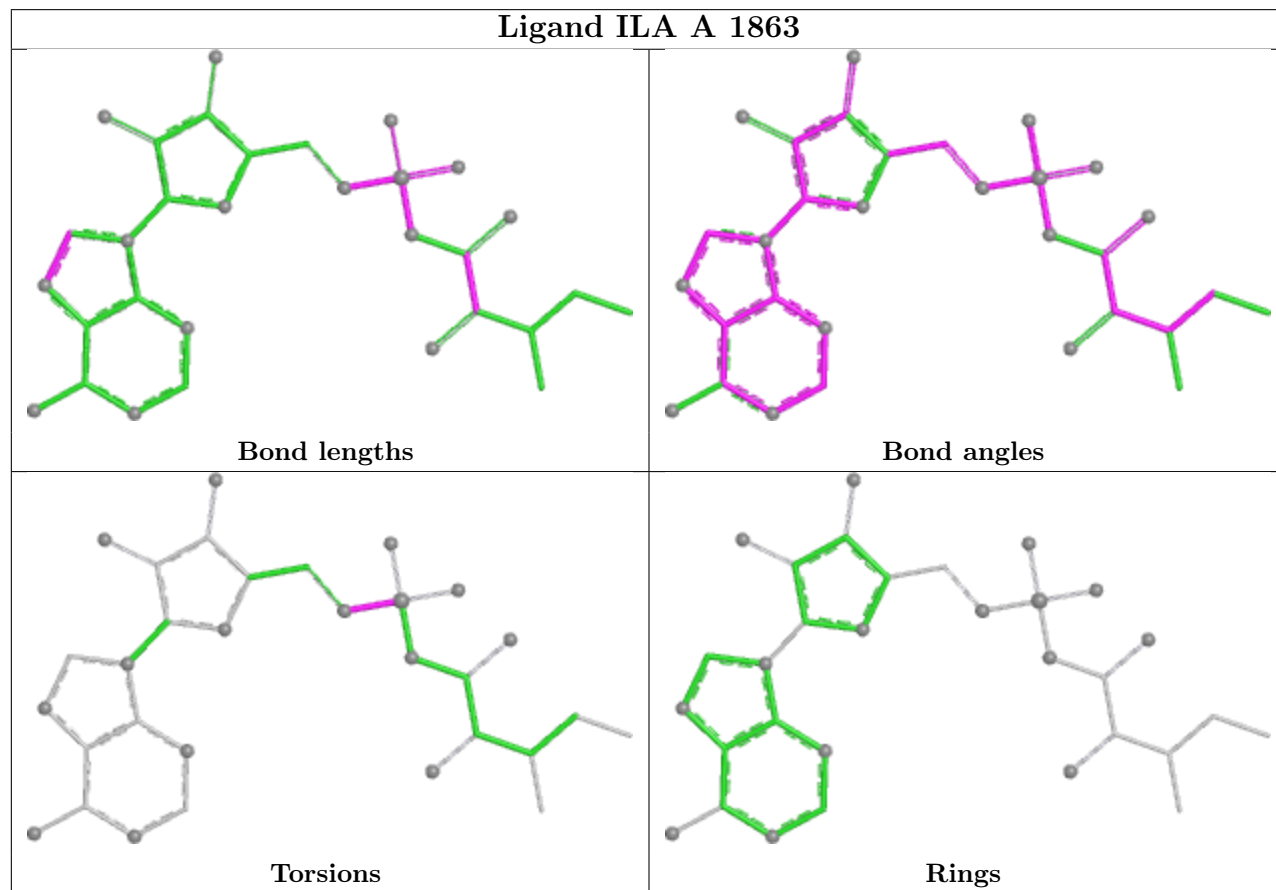
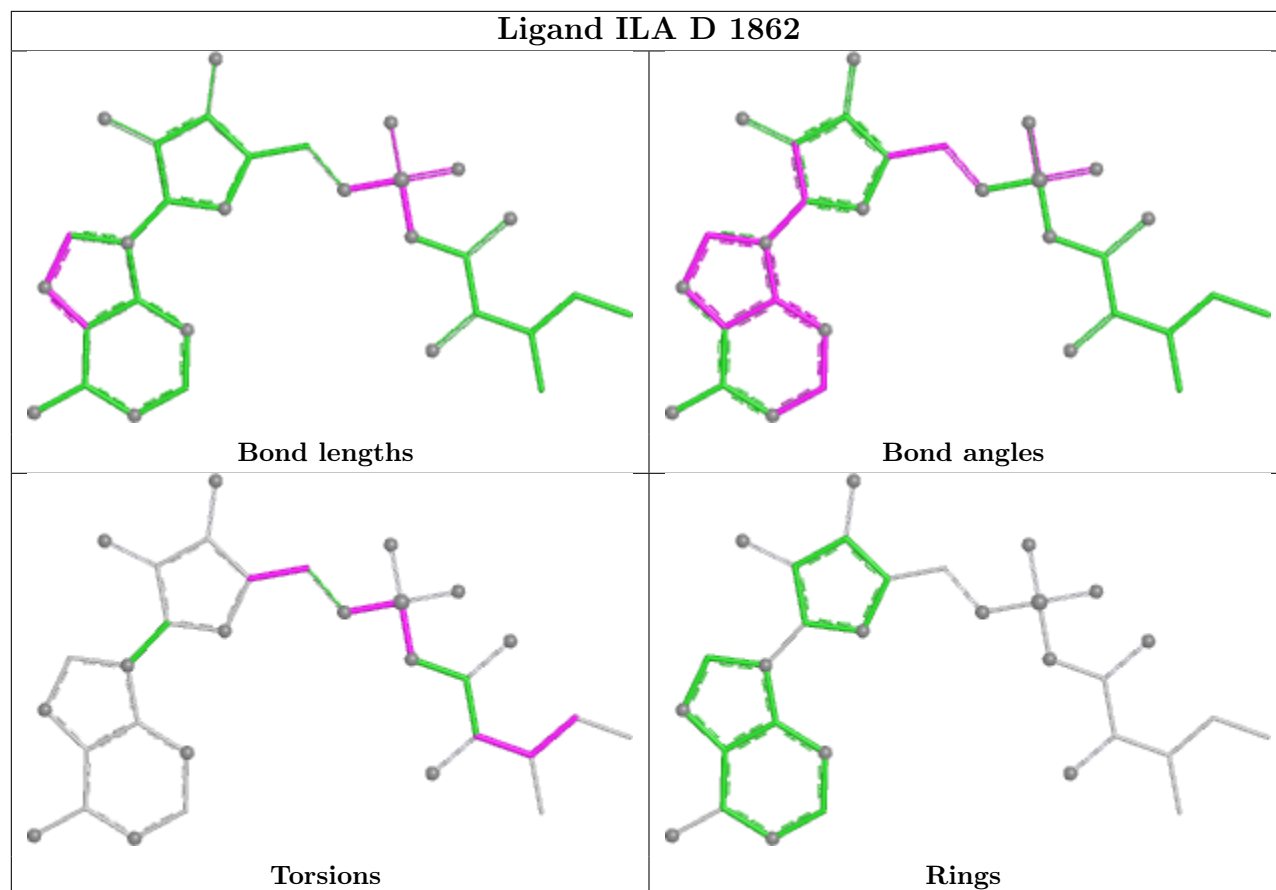
There are no ring outliers.

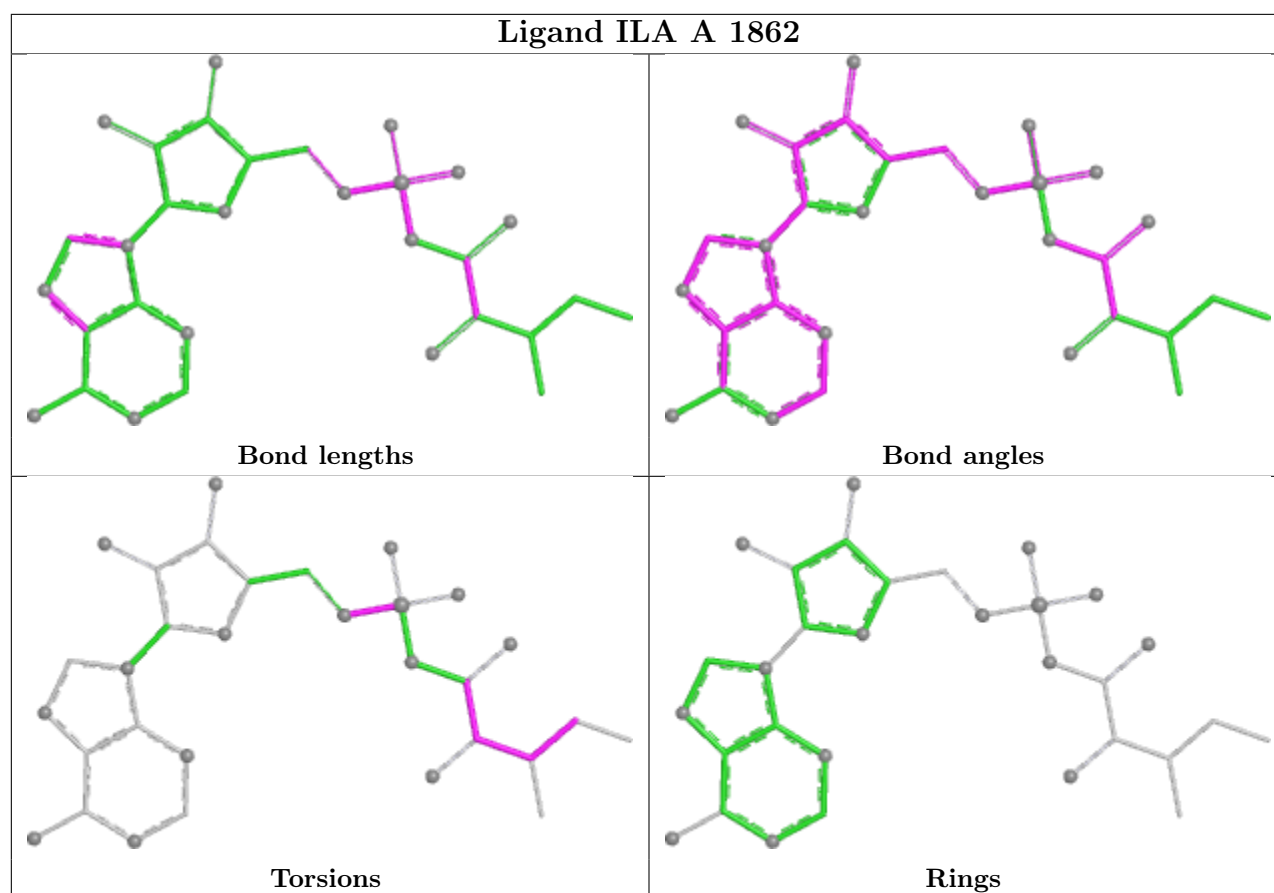
4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1863	ILA	4	0
4	D	1862	ILA	3	0
4	A	1863	ILA	11	0
4	A	1862	ILA	1	0

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







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
2	B	2
2	E	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	B	33:U	O3'	37:A	P	11.93
1	B	47(A):G	O3'	47(D):C	P	10.54
1	E	47(A):G	O3'	47(D):C	P	9.54

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, 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	860/880 (97%)	-0.39	4 (0%) 87 85	6, 19, 48, 99	2 (0%)
1	D	860/880 (97%)	0.96	97 (11%) 10 8	36, 71, 111, 142	0
2	B	82/82 (100%)	-0.60	3 (3%) 45 40	9, 21, 72, 116	0
2	E	79/82 (96%)	0.56	0 100 100	56, 79, 125, 142	0
All	All	1881/1924 (97%)	0.26	104 (5%) 30 27	6, 47, 105, 142	2 (0%)

All (104) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	322	ALA	4.7
1	D	290	VAL	4.2
1	D	810	VAL	4.0
1	D	291	ALA	3.8
1	D	858	VAL	3.7
1	D	691	VAL	3.5
1	D	857	LEU	3.5
1	D	286	ARG	3.4
1	D	253	PHE	3.3
1	D	256	CYS	3.2
1	D	379	GLY	3.2
1	D	859	VAL	3.2
1	D	295	MET	3.1
1	D	321	TRP	3.1
1	D	310	VAL	3.1
1	D	847	VAL	3.1
1	D	258	TYR	3.0
1	D	459	VAL	3.0
1	D	330	TYR	2.9
1	D	860	GLY	2.9
1	D	835	VAL	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	794	ALA	2.9
1	A	177	TRP	2.9
1	D	808	GLY	2.9
1	D	598	LYS	2.8
1	D	288	THR	2.8
1	A	580	ASN	2.8
1	D	599	GLY	2.7
1	D	814	ILE	2.7
1	D	325	PHE	2.7
1	D	834	LEU	2.7
1	D	490	PHE	2.7
1	D	36	TYR	2.7
1	D	686	VAL	2.6
1	D	260	ALA	2.6
2	B	33	U	2.6
1	D	680	HIS	2.6
1	D	293	ALA	2.6
1	D	303	VAL	2.6
2	B	17	C	2.5
1	D	844	VAL	2.5
1	A	599	GLY	2.5
1	D	166	LEU	2.5
1	D	420	TRP	2.5
1	D	324	ASN	2.4
1	D	856	ASN	2.4
1	D	155	ALA	2.4
1	D	164	THR	2.4
1	D	93	ASN	2.4
1	D	177	TRP	2.4
1	D	352	TYR	2.4
1	D	368	PRO	2.4
1	D	777	LYS	2.4
1	D	331	GLY	2.4
1	D	852	GLY	2.4
1	D	359	VAL	2.3
1	D	158	TRP	2.3
1	D	206	LEU	2.3
1	D	705	VAL	2.3
1	D	349	ALA	2.3
1	D	701	LEU	2.3
1	D	848	ILE	2.3
1	D	540	TYR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	384	SER	2.3
1	D	370	LEU	2.3
1	D	463	ILE	2.3
1	D	789	VAL	2.3
1	D	96	ALA	2.2
1	D	830	GLY	2.2
1	D	375	LEU	2.2
1	D	183	VAL	2.2
1	D	63	ALA	2.2
1	D	362	ALA	2.2
1	D	821	THR	2.2
1	D	833	HIS	2.2
1	D	366	SER	2.2
1	D	160	PRO	2.2
1	D	320	VAL	2.2
1	D	337	ALA	2.2
1	D	753	ALA	2.2
1	D	681	THR	2.2
1	D	353	GLY	2.2
1	D	855	LEU	2.2
1	D	165	VAL	2.2
1	D	263	ALA	2.2
1	D	755	LEU	2.2
1	D	768	ILE	2.2
1	D	334	ALA	2.1
1	D	229	GLY	2.1
1	D	318	ILE	2.1
1	D	234	PHE	2.1
1	D	363	ALA	2.1
1	D	361	LEU	2.1
1	D	224	ILE	2.1
1	D	254	MET	2.1
1	D	787	TRP	2.1
1	D	432	ILE	2.1
1	D	380	VAL	2.0
1	D	314	THR	2.0
2	B	37	A	2.0
1	A	178	ARG	2.0
1	D	796	VAL	2.0
1	D	287	ASN	2.0
1	D	706	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

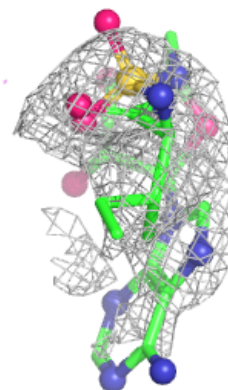
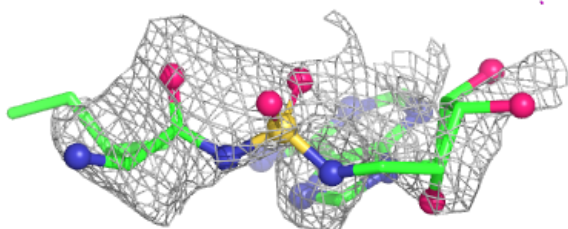
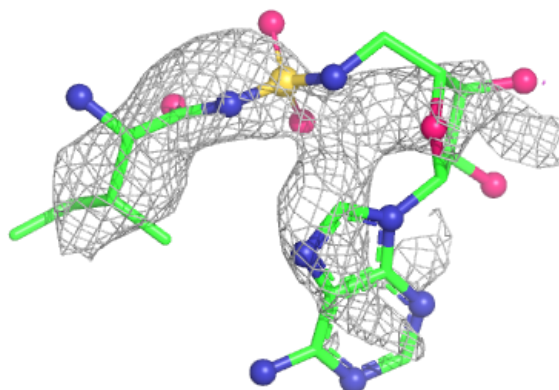
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
4	ILA	D	1863	31/31	0.72	0.17	104,151,160,160	0
5	MG	E	1077	1/1	0.89	0.07	52,52,52,52	0
4	ILA	D	1862	31/31	0.91	0.09	38,48,56,61	0
3	ZN	D	1861	1/1	0.93	0.05	100,100,100,100	0
4	ILA	A	1863	31/31	0.94	0.08	21,28,32,36	0
5	MG	B	1077	1/1	0.96	0.05	25,25,25,25	0
4	ILA	A	1862	31/31	0.97	0.06	7,10,11,11	0
3	ZN	A	1861	1/1	0.98	0.04	65,65,65,65	0

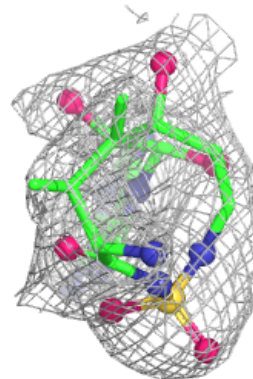
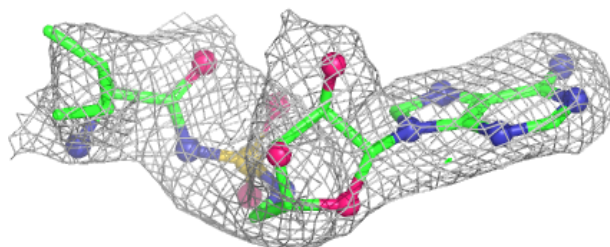
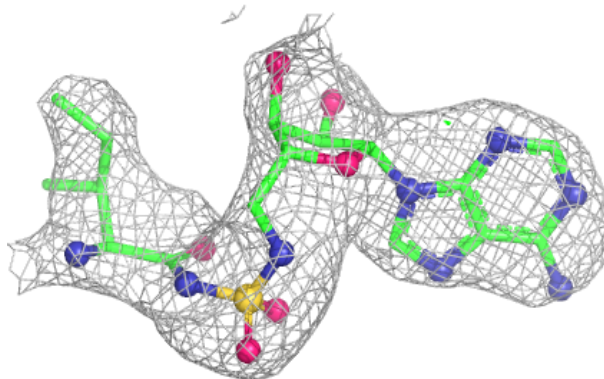
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around ILA D 1863:

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

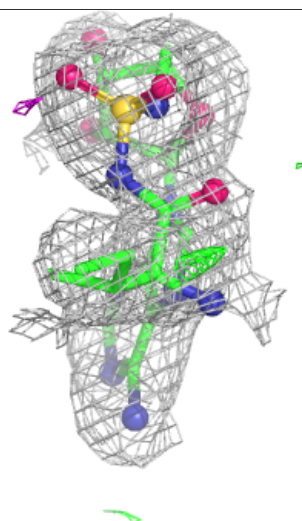
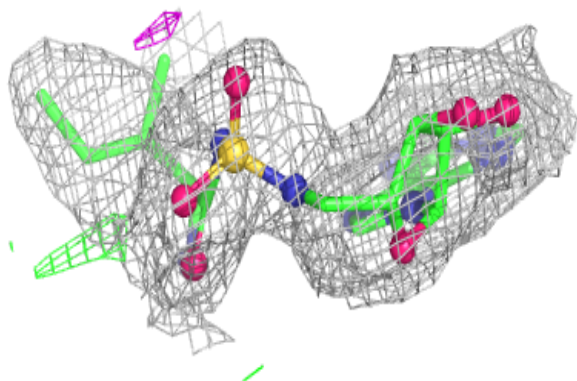
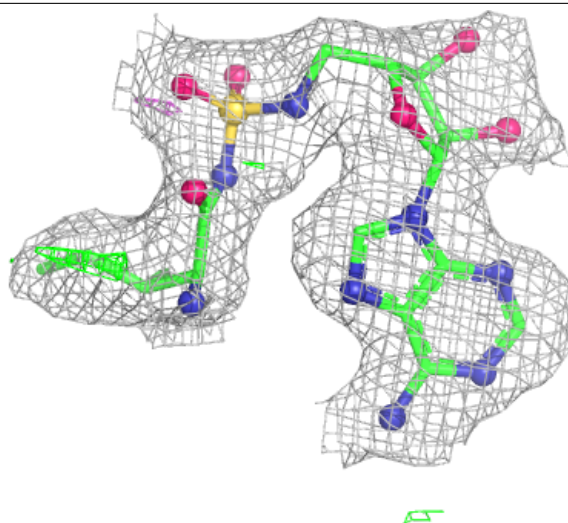
**Electron density around ILA D 1862:**

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



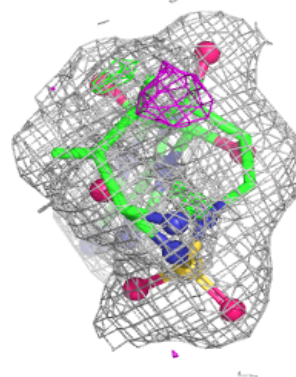
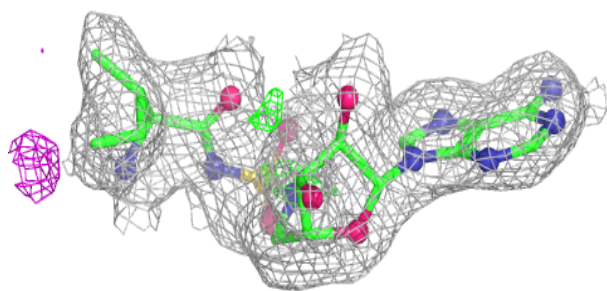
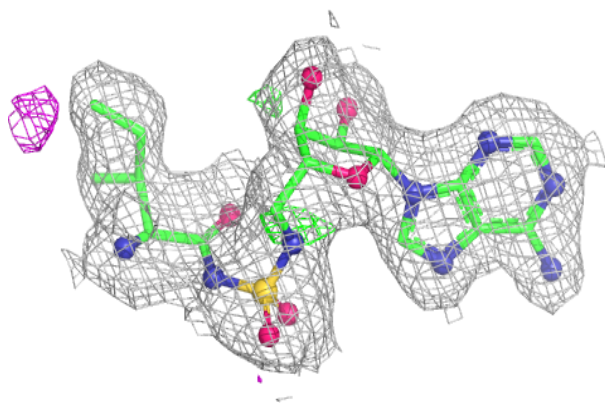
Electron density around ILA A 1863:

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



Electron density around ILA A 1862:

$2mF_o-DF_c$ (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.