



Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 09:58 pm BST

PDB ID : 4CQN
Title : Crystal structure of the E.coli LeuRS-tRNA complex with the non- cognate
isoleucyl adenylate analogue
Authors : Palencia, A.; Cusack, S.; Cvetesic, 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.11
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.11

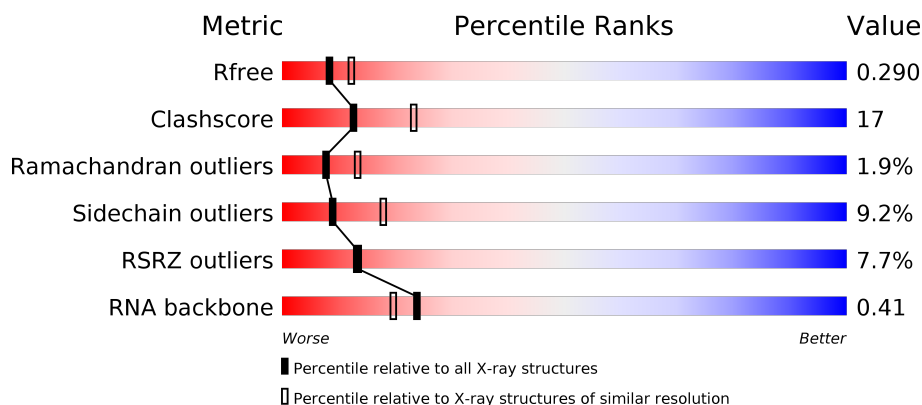
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)
RNA backbone	3102	1008 (2.84-2.16)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 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	<div> <div>%</div> <div> <div></div> <div>58%</div> <div>36%</div> <div>• •</div> </div> </div>
1	D	880	<div> <div>15%</div> <div> <div></div> <div>59%</div> <div>34%</div> <div>• •</div> </div> </div>
2	B	82	<div> <div>%</div> <div> <div></div> <div>45%</div> <div>38%</div> <div>17%</div> </div> </div>
2	E	82	<div> <div>10%</div> <div> <div></div> <div>32%</div> <div>51%</div> <div>13%</div> <div>•</div> </div> </div>

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

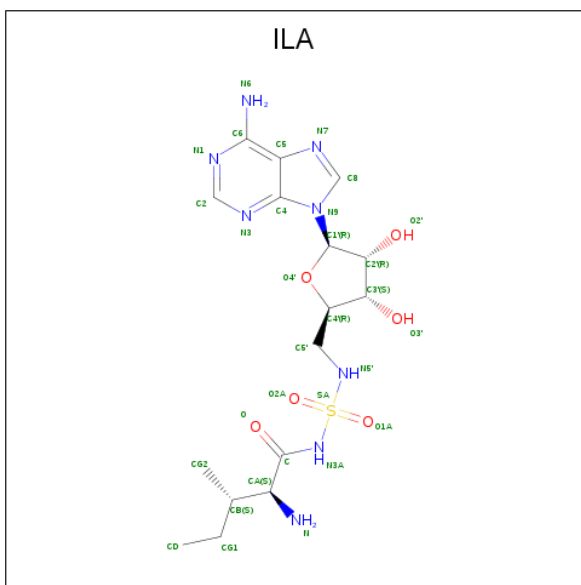
- Molecule 2 is a RNA chain called ESCHERICHIA COLI TRNA-LEU UAA ISOACCEPTOR.

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 (three-letter code: 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 (three-letter code: 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 (three-letter code: 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

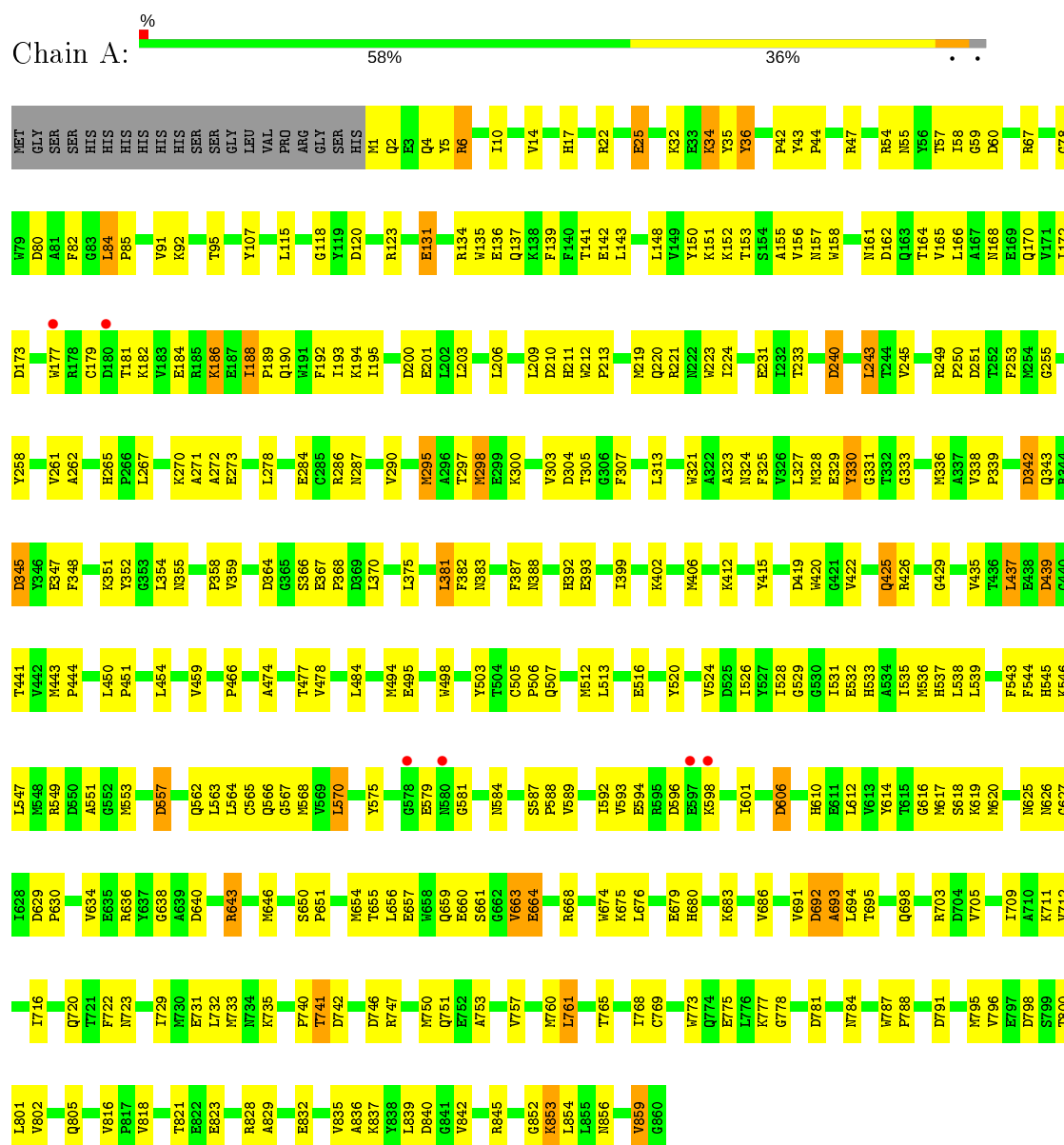
- Molecule 6 is water.

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

3 Residue-property plots

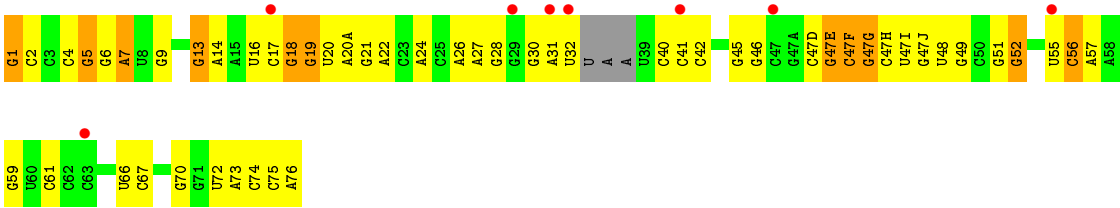
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($\text{RSRZ} > 2$). 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: LEUCINE-TRNA LIGASE



- Molecule 1: LEUCINE-TRNA LIGASE





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 46.45 – 2.50	Depositor EDS
% Data completeness (in resolution range)	97.1 (46.49-2.50) 97.1 (46.45-2.50)	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)	0.29 , 45.5	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

5.1 Standard geometry

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

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	0.71	0/7014	0.88	7/9520 (0.1%)
1	D	0.38	0/6995	0.60	1/9495 (0.0%)
2	B	0.61	2/1959 (0.1%)	0.90	4/3047 (0.1%)
2	E	0.37	1/1887 (0.1%)	0.64	0/2935
All	All	0.56	3/17855 (0.0%)	0.76	12/24997 (0.0%)

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

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	G	OP3-P	-9.82	1.49	1.61
2	B	1	G	OP3-P	-9.46	1.49	1.61
2	B	12	G	O3'-P	-6.47	1.53	1.61

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	58	A	O5'-P-OP2	-7.04	99.36	105.70
1	A	345	ASP	CB-CG-OD1	6.49	124.14	118.30
2	B	72	U	O5'-P-OP2	6.16	118.09	110.70
1	A	345	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	A	791	ASP	CB-CG-OD1	5.62	123.36	118.30
1	A	643	ARG	NE-CZ-NH1	-5.58	117.51	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	437	LEU	CA-CB-CG	5.24	127.36	115.30
2	B	65	C	C2'-C3'-O3'	5.12	121.89	113.70
1	A	166	LEU	CB-CG-CD1	-5.11	102.32	111.00
1	D	84	LEU	CA-CB-CG	5.09	127.00	115.30
1	A	557	ASP	CB-CG-OD1	5.08	122.88	118.30
2	B	74	C	O5'-P-OP1	-5.07	101.14	105.70

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	258	0
1	D	6834	0	6683	216	0
2	B	1755	0	890	37	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
6	B	57	0	0	1	0
6	D	16	0	0	2	0
All	All	17558	0	15231	537	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 17.

All (537) 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	1.35	1.07
1:A:267:LEU:HD21	1:A:305:THR:HG21	1.40	1.00
1:A:553:MET:CE	6:A:2052:HOH:O	2.10	0.99
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:HE1	6:A:2052:HOH:O	1.64	0.94
2:B:40:C:H2'	2:B:41:C:H5''	1.51	0.93
1:A:801:LEU:HD23	1:A:801:LEU:C	1.90	0.92
1:A:342:ASP:OD2	4:A:1863:ILA:HG22	1.72	0.89
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:342:ASP:HB2	4:A:1863:ILA:HG21	1.57	0.85
1:A:34:LYS:O	1:A:34:LYS:HD3	1.75	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
2:B:41:C:C5'	2:B:41:C:H6	1.93	0.80
1:A:512:MET:O	1:A:513:LEU:HD23	1.81	0.80
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:139:PHE:HE1	1:A:553:MET:HE3	1.49	0.77
1:A:422:VAL:HG11	1:A:494:MET:CE	2.13	0.77
1:A:507:GLN:OE1	1:A:507:GLN:HA	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
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
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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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: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:295:MET:HA	1:A:295:MET:HE3	1.73	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:139:PHE:HE1	1:A:553:MET:CE	2.05	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:C6	2:B:41:C:C5'	2.75	0.68
1:D:134:ARG:HH11	1:D:451:PRO:HD3	1.57	0.68
1:D:57:THR:O	1:D:61:VAL:HG23	1.93	0.68
1:D:17:HIS:O	1:D:21:LYS:HB2	1.94	0.68
1:A:532:GLU:H	1:A:568:MET:HE1	1.58	0.68
1:D:651:PRO:HG3	2:E:14:A:OP1	1.94	0.68
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:258:TYR:HH	1:A:348:PHE:HB3	1.59	0.67
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:A:34:LYS:C	1:A:34:LYS:HD3	2.15	0.66
1:D:44:PRO:HA	1:D:108:MET:SD	2.36	0.65
1:A:200:ASP:OD1	1:A:415:TYR:OH	2.12	0.65
1:A:271:ALA:CB	1:A:305:THR:HG23	2.26	0.65
2:B:37:A:H2'	2:B:37:A:N3	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:A:606:ASP:CG	1:A:610:HIS:HB2	2.17	0.64
1:A:801:LEU:C	1:A:801:LEU:CD2	2.66	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:42:PRO:HD2	1:A:78:GLY:O	1.98	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: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:A:139:PHE:CE1	1:A:553:MET:CE	2.82	0.62
1:D:422:VAL:HG11	1:D:494:MET:HE1	1.82	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:D:446:PRO:HB2	1:D:448:ASP:OD1	1.99	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:A:617:MET:HE1	1:A:657:GLU:HB3	1.83	0.61
1:D:817:PRO:HB2	1:D:820:ALA:HB2	1.81	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
1:A:342:ASP:CB	4:A:1863:ILA:CG2	2.77	0.60
1:A:270:LYS:O	1:A:273:GLU:HB2	2.00	0.60
1:D:153:THR:HG23	1:D:187:GLU:HB3	1.83	0.60
2:B:41:C:C6	2:B:41:C:H5'	2.24	0.60
1:A:587:SER:OG	1:A:589:VAL:HG23	2.02	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:378:LYS:HB3	1:D:392:HIS:CG	2.37	0.60
1:D:60:ASP:OD2	1:D:117:PHE:HA	2.02	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:553:MET:HE2	6:A:2052:HOH:O	1.84	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:75:C:H2'	2:E:76:A:O4'	2.02	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:O2	2:B:17:C:H2'	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:478:VAL:C	1:D:480:GLY:H	2.05	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: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:435:VAL:HG11	1:A:478:VAL:HG21	1.86	0.57
1:A:136:GLU:OE2	1:A:495:GLU:OE2	2.21	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
2:E:56:C:H2'	2:E:57:A:C8	2.39	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:A:630:PRO:O	1:A:634:VAL:HG23	2.05	0.56
1:A:402:LYS:O	1:A:406:MET:HG3	2.04	0.56
1:D:236:VAL:HG21	1:D:239:TYR:HD2	1.70	0.56
1:A:351:LYS:HD3	1:A:352:TYR:CE2	2.41	0.56
1:A:686:VAL:HG21	1:A:751:GLN:HG2	1.88	0.56
1:A:295:MET:HE1	1:A:325:PHE:HA	1.87	0.56
1:D:685:ASP:O	1:D:747:ARG:NH2	2.39	0.56
1:A:852:GLY:C	1:A:853:LYS:HE3	2.26	0.56
1:A:165:VAL:HG21	1:A:425:GLN:CG	2.32	0.56
1:A:139:PHE:CE1	1:A:553:MET:HE3	2.38	0.56
1:A:845:ARG:HH11	1:A:845:ARG:HG3	1.70	0.56
1:A:426:ARG:HH11	1:A:426:ARG:CB	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:468:LYS:HG2	1:D:487:THR:HB	1.88	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:82:PHE:HB2	1:D:492:THR:HG22	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: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:D:134:ARG:CB	1:D:451:PRO:HB3	2.37	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:D:68:MET:HE1	1:D:759:ARG:HB3	1.90	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
1:A:676:LEU:CD2	1:A:733:MET:HE3	2.37	0.54
4:D:1863:ILA:HN5	4:D:1863:ILA:H8	1.73	0.54
2:E:40:C:O2	2:E:40:C:H2'	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: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
4:A:1863:ILA:HG23	4:A:1863:ILA:HNA	1.73	0.54
2:B:10:G:C2'	2:B:11:U:H5'	2.38	0.54
2:E:5:G:H2'	2:E:6:G:H8	1.72	0.54
1:A:422:VAL:CG1	1:A:494:MET:HE1	2.25	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: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:253:PHE:C	1:D:255:GLY:H	2.11	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: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:342:ASP:CG	4:A:1863:ILA:HG22	2.28	0.52
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:192:PHE:HA	1:A:420:TRP:O	2.08	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:712:VAL:O	1:A:716:ILE:HG13	2.10	0.52
1:A:240:ASP:OD1	1:A:240:ASP:N	2.43	0.52
1:A:437:LEU:HB2	1:A:439:ASP:HB2	1.92	0.52
1:D:305:THR:C	1:D:307:PHE:H	2.13	0.52
1:D:777:LYS:HA	6:D:2015:HOH:O	2.09	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:HB2	1:A:426:ARG:HH11	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
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:D:695:THR:C	1:D:697:ASN:H	2.13	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:295:MET:CE	1:A:325:PHE:HA	2.40	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
1:A:139:PHE:CE1	1:A:553:MET:HE1	2.46	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:A:676:LEU:HD23	1:A:733:MET:CE	2.40	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:157:ASN:ND2	1:D:157:ASN:H	2.09	0.51
1:D:98:ALA:HA	1:D:428:TRP:CH2	2.45	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:A:212:TRP:CH2	1:A:538:LEU:HD22	2.46	0.50
1:A:823:GLU:CD	1:A:823:GLU:H	2.14	0.50
1:D:543:PHE:CZ	1:D:547:LEU:HD11	2.47	0.50
1:D:424:ARG:NH2	2:E:74:C:OP2	2.44	0.50
1:D:42:PRO:HD2	1:D:78:GLY:O	2.11	0.50
2:E:14:A:O4'	2:E:22:A:C6	2.64	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:262:ALA:HB3	1:A:328:MET:HG2	1.94	0.50
1:A:328:MET:HE2	1:A:333:GLY:HA3	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:102:TYR:HA	1:D:105:ILE:HD12	1.94	0.49
1:D:43:TYR:HE2	1:D:82:PHE:O	1.95	0.49
1:A:367:GLU:HG2	1:A:382:PHE:CZ	2.47	0.49
1:A:422:VAL:CG1	1:A:494:MET:CE	2.87	0.49
1:A:588:PRO:HD2	1:A:626:ASN:HA	1.95	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:D:681:THR:C	1:D:683:LYS:H	2.16	0.49
1:A:544:PHE:O	1:A:545:HIS:C	2.51	0.49
1:A:854:LEU:HD13	2:B:19:G:H1'	1.95	0.49
1:A:775:GLU:C	1:A:777:LYS:H	2.15	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:A:676:LEU:HD22	1:A:733:MET:HE3	1.95	0.48
1:D:190:GLN:HE22	2:E:74:C:H41	1.61	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:D:148:LEU:O	1:D:194:LYS:HB2	2.14	0.48
1:A:91:VAL:O	1:A:92:LYS:C	2.53	0.47
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: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:25:GLU:HA	1:A:120:ASP:CG	2.34	0.47
1:A:835:VAL:O	1:A:839:LEU:HG	2.14	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:D:536:MET:O	1:D:540:TYR:CD2	2.67	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:606:ASP:OD2	1:D:610:HIS:ND1	2.37	0.47
1:A:342:ASP:OD1	1:A:345:ASP:N	2.31	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:47:ARG:NH1	1:D:579:GLU:OE1	2.47	0.47
1:D:90:ALA:HB1	1:D:95:THR:O	2.15	0.47
1:A:533:HIS:HB3	1:A:537:HIS:HB3	1.97	0.47
1:A:258:TYR:HH	1:A:348:PHE:CB	2.28	0.47
2:B:47(G):G:C2	2:B:47(H):C:C2	3.03	0.47
1:D:514:ASP:C	1:D:514:ASP:OD1	2.52	0.47
4:A:1863:ILA:N3A	4:A:1863:ILA:HG23	2.30	0.47
1:A:206:LEU:HD23	1:A:209:LEU:HD12	1.97	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:O2	2:E:47(D):C:O4'	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: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:551:ALA:CB	1:A:553:MET:HE3	2.44	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:673:VAL:HG22	1:D:733:MET:HE2	1.96	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: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:CD1	1:A:330:TYR:N	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: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:D:36:TYR:CE1	1:D:38:LEU:HB2	2.51	0.46
1:A:137:GLN:O	1:A:141:THR:HG23	2.16	0.46
1:A:135:TRP:HB2	1:A:498:TRP:CH2	2.50	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:172:ILE:O	1:A:172:ILE:HG13	2.16	0.46
1:A:828:ARG:O	1:A:829:ALA:C	2.54	0.46
1:D:175:CYS:HB3	1:D:182:LYS:HA	1.97	0.46
2:E:5:G:H2'	2:E:6:G:C8	2.51	0.46
1:A:131:GLU:CD	1:A:131:GLU:H	2.19	0.45
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:A:60:ASP:OD1	1:A:118:GLY:N	2.35	0.45
1:D:235:ASN:O	1:D:309:ALA:HA	2.15	0.45
1:D:76:PRO:HG2	1:D:503:TYR:CE2	2.51	0.45
4:A:1863:ILA:H8	4:A:1863:ILA:HN5	1.79	0.45
1:A:845:ARG:NH1	1:A:845:ARG:HG3	2.31	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:D:313:LEU:C	1:D:315:GLY:H	2.18	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: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:D:77:ILE:O	1:D:503:TYR:HE1	2.00	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:733:MET:HA	1:D:736:LEU:HD12	1.99	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:676:LEU:HG	1:D:754:LEU:HD11	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:650:SER:HB2	1:A:651:PRO:HD3	1.97	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:543:PHE:CE2	1:A:547:LEU:HD11	2.53	0.44
1:D:633:MET:HE2	1:D:642:VAL:HG13	2.00	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:D:606:ASP:CG	1:D:610:HIS:HD1	2.16	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
1:A:295:MET:CA	1:A:295:MET:HE3	2.45	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:385:GLY:C	1:D:387:PHE:H	2.20	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:575:TYR:HA	1:A:584:ASN:O	2.18	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:A:532:GLU:H	1:A:568:MET:HE3	1.81	0.43
1:D:693:ALA:O	1:D:694:LEU:HG	2.18	0.43
1:A:723:ASN:N	1:A:723:ASN:OD1	2.52	0.43
1:A:358:PRO:HB3	1:A:370:LEU:HD11	2.00	0.43
1:A:67:ARG:NH2	6:A:2025:HOH:O	2.48	0.43
1:D:52:HIS:O	1:D:56:TYR:CD2	2.71	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
2:B:47(G):G:H2'	2:B:47(H):C:O4'	2.19	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)
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:123:ARG:HD3	1:A:503:TYR:O	2.18	0.43
1:A:54:ARG:HD3	1:A:54:ARG:HH11	1.71	0.43
1:A:339:PRO:HG3	1:A:355:ASN:O	2.19	0.43
1:A:375:LEU:HA	1:A:375:LEU:HD12	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:130:PRO:C	1:D:132:TYR:H	2.22	0.43
1:D:190:GLN:HE22	2:E:74:C:N4	2.17	0.43
1:D:532:GLU:H	1:D:568:MET:HE3	1.83	0.43
1:A:683:LYS:HB2	1:A:747:ARG:NH2	2.33	0.42
1:A:836:ALA:O	1:A:837:LYS:C	2.57	0.42
1:A:255:GLY:C	1:A:338:VAL:HG22	2.40	0.42
1:A:364:ASP:OD1	1:A:364:ASP:C	2.57	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
1:D:673:VAL:HA	1:D:733:MET:HE1	2.00	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: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:438:GLU:HB3	1:D:481:MET:CE	2.49	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:D:185:ARG:NH1	1:D:289:LYS:O	2.52	0.42
1:D:289:LYS:HD2	1:D:289:LYS:HA	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:450:LEU:HA	1:A:451:PRO:C	2.40	0.42
1:A:703:ARG:HG3	1:A:795:MET:HA	2.02	0.42
1:A:84:LEU:HD21	1:A:170:GLN:NE2	2.35	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:O	1:D:84:LEU:HD22	2.20	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:328:MET:N	1:D:328:MET:SD	2.93	0.42
1:A:676:LEU:HD23	1:A:733:MET:HE3	2.01	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
1:A:17:HIS:NE2	1:A:781:ASP:OD2	2.44	0.42
2:B:47(H):C:O2'	2:B:47(I):U:H5'	2.20	0.42
1:A:520:TYR:C	1:A:520:TYR:CD1	2.92	0.42
1:A:201:GLU:OE2	1:A:546:LYS:HD3	2.19	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
1:A:300:LYS:HD3	6:A:2123:HOH:O	2.19	0.41
1:D:276:PRO:HA	6:D:2008:HOH:O	2.20	0.41
1:D:49:HIS:CD2	1:D:52:HIS:CE1	3.08	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:D:54:ARG:NH2	1:D:650:SER:HB3	2.34	0.41
1:A:295:MET:HE1	1:A:324:ASN:O	2.20	0.41
1:A:538:LEU:HA	1:A:538:LEU:HD23	1.79	0.41
1:A:57:THR:O	1:A:58:ILE:C	2.58	0.41
2:E:72:U:H5''	2:E:73:A:H5'	2.01	0.41
1:A:265:HIS:CD2	1:A:328:MET:HE1	2.56	0.41
1:A:313:LEU:HD11	1:A:399:ILE:HG23	2.01	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:643:ARG:NH2	1:D:766:PRO:HD3	2.34	0.41
1:D:71:LYS:O	1:D:73:VAL:HG23	2.20	0.41
1:A:34:LYS:HB3	1:A:520:TYR:CE1	2.55	0.41
1:A:629:ASP:HA	1:A:630:PRO:HD2	1.87	0.41
1:D:351:LYS:HD3	1:D:351:LYS:HA	1.90	0.41
1:D:77:ILE:HG13	1:D:78:GLY:N	2.36	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: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
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: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
1:A:823:GLU:CD	1:A:823:GLU:N	2.74	0.41
1:A:84:LEU:HB3	1:A:85:PRO:HD3	2.03	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47(I):U:H2'	2:B:47(J):G:O5'	2.20	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:383:ASN:N	1:A:388:ASN:OD1	2.53	0.41
1:A:5:TYR:CE1	1:A:768:ILE:HD12	2.56	0.41
2:B:14:A:C2'	2:B:15:A:O5'	2.68	0.41
1:D:669:PHE:HA	1:D:672:ARG:CZ	2.50	0.41
1:D:756:ALA:O	1:D:757:VAL:C	2.58	0.41
1:A:243:LEU:CD1	1:A:265:HIS:CE1	3.04	0.41
1:A:634:VAL:O	1:A:638:GLY:N	2.51	0.41
2:B:3:C:C2'	2:B:4:C:H5'	2.51	0.41
1:D:76:PRO:CG	1:D:503:TYR:CD2	3.01	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:681:THR:C	1:D:683:LYS:N	2.74	0.41
2:E:47(E):G:H4'	2:E:47(F):C:OP2	2.20	0.41
1:A:298:MET:HE3	1:A:298:MET:HB3	1.90	0.40
1:D:249:ARG:HA	1:D:249:ARG:HD2	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:134:ARG:HG3	1:A:135:TRP:N	2.36	0.40
1:A:35:TYR:CE2	1:A:526:ILE:HG22	2.57	0.40
1:A:136:GLU:HB3	1:A:498:TRP:NE1	2.36	0.40
1:A:618:SER:O	1:A:619:LYS:C	2.59	0.40
1:D:172:ILE:HG22	1:D:173:ASP:N	2.35	0.40
1:D:58:ILE:HG13	1:D:647:MET:CE	2.51	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
1:A:313:LEU:HD13	1:A:387:PHE:CE2	2.57	0.40
1:A:155:ALA:HB3	1:A:329:GLU:OE2	2.21	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:223:TRP:CD2	1:D:535:ILE:HG21	2.56	0.40
1:D:5:TYR:CE2	1:D:7:PRO:HG3	2.56	0.40
1:A:732:LEU:HD23	1:A:757:VAL:HG22	2.03	0.40
1:A:731:GLU:O	1:A:735:LYS:HG3	2.22	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:249:ARG:C	1:A:251:ASP:N	2.75	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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 [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	860/880 (98%)	797 (93%)	54 (6%)	9 (1%)	15	28
1	D	858/880 (98%)	716 (83%)	119 (14%)	23 (3%)	5	7
All	All	1718/1760 (98%)	1513 (88%)	173 (10%)	32 (2%)	8	13

All (32) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	439	ASP
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	726/741 (98%)	661 (91%)	65 (9%)	9	19
1	D	723/741 (98%)	655 (91%)	68 (9%)	8	17
All	All	1449/1482 (98%)	1316 (91%)	133 (9%)	9	18

All (133) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	25	GLU
1	A	32	LYS
1	A	34	LYS
1	A	36	TYR
1	A	55	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	84	LEU
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	177	TRP
1	A	182	LYS
1	A	184	GLU
1	A	186	LYS
1	A	188	ILE
1	A	210	ASP
1	A	240	ASP
1	A	243	LEU
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
1	A	342	ASP
1	A	381	LEU
1	A	393	GLU
1	A	412	LYS
1	A	425	GLN
1	A	459	VAL
1	A	466	PRO
1	A	477	THR
1	A	516	GLU
1	A	570	LEU
1	A	579	GLU
1	A	594	GLU
1	A	598	LYS
1	A	606	ASP
1	A	625	ASN
1	A	636	ARG
1	A	646	MET
1	A	656	LEU
1	A	659	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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	750	MET
1	A	761	LEU
1	A	796	VAL
1	A	798	ASP
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	34	LYS
1	D	36	TYR
1	D	55	ASN
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	228	GLU
1	D	241	ASN
1	D	243	LEU
1	D	261	VAL
1	D	269	GLN
1	D	273	GLU
1	D	275	ASN
1	D	289	LYS
1	D	294	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	300	LYS
1	D	312	PRO
1	D	318	ILE
1	D	324	ASN
1	D	327	LEU
1	D	336	MET
1	D	356	ILE
1	D	372	GLN
1	D	373	GLN
1	D	375	LEU
1	D	376	THR
1	D	391	ASP
1	D	396	PHE
1	D	427	TYR
1	D	448	ASP
1	D	465	SER
1	D	479	ASN
1	D	488	ASP
1	D	491	ASP
1	D	513	LEU
1	D	527	TYR
1	D	531	ILE
1	D	541	PHE
1	D	544	PHE
1	D	621	SER
1	D	622	LYS
1	D	646	MET
1	D	650	SER
1	D	659	GLN
1	D	660	GLU
1	D	692	ASP
1	D	701	LEU
1	D	702	ARG
1	D	708	THR
1	D	742	ASP
1	D	768	ILE
1	D	793	LYS
1	D	798	ASP
1	D	805	GLN
1	D	816	VAL
1	D	823	GLU
1	D	828	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	842	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	110	ASN
1	A	555	ASN
1	A	774	GLN
1	A	831	GLN
1	D	110	ASN
1	D	157	ASN
1	D	190	GLN
1	D	222	ASN
1	D	355	ASN
1	D	425	GLN
1	D	507	GLN
1	D	533	HIS
1	D	562	GLN
1	D	680	HIS

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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	41	C
2	B	47	C
2	B	47(E)	G
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 [i](#)

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	ILA	A	1862	-	29,33,33	2.19	6 (20%)	31,49,49	3.00	11 (35%)
4	ILA	D	1862	-	29,33,33	1.79	3 (10%)	31,49,49	1.86	3 (9%)
4	ILA	D	1863	-	29,33,33	1.82	6 (20%)	31,49,49	1.86	3 (9%)
4	ILA	A	1863	-	29,33,33	2.00	4 (13%)	31,49,49	2.75	12 (38%)

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	A	1862	-	-	6/21/41/41	0/3/3/3
4	ILA	D	1862	-	-	9/21/41/41	0/3/3/3
4	ILA	D	1863	-	1/1/8/10	7/21/41/41	0/3/3/3
4	ILA	A	1863	-	1/1/8/10	1/21/41/41	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1862	ILA	SA-N5'	-8.47	1.51	1.61

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1862	ILA	SA-N5'	-7.05	1.52	1.61
4	D	1863	ILA	SA-N5'	-6.69	1.53	1.61
4	A	1863	ILA	SA-N5'	-6.65	1.53	1.61
4	A	1863	ILA	O1A-SA	5.34	1.51	1.43
4	A	1862	ILA	O2A-SA	4.76	1.50	1.43
4	A	1863	ILA	O2A-SA	3.91	1.49	1.43
4	D	1863	ILA	O2A-SA	3.73	1.48	1.43
4	D	1862	ILA	O1A-SA	3.70	1.48	1.43
4	A	1862	ILA	O1A-SA	3.63	1.48	1.43
4	D	1863	ILA	O1A-SA	3.52	1.48	1.43
4	D	1862	ILA	O2A-SA	3.40	1.48	1.43
4	A	1863	ILA	CA-C	-3.14	1.50	1.53
4	A	1862	ILA	O4'-C1'	2.95	1.45	1.41
4	A	1862	ILA	CA-C	-2.78	1.50	1.53
4	D	1863	ILA	CA-C	-2.40	1.50	1.53
4	D	1863	ILA	O4'-C1'	2.20	1.44	1.41
4	D	1863	ILA	C-N3A	-2.10	1.33	1.37
4	A	1862	ILA	C5'-N5'	-2.07	1.43	1.47

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1862	ILA	O2A-SA-O1A	-11.04	103.88	120.40
4	D	1862	ILA	O2A-SA-O1A	-7.24	109.57	120.40
4	D	1863	ILA	O2A-SA-O1A	-6.98	109.95	120.40
4	A	1863	ILA	N3-C2-N1	-6.80	118.05	128.68
4	A	1863	ILA	O2A-SA-O1A	-6.76	110.28	120.40
4	A	1862	ILA	C4'-C5'-N5'	-5.66	101.17	112.51
4	A	1862	ILA	N3-C2-N1	-5.03	120.82	128.68
4	D	1863	ILA	N3-C2-N1	-4.87	121.07	128.68
4	A	1863	ILA	O-C-CA	-4.72	117.01	120.73
4	A	1863	ILA	C3'-C2'-C1'	4.24	107.36	100.98
4	D	1862	ILA	N3-C2-N1	-4.20	122.11	128.68
4	A	1862	ILA	C4-C5-N7	-4.14	105.09	109.40
4	A	1862	ILA	O2A-SA-N5'	4.06	113.88	106.73
4	A	1863	ILA	O1A-SA-N5'	3.83	113.48	106.73
4	A	1863	ILA	C4'-C5'-N5'	-3.52	105.45	112.51
4	A	1862	ILA	O-C-CA	-3.50	117.98	120.73
4	A	1863	ILA	O3'-C3'-C2'	-3.47	100.60	111.82
4	A	1862	ILA	O3'-C3'-C4'	-3.25	101.67	111.05
4	A	1863	ILA	C4-C5-N7	-3.12	106.14	109.40
4	D	1863	ILA	C3'-C2'-C1'	2.99	105.48	100.98

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1863	ILA	N3A-SA-N5'	-2.89	103.78	110.88
4	A	1862	ILA	C5-C6-N6	2.62	124.33	120.35
4	D	1862	ILA	C4'-C5'-N5'	-2.54	107.41	112.51
4	A	1863	ILA	O2A-SA-N3A	2.52	114.80	106.85
4	A	1862	ILA	O3'-C3'-C2'	-2.46	103.88	111.82
4	A	1863	ILA	C2-N1-C6	2.39	122.84	118.75
4	A	1863	ILA	CG1-CB-CA	2.32	117.03	111.18
4	A	1862	ILA	O-C-N3A	2.24	127.30	123.00
4	A	1862	ILA	O4'-C1'-C2'	-2.11	103.84	106.93

All (2) chirality outliers are listed below:

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

All (23) torsion outliers are listed below:

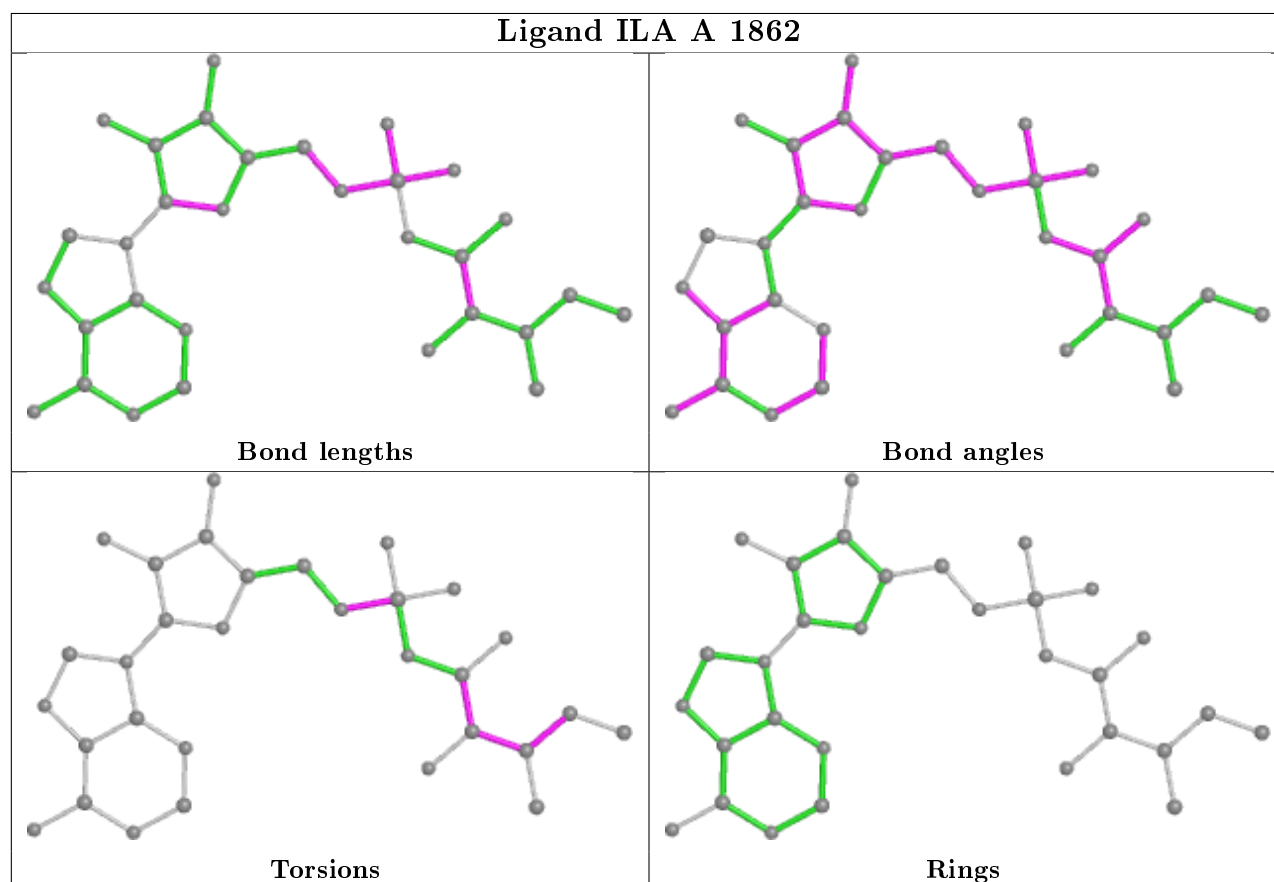
Mol	Chain	Res	Type	Atoms
4	D	1863	ILA	C-N3A-SA-N5'
4	D	1863	ILA	C5'-N5'-SA-O2A
4	D	1863	ILA	C5'-N5'-SA-N3A
4	D	1862	ILA	CG2-CB-CG1-CD
4	D	1862	ILA	C-N3A-SA-O1A
4	D	1862	ILA	C-N3A-SA-O2A
4	D	1862	ILA	C5'-N5'-SA-O1A
4	D	1862	ILA	C5'-N5'-SA-O2A
4	D	1862	ILA	C5'-N5'-SA-N3A
4	A	1862	ILA	O-C-CA-CB
4	A	1862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

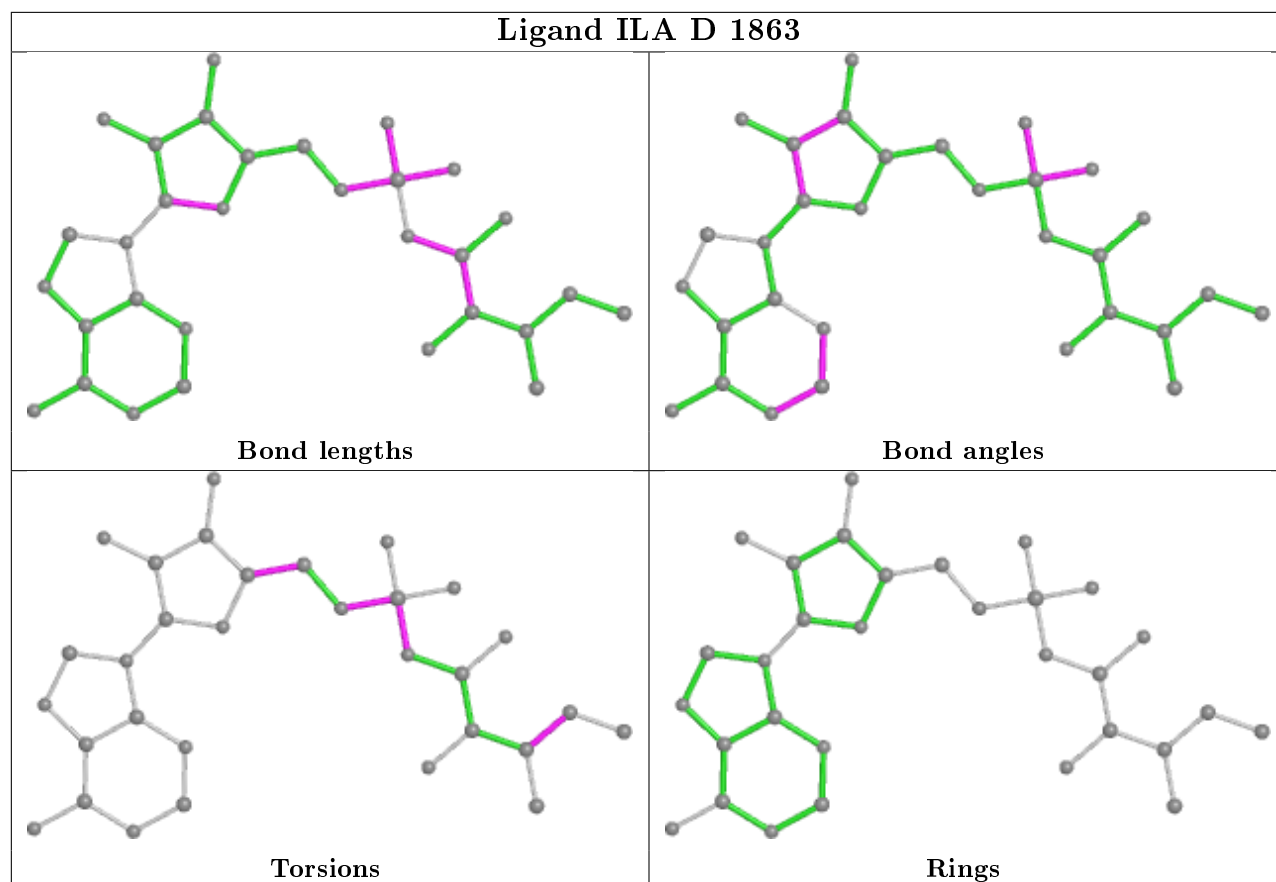
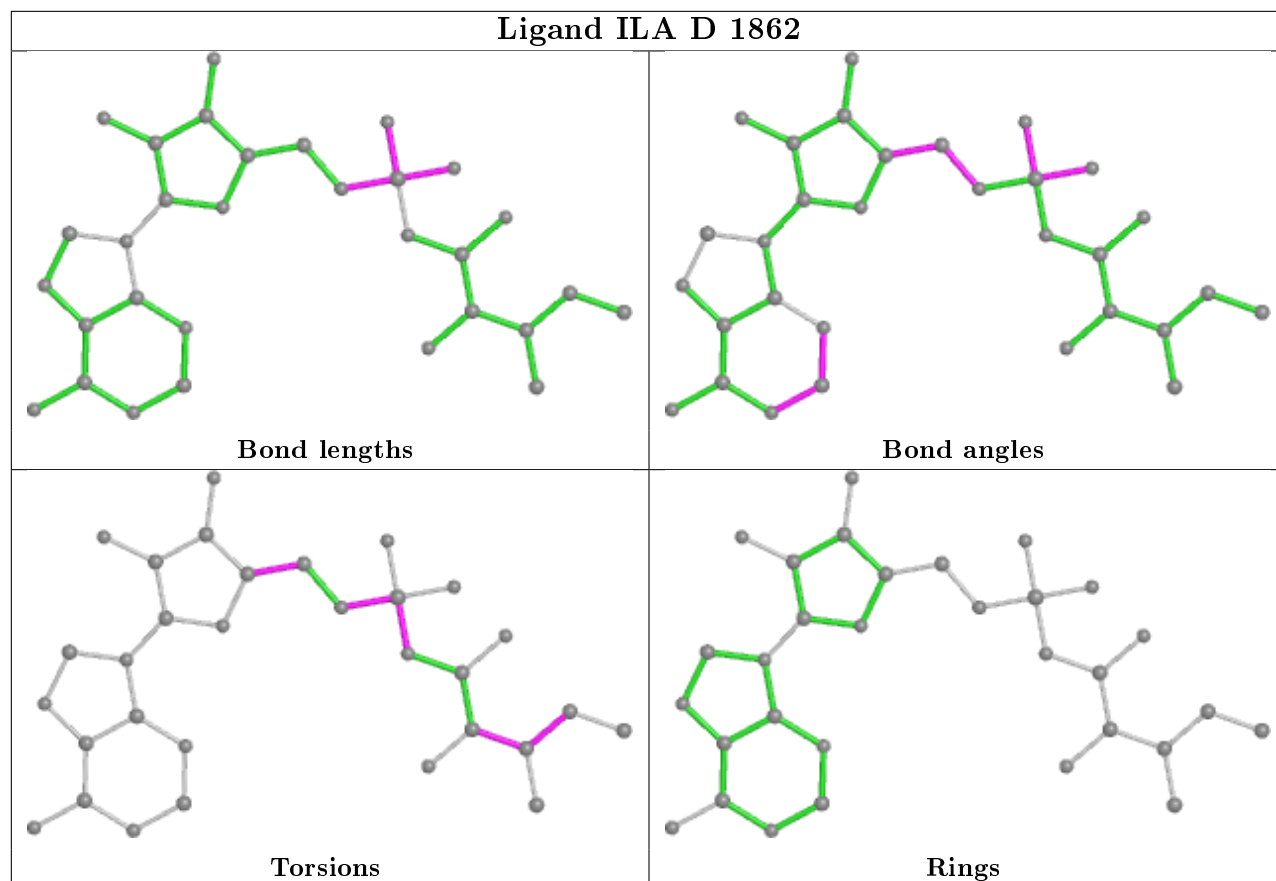
There are no ring outliers.

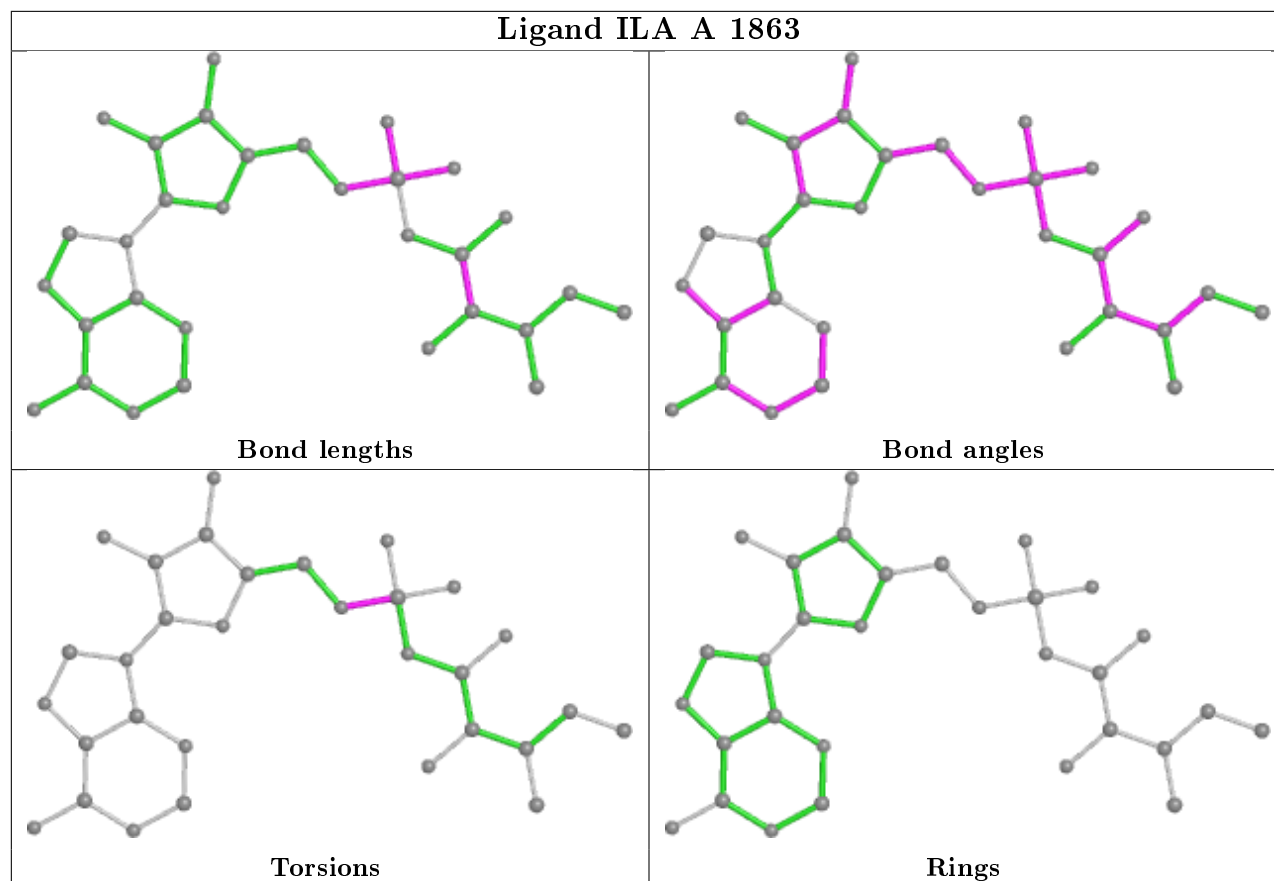
4 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1862	ILA	1	0
4	D	1862	ILA	3	0
4	D	1863	ILA	4	0
4	A	1863	ILA	11	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%)	-0.29	6 (0%) 87 89	6, 19, 48, 99	0
1	D	860/880 (97%)	0.95	129 (15%) 2 2	36, 71, 111, 142	0
2	B	82/82 (100%)	-0.61	1 (1%) 79 80	9, 21, 72, 116	0
2	E	79/82 (96%)	0.62	8 (10%) 7 6	56, 79, 125, 142	0
All	All	1881/1924 (97%)	0.30	144 (7%) 13 13	6, 47, 105, 142	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	860	GLY	12.7
1	D	809	LYS	6.0
1	D	330	TYR	5.8
1	D	322	ALA	5.6
1	D	352	TYR	5.6
1	D	321	TRP	5.5
1	D	348	PHE	5.4
1	D	324	ASN	5.1
1	D	846	LYS	5.0
1	D	279	ALA	5.0
1	D	178	ARG	4.9
1	D	847	VAL	4.9
1	D	379	GLY	4.9
2	E	31	A	4.8
1	D	281	PHE	4.7
1	D	820	ALA	4.7
1	D	845	ARG	4.6
1	D	295	MET	4.5
1	D	287	ASN	4.4
1	D	598	LYS	4.4
1	D	320	VAL	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	810	VAL	4.2
1	D	303	VAL	4.2
1	D	691	VAL	4.2
1	D	368	PRO	4.2
1	D	808	GLY	4.1
1	D	253	PHE	4.1
2	E	32	U	4.0
1	D	310	VAL	4.0
1	D	259	LEU	3.9
1	D	319	PRO	3.9
1	D	858	VAL	3.9
1	D	325	PHE	3.8
1	D	463	ILE	3.8
1	D	256	CYS	3.8
1	D	851	PRO	3.8
1	D	848	ILE	3.7
1	D	370	LEU	3.7
1	D	362	ALA	3.7
1	A	598	LYS	3.6
1	A	580	ASN	3.6
1	D	597	GLU	3.6
1	D	258	TYR	3.5
1	D	852	GLY	3.5
1	D	291	ALA	3.5
1	D	601	ILE	3.5
1	D	286	ARG	3.5
1	D	859	VAL	3.5
1	D	276	PRO	3.4
1	D	599	GLY	3.4
1	D	600	ARG	3.3
1	D	843	THR	3.3
1	D	736	LEU	3.3
1	D	354	LEU	3.2
1	D	313	LEU	3.2
1	D	363	ALA	3.1
1	D	351	LYS	3.1
1	D	459	VAL	3.1
1	D	855	LEU	3.1
1	D	160	PRO	3.1
1	D	271	ALA	3.0
1	D	288	THR	3.0
1	D	172	ILE	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	353	GLY	3.0
1	D	694	LEU	3.0
1	D	302	GLY	3.0
1	D	366	SER	2.9
1	D	367	GLU	2.9
1	D	835	VAL	2.9
1	D	742	ASP	2.9
1	D	841	GLY	2.9
1	D	405	ALA	2.8
1	D	582	GLU	2.8
1	A	578	GLY	2.8
1	D	177	TRP	2.8
1	D	364	ASP	2.8
2	E	17	C	2.8
1	D	380	VAL	2.7
1	D	378	LYS	2.7
1	D	318	ILE	2.7
1	D	166	LEU	2.7
1	D	789	VAL	2.7
1	D	844	VAL	2.6
1	D	850	VAL	2.6
1	D	365	GLY	2.6
1	D	297	THR	2.6
1	D	356	ILE	2.6
1	D	811	ARG	2.6
1	D	807	ASN	2.5
1	D	856	ASN	2.5
1	D	602	VAL	2.5
1	D	699	LYS	2.5
1	D	737	ALA	2.5
1	D	93	ASN	2.5
1	D	349	ALA	2.5
1	D	267	LEU	2.4
1	D	361	LEU	2.4
1	D	539	LEU	2.4
1	D	306	GLY	2.4
1	D	684	GLY	2.4
1	D	164	THR	2.4
1	D	290	VAL	2.4
1	D	161	ASN	2.4
2	E	29	G	2.4
1	D	821	THR	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	D	458	VAL	2.4
1	D	689	LEU	2.4
1	D	831	GLN	2.4
1	D	270	LYS	2.3
1	D	369	ASP	2.3
1	D	283	ASP	2.3
1	D	331	GLY	2.3
1	D	73	VAL	2.3
1	D	536	MET	2.3
1	D	309	ALA	2.3
1	D	344	ARG	2.3
2	E	63	C	2.3
1	D	849	TYR	2.3
1	D	777	LYS	2.2
2	E	41	C	2.2
2	E	47	C	2.2
1	D	517	ALA	2.2
1	D	359	VAL	2.2
1	D	294	GLU	2.2
1	A	177	TRP	2.2
1	D	346	TYR	2.2
1	D	686	VAL	2.2
1	D	755	LEU	2.2
1	A	597	GLU	2.2
1	D	680	HIS	2.1
1	D	857	LEU	2.1
2	E	55	U	2.1
1	A	180	ASP	2.1
1	D	181	THR	2.1
1	D	307	PHE	2.1
1	D	373	GLN	2.1
1	D	375	LEU	2.1
1	D	269	GLN	2.1
1	D	337	ALA	2.1
1	D	781	ASP	2.0
1	D	255	GLY	2.0
1	D	299	GLU	2.0
2	B	17	C	2.0
1	D	481	MET	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 carbohydrates in this entry.

6.4 Ligands [i](#)

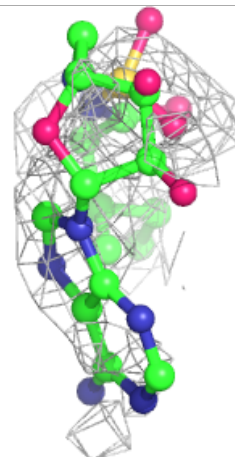
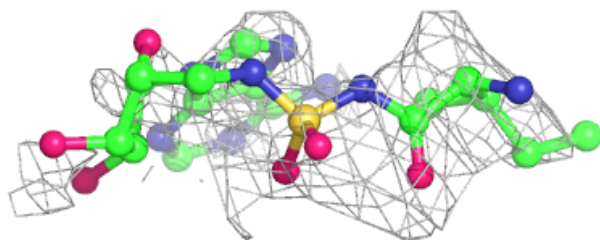
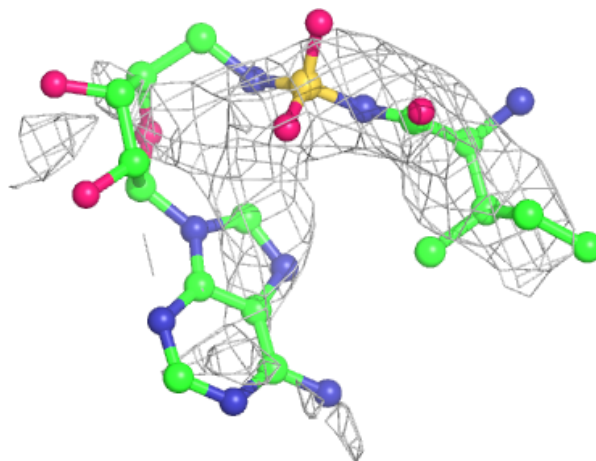
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
4	ILA	D	1863	31/31	0.65	0.31	104,151,160,160	0
3	ZN	D	1861	1/1	0.86	0.06	100,100,100,100	0
5	MG	B	1077	1/1	0.93	0.09	25,25,25,25	0
5	MG	E	1077	1/1	0.93	0.22	52,52,52,52	0
4	ILA	D	1862	31/31	0.95	0.16	38,48,56,61	0
4	ILA	A	1863	31/31	0.95	0.14	21,28,32,36	0
3	ZN	A	1861	1/1	0.96	0.05	65,65,65,65	0
4	ILA	A	1862	31/31	0.97	0.15	7,10,11,11	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.

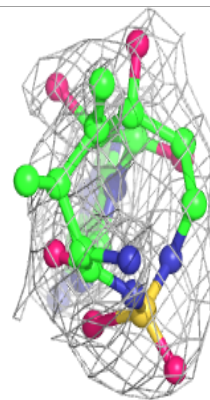
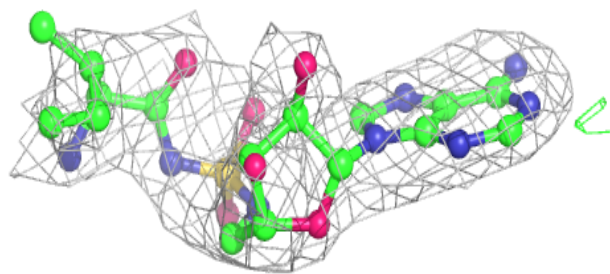
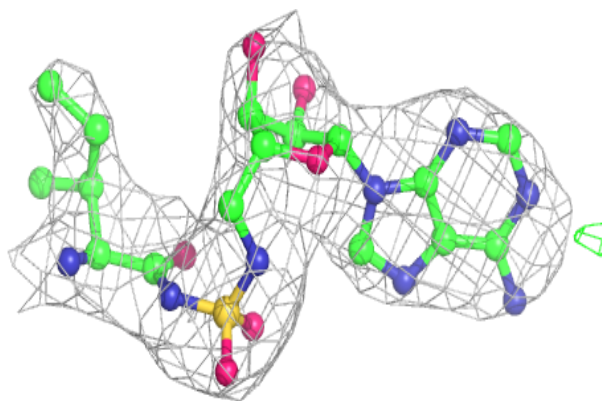
Electron density around ILA D 1863:

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



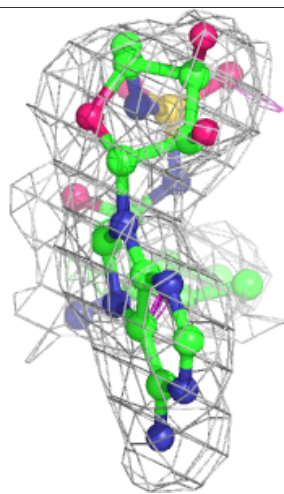
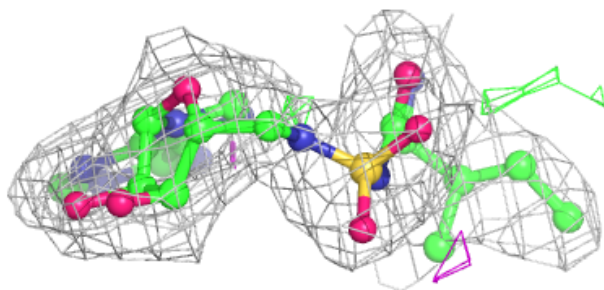
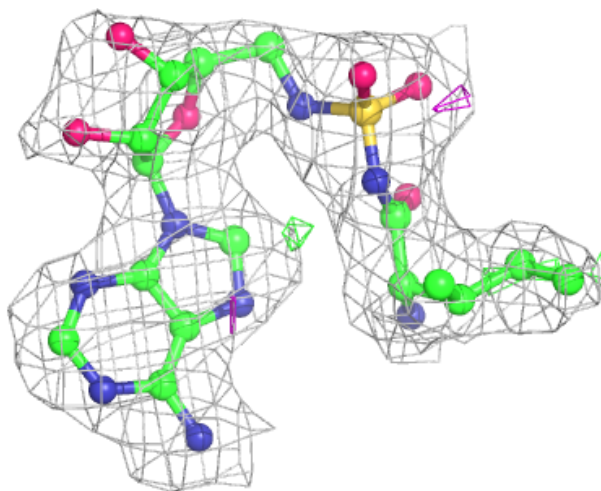
Electron density around ILA D 1862:

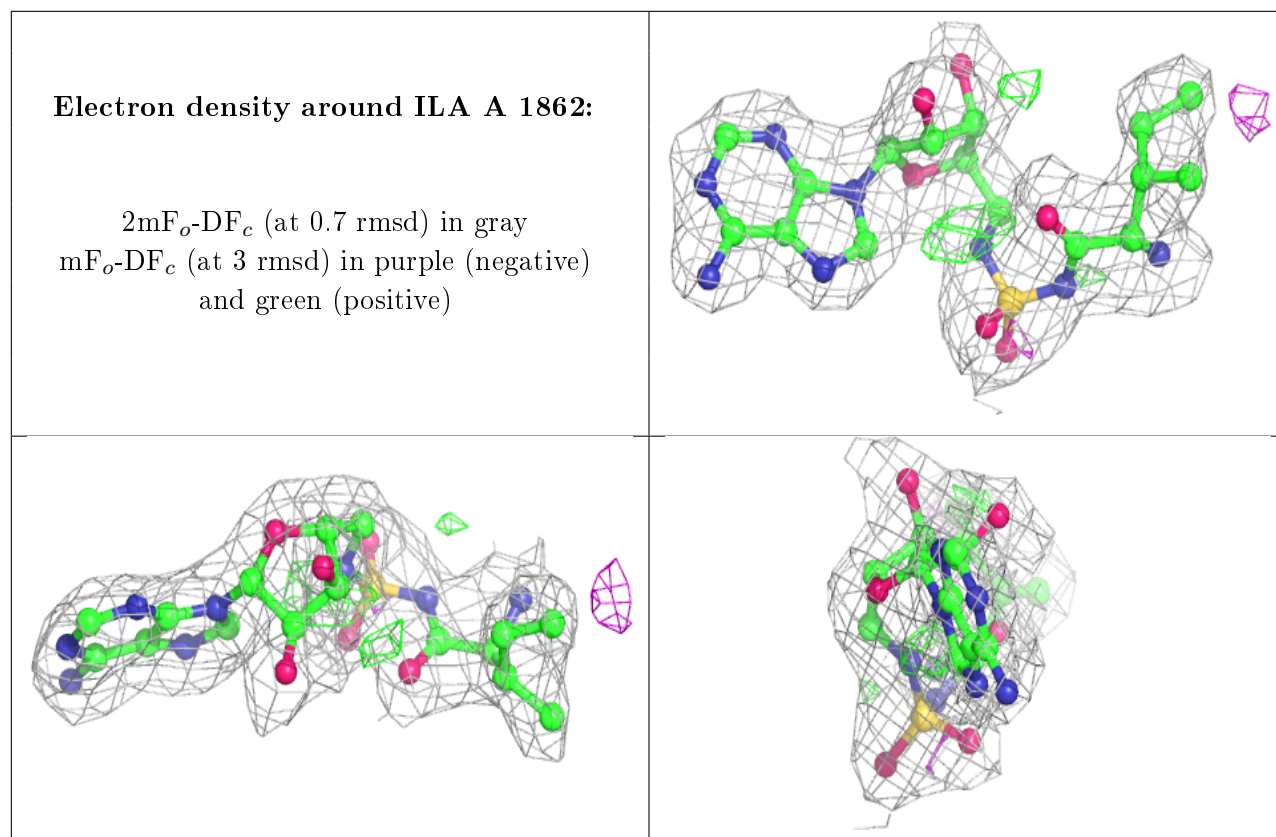
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



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)





6.5 Other polymers [i](#)

There are no such residues in this entry.