



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 03:36 PM GMT

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
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

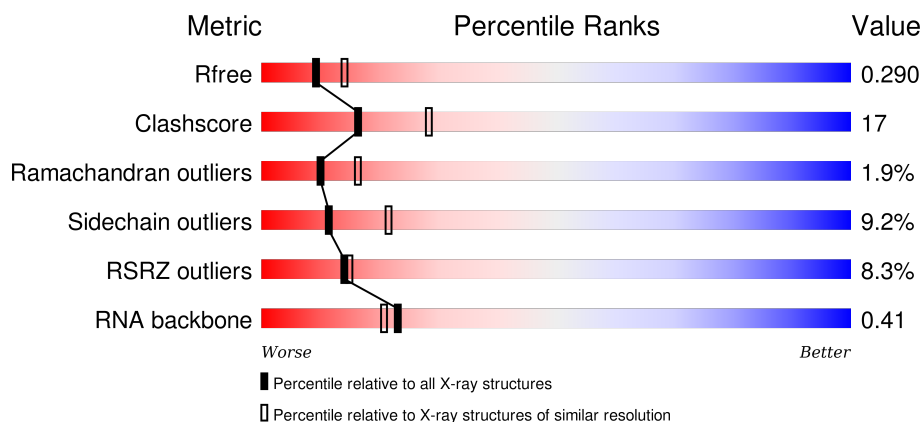
1 Overall quality at a glance

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}	91344	3553 (2.50-2.50)
Clashscore	102246	4242 (2.50-2.50)
Ramachandran outliers	100387	4156 (2.50-2.50)
Sidechain outliers	100360	4158 (2.50-2.50)
RSRZ outliers	91569	3562 (2.50-2.50)
RNA backbone	2183	1172 (3.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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>16%</div> <div>58%</div> <div>36%</div> <div>• •</div> </div>
1	D	880	<div> <div>16%</div> <div>59%</div> <div>34%</div> <div>• •</div> </div>
2	B	82	<div> <div>45%</div> <div>38%</div> <div>17%</div> </div>
2	E	82	<div> <div>11%</div> <div>32%</div> <div>51%</div> <div>13%</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

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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

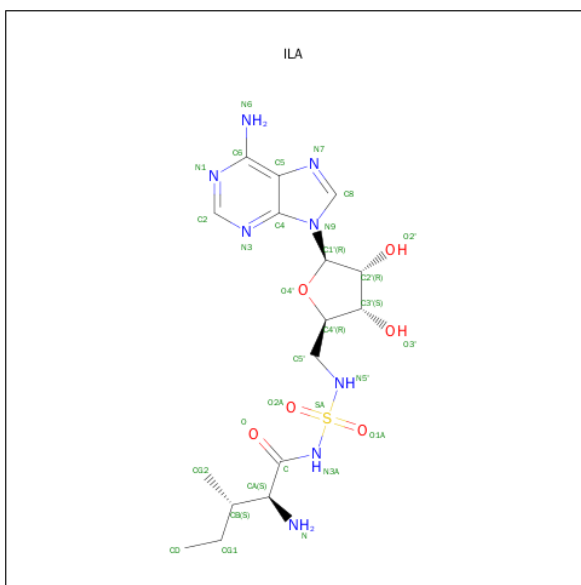
- Molecule 2 is a RNA chain called ESCHERICHIA COLI TRNA-LEU UAA ISOACCEPTOR.

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	C	N	O	S	0	0
			31	16	8	6	1		
4	A	1	Total	C	N	O	S	0	0
			31	16	8	6	1		
4	D	1	Total	C	N	O	S	0	0
			31	16	8	6	1		
4	D	1	Total	C	N	O	S	0	0
			31	16	8	6	1		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

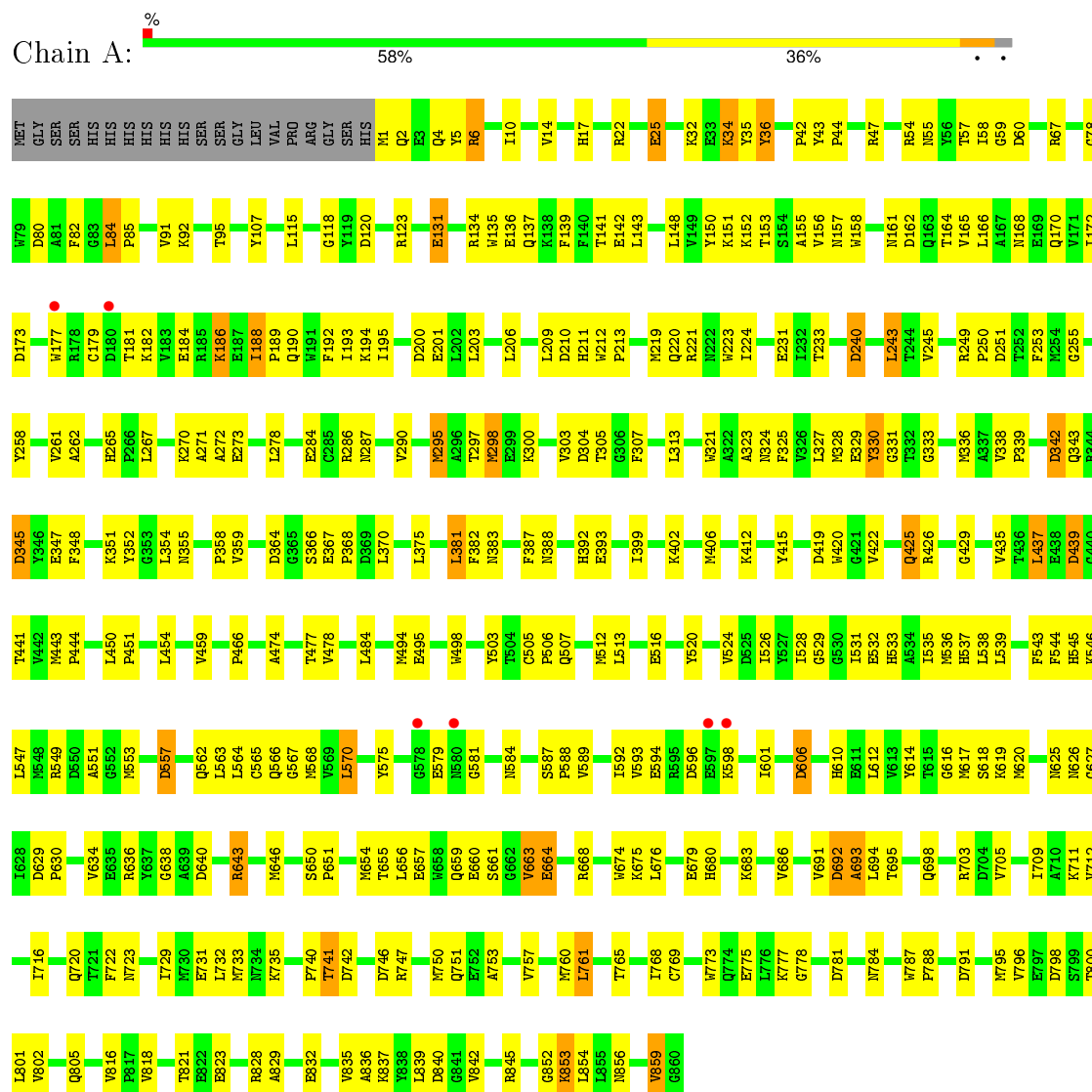
- Molecule 6 is water.

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

3 Residue-property plots [i](#)

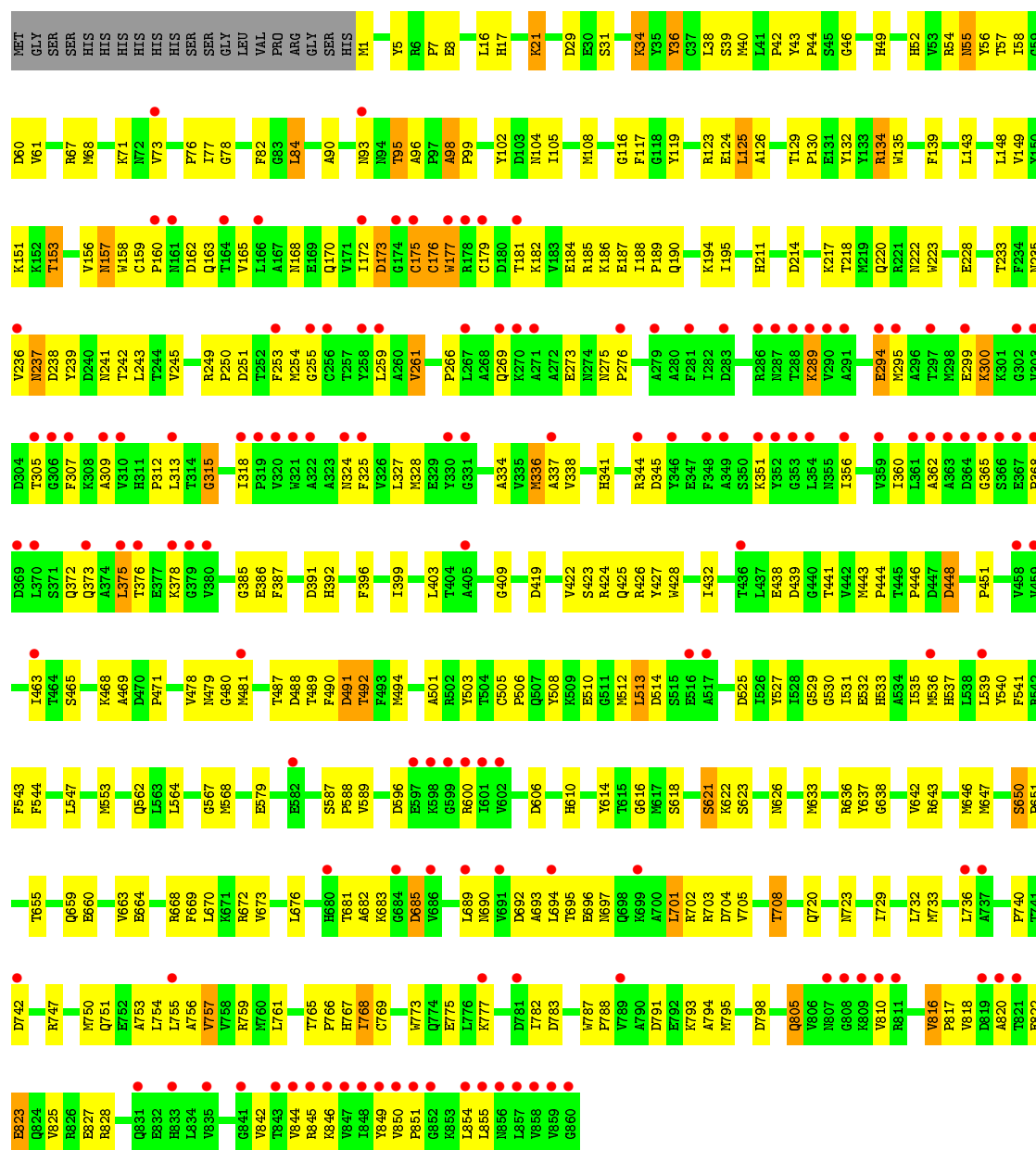
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: LEUCINE-TRNA LIGASE

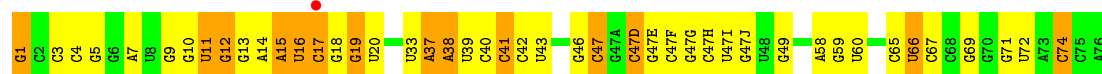
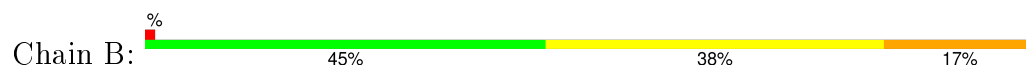


• Molecule 1: LEUCINE-TRNA LIGASE

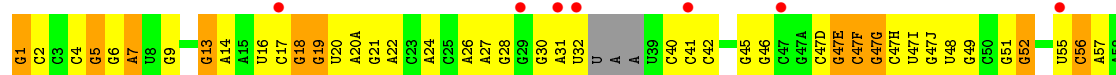


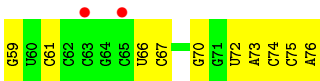


• Molecule 2: ESCHERICHIA COLI TRNA-LEU UAA ISOACCEPTOR



• 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 46.45 – 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 (5.29%)	DCC
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
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.27$	Xtriage
Outliers	0 of 76243 reflections	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, 0.375 respectively for untwinned datasets, and 0.333, 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: 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-OP1	-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-OP1	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

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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-OP2	-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:305:THR:HG22	1:A:307:PHE:HD2	1.52	0.74
1:A:136:GLU:OE1	1:A:495:GLU:HG3	1.87	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:223:TRP:CH2	2:E:72:U:H4'	2.22	0.73
1:D:195:ILE:HG22	1:D:419:ASP:HA	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

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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:D:76:PRO:HG2	1:D:503:TYR:CD2	2.30	0.66
1:A:821:THR:HB	1:A:823:GLU:OE1	1.96	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
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
2:B:37:A:H2'	2:B:37:A:N3	2.12	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

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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
2:E:55:U:C2	2:E:57:A:OP1	2.52	0.63
1:D:469:ALA:O	1:D:471:PRO:HD3	1.98	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:D:77:ILE:HB	1:D:119:TYR:CD2	2.34	0.62
1:A:654:MET:HG3	6:A:2198:HOH:O	1.99	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:D:596:ASP:HB2	1:D:600:ARG:O	1.99	0.61
1:A:680:HIS:O	1:A:747:ARG:NH2	2.33	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:D:67:ARG:HG2	1:D:783:ASP:O	2.02	0.60
1:A:284:GLU:HB2	6:A:2107:HOH:O	2.01	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:664:GLU:HG3	1:D:668:ARG:NE	2.17	0.59
1:D:40:MET:HB2	4:D:1862:ILA:O3'	2.02	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

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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:D:368:PRO:HB2	1:D:375:LEU:HD13	1.85	0.58
1:D:170:GLN:O	1:D:177:TRP:HB3	2.03	0.58
1:A:115:LEU:O	1:A:643:ARG:NH1	2.36	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: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
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:D:236:VAL:HG21	1:D:239:TYR:HD2	1.70	0.56
1:A:402:LYS:O	1:A:406:MET:HG3	2.04	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:139:PHE:CE1	1:A:553:MET:HE3	2.38	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: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:82:PHE:HB2	1:D:492:THR:HG22	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:468:LYS:HG2	1:D:487:THR:HB	1.88	0.55
1:D:96:ALA:HB3	1:D:99:PRO:HD2	1.86	0.55
1:A:761:LEU:HB3	1:A:769:CYS:SG	2.45	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:D:134:ARG:CB	1:D:451:PRO:HB3	2.37	0.55
1:A:664:GLU:O	1:A:668:ARG:HG3	2.06	0.55
1:D:77:ILE:HD13	1:D:119:TYR:CE2	2.41	0.54
1:A:195:ILE:HG22	1:A:419:ASP:HA	1.89	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
4:D:1863:ILA:HN5	4:D:1863:ILA:H8	1.73	0.54
1:A:676:LEU:CD2	1:A:733:MET:HE3	2.37	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:D:98:ALA:HB3	1:D:99:PRO:CD	2.39	0.53
1:A:5:TYR:HB2	1:A:674:TRP:CG	2.44	0.53
1:D:587:SER:OG	1:D:589:VAL:HG23	2.09	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:A:342:ASP:CG	4:A:1863:ILA:HG22	2.28	0.52
1:D:426:ARG:NH2	2:E:74:C:O2	2.42	0.52
1:A:828:ARG:NH1	1:A:832:GLU:OE2	2.38	0.52
1:D:151:LYS:HG3	1:D:190:GLN:O	2.09	0.52
1:D:300:LYS:HB3	1:D:325:PHE:HE2	1.75	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:PHE:HA	1:A:420:TRP:O	2.08	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:D:305:THR:C	1:D:307:PHE:H	2.13	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
1:A:240:ASP:OD1	1:A:240:ASP:N	2.43	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:D:424:ARG:CZ	1:D:491:ASP:HB2	2.40	0.51
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:695:THR:C	1:D:697:ASN:H	2.13	0.51
1:D:233:THR:HG22	1:D:242:THR:HB	1.92	0.51
2:B:47(D):C:O2	2:B:47(D):C:O4'	2.28	0.51
1:A:570:LEU:HD12	1:A:657:GLU:HG2	1.92	0.51
1:A:224:ILE:HD11	1:A:539:LEU:HD11	1.93	0.51
1:A:295:MET:CE	1:A:325:PHE:HA	2.40	0.51
1:A:10:ILE:O	1:A:14:VAL:HG23	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: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: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:676:LEU:HD23	1:A:733:MET:CE	2.40	0.51
1:D:98:ALA:HA	1:D:428:TRP:CH2	2.45	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:670:LEU:HD21	1:D:765:THR:HG21	1.93	0.51
4:A:1862:ILA:H8	4:A:1862:ILA:HN5	1.76	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:OP1	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

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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
1:D:43:TYR:HE2	1:D:82:PHE:O	1.95	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:A:422:VAL:CG1	1:A:494:MET:CE	2.87	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
1:A:614:TYR:CZ	1:A:616:GLY:HA2	2.48	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:692:ASP:O	1:A:693:ALA:HB2	2.12	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:D:143:LEU:HB3	1:D:149:VAL:CG2	2.44	0.48
1:A:775:GLU:C	1:A:777:LYS:H	2.15	0.48
1:A:842:VAL:HB	1:A:859:VAL:HG13	1.95	0.48
1:A:675:LYS:HE3	1:A:679:GLU:OE2	2.13	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
2:E:4:C:C2	2:E:5:G:C8	3.01	0.47
1:A:91:VAL:O	1:A:92:LYS:C	2.53	0.47
1:D:77:ILE:HG13	1:D:78:GLY:H	1.79	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: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: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:835:VAL:O	1:A:839:LEU:HG	2.14	0.47
1:D:536:MET:O	1:D:540:TYR:CD2	2.67	0.47

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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:237:ASN:HB2	1:D:307:PHE:HD1	1.80	0.47
1:D:90:ALA:HB1	1:D:95:THR:O	2.15	0.47
1:A:47:ARG:NH1	1:D:579:GLU:OE1	2.47	0.47
1:D:135:TRP:CD2	1:D:512:MET:HA	2.49	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:HG23	4:A:1863:ILA:N3A	2.30	0.47
1:A:206:LEU:HD23	1:A:209:LEU:HD12	1.97	0.47
1:A:258:TYR:CE1	1:A:354:LEU:HD12	2.50	0.47
1:A:148:LEU:HA	1:A:194:LYS:HD2	1.97	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:D:249:ARG:HD3	1:D:378:LYS:HE2	1.97	0.46
1:A:800:THR:HG22	1:A:818:VAL:HA	1.97	0.46
1:A:364:ASP:OD1	1:A:366:SER:N	2.48	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:823:GLU:O	1:D:827:GLU:HG2	2.15	0.46
1:D:567:GLY:CA	1:D:655:THR:HG22	2.46	0.46
1:D:123:ARG:O	1:D:125:LEU:HD23	2.15	0.46
1:A:740:PRO:HB2	1:A:746:ASP:OD2	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:729:ILE:HG21	1:D:761:LEU:CD2	2.44	0.46
1:D:588:PRO:HD2	1:D:626:ASN:HA	1.96	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:330:TYR:CD1	1:A:330:TYR:N	2.84	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:135:TRP:HB2	1:A:498:TRP:CH2	2.50	0.46
1:D:362:ALA:HB2	1:D:368:PRO:HB3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:773:TRP:HB2	1:D:782:ILE:HD12	1.97	0.46
1:D:344:ARG:HH12	4:D:1863:ILA:H2'	1.81	0.46
1:A:137:GLN:O	1:A:141:THR:HG23	2.16	0.46
2:E:5:G:H2'	2:E:6:G:C8	2.51	0.46
1:A:828:ARG:O	1:A:829:ALA:C	2.54	0.46
1:A:172:ILE:O	1:A:172:ILE:HG13	2.16	0.46
1:D:175:CYS:HB3	1:D:182:LYS:HA	1.97	0.46
1:D:501:ALA:HB1	1:D:513:LEU:HD22	1.97	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
1:D:218:THR:HG22	1:D:222:ASN:HD21	1.81	0.45
2:B:1:G:OP1	6:B:2003:HOH:O	2.21	0.45
1:A:131:GLU:CD	1:A:131:GLU:H	2.19	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:60:ASP:OD1	1:A:118:GLY:N	2.35	0.45
4:A:1863:ILA:H8	4:A:1863:ILA:HN5	1.79	0.45
1:D:84:LEU:HD21	1:D:170:GLN:NE2	2.31	0.45
1:A:845:ARG:NH1	1:A:845:ARG:HG3	2.31	0.45
1:D:55:ASN:OD1	1:D:529:GLY:HA2	2.15	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:58:ILE:HG13	1:D:647:MET:SD	2.56	0.45
1:D:77:ILE:O	1:D:503:TYR:HE1	2.00	0.45
1:D:705:VAL:HG22	1:D:732:LEU:HD11	1.97	0.45
1:D:690:ASN:HB3	1:D:693:ALA:HB3	1.98	0.45
1:A:141:THR:HB	1:A:444:PRO:HB3	1.98	0.45
1:D:300:LYS:HB3	1:D:325:PHE:CE2	2.51	0.45
1:A:231:GLU:HA	1:A:245:VAL:O	2.15	0.45
1:A:150:TYR:HE2	1:A:152:LYS:HD3	1.81	0.45
1:D:250:PRO:O	1:D:253:PHE:HB2	2.17	0.45
1:A:692:ASP:OD1	1:A:692:ASP:N	2.45	0.45
1:D:733:MET:HA	1:D:736:LEU:HD12	1.99	0.45
1:A:4:GLN:HB3	1:A:6:ARG:HD2	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:D:39:SER:HB3	1:D:55:ASN:ND2	2.32	0.45
1:A:47:ARG:NE	1:A:107:TYR:CE1	2.85	0.45
1:D:676:LEU:HG	1:D:754:LEU:HD11	1.99	0.45
1:A:223:TRP:CD2	1:A:535:ILE:HG21	2.51	0.45

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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:OP1	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
2:B:3:C:H2'	2:B:4:C:H5'	1.99	0.44
1:D:606:ASP:CG	1:D:610:HIS:HD1	2.16	0.44
1:A:219:MET:HB3	1:A:535:ILE:HD11	1.98	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
1:D:663:VAL:HG23	1:D:664:GLU:N	2.33	0.44
1:A:295:MET:CA	1:A:295:MET:HE3	2.45	0.44
1:D:159:CYS:HA	1:D:160:PRO:HD2	1.86	0.44
2:B:42:C:H2'	2:B:43:U:H6	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: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: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:532:GLU:H	1:A:568:MET:HE3	1.81	0.43
1:A:300:LYS:CD	6:A:2114:HOH:O	2.63	0.43
1:D:693:ALA:O	1:D:694:LEU:HG	2.18	0.43
1:A:505:CYS:N	1:A:506:PRO:CD	2.81	0.43
1:A:723:ASN:N	1:A:723:ASN:OD1	2.52	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:751:GLN:O	1:D:755:LEU:HB2	2.19	0.43
1:A:566:GLN:HG3	1:A:567:GLY:O	2.18	0.43
1:A:426:ARG:HB2	1:A:426:ARG:NH1	2.33	0.43
1:A:186:LYS:HG2	1:A:188:ILE:HD11	2.01	0.43
1:A:186:LYS:HG2	1:A:188:ILE:HD12	2.00	0.43
2:B:47(G):G:H2'	2:B:47(H):C:O4'	2.19	0.43
1:A:381:LEU:HD12	1:A:387:PHE:HB2	2.01	0.43
1:A:619:LYS:HE2	2:B:71:G:OP2	2.19	0.43

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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:54:ARG:HD3	1:A:54:ARG:HH11	1.71	0.43
1:A:123:ARG:HD3	1:A:503:TYR:O	2.18	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:375:LEU:HA	1:A:375:LEU:HD12	1.91	0.43
1:A:339:PRO:HG3	1:A:355:ASN:O	2.19	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:D:130:PRO:C	1:D:132:TYR:H	2.22	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:D:188:ILE:O	1:D:190:GLN:HG3	2.19	0.42
1:A:364:ASP:C	1:A:364:ASP:OD1	2.57	0.42
1:D:673:VAL:HA	1:D:733:MET:HE1	2.00	0.42
1:A:255:GLY:C	1:A:338:VAL:HG22	2.40	0.42
1:A:787:TRP:CD2	1:A:788:PRO:HD2	2.55	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: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:D:438:GLU:HB3	1:D:481:MET:CE	2.49	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:567:GLY:HA2	1:D:655:THR:HG22	2.00	0.42
1:A:443:MET:HB2	1:A:444:PRO:HD2	2.01	0.42
1:D:432:ILE:HG12	1:D:490:PHE:CE1	2.54	0.42
1:D:385:GLY:O	1:D:387:PHE:N	2.50	0.42
1:A:450:LEU:HA	1:A:451:PRO:C	2.40	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:A:151:LYS:HA	1:A:190:GLN:O	2.20	0.42
1:D:40:MET:HB3	4:D:1862:ILA:HD1	2.01	0.42
1:A:323:ALA:HB1	1:A:325:PHE:CE2	2.55	0.42
1:D:84:LEU:O	1:D:84:LEU:HD22	2.20	0.42
1:A:650:SER:CB	1:A:651:PRO:CD	2.97	0.42

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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:729:ILE:HD13	1:A:761:LEU:HD13	2.02	0.42
1:A:676:LEU:HD23	1:A:733:MET:HE3	2.01	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:773:TRP:CE2	1:A:778:GLY:HA3	2.55	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:508:TYR:CE1	1:D:510:GLU:HG2	2.55	0.41
1:D:49:HIS:CD2	1:D:52:HIS:CE1	3.08	0.41
1:D:533:HIS:HB3	1:D:537:HIS:HB3	2.02	0.41
1:D:276:PRO:HA	6:D:2008:HOH:O	2.20	0.41
1:D:54:ARG:NH2	1:D:650:SER:HB3	2.34	0.41
2:E:72:U:H5''	2:E:73:A:H5'	2.01	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
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: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:71:LYS:O	1:D:73:VAL:HG23	2.20	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:D:77:ILE:HG13	1:D:78:GLY:N	2.36	0.41
1:A:629:ASP:HA	1:A:630:PRO:HD2	1.87	0.41
2:E:47(H):C:H2'	2:E:47(I):U:O4'	2.21	0.41
1:D:351:LYS:HD3	1:D:351:LYS:HA	1.90	0.41
2:E:18:G:H1	2:E:55:U:H1'	1.85	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
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:D:729:ILE:HD13	1:D:761:LEU:HD22	2.03	0.41
1:A:823:GLU:CD	1:A:823:GLU:N	2.74	0.41
1:A:14:VAL:O	1:A:17:HIS:HB3	2.21	0.41
2:B:47(I):U:H2'	2:B:47(J):G:O5'	2.20	0.41
1:A:84:LEU:HB3	1:A:85:PRO:HD3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:816:VAL:HG21	1:D:825:VAL:HG22	2.02	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:D:756:ALA:O	1:D:757:VAL:C	2.58	0.41
1:D:76:PRO:CG	1:D:503:TYR:CD2	3.01	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: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
2:B:14:A:C2'	2:B:15:A:O5'	2.68	0.41
1:A:383:ASN:N	1:A:388:ASN:OD1	2.53	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: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
1:A:364:ASP:OD1	1:A:366:SER:OG	2.38	0.41
2:E:47(E):G:H4'	2:E:47(F):C:OP1	2.20	0.41
1:D:261:VAL:HG23	1:D:334:ALA:CB	2.39	0.40
1:D:249:ARG:HA	1:D:249:ARG:HD2	1.96	0.40
1:D:850:VAL:HA	1:D:851:PRO:HD3	1.91	0.40
1:A:298:MET:HE3	1:A:298:MET:HB3	1.90	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
2:E:51:G:H2'	2:E:52:G:O4'	2.21	0.40
1:D:765:THR:O	1:D:768:ILE:HG22	2.21	0.40
1:D:58:ILE:HG13	1:D:647:MET:CE	2.51	0.40
1:A:618:SER:O	1:A:619:LYS:C	2.59	0.40
1:A:35:TYR:CE2	1:A:526:ILE:HG22	2.57	0.40
1:D:172:ILE:HG22	1:D:173:ASP:N	2.35	0.40
1:D:223:TRP:CD2	1:D:535:ILE:HG21	2.56	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:313:LEU:HD13	1:A:387:PHE:CE2	2.57	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: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:OP2	2.21	0.40
1:D:810:VAL:HG21	2:E:20:U:H4'	2.02	0.40
1:D:822:GLU:HG3	1:D:849:TYR:CG	2.56	0.40
1:A:284:GLU:O	1:A:287:ASN:HB2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:345:ASP:OD1	4:D:1863:ILA:N6	2.54	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

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%)	19	34
1	D	858/880 (98%)	716 (83%)	119 (14%)	23 (3%)	6	9
All	All	1718/1760 (98%)	1513 (88%)	173 (10%)	32 (2%)	10	16

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

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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%)	12	22
1	D	723/741 (98%)	655 (91%)	68 (9%)	11	20
All	All	1449/1482 (98%)	1316 (91%)	133 (9%)	11	21

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

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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

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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

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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

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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

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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 ⓘ

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

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	-	27,33,33	2.84	5 (18%)	31,49,49	3.36	10 (32%)
4	ILA	A	1863	-	27,33,33	2.57	5 (18%)	31,49,49	3.43	14 (45%)
4	ILA	D	1862	-	27,33,33	2.40	5 (18%)	31,49,49	2.36	5 (16%)
4	ILA	D	1863	-	27,33,33	2.41	6 (22%)	31,49,49	2.43	3 (9%)

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	-	-	0/19/41/41	0/3/3/3
4	ILA	A	1863	-	1/1/8/10	1/19/41/41	0/3/3/3
4	ILA	D	1862	-	-	0/19/41/41	0/3/3/3
4	ILA	D	1863	-	1/1/8/10	1/19/41/41	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1862	ILA	SA-N5'	-10.39	1.51	1.61
4	D	1862	ILA	SA-N5'	-8.69	1.52	1.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	1863	ILA	SA-N5'	-8.25	1.53	1.61
4	A	1863	ILA	SA-N5'	-8.21	1.53	1.61
4	A	1862	ILA	SA-N3A	-5.57	1.52	1.63
4	D	1863	ILA	SA-N3A	-5.30	1.52	1.63
4	D	1862	ILA	SA-N3A	-5.05	1.53	1.63
4	A	1863	ILA	SA-N3A	-5.02	1.53	1.63
4	D	1863	ILA	C-N3A	-2.67	1.33	1.37
4	D	1862	ILA	C-N3A	-2.30	1.34	1.37
4	A	1863	ILA	O4'-C1'	2.01	1.43	1.41
4	D	1863	ILA	O4'-C1'	2.33	1.44	1.41
4	A	1862	ILA	O4'-C1'	3.16	1.45	1.41
4	D	1862	ILA	O2A-SA	4.20	1.48	1.43
4	D	1863	ILA	O1A-SA	4.36	1.48	1.43
4	A	1862	ILA	O1A-SA	4.50	1.48	1.43
4	D	1862	ILA	O1A-SA	4.59	1.48	1.43
4	D	1863	ILA	O2A-SA	4.63	1.48	1.43
4	A	1863	ILA	O2A-SA	4.86	1.49	1.43
4	A	1862	ILA	O2A-SA	5.97	1.50	1.43
4	A	1863	ILA	O1A-SA	6.72	1.51	1.43

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1863	ILA	N3-C2-N1	-14.16	118.05	128.89
4	A	1862	ILA	N3-C2-N1	-10.55	120.82	128.89
4	D	1863	ILA	N3-C2-N1	-10.22	121.07	128.89
4	A	1862	ILA	O2A-SA-O1A	-9.90	103.88	120.04
4	D	1862	ILA	N3-C2-N1	-8.86	122.11	128.89
4	D	1862	ILA	O2A-SA-O1A	-6.42	109.57	120.04
4	D	1863	ILA	O2A-SA-O1A	-6.18	109.95	120.04
4	A	1863	ILA	O2A-SA-O1A	-5.98	110.28	120.04
4	A	1862	ILA	C4'-C5'-N5'	-5.38	101.17	112.56
4	A	1863	ILA	C2'-C1'-N9	-5.19	106.37	114.29
4	A	1862	ILA	C4-C5-N7	-4.78	105.09	109.48
4	A	1862	ILA	C2'-C1'-N9	-4.72	107.08	114.29
4	D	1862	ILA	C2'-C1'-N9	-4.52	107.39	114.29
4	A	1863	ILA	C4-C5-N7	-3.63	106.14	109.48
4	A	1863	ILA	O3'-C3'-C2'	-3.45	100.60	111.83
4	A	1863	ILA	C4'-C5'-N5'	-3.36	105.45	112.56
4	A	1862	ILA	O3'-C3'-C4'	-3.13	101.67	111.05
4	A	1862	ILA	O3'-C3'-C2'	-2.44	103.88	111.83
4	D	1862	ILA	C4'-C5'-N5'	-2.43	107.41	112.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1863	ILA	C1'-N9-C4	-2.18	123.66	126.94
4	A	1863	ILA	C-N3A-SA	-2.00	121.24	124.05
4	D	1862	ILA	O4'-C4'-C5'	2.16	111.84	108.70
4	A	1863	ILA	CG1-CB-CA	2.19	117.03	111.12
4	A	1862	ILA	O4'-C4'-C5'	2.23	111.93	108.70
4	A	1863	ILA	O-C-N3A	2.27	125.60	121.62
4	A	1863	ILA	C2-N1-C6	2.28	122.84	118.77
4	A	1863	ILA	O4'-C1'-N9	2.30	112.91	108.10
4	A	1863	ILA	O2A-SA-N3A	2.68	114.80	106.72
4	D	1863	ILA	O4'-C4'-C5'	2.91	112.94	108.70
4	A	1862	ILA	O-C-N3A	3.24	127.30	121.62
4	A	1863	ILA	O1A-SA-N5'	3.28	113.48	106.83
4	A	1862	ILA	O2A-SA-N5'	3.47	113.88	106.83

All (2) chirality outliers are listed below:

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

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	D	1863	ILA	N3A-SA-N5'-C5'
4	A	1863	ILA	N3A-SA-N5'-C5'

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	A	1863	ILA	11	0
4	D	1862	ILA	3	0
4	D	1863	ILA	4	0

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.24	6 (0%) 89 90	6, 19, 48, 99	0
1	D	860/880 (97%)	1.04	141 (16%) 2 2	36, 71, 111, 142	0
2	B	82/82 (100%)	-0.43	1 (1%) 81 83	9, 21, 72, 116	0
2	E	79/82 (96%)	0.79	9 (11%) 7 6	56, 79, 125, 142	0
All	All	1881/1924 (97%)	0.38	157 (8%) 14 15	6, 47, 105, 142	0

All (157) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	860	GLY	13.2
1	D	809	LYS	6.1
1	D	330	TYR	5.9
1	D	322	ALA	5.9
1	D	321	TRP	5.7
1	D	352	TYR	5.7
1	D	348	PHE	5.5
1	D	324	ASN	5.3
1	D	279	ALA	5.2
1	D	847	VAL	5.2
1	D	846	LYS	5.1
1	D	178	ARG	5.1
1	D	379	GLY	5.1
2	E	31	A	5.0
1	D	820	ALA	4.9
1	D	281	PHE	4.8
1	D	845	ARG	4.7
1	D	295	MET	4.7
1	D	287	ASN	4.6
1	D	320	VAL	4.6
1	D	598	LYS	4.6

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Mol	Chain	Res	Type	RSRZ
1	D	691	VAL	4.4
1	D	303	VAL	4.4
1	D	810	VAL	4.4
1	D	368	PRO	4.4
1	D	808	GLY	4.3
1	D	253	PHE	4.2
1	D	310	VAL	4.2
1	D	319	PRO	4.1
1	D	858	VAL	4.1
1	D	259	LEU	4.1
2	E	32	U	4.0
1	D	256	CYS	4.0
1	D	463	ILE	4.0
1	D	325	PHE	4.0
1	D	851	PRO	4.0
1	D	370	LEU	3.9
1	D	848	ILE	3.9
1	D	362	ALA	3.9
1	A	580	ASN	3.8
1	A	598	LYS	3.8
1	D	597	GLU	3.7
1	D	859	VAL	3.7
1	D	852	GLY	3.7
1	D	291	ALA	3.7
1	D	258	TYR	3.6
1	D	276	PRO	3.6
1	D	601	ILE	3.6
1	D	286	ARG	3.6
1	D	599	GLY	3.6
1	D	600	ARG	3.5
1	D	843	THR	3.5
1	D	736	LEU	3.4
1	D	313	LEU	3.4
1	D	354	LEU	3.4
1	D	363	ALA	3.3
1	D	855	LEU	3.3
1	D	459	VAL	3.3
1	D	160	PRO	3.3
1	D	353	GLY	3.2
1	D	351	LYS	3.2
1	D	288	THR	3.2
1	D	271	ALA	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	172	ILE	3.2
1	D	694	LEU	3.2
1	D	302	GLY	3.1
1	D	366	SER	3.1
1	D	835	VAL	3.1
1	D	367	GLU	3.0
1	D	742	ASP	3.0
1	D	841	GLY	3.0
1	A	578	GLY	3.0
1	D	405	ALA	3.0
1	D	364	ASP	3.0
1	D	582	GLU	3.0
1	D	177	TRP	2.9
2	E	17	C	2.9
1	D	380	VAL	2.9
1	D	166	LEU	2.8
1	D	789	VAL	2.8
1	D	318	ILE	2.8
1	D	850	VAL	2.8
1	D	378	LYS	2.8
1	D	844	VAL	2.8
1	D	365	GLY	2.8
1	D	297	THR	2.7
1	D	602	VAL	2.7
1	D	356	ILE	2.7
1	D	807	ASN	2.7
1	D	811	ARG	2.7
1	D	856	ASN	2.7
1	D	306	GLY	2.6
1	D	349	ALA	2.6
1	D	699	LYS	2.6
1	D	737	ALA	2.6
1	D	361	LEU	2.6
1	D	684	GLY	2.6
1	D	267	LEU	2.6
1	D	539	LEU	2.6
1	D	164	THR	2.6
1	D	290	VAL	2.6
2	E	29	G	2.6
1	D	93	ASN	2.6
1	D	458	VAL	2.5
1	D	161	ASN	2.5

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Mol	Chain	Res	Type	RSRZ
1	D	689	LEU	2.5
1	D	821	THR	2.5
1	D	831	GLN	2.5
1	D	369	ASP	2.5
1	D	331	GLY	2.5
1	D	283	ASP	2.5
1	D	73	VAL	2.5
1	D	536	MET	2.5
1	D	270	LYS	2.4
1	D	309	ALA	2.4
2	E	63	C	2.4
2	E	41	C	2.4
1	D	344	ARG	2.4
2	E	47	C	2.4
1	D	849	TYR	2.4
1	D	359	VAL	2.4
1	D	517	ALA	2.3
1	D	777	LYS	2.3
1	D	294	GLU	2.3
1	A	177	TRP	2.3
1	D	346	TYR	2.3
1	D	686	VAL	2.3
1	D	755	LEU	2.3
1	A	597	GLU	2.3
1	D	857	LEU	2.3
1	A	180	ASP	2.2
1	D	181	THR	2.2
1	D	680	HIS	2.2
1	D	307	PHE	2.2
1	D	375	LEU	2.2
1	D	373	GLN	2.2
1	D	337	ALA	2.2
2	E	55	U	2.2
1	D	269	GLN	2.2
1	D	255	GLY	2.2
2	B	17	C	2.2
1	D	781	ASP	2.2
1	D	481	MET	2.1
1	D	179	CYS	2.1
1	D	299	GLU	2.1
1	D	376	THR	2.1
1	D	833	HIS	2.1

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Mol	Chain	Res	Type	RSRZ
2	E	65	C	2.1
1	D	174	GLY	2.1
1	D	436	THR	2.1
1	D	289	LYS	2.1
1	D	854	LEU	2.1
1	D	236	VAL	2.0
1	D	175	CYS	2.0
1	D	819	ASP	2.0
1	D	305	THR	2.0
1	D	516	GLU	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å ²)	Q<0.9
4	ILA	A	1863	31/31	0.95	0.14	1.00	21,28,32,36	0
4	ILA	D	1863	31/31	0.65	0.31	0.64	104,151,160,160	0
4	ILA	A	1862	31/31	0.97	0.15	0.38	7,10,11,11	0
4	ILA	D	1862	31/31	0.95	0.16	-0.68	38,48,56,61	0
3	ZN	D	1861	1/1	0.86	0.06	-1.45	100,100,100,100	0
3	ZN	A	1861	1/1	0.96	0.05	-3.07	65,65,65,65	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

6.5 Other polymers

There are no such residues in this entry.