



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 15, 2020 – 11:02 pm BST

PDB ID : 2BYT  
Title : Thermus thermophilus Leucyl-tRNA synthetase complexed with a tRNA<sup>Leu</sup> transcript in the post-editing conformation  
Authors : Cusack, S.; Tukalo, M.; Yaremchuk, A.; Fukunaga, R.; Yokoyama, S.  
Deposited on : 2005-08-04  
Resolution : 3.30 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

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

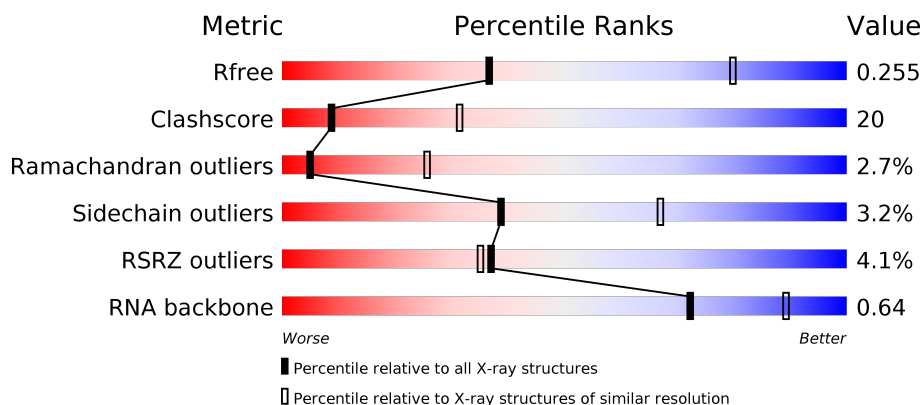
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.30 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	1149 (3.34-3.26)
Clashscore	141614	1205 (3.34-3.26)
Ramachandran outliers	138981	1183 (3.34-3.26)
Sidechain outliers	138945	1182 (3.34-3.26)
RSRZ outliers	127900	1115 (3.34-3.26)
RNA backbone	3102	1117 (3.70-2.90)

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

Mol	Chain	Length	Quality of chain
1	A	878	<div> <div>2%</div> <div> <div></div> <div>59%</div> <div>37%</div> <div>.</div> </div> </div>
1	D	878	<div> <div>6%</div> <div> <div></div> <div>58%</div> <div>39%</div> <div>.</div> </div> </div>
2	B	83	<div> <div>4%</div> <div> <div></div> <div>42%</div> <div>39%</div> <div>11%</div> <div>6%</div> <div>.</div> </div> </div>
2	E	83	<div> <div>5%</div> <div> <div></div> <div>46%</div> <div>39%</div> <div>8%</div> <div>6%</div> <div>.</div> </div> </div>

## 2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 17697 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.

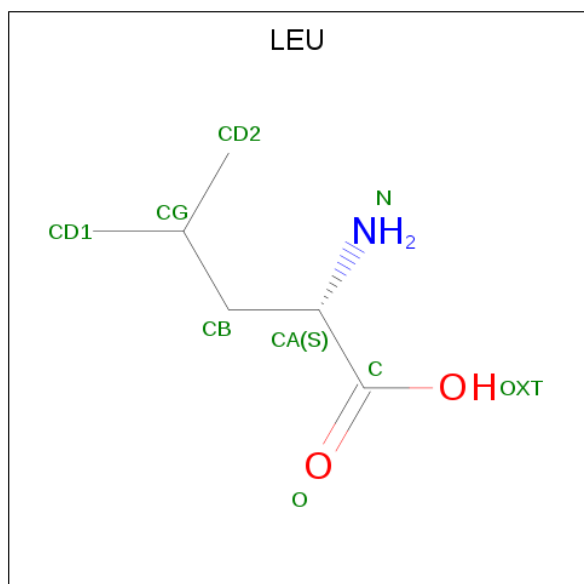
- Molecule 1 is a protein called LEUCYL-TRNA SYNTHETASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	876	Total	C	N	O	S	0	0	0
			7122	4593	1223	1275	31			
1	D	876	Total	C	N	O	S	0	0	0
			7122	4593	1223	1275	31			

- Molecule 2 is a RNA chain called TRNALEU TRANSCRIPT WITH ANTICODON CAG.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	78	Total	C	N	O	P	0	0	0
			1677	745	309	545	78			
2	E	78	Total	C	N	O	P	0	0	0
			1677	745	309	545	78			

- Molecule 3 is LEUCINE (three-letter code: LEU) (formula: C<sub>6</sub>H<sub>13</sub>NO<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C N O 9 6 1 2	0	0
3	D	1	Total C N O 9 6 1 2	0	0

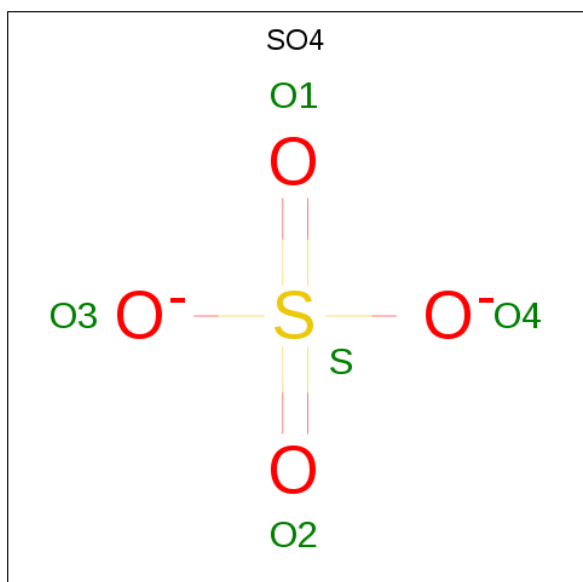
- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	2	Total Zn 2 2	0	0
4	D	2	Total Zn 2 2	0	0

- Molecule 5 is MERCURY (II) ION (three-letter code: HG) (formula: Hg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total Hg 1 1	0	0
5	D	1	Total Hg 1 1	0	0

- Molecule 6 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1	Total O S 5 4 1	0	0

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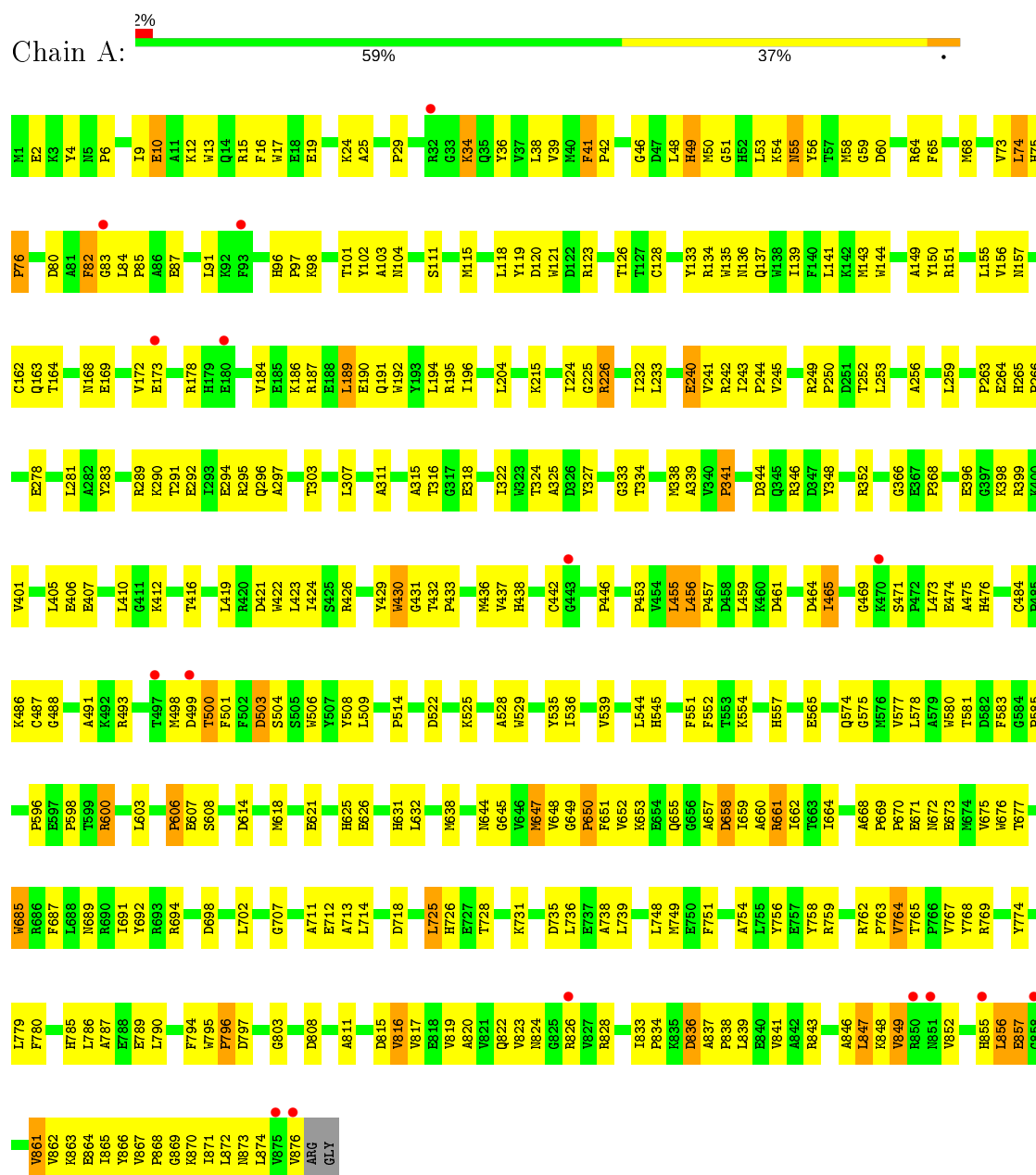
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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	A	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		
6	D	1	Total	O	S	0	0
			5	4	1		

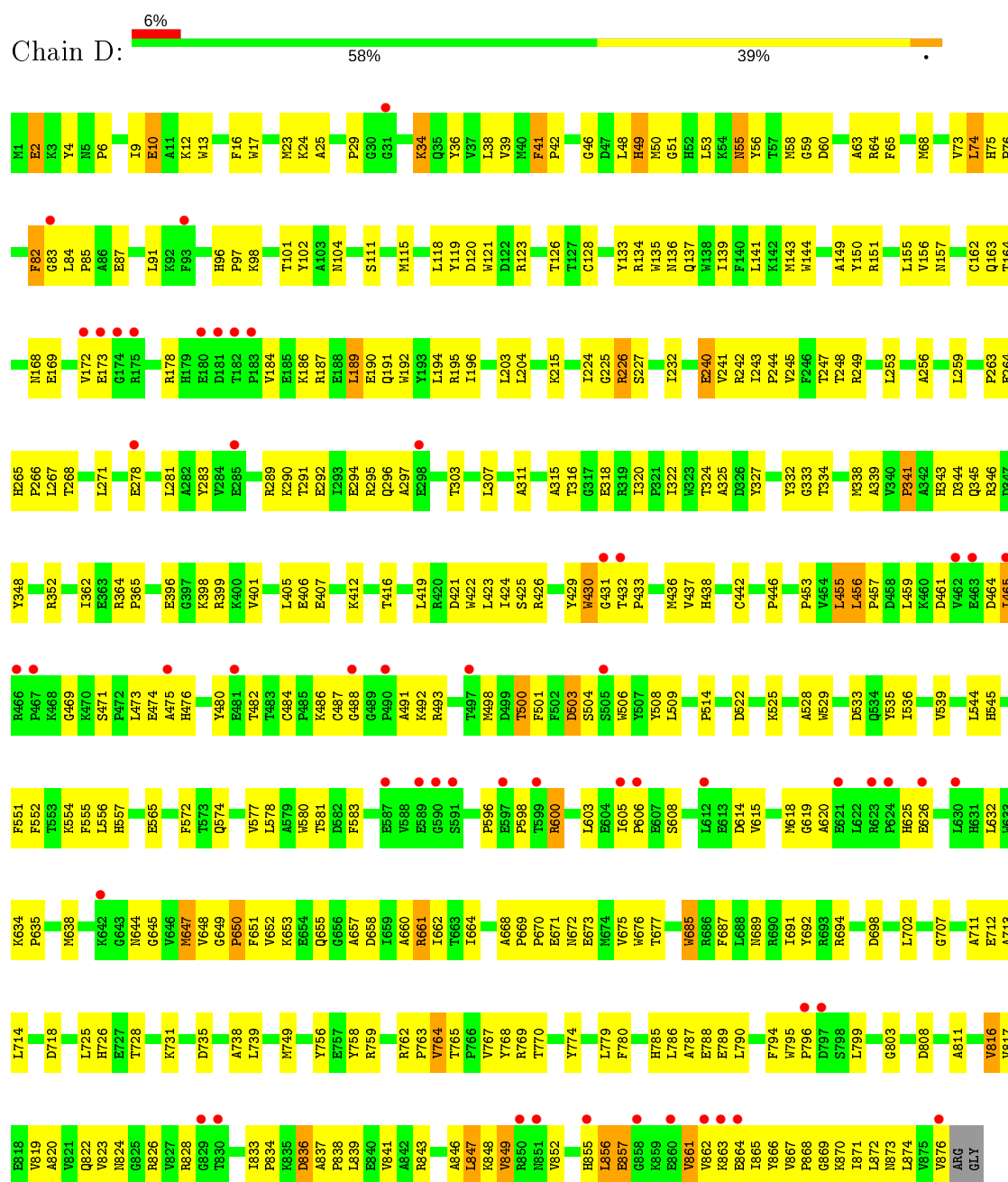
### 3 Residue-property plots

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

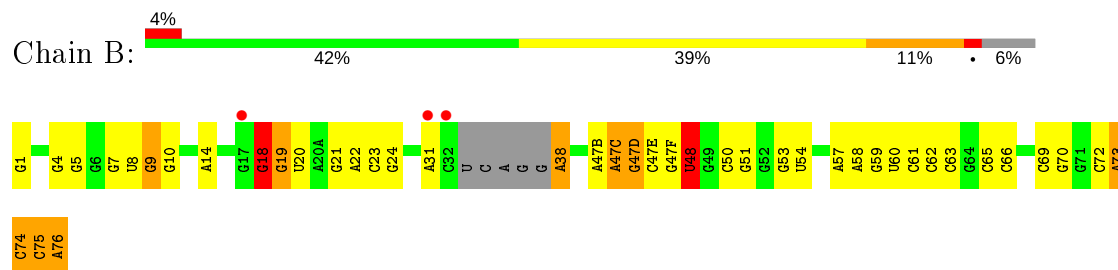
#### • Molecule 1: LEUCYL-TRNA SYNTHETASE



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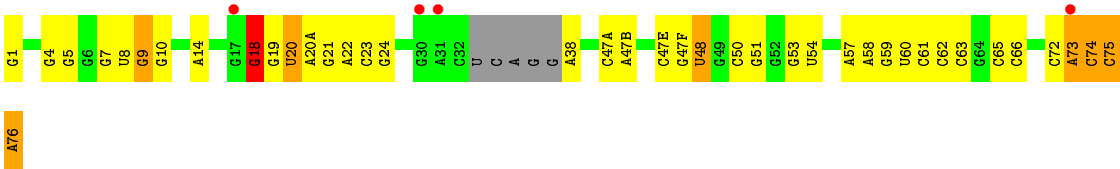


• Molecule 2: TRNALEU TRANSCRIPT WITH ANTICODON CAG



• Molecule 2: TRNALEU TRANSCRIPT WITH ANTICODON CAG







## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	203.87Å 125.58Å 172.98Å 90.00° 118.44° 90.00°	Depositor
Resolution (Å)	24.45 – 3.30 24.45 – 3.30	Depositor EDS
% Data completeness (in resolution range)	99.1 (24.45-3.30) 99.3 (24.45-3.30)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.65 (at 3.30Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.243 , 0.282 0.225 , 0.255	Depositor DCC
$R_{free}$ test set	2289 reflections (4.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	83.7	Xtriage
Anisotropy	0.197	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.28 , 76.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	17697	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	87.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ZN, SO4, HG

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	0.48	0/7327	0.60	0/9945
1	D	0.40	0/7327	0.57	0/9945
2	B	0.64	2/1874 (0.1%)	0.80	3/2917 (0.1%)
2	E	0.58	2/1874 (0.1%)	0.79	2/2917 (0.1%)
All	All	0.48	4/18402 (0.0%)	0.64	5/25724 (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
2	B	1	0
2	E	1	0
All	All	2	0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	38	A	OP3-P	-7.26	1.52	1.61
2	B	38	A	OP3-P	-7.17	1.52	1.61
2	B	1	G	OP3-P	-7.15	1.52	1.61
2	E	1	G	OP3-P	-7.03	1.52	1.61

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	9	G	C2'-C3'-O3'	10.45	132.48	109.50
2	B	9	G	C2'-C3'-O3'	10.35	132.26	109.50
2	B	18	G	C2'-C3'-O3'	5.61	122.67	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	18	G	C2'-C3'-O3'	5.44	122.41	113.70
2	B	48	U	C5'-C4'-C3'	-5.22	107.64	116.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	9	G	C3'
2	E	9	G	C3'

There are no planarity outliers.

## 5.2 Too-close contacts [i](#)

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	7122	0	7031	311	0
1	D	7122	0	7031	316	0
2	B	1677	0	849	34	0
2	E	1677	0	849	40	0
3	A	9	0	10	0	0
3	D	9	0	10	1	0
4	A	2	0	0	0	0
4	D	2	0	0	0	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
6	A	45	0	0	0	0
6	D	30	0	0	0	0
All	All	17697	0	15780	686	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 20.

All (686) 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:D:826:ARG:HD2	1:D:828:ARG:HH22	1.07	1.16

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:826:ARG:HD2	1:A:828:ARG:HH22	1.09	1.16
1:D:826:ARG:HD2	1:D:828:ARG:NH2	1.68	1.07
1:A:826:ARG:HD2	1:A:828:ARG:NH2	1.69	1.05
1:A:346:ARG:HH22	2:B:76:A:H1'	1.21	1.02
1:A:25:ALA:HB3	1:A:123:ARG:HE	1.34	0.93
1:D:25:ALA:HB3	1:D:123:ARG:HE	1.35	0.92
1:A:694:ARG:HB2	1:A:756:TYR:HE1	1.35	0.90
1:D:694:ARG:HB2	1:D:756:TYR:HE1	1.37	0.90
1:A:38:LEU:HD23	1:A:535:TYR:CE1	2.08	0.88
1:D:852:VAL:HG12	1:D:855:HIS:HB2	1.57	0.87
1:A:852:VAL:HG12	1:A:855:HIS:HB2	1.58	0.86
1:D:38:LEU:HD23	1:D:535:TYR:CE1	2.13	0.84
1:A:839:LEU:H	1:A:839:LEU:HD12	1.45	0.82
1:A:694:ARG:HD2	1:A:756:TYR:CE1	2.14	0.82
1:A:82:PHE:CD2	1:A:128:CYS:HA	2.16	0.80
1:D:839:LEU:H	1:D:839:LEU:HD12	1.48	0.79
1:A:346:ARG:NH2	2:B:76:A:H1'	1.97	0.79
1:A:17:TRP:HB3	1:A:118:LEU:HD21	1.63	0.79
1:D:694:ARG:HD2	1:D:756:TYR:CE1	2.18	0.79
1:D:17:TRP:HB3	1:D:118:LEU:HD21	1.64	0.79
1:A:29:PRO:HG3	1:A:529:TRP:CZ2	2.18	0.78
1:D:82:PHE:CD2	1:D:128:CYS:HA	2.19	0.77
1:D:867:VAL:HB	1:D:871:ILE:HG22	1.65	0.76
1:A:867:VAL:HB	1:A:871:ILE:HG22	1.68	0.76
1:D:687:PHE:O	1:D:691:ILE:HG13	1.86	0.76
1:D:316:THR:OG1	1:D:318:GLU:HG2	1.85	0.76
1:A:687:PHE:O	1:A:691:ILE:HG13	1.86	0.75
1:D:247:THR:HA	2:E:76:A:O3'	1.87	0.75
1:D:39:VAL:HG12	1:D:536:ILE:HB	1.68	0.75
1:D:346:ARG:HD2	2:E:74:C:O2'	1.87	0.75
1:A:316:THR:OG1	1:A:318:GLU:HG2	1.88	0.74
1:A:649:GLY:O	1:A:653:LYS:HG2	1.87	0.74
1:A:822:GLN:O	1:A:873:ASN:HA	1.88	0.74
1:D:29:PRO:HG3	1:D:529:TRP:CZ2	2.23	0.74
1:D:822:GLN:O	1:D:873:ASN:HA	1.88	0.73
1:A:838:PRO:HD2	1:A:841:VAL:HG21	1.70	0.73
1:A:34:LYS:C	1:A:34:LYS:HD2	2.10	0.72
1:A:442:CYS:HB3	1:A:486:LYS:HD3	1.70	0.72
1:D:649:GLY:O	1:D:653:LYS:HG2	1.89	0.72
1:D:34:LYS:HD2	1:D:34:LYS:C	2.09	0.72
1:D:332:TYR:CZ	2:E:75:C:O2'	2.40	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:47(C):A:H5'	2:B:47(D):G:OP2	1.89	0.71
1:D:442:CYS:HB3	1:D:486:LYS:HD3	1.70	0.71
1:D:658:ASP:OD2	1:D:785:HIS:HB2	1.91	0.71
1:D:83:GLY:HA3	1:D:500:THR:HB	1.72	0.71
1:D:647:MET:HB3	1:D:650:PRO:HD2	1.72	0.71
1:A:189:LEU:HD22	1:A:191:GLN:NE2	2.06	0.70
1:A:83:GLY:HA3	1:A:500:THR:HB	1.73	0.70
1:D:96:HIS:ND1	1:D:97:PRO:HD2	2.06	0.70
1:D:826:ARG:HB2	1:D:828:ARG:CZ	2.20	0.70
2:B:47(D):G:O2'	2:B:47(E):C:H5'	1.91	0.69
1:A:866:TYR:HD1	1:A:872:LEU:HD13	1.57	0.69
2:E:74:C:HO2'	2:E:75:C:P	2.16	0.69
1:A:39:VAL:HG12	1:A:536:ILE:HB	1.74	0.69
1:D:535:TYR:HH	1:D:545:HIS:HE2	1.41	0.69
1:A:38:LEU:HD23	1:A:535:TYR:CD1	2.27	0.68
2:B:47(C):A:N3	2:E:66:C:H1'	2.07	0.68
1:A:96:HIS:ND1	1:A:97:PRO:HD2	2.09	0.68
1:D:685:TRP:HE3	1:D:689:ASN:ND2	1.91	0.68
1:A:685:TRP:HE3	1:A:689:ASN:ND2	1.92	0.68
1:A:826:ARG:HB2	1:A:828:ARG:CZ	2.24	0.68
1:A:856:LEU:O	1:A:857:GLU:HG2	1.93	0.67
1:D:455:LEU:HD12	1:D:455:LEU:H	1.59	0.67
1:D:620:ALA:HB2	1:D:634:LYS:HB2	1.75	0.67
1:A:694:ARG:HB2	1:A:756:TYR:CE1	2.26	0.67
1:A:647:MET:HB3	1:A:650:PRO:HD2	1.74	0.67
1:A:658:ASP:OD2	1:A:785:HIS:HB2	1.94	0.67
1:D:856:LEU:O	1:D:857:GLU:HG2	1.93	0.67
1:D:189:LEU:HD22	1:D:191:GLN:NE2	2.08	0.67
1:A:455:LEU:H	1:A:455:LEU:HD12	1.58	0.67
1:D:580:TRP:CZ3	1:D:635:PRO:HD3	2.29	0.66
1:A:136:ASN:OD1	1:A:503:ASP:HB3	1.95	0.66
1:A:346:ARG:HD2	2:B:74:C:O2'	1.96	0.66
1:A:46:GLY:N	1:A:104:ASN:HD21	1.94	0.66
2:E:7:G:H3'	2:E:8:U:H5'	1.76	0.66
1:D:866:TYR:HD1	1:D:872:LEU:HD13	1.60	0.66
1:D:694:ARG:HB2	1:D:756:TYR:CE1	2.27	0.66
1:D:46:GLY:N	1:D:104:ASN:HD21	1.94	0.65
1:D:581:THR:OG1	1:D:644:ASN:ND2	2.28	0.65
1:A:38:LEU:HD23	1:A:535:TYR:HE1	1.57	0.65
2:B:60:U:H5'	2:B:61:C:H5	1.60	0.64
1:D:833:ILE:HD13	1:D:837:ALA:HB3	1.78	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:843:ARG:O	1:D:847:LEU:HG	1.97	0.64
1:D:855:HIS:C	1:D:857:GLU:H	2.01	0.64
1:A:583:PHE:CD1	1:A:603:LEU:HD23	2.33	0.64
1:D:136:ASN:OD1	1:D:503:ASP:HB3	1.98	0.64
1:A:833:ILE:HD13	1:A:837:ALA:HB3	1.80	0.64
1:A:34:LYS:O	1:A:34:LYS:HD2	1.96	0.64
1:A:668:ALA:HB1	1:A:669:PRO:CD	2.28	0.64
1:A:855:HIS:C	1:A:857:GLU:H	2.00	0.64
1:D:838:PRO:HD2	1:D:841:VAL:HG21	1.79	0.64
1:D:38:LEU:HD23	1:D:535:TYR:HE1	1.61	0.63
1:D:38:LEU:HD23	1:D:535:TYR:CD1	2.33	0.63
1:A:685:TRP:CE3	1:A:689:ASN:ND2	2.66	0.63
1:D:864:GLU:OE2	1:D:874:LEU:HD22	1.99	0.63
1:A:48:LEU:HD12	1:A:111:SER:HB2	1.81	0.63
1:A:406:GLU:HG3	1:A:412:LYS:HA	1.80	0.63
1:A:843:ARG:O	1:A:847:LEU:HG	1.98	0.63
2:B:7:G:H3'	2:B:8:U:H5'	1.79	0.63
1:D:726:HIS:HD2	1:D:808:ASP:H	1.47	0.63
1:A:41:PHE:HD1	1:A:41:PHE:O	1.82	0.62
1:A:133:TYR:HB2	1:A:432:THR:HG23	1.80	0.62
1:D:133:TYR:HB2	1:D:432:THR:HG23	1.82	0.62
1:D:668:ALA:HB1	1:D:669:PRO:CD	2.29	0.62
2:E:60:U:H5'	2:E:61:C:H5	1.64	0.62
1:D:406:GLU:HG3	1:D:412:LYS:HA	1.81	0.62
1:A:726:HIS:HD2	1:A:808:ASP:H	1.48	0.61
1:A:864:GLU:OE2	1:A:874:LEU:HD22	2.00	0.61
1:A:456:LEU:HD23	1:A:457:PRO:HD2	1.82	0.61
1:A:694:ARG:HD2	1:A:756:TYR:CD1	2.34	0.61
1:D:311:ALA:HB2	1:D:322:ILE:HD11	1.83	0.61
1:D:685:TRP:CE3	1:D:689:ASN:ND2	2.65	0.61
1:A:291:THR:O	1:A:295:ARG:HG3	2.01	0.61
1:D:34:LYS:HD2	1:D:34:LYS:O	1.99	0.61
1:D:826:ARG:HD2	1:D:828:ARG:CZ	2.29	0.61
1:D:29:PRO:HD2	1:D:528:ALA:HB1	1.83	0.61
1:D:583:PHE:CD1	1:D:603:LEU:HD23	2.35	0.61
1:D:291:THR:O	1:D:295:ARG:HG3	2.01	0.60
1:D:332:TYR:CD1	2:E:75:C:H1'	2.36	0.60
1:D:46:GLY:H	1:D:104:ASN:HD21	1.48	0.60
1:D:456:LEU:HD23	1:D:457:PRO:HD2	1.83	0.60
1:A:574:GLN:HE21	1:A:574:GLN:HA	1.66	0.60
1:A:577:VAL:O	1:A:578:LEU:HD12	2.01	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:664:ILE:HG13	1:A:676:TRP:HZ3	1.66	0.60
1:A:855:HIS:O	1:A:857:GLU:N	2.35	0.60
1:D:189:LEU:HD22	1:D:191:GLN:HE21	1.66	0.60
1:D:580:TRP:CZ3	1:D:634:LYS:HA	2.37	0.60
1:D:442:CYS:SG	1:D:486:LYS:HD3	2.42	0.60
1:A:826:ARG:HD2	1:A:828:ARG:CZ	2.29	0.59
1:A:442:CYS:SG	1:A:486:LYS:HD3	2.42	0.59
1:D:48:LEU:HD12	1:D:111:SER:HB2	1.83	0.59
1:A:442:CYS:CB	1:A:486:LYS:HD3	2.33	0.59
1:D:694:ARG:HD2	1:D:756:TYR:CD1	2.37	0.59
1:A:189:LEU:HD22	1:A:191:GLN:HE21	1.65	0.59
2:B:60:U:H5'	2:B:61:C:C5	2.37	0.59
1:D:41:PHE:O	1:D:41:PHE:HD1	1.86	0.59
1:D:664:ILE:HG13	1:D:676:TRP:HZ3	1.68	0.59
1:D:638:MET:HG3	1:D:645:GLY:HA2	1.84	0.59
1:D:855:HIS:O	1:D:857:GLU:N	2.36	0.59
1:A:46:GLY:H	1:A:104:ASN:HD21	1.50	0.58
1:A:673:GLU:HG3	1:A:673:GLU:O	2.03	0.58
1:A:675:VAL:O	1:A:677:THR:HG23	2.03	0.58
1:D:442:CYS:CB	1:D:486:LYS:HD3	2.33	0.58
1:D:574:GLN:HE21	1:D:574:GLN:HA	1.68	0.58
1:A:172:VAL:HG12	1:A:173:GLU:HG3	1.83	0.58
1:D:204:LEU:HD12	1:D:204:LEU:O	2.01	0.58
2:E:14:A:H1'	2:E:22:A:C5	2.38	0.58
1:D:195:ARG:HA	1:D:421:ASP:OD1	2.04	0.58
1:D:580:TRP:CH2	1:D:635:PRO:HD3	2.39	0.58
2:E:72:C:H3'	2:E:73:A:H5''	1.84	0.58
1:A:786:LEU:HD12	1:A:786:LEU:O	2.02	0.58
2:B:53:G:O2'	2:B:54:U:H5'	2.03	0.58
1:D:194:LEU:HB2	1:D:422:TRP:HB3	1.84	0.58
1:A:29:PRO:HD2	1:A:528:ALA:HB1	1.86	0.57
2:B:72:C:H3'	2:B:73:A:H5''	1.84	0.57
1:D:620:ALA:CB	1:D:634:LYS:HB2	2.34	0.57
2:E:53:G:O2'	2:E:54:U:H5'	2.04	0.57
1:A:423:LEU:HD23	1:A:423:LEU:C	2.25	0.57
1:A:195:ARG:HA	1:A:421:ASP:OD1	2.04	0.57
1:A:557:HIS:ND1	1:A:565:GLU:HG2	2.19	0.57
1:A:10:GLU:HG2	1:A:785:HIS:CG	2.40	0.57
1:A:838:PRO:HD2	1:A:841:VAL:CG2	2.35	0.57
1:D:172:VAL:HG12	1:D:173:GLU:HG3	1.85	0.57
1:D:786:LEU:O	1:D:786:LEU:HD12	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:638:MET:HG3	1:A:645:GLY:HA2	1.86	0.57
1:A:50:MET:HE1	1:A:648:VAL:HG22	1.86	0.57
1:D:55:ASN:ND2	1:D:574:GLN:HG3	2.19	0.57
1:D:50:MET:HE1	1:D:648:VAL:HG22	1.87	0.57
1:D:137:GLN:NE2	1:D:433:PRO:O	2.37	0.56
2:B:60:U:C5'	2:B:61:C:H5	2.18	0.56
1:D:215:LYS:HE2	1:D:539:VAL:HG11	1.87	0.56
1:A:324:THR:O	1:A:324:THR:HG23	2.06	0.56
1:D:557:HIS:ND1	1:D:565:GLU:HG2	2.21	0.56
1:A:58:MET:HE1	1:A:670:PRO:HB3	1.88	0.56
1:D:87:GLU:O	1:D:91:LEU:HD13	2.05	0.56
2:E:60:U:H5'	2:E:61:C:C5	2.41	0.55
2:E:65:C:O2'	2:E:66:C:H5'	2.06	0.55
1:D:248:THR:HG23	2:E:76:A:H5'	1.87	0.55
2:E:7:G:H3'	2:E:8:U:C5'	2.36	0.55
1:D:134:ARG:HG3	1:D:135:TRP:N	2.21	0.55
1:D:10:GLU:HG2	1:D:785:HIS:CG	2.41	0.55
1:D:600:ARG:HD2	1:D:608:SER:OG	2.06	0.55
2:E:47(E):C:H2'	2:E:47(F):G:O4'	2.07	0.55
2:B:65:C:O2'	2:B:66:C:H5'	2.07	0.55
1:D:58:MET:HE1	1:D:670:PRO:HB3	1.88	0.55
1:A:55:ASN:ND2	1:A:574:GLN:HG3	2.21	0.55
1:A:194:LEU:HB2	1:A:422:TRP:HB3	1.89	0.55
1:A:426:ARG:HG2	1:A:426:ARG:HH11	1.71	0.54
2:E:60:U:C5'	2:E:61:C:H5	2.19	0.54
1:D:324:THR:HG23	1:D:324:THR:O	2.06	0.54
2:B:14:A:H1'	2:B:22:A:C5	2.43	0.54
1:D:763:PRO:O	1:D:765:THR:HG23	2.08	0.54
1:A:49:HIS:CD2	1:A:49:HIS:N	2.76	0.54
1:D:4:TYR:CZ	1:D:6:PRO:HG3	2.43	0.54
1:D:648:VAL:O	1:D:652:VAL:HG23	2.07	0.54
1:D:765:THR:OG1	1:D:767:VAL:HG12	2.07	0.54
1:A:137:GLN:NE2	1:A:433:PRO:O	2.35	0.54
1:D:346:ARG:NH1	2:E:75:C:OP1	2.41	0.54
1:A:82:PHE:CE2	1:A:128:CYS:HA	2.43	0.54
1:A:204:LEU:HD12	1:A:204:LEU:O	2.09	0.53
2:B:47(D):G:C2'	2:B:47(E):C:H5'	2.38	0.53
1:A:134:ARG:HG3	1:A:135:TRP:N	2.22	0.53
1:D:675:VAL:O	1:D:677:THR:HG23	2.08	0.53
1:A:648:VAL:O	1:A:652:VAL:HG23	2.09	0.53
1:A:817:VAL:CG1	1:A:870:LYS:HE2	2.39	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:9:ILE:O	1:D:12:LYS:HB3	2.08	0.53
1:A:4:TYR:HB3	1:A:689:ASN:OD1	2.09	0.53
2:B:7:G:H3'	2:B:8:U:C5'	2.39	0.53
1:D:846:ALA:O	1:D:849:VAL:HG13	2.09	0.53
2:B:18:G:H8	2:B:18:G:H5'	1.74	0.53
1:D:163:GLN:NE2	1:D:469:GLY:HA2	2.23	0.53
1:D:471:SER:O	1:D:474:GLU:HB2	2.09	0.53
1:A:195:ARG:HH11	1:A:195:ARG:HG3	1.74	0.53
1:A:4:TYR:CZ	1:A:6:PRO:HG3	2.44	0.53
1:A:657:ALA:O	1:A:660:ALA:N	2.41	0.53
1:A:459:LEU:HD21	1:A:476:HIS:NE2	2.24	0.53
1:A:759:ARG:NH1	1:A:764:VAL:HG23	2.24	0.53
1:D:574:GLN:HE22	1:D:670:PRO:HB2	1.73	0.53
1:A:196:ILE:HG13	1:A:551:PHE:CG	2.43	0.52
1:D:657:ALA:O	1:D:660:ALA:N	2.42	0.52
1:D:68:MET:O	1:D:803:GLY:HA2	2.09	0.52
2:E:65:C:H2'	2:E:66:C:H6	1.74	0.52
1:A:536:ILE:HD12	1:A:536:ILE:N	2.24	0.52
1:A:763:PRO:O	1:A:765:THR:HG23	2.08	0.52
1:A:311:ALA:HB2	1:A:322:ILE:HD11	1.90	0.52
1:A:765:THR:OG1	1:A:767:VAL:HG12	2.09	0.52
1:A:82:PHE:CE1	1:A:431:GLY:N	2.78	0.52
1:A:50:MET:CE	1:A:648:VAL:HG22	2.40	0.52
1:D:215:LYS:CE	1:D:539:VAL:HG11	2.40	0.52
1:A:194:LEU:HD12	1:A:424:ILE:HG21	1.92	0.52
1:A:794:PHE:HB2	1:A:795:TRP:CE3	2.45	0.52
1:A:163:GLN:NE2	1:A:469:GLY:HA2	2.25	0.52
1:D:50:MET:CE	1:D:648:VAL:HG22	2.40	0.52
1:A:614:ASP:O	1:A:618:MET:HG2	2.10	0.52
1:A:68:MET:O	1:A:803:GLY:HA2	2.09	0.52
1:D:263:PRO:HD3	1:D:325:ALA:O	2.09	0.52
1:D:169:GLU:HB3	1:D:544:LEU:HD23	1.92	0.52
1:A:187:ARG:HH11	1:A:187:ARG:HG3	1.74	0.52
1:A:846:ALA:O	1:A:849:VAL:HG13	2.09	0.52
1:D:194:LEU:HD12	1:D:424:ILE:HG21	1.91	0.52
1:A:291:THR:OG1	1:A:294:GLU:HG3	2.10	0.52
1:A:855:HIS:C	1:A:857:GLU:N	2.62	0.52
1:D:240:GLU:CD	1:D:240:GLU:H	2.14	0.52
1:D:346:ARG:HH22	2:E:76:A:H1'	1.74	0.52
1:A:215:LYS:HE2	1:A:539:VAL:HG11	1.92	0.52
1:D:291:THR:OG1	1:D:294:GLU:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:817:VAL:CG1	1:D:870:LYS:HE2	2.40	0.52
1:A:484:CYS:SG	1:A:486:LYS:HB3	2.50	0.51
1:A:820:ALA:HB3	1:A:871:ILE:HD12	1.90	0.51
1:D:136:ASN:ND2	1:D:506:TRP:HE1	2.08	0.51
1:A:38:LEU:CD2	1:A:535:TYR:HE1	2.23	0.51
1:A:436:MET:SD	1:A:446:PRO:HA	2.50	0.51
1:A:471:SER:O	1:A:474:GLU:HB2	2.11	0.51
1:D:187:ARG:HH11	1:D:187:ARG:HG3	1.76	0.51
1:D:580:TRP:CE2	1:D:635:PRO:HG3	2.46	0.51
1:A:712:GLU:C	1:A:714:LEU:H	2.13	0.51
1:D:423:LEU:HD23	1:D:423:LEU:C	2.30	0.51
1:D:658:ASP:OD1	1:D:785:HIS:ND1	2.41	0.51
1:D:855:HIS:C	1:D:857:GLU:N	2.63	0.51
1:A:577:VAL:C	1:A:578:LEU:HD12	2.31	0.51
1:D:196:ILE:HG13	1:D:551:PHE:CG	2.45	0.51
1:D:536:ILE:HD12	1:D:536:ILE:N	2.25	0.51
1:A:240:GLU:H	1:A:240:GLU:CD	2.13	0.51
1:A:726:HIS:CD2	1:A:808:ASP:H	2.28	0.51
1:A:751:PHE:O	1:A:754:ALA:HB3	2.11	0.51
1:D:484:CYS:SG	1:D:486:LYS:HB3	2.51	0.51
1:D:4:TYR:HB3	1:D:689:ASN:OD1	2.11	0.51
1:D:725:LEU:HD21	1:D:774:TYR:CD2	2.46	0.51
1:D:673:GLU:O	1:D:673:GLU:HG3	2.11	0.51
1:A:574:GLN:HE22	1:A:670:PRO:HB2	1.75	0.51
2:B:48:U:H2'	2:B:59:G:H4'	1.93	0.51
1:D:65:PHE:O	1:D:68:MET:HB2	2.11	0.51
1:D:726:HIS:CD2	1:D:808:ASP:H	2.29	0.51
1:D:536:ILE:HD12	1:D:536:ILE:H	1.76	0.51
1:A:459:LEU:HD21	1:A:476:HIS:CD2	2.46	0.50
1:A:536:ILE:H	1:A:536:ILE:HD12	1.75	0.50
1:A:554:LYS:O	1:A:557:HIS:HB3	2.11	0.50
1:A:823:VAL:HG22	1:A:874:LEU:HB2	1.94	0.50
1:A:294:GLU:O	1:A:297:ALA:HB3	2.11	0.50
1:D:581:THR:HB	1:D:583:PHE:HE2	1.76	0.50
1:D:712:GLU:C	1:D:714:LEU:H	2.13	0.50
1:D:577:VAL:O	1:D:578:LEU:HD12	2.12	0.50
1:A:816:VAL:HA	1:A:834:PRO:HA	1.92	0.50
1:D:82:PHE:CE2	1:D:128:CYS:HA	2.45	0.50
1:A:457:PRO:HG2	1:A:473:LEU:HD22	1.94	0.50
1:D:157:ASN:HB3	1:D:184:VAL:HG11	1.93	0.50
1:D:578:LEU:O	1:D:676:TRP:N	2.45	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:794:PHE:HB2	1:D:795:TRP:CE3	2.46	0.50
1:A:689:ASN:O	1:A:692:TYR:N	2.45	0.50
2:B:74:C:O2'	2:B:75:C:OP1	2.28	0.50
2:B:18:G:C8	2:B:18:G:H5'	2.47	0.50
1:D:457:PRO:HG2	1:D:473:LEU:HD22	1.93	0.50
1:D:53:LEU:CD1	1:D:115:MET:HG3	2.42	0.50
1:A:58:MET:O	1:A:59:GLY:C	2.50	0.50
1:A:600:ARG:HD2	1:A:608:SER:OG	2.12	0.50
1:A:651:PHE:CE1	1:A:655:GLN:HG3	2.47	0.50
1:A:74:LEU:C	1:A:74:LEU:HD12	2.32	0.50
2:B:4:G:O2'	2:B:5:G:H5'	2.12	0.49
1:D:256:ALA:HA	1:D:339:ALA:O	2.12	0.49
1:D:9:ILE:HG21	1:D:789:GLU:CD	2.33	0.49
1:A:711:ALA:HB3	1:A:712:GLU:OE1	2.12	0.49
1:D:46:GLY:H	1:D:104:ASN:ND2	2.09	0.49
1:D:9:ILE:HD13	1:D:789:GLU:HG2	1.93	0.49
1:D:816:VAL:HA	1:D:834:PRO:HA	1.92	0.49
1:A:725:LEU:HD21	1:A:774:TYR:CD2	2.48	0.49
1:A:87:GLU:O	1:A:91:LEU:HD13	2.12	0.49
2:E:18:G:H5'	2:E:18:G:H8	1.77	0.49
2:E:4:G:O2'	2:E:5:G:H5'	2.12	0.49
1:A:9:ILE:HG21	1:A:789:GLU:CD	2.32	0.49
1:A:833:ILE:HD12	1:A:834:PRO:O	2.12	0.49
2:B:65:C:H2'	2:B:66:C:H6	1.78	0.49
1:D:459:LEU:HD21	1:D:476:HIS:NE2	2.27	0.49
2:E:48:U:H2'	2:E:59:G:H4'	1.95	0.49
1:A:151:ARG:NH2	1:A:190:GLU:OE1	2.45	0.49
1:D:38:LEU:HD12	1:D:76:PRO:HG2	1.94	0.49
1:D:192:TRP:CZ2	1:D:436:MET:HG3	2.47	0.49
1:D:294:GLU:O	1:D:297:ALA:HB3	2.13	0.49
1:D:459:LEU:HD21	1:D:476:HIS:CD2	2.47	0.49
1:A:192:TRP:CZ2	1:A:436:MET:HG3	2.48	0.48
1:A:265:HIS:ND1	1:A:266:PRO:HD2	2.28	0.48
1:A:866:TYR:CD1	1:A:872:LEU:HD13	2.43	0.48
1:A:74:LEU:CD1	1:A:76:PRO:HD3	2.44	0.48
1:D:661:ARG:O	1:D:662:ILE:C	2.51	0.48
1:D:711:ALA:HB3	1:D:712:GLU:OE1	2.13	0.48
1:A:263:PRO:HD3	1:A:325:ALA:O	2.13	0.48
1:A:46:GLY:H	1:A:104:ASN:ND2	2.10	0.48
2:B:62:C:O2'	2:B:63:C:H5'	2.13	0.48
1:A:53:LEU:CD1	1:A:115:MET:HG3	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:GLU:HB3	1:A:544:LEU:HD23	1.95	0.48
1:A:647:MET:HE1	1:A:647:MET:H	1.79	0.48
1:A:671:GLU:HG2	1:A:672:ASN:N	2.27	0.48
1:A:281:LEU:O	1:A:281:LEU:HD23	2.13	0.48
1:D:341:PRO:O	1:D:348:TYR:HB2	2.13	0.48
1:D:49:HIS:N	1:D:49:HIS:CD2	2.82	0.48
1:D:615:VAL:HG13	1:D:632:LEU:HD11	1.96	0.48
1:D:651:PHE:CE1	1:D:655:GLN:HG3	2.49	0.48
2:E:62:C:O2'	2:E:63:C:H5'	2.14	0.48
1:A:215:LYS:CE	1:A:539:VAL:HG11	2.43	0.48
1:A:123:ARG:HA	1:A:514:PRO:HG3	1.96	0.48
1:A:157:ASN:HB3	1:A:184:VAL:HG11	1.95	0.48
1:A:38:LEU:HD12	1:A:76:PRO:HG2	1.95	0.48
1:D:281:LEU:O	1:D:281:LEU:HD23	2.13	0.48
1:D:554:LYS:O	1:D:557:HIS:HB3	2.13	0.48
1:D:738:ALA:O	1:D:739:LEU:HB2	2.13	0.48
2:E:18:G:C8	2:E:18:G:H5'	2.49	0.48
1:D:671:GLU:HG2	1:D:672:ASN:N	2.28	0.48
1:A:51:GLY:HA2	1:A:577:VAL:HG21	1.95	0.47
1:A:661:ARG:O	1:A:662:ILE:C	2.51	0.47
1:D:759:ARG:NH1	1:D:764:VAL:HG23	2.28	0.47
1:D:849:VAL:HG23	1:D:852:VAL:N	2.29	0.47
1:A:863:LYS:HE2	1:A:865:ILE:HD11	1.95	0.47
2:B:14:A:C2	2:B:21:G:H4'	2.49	0.47
1:D:307:LEU:HD12	1:D:322:ILE:HG22	1.96	0.47
1:D:863:LYS:HE2	1:D:865:ILE:HD11	1.96	0.47
1:A:487:CYS:SG	1:A:488:GLY:N	2.87	0.47
1:A:136:ASN:ND2	1:A:506:TRP:HE1	2.12	0.47
1:D:17:TRP:CB	1:D:118:LEU:HD21	2.41	0.47
1:D:259:LEU:HD23	1:D:338:MET:HA	1.96	0.47
1:D:820:ALA:HB3	1:D:871:ILE:HD12	1.95	0.47
1:D:493:ARG:HG2	1:D:493:ARG:HH11	1.80	0.47
1:A:461:ASP:O	1:A:464:ASP:HB3	2.14	0.47
1:D:265:HIS:ND1	1:D:266:PRO:HD2	2.29	0.47
1:A:24:LYS:HA	1:A:120:ASP:OD1	2.15	0.47
1:A:256:ALA:HA	1:A:339:ALA:O	2.15	0.47
1:A:738:ALA:O	1:A:739:LEU:HB2	2.13	0.47
1:D:574:GLN:NE2	1:D:574:GLN:HA	2.30	0.47
1:D:501:PHE:HA	1:D:504:SER:OG	2.13	0.47
1:D:123:ARG:HA	1:D:514:PRO:HG3	1.96	0.47
1:D:614:ASP:O	1:D:618:MET:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:596:PRO:HB2	1:D:598:PRO:HD2	1.96	0.47
1:D:638:MET:HA	1:D:644:ASN:OD1	2.15	0.47
1:D:767:VAL:HG13	1:D:768:TYR:N	2.30	0.47
1:D:838:PRO:HD2	1:D:841:VAL:CG2	2.43	0.47
1:A:405:LEU:C	1:A:407:GLU:H	2.18	0.47
1:A:817:VAL:HG12	1:A:870:LYS:HE2	1.97	0.47
1:D:82:PHE:CE1	1:D:431:GLY:N	2.83	0.47
1:A:149:ALA:O	1:A:150:TYR:HB3	2.15	0.47
1:A:581:THR:HB	1:A:583:PHE:HE2	1.80	0.47
1:D:348:TYR:C	1:D:348:TYR:CD1	2.88	0.47
1:D:461:ASP:O	1:D:464:ASP:HB3	2.15	0.47
1:D:49:HIS:HE1	1:D:638:MET:O	1.98	0.47
1:A:465:ILE:HG13	1:A:465:ILE:O	2.15	0.47
1:A:658:ASP:OD1	1:A:785:HIS:ND1	2.43	0.47
1:A:725:LEU:O	1:A:728:THR:N	2.48	0.47
1:D:51:GLY:HA2	1:D:577:VAL:HG21	1.97	0.47
1:A:574:GLN:HA	1:A:574:GLN:NE2	2.28	0.46
1:A:849:VAL:HG23	1:A:852:VAL:N	2.30	0.46
1:A:484:CYS:HB2	1:A:491:ALA:HB2	1.98	0.46
1:D:163:GLN:HE22	1:D:469:GLY:HA2	1.80	0.46
1:D:707:GLY:CA	1:D:769:ARG:HD3	2.45	0.46
2:E:23:C:H2'	2:E:24:G:O4'	2.15	0.46
1:D:101:THR:HG22	1:D:102:TYR:N	2.31	0.46
1:D:133:TYR:O	1:D:136:ASN:HB2	2.14	0.46
1:D:151:ARG:NH2	1:D:190:GLU:OE1	2.45	0.46
1:D:426:ARG:HH11	1:D:426:ARG:HG2	1.81	0.46
1:A:101:THR:HG22	1:A:102:TYR:N	2.30	0.46
1:A:493:ARG:HH11	1:A:493:ARG:HG2	1.80	0.46
1:A:836:ASP:O	1:A:837:ALA:C	2.54	0.46
1:D:195:ARG:HH11	1:D:195:ARG:HG3	1.78	0.46
1:D:508:TYR:CE1	1:D:509:LEU:HG	2.51	0.46
1:D:647:MET:H	1:D:647:MET:HE1	1.80	0.46
1:A:348:TYR:C	1:A:348:TYR:CD1	2.89	0.46
1:A:638:MET:CG	1:A:645:GLY:HA2	2.45	0.46
1:D:487:CYS:SG	1:D:488:GLY:N	2.89	0.46
1:D:638:MET:CG	1:D:645:GLY:HA2	2.45	0.46
1:A:163:GLN:HE22	1:A:469:GLY:HA2	1.81	0.46
1:A:55:ASN:N	1:A:55:ASN:HD22	2.13	0.46
1:A:638:MET:HA	1:A:644:ASN:OD1	2.16	0.46
1:A:819:VAL:HG22	1:A:870:LYS:HA	1.97	0.46
1:A:9:ILE:O	1:A:12:LYS:HB3	2.15	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:134:ARG:HB2	1:D:453:PRO:HB3	1.98	0.46
1:D:283:TYR:OH	1:D:303:THR:O	2.33	0.46
1:D:687:PHE:CE1	1:D:749:MET:HG2	2.51	0.46
1:A:759:ARG:HD3	1:A:768:TYR:CE1	2.51	0.46
2:B:23:C:H2'	2:B:24:G:O4'	2.16	0.46
1:D:24:LYS:HA	1:D:120:ASP:OD1	2.15	0.46
1:D:245:VAL:HA	1:D:334:THR:OG1	2.16	0.46
1:A:232:ILE:HD13	1:A:253:LEU:HD13	1.98	0.46
1:A:430:TRP:HA	1:A:430:TRP:CE3	2.51	0.46
1:D:817:VAL:HG12	1:D:870:LYS:HE2	1.98	0.46
1:D:833:ILE:HD12	1:D:834:PRO:O	2.16	0.46
1:D:139:ILE:O	1:D:143:MET:HG3	2.15	0.46
1:D:436:MET:SD	1:D:446:PRO:HA	2.56	0.46
2:B:19:G:OP1	2:B:60:U:N3	2.49	0.45
1:D:292:GLU:O	1:D:296:GLN:HG2	2.16	0.45
1:A:283:TYR:OH	1:A:303:THR:O	2.32	0.45
1:A:456:LEU:CD2	1:A:457:PRO:HD2	2.46	0.45
1:D:461:ASP:HB3	1:D:464:ASP:HB2	1.98	0.45
1:D:577:VAL:C	1:D:578:LEU:HD12	2.37	0.45
2:E:20:U:O2'	2:E:20(A):A:H5'	2.16	0.45
1:A:292:GLU:O	1:A:296:GLN:HG2	2.15	0.45
1:A:74:LEU:HD12	1:A:76:PRO:HD3	1.97	0.45
1:D:824:ASN:ND2	1:D:876:VAL:HB	2.31	0.45
1:A:432:THR:HB	1:A:498:MET:HB2	1.98	0.45
1:A:508:TYR:CE1	1:A:509:LEU:HG	2.51	0.45
1:A:647:MET:CE	1:A:647:MET:H	2.29	0.45
2:B:47(E):C:H2'	2:B:47(F):G:O4'	2.17	0.45
1:D:779:LEU:HD23	1:D:787:ALA:HB2	1.97	0.45
1:A:856:LEU:C	1:A:857:GLU:CG	2.85	0.45
1:D:38:LEU:CD2	1:D:535:TYR:HE1	2.27	0.45
1:A:259:LEU:HD23	1:A:338:MET:HA	1.98	0.45
1:A:786:LEU:O	1:A:790:LEU:HG	2.17	0.45
1:D:456:LEU:CD2	1:D:457:PRO:HD2	2.47	0.45
1:D:74:LEU:HD12	1:D:74:LEU:C	2.37	0.45
1:D:786:LEU:O	1:D:790:LEU:HG	2.17	0.45
1:A:596:PRO:HB2	1:A:598:PRO:HD2	1.98	0.45
1:A:707:GLY:CA	1:A:769:ARG:HD3	2.47	0.45
1:D:484:CYS:HB2	1:D:491:ALA:HB2	1.99	0.45
1:A:333:GLY:HA2	1:A:416:THR:HG21	1.99	0.45
1:A:144:TRP:CE3	1:A:436:MET:HE2	2.52	0.45
1:D:836:ASP:O	1:D:837:ALA:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:501:PHE:HA	1:A:504:SER:OG	2.16	0.45
1:D:758:TYR:CZ	1:D:762:ARG:HG2	2.52	0.45
1:A:75:HIS:CE1	1:A:119:TYR:CE1	3.04	0.45
1:A:426:ARG:NH1	1:A:426:ARG:HG2	2.32	0.45
1:D:155:LEU:HD12	1:D:264:GLU:HG2	1.99	0.45
2:E:74:C:H4'	2:E:75:C:OP2	2.17	0.45
1:A:134:ARG:CG	1:A:135:TRP:N	2.80	0.44
1:A:725:LEU:O	1:A:728:THR:HB	2.17	0.44
1:A:85:PRO:HA	1:A:178:ARG:HH21	1.82	0.44
1:D:134:ARG:CG	1:D:135:TRP:N	2.80	0.44
1:D:58:MET:O	1:D:59:GLY:C	2.55	0.44
1:D:689:ASN:O	1:D:692:TYR:N	2.50	0.44
1:D:332:TYR:OH	2:E:76:A:OP2	2.33	0.44
1:A:341:PRO:O	1:A:348:TYR:HB2	2.16	0.44
1:A:731:LYS:HZ2	1:A:735:ASP:CG	2.19	0.44
2:B:18:G:N2	2:B:57:A:H2'	2.33	0.44
1:A:762:ARG:HA	1:A:763:PRO:HD3	1.87	0.44
1:A:856:LEU:C	1:A:857:GLU:HG2	2.38	0.44
2:B:74:C:H4'	2:B:75:C:OP2	2.18	0.44
1:D:2:GLU:H	1:D:2:GLU:HG2	1.52	0.44
1:D:430:TRP:CE3	1:D:430:TRP:HA	2.52	0.44
1:D:687:PHE:CE2	1:D:691:ILE:HD11	2.52	0.44
1:D:856:LEU:C	1:D:857:GLU:HG2	2.37	0.44
1:A:155:LEU:HD12	1:A:264:GLU:HG2	2.00	0.44
1:A:29:PRO:HG3	1:A:529:TRP:CE2	2.53	0.44
1:A:522:ASP:HB3	1:A:525:LYS:HG2	2.00	0.44
1:D:731:LYS:HZ2	1:D:735:ASP:CG	2.21	0.44
1:D:698:ASP:OD1	1:D:759:ARG:NH2	2.51	0.44
2:E:47(A):C:H2'	2:E:47(B):A:O4'	2.18	0.44
1:A:250:PRO:C	1:A:252:THR:H	2.21	0.44
1:A:649:GLY:O	1:A:650:PRO:C	2.56	0.44
1:A:687:PHE:CE2	1:A:691:ILE:HD11	2.53	0.44
1:A:824:ASN:HD21	1:A:876:VAL:HB	1.83	0.44
1:D:405:LEU:C	1:D:407:GLU:H	2.19	0.44
1:D:84:LEU:HB2	1:D:85:PRO:HD3	1.99	0.44
1:D:856:LEU:C	1:D:857:GLU:CG	2.86	0.44
1:D:332:TYR:CE1	2:E:75:C:H1'	2.52	0.44
1:A:506:TRP:O	1:A:509:LEU:HB2	2.17	0.44
1:A:838:PRO:O	1:A:841:VAL:N	2.47	0.44
1:A:861:VAL:HA	1:A:876:VAL:HA	2.00	0.44
1:A:861:VAL:HG12	1:A:862:VAL:N	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:839:LEU:H	1:D:839:LEU:CD1	2.26	0.44
1:A:473:LEU:C	1:A:475:ALA:H	2.21	0.44
1:A:51:GLY:HA2	1:A:577:VAL:CG2	2.47	0.44
1:D:432:THR:HB	1:D:498:MET:HB2	2.00	0.44
1:A:156:VAL:O	1:A:186:LYS:HA	2.18	0.44
1:A:65:PHE:O	1:A:68:MET:HB2	2.18	0.44
1:A:73:VAL:HG12	1:A:74:LEU:N	2.33	0.44
2:E:48:U:C6	2:E:59:G:H5'	2.53	0.44
1:A:134:ARG:HB2	1:A:453:PRO:HB3	1.99	0.43
1:A:224:ILE:HA	1:A:419:LEU:HB2	2.00	0.43
1:A:41:PHE:O	1:A:41:PHE:CD1	2.68	0.43
1:D:194:LEU:HD11	1:D:424:ILE:HD13	1.99	0.43
1:D:401:VAL:O	1:D:405:LEU:HG	2.18	0.43
1:D:759:ARG:NH1	1:D:764:VAL:N	2.65	0.43
1:D:838:PRO:O	1:D:841:VAL:N	2.50	0.43
1:D:846:ALA:O	1:D:848:LYS:N	2.51	0.43
1:D:819:VAL:HG13	1:D:871:ILE:N	2.33	0.43
1:A:84:LEU:HB2	1:A:85:PRO:HD3	1.99	0.43
1:D:522:ASP:HB3	1:D:525:LYS:HG2	1.99	0.43
1:D:824:ASN:HD21	1:D:876:VAL:HB	1.82	0.43
1:A:25:ALA:H	1:A:120:ASP:CG	2.22	0.43
1:A:346:ARG:HD2	2:B:74:C:HO2'	1.81	0.43
1:A:535:TYR:OH	1:A:545:HIS:NE2	2.43	0.43
1:A:824:ASN:ND2	1:A:876:VAL:HB	2.32	0.43
1:D:861:VAL:HA	1:D:876:VAL:HA	2.00	0.43
1:D:248:THR:CG2	2:E:76:A:H5'	2.47	0.43
1:A:60:ASP:OD1	1:A:64:ARG:NE	2.47	0.43
1:A:580:TRP:CZ3	1:A:621:GLU:HG2	2.53	0.43
1:A:767:VAL:HG13	1:A:768:TYR:N	2.32	0.43
1:A:786:LEU:HD11	1:A:790:LEU:HD11	2.01	0.43
1:D:333:GLY:HA2	1:D:416:THR:HG21	1.99	0.43
1:D:134:ARG:CB	1:D:453:PRO:HB3	2.48	0.43
1:D:603:LEU:O	1:D:605:ILE:HG23	2.17	0.43
1:A:289:ARG:HB2	1:A:289:ARG:CZ	2.49	0.43
1:A:429:TYR:CE1	1:A:456:LEU:HD22	2.53	0.43
1:A:632:LEU:O	1:A:632:LEU:HD23	2.18	0.43
1:A:846:ALA:O	1:A:848:LYS:N	2.51	0.43
1:D:241:VAL:HG22	1:D:242:ARG:N	2.34	0.43
1:D:647:MET:H	1:D:647:MET:CE	2.32	0.43
1:D:826:ARG:CB	1:D:828:ARG:CZ	2.93	0.43
1:A:241:VAL:HG22	1:A:242:ARG:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:ASP:HB3	1:A:464:ASP:HB2	1.99	0.43
1:A:826:ARG:CB	1:A:828:ARG:CZ	2.96	0.43
1:D:53:LEU:HD12	1:D:115:MET:HG3	2.01	0.43
1:D:224:ILE:HA	1:D:419:LEU:HB2	2.00	0.43
1:D:51:GLY:HA2	1:D:577:VAL:CG2	2.48	0.43
2:E:50:C:H2'	2:E:51:G:H8	1.84	0.43
1:A:437:VAL:HG12	1:A:438:HIS:N	2.34	0.43
1:A:823:VAL:HG13	1:A:874:LEU:O	2.19	0.43
1:A:849:VAL:HG23	1:A:852:VAL:CA	2.49	0.43
2:B:58:A:H2	2:B:60:U:H2'	1.84	0.43
1:D:289:ARG:HB2	1:D:289:ARG:CZ	2.48	0.43
1:A:133:TYR:O	1:A:136:ASN:HB2	2.19	0.43
1:A:243:ILE:HA	1:A:244:PRO:HD3	1.86	0.43
1:A:401:VAL:O	1:A:405:LEU:HG	2.19	0.43
1:A:41:PHE:CE1	1:A:80:ASP:HB2	2.54	0.43
1:D:473:LEU:C	1:D:475:ALA:H	2.22	0.43
1:D:75:HIS:CE1	1:D:119:TYR:CE1	3.06	0.43
1:D:866:TYR:CD1	1:D:872:LEU:HD13	2.46	0.43
1:D:364:ARG:HA	1:D:365:PRO:HD3	1.91	0.43
1:D:429:TYR:CE1	1:D:456:LEU:HD22	2.54	0.43
1:D:619:GLY:O	1:D:634:LYS:HG3	2.19	0.43
1:D:849:VAL:HG23	1:D:852:VAL:CA	2.49	0.43
1:A:29:PRO:HG3	1:A:529:TRP:CH2	2.54	0.43
1:D:74:LEU:CD1	1:D:76:PRO:HD3	2.49	0.43
1:A:290:LYS:HA	1:A:294:GLU:OE2	2.19	0.42
1:A:668:ALA:HB1	1:A:669:PRO:HD3	1.98	0.42
1:A:852:VAL:O	1:A:852:VAL:HG12	2.19	0.42
1:D:42:PRO:HB3	1:D:56:TYR:OH	2.19	0.42
1:D:144:TRP:CE3	1:D:436:MET:HE2	2.53	0.42
1:D:96:HIS:CD2	1:D:98:LYS:HB3	2.54	0.42
1:A:698:ASP:OD1	1:A:759:ARG:NH2	2.52	0.42
1:D:819:VAL:HG22	1:D:870:LYS:HA	2.00	0.42
2:E:72:C:H3'	2:E:73:A:C5'	2.49	0.42
1:A:659:ILE:HD13	1:A:685:TRP:CD1	2.55	0.42
1:D:808:ASP:OD2	1:D:811:ALA:HB2	2.19	0.42
1:A:606:PRO:HG2	1:A:607:GLU:H	1.84	0.42
1:A:748:LEU:HA	1:A:748:LEU:HD23	1.72	0.42
1:A:9:ILE:HD13	1:A:789:GLU:HG2	2.00	0.42
1:D:437:VAL:HG12	1:D:438:HIS:N	2.34	0.42
1:A:650:PRO:O	1:A:653:LYS:N	2.52	0.42
1:D:141:LEU:O	1:D:144:TRP:N	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:13:TRP:O	1:D:16:PHE:HB3	2.19	0.42
1:A:139:ILE:O	1:A:143:MET:HG3	2.19	0.42
1:D:41:PHE:O	1:D:41:PHE:CD1	2.70	0.42
2:E:58:A:H2	2:E:60:U:H2'	1.84	0.42
1:A:808:ASP:OD2	1:A:811:ALA:HB2	2.19	0.42
1:D:572:PHE:HZ	1:D:670:PRO:HG2	1.84	0.42
1:D:60:ASP:OD1	1:D:64:ARG:NE	2.48	0.42
1:D:615:VAL:HG12	1:D:620:ALA:O	2.20	0.42
1:A:141:LEU:O	1:A:144:TRP:N	2.52	0.42
1:D:25:ALA:H	1:D:120:ASP:CG	2.22	0.42
1:D:249:ARG:HD2	1:D:398:LYS:HE2	2.02	0.42
1:A:249:ARG:HD2	1:A:398:LYS:HE2	2.01	0.42
1:A:583:PHE:HB2	1:A:632:LEU:O	2.20	0.42
1:A:759:ARG:NH1	1:A:764:VAL:N	2.67	0.42
1:D:191:GLN:HB3	1:D:425:SER:OG	2.20	0.42
1:D:465:ILE:O	1:D:465:ILE:HG13	2.18	0.42
1:D:625:HIS:CG	1:D:626:GLU:H	2.38	0.42
1:D:861:VAL:HG12	1:D:862:VAL:N	2.34	0.42
2:E:65:C:H2'	2:E:66:C:C6	2.55	0.42
1:A:13:TRP:O	1:A:16:PHE:HB3	2.20	0.42
1:A:278:GLU:O	1:A:278:GLU:HG2	2.19	0.42
1:A:194:LEU:CD1	1:A:424:ILE:HG21	2.49	0.42
1:A:687:PHE:CE1	1:A:749:MET:HG2	2.55	0.42
1:D:194:LEU:CD1	1:D:424:ILE:HG21	2.49	0.42
1:D:320:ILE:HG13	1:D:320:ILE:O	2.19	0.42
1:D:725:LEU:O	1:D:728:THR:HB	2.20	0.42
1:A:53:LEU:HD12	1:A:115:MET:HG3	2.02	0.41
1:D:41:PHE:O	3:D:1601:LEU:N	2.53	0.41
1:D:55:ASN:HD22	1:D:55:ASN:N	2.18	0.41
2:E:14:A:C2	2:E:21:G:H4'	2.55	0.41
1:A:253:LEU:HG	1:A:315:ALA:HB2	2.02	0.41
1:A:245:VAL:HA	1:A:334:THR:OG1	2.20	0.41
1:A:702:LEU:HD22	1:A:769:ARG:HG3	2.00	0.41
1:D:29:PRO:HG3	1:D:529:TRP:CE2	2.54	0.41
1:D:345:GLN:O	1:D:346:ARG:C	2.57	0.41
1:A:366:GLY:O	1:A:368:PRO:HD3	2.20	0.41
1:A:815:ASP:C	1:A:816:VAL:HG23	2.41	0.41
1:A:819:VAL:HG13	1:A:871:ILE:N	2.35	0.41
1:D:149:ALA:O	1:D:150:TYR:HB3	2.19	0.41
1:D:85:PRO:HA	1:D:178:ARG:HH21	1.85	0.41
1:D:203:LEU:HD23	1:D:203:LEU:HA	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:134:ARG:CB	1:A:453:PRO:HB3	2.50	0.41
1:A:779:LEU:HD23	1:A:787:ALA:HB2	2.02	0.41
1:A:96:HIS:CD2	1:A:98:LYS:HB3	2.55	0.41
1:D:23:MET:CE	1:D:63:ALA:HB1	2.51	0.41
1:A:195:ARG:NH1	1:A:195:ARG:HG3	2.36	0.41
1:A:341:PRO:HB3	1:A:348:TYR:HA	2.02	0.41
1:A:42:PRO:HB3	1:A:56:TYR:OH	2.20	0.41
1:D:156:VAL:O	1:D:186:LYS:HA	2.20	0.41
1:D:625:HIS:CG	1:D:626:GLU:N	2.88	0.41
1:D:852:VAL:HG12	1:D:852:VAL:O	2.20	0.41
2:E:14:A:H1'	2:E:22:A:N7	2.35	0.41
1:A:15:ARG:O	1:A:19:GLU:HG3	2.20	0.41
1:A:338:MET:HG3	1:A:338:MET:O	2.20	0.41
1:D:29:PRO:HG3	1:D:529:TRP:CH2	2.55	0.41
1:D:341:PRO:HB3	1:D:348:TYR:HA	2.01	0.41
1:D:438:HIS:N	1:D:492:LYS:O	2.51	0.41
1:A:119:TYR:HD2	1:A:121:TRP:CZ2	2.38	0.41
1:A:796:PRO:HG2	1:A:797:ASP:H	1.85	0.41
2:E:18:G:N2	2:E:57:A:H2'	2.35	0.41
1:A:25:ALA:HB3	1:A:123:ARG:NE	2.17	0.41
1:A:426:ARG:NH1	1:A:499:ASP:HB2	2.36	0.41
1:A:585:PRO:HA	1:A:631:HIS:CD2	2.55	0.41
1:A:758:TYR:CZ	1:A:762:ARG:HG2	2.56	0.41
2:B:69:C:O2'	2:B:70:G:H5'	2.21	0.41
1:A:307:LEU:HD12	1:A:322:ILE:HG22	2.01	0.41
1:A:432:THR:HA	1:A:433:PRO:HD3	1.90	0.41
1:D:823:VAL:HG22	1:D:874:LEU:HB2	2.02	0.41
1:A:101:THR:O	1:A:103:ALA:N	2.54	0.41
1:A:162:CYS:HB3	1:A:164:THR:HG22	2.02	0.41
1:A:396:GLU:HA	1:A:399:ARG:HE	1.86	0.41
1:A:29:PRO:CG	1:A:529:TRP:CE2	3.03	0.41
1:D:278:GLU:HG2	1:D:278:GLU:O	2.20	0.41
1:D:556:LEU:HD23	1:D:556:LEU:HA	1.89	0.41
1:D:759:ARG:HD3	1:D:768:TYR:CE1	2.56	0.41
1:D:74:LEU:HD12	1:D:76:PRO:HD3	2.03	0.41
1:D:84:LEU:N	1:D:85:PRO:CD	2.84	0.41
1:A:226:ARG:HH11	1:A:226:ARG:HG3	1.85	0.41
1:D:119:TYR:HD2	1:D:121:TRP:CZ2	2.39	0.41
1:D:265:HIS:HB3	1:D:268:THR:OG1	2.21	0.41
1:D:73:VAL:HG12	1:D:74:LEU:N	2.35	0.41
1:A:249:ARG:HD2	1:A:249:ARG:HA	1.94	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:233:LEU:HB2	1:A:410:LEU:O	2.21	0.40
1:A:65:PHE:CD1	1:A:736:LEU:HD13	2.56	0.40
1:D:162:CYS:HB3	1:D:164:THR:HG22	2.03	0.40
1:D:396:GLU:HA	1:D:399:ARG:HE	1.86	0.40
1:D:788:GLU:OE2	1:D:799:LEU:HB2	2.20	0.40
1:A:625:HIS:CG	1:A:626:GLU:H	2.40	0.40
1:D:243:ILE:HA	1:D:244:PRO:HD3	1.85	0.40
1:D:290:LYS:HA	1:D:294:GLU:OE2	2.21	0.40
1:D:34:LYS:NZ	1:D:533:ASP:OD1	2.52	0.40
1:D:702:LEU:HD22	1:D:769:ARG:HG3	2.02	0.40
1:A:54:LYS:HE2	1:A:575:GLY:H	1.86	0.40
1:A:625:HIS:CG	1:A:626:GLU:N	2.89	0.40
1:D:267:LEU:O	1:D:271:LEU:HB2	2.21	0.40
1:A:194:LEU:HD23	1:A:194:LEU:HA	1.90	0.40
1:D:343:HIS:CE1	1:D:362:ILE:HB	2.57	0.40
1:D:456:LEU:HD23	1:D:457:PRO:CD	2.49	0.40
1:D:480:TYR:O	1:D:482:THR:N	2.50	0.40
1:A:253:LEU:CD2	1:A:315:ALA:HB2	2.52	0.40
1:A:194:LEU:HD11	1:A:424:ILE:HD13	2.04	0.40
1:A:823:VAL:HG13	1:A:876:VAL:HG23	2.03	0.40
1:A:84:LEU:N	1:A:85:PRO:CD	2.83	0.40
2:B:31:A:H61	2:B:38:A:H62	1.70	0.40
2:B:50:C:H2'	2:B:51:G:H8	1.86	0.40
1:D:226:ARG:HG2	1:D:227:SER:N	2.37	0.40
1:D:232:ILE:HD13	1:D:253:LEU:HD13	2.02	0.40
1:D:267:LEU:HB3	1:D:271:LEU:HD12	2.03	0.40
1:D:253:LEU:HG	1:D:315:ALA:HB2	2.03	0.40
1:D:143:MET:HG2	1:D:555:PHE:CZ	2.57	0.40
1:D:632:LEU:O	1:D:632:LEU:HD23	2.21	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	874/878 (100%)	728 (83%)	121 (14%)	25 (3%)	4	24
1	D	874/878 (100%)	734 (84%)	117 (13%)	23 (3%)	5	27
All	All	1748/1756 (100%)	1462 (84%)	238 (14%)	48 (3%)	5	26

All (48) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	796	PRO
1	A	861	VAL
1	D	856	LEU
1	D	861	VAL
1	A	847	LEU
1	A	856	LEU
1	A	869	GLY
1	D	796	PRO
1	D	847	LEU
1	D	869	GLY
1	A	10	GLU
1	A	55	ASN
1	A	661	ARG
1	A	713	ALA
1	D	10	GLU
1	D	55	ASN
1	D	661	ARG
1	D	713	ALA
1	A	344	ASP
1	A	455	LEU
1	A	650	PRO
1	A	658	ASP
1	A	816	VAL
1	D	344	ASP
1	D	455	LEU
1	D	465	ILE
1	D	650	PRO
1	D	816	VAL
1	A	465	ILE
1	A	725	LEU
1	D	2	GLU
1	A	2	GLU
1	A	606	PRO
1	A	780	PHE
1	A	857	GLU

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Mol	Chain	Res	Type
1	D	857	GLU
1	A	225	GLY
1	A	849	VAL
1	D	606	PRO
1	D	764	VAL
1	D	780	PHE
1	D	849	VAL
1	A	341	PRO
1	D	225	GLY
1	A	868	PRO
1	D	341	PRO
1	A	764	VAL
1	D	868	PRO

### 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	741/742 (100%)	717 (97%)	24 (3%)	39	67
1	D	741/742 (100%)	717 (97%)	24 (3%)	39	67
All	All	1482/1484 (100%)	1434 (97%)	48 (3%)	39	67

All (48) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	LYS
1	A	36	TYR
1	A	41	PHE
1	A	49	HIS
1	A	74	LEU
1	A	76	PRO
1	A	82	PHE
1	A	126	THR
1	A	168	ASN
1	A	189	LEU

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Mol	Chain	Res	Type
1	A	226	ARG
1	A	240	GLU
1	A	327	TYR
1	A	352	ARG
1	A	430	TRP
1	A	456	LEU
1	A	500	THR
1	A	503	ASP
1	A	552	PHE
1	A	600	ARG
1	A	647	MET
1	A	685	TRP
1	A	718	ASP
1	A	836	ASP
1	D	34	LYS
1	D	36	TYR
1	D	41	PHE
1	D	49	HIS
1	D	74	LEU
1	D	82	PHE
1	D	126	THR
1	D	168	ASN
1	D	189	LEU
1	D	226	ARG
1	D	240	GLU
1	D	327	TYR
1	D	352	ARG
1	D	430	TRP
1	D	456	LEU
1	D	500	THR
1	D	503	ASP
1	D	552	PHE
1	D	600	ARG
1	D	647	MET
1	D	685	TRP
1	D	718	ASP
1	D	770	THR
1	D	836	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	ASN
1	A	104	ASN
1	A	107	GLN
1	A	163	GLN
1	A	179	HIS
1	A	574	GLN
1	A	682	GLN
1	A	726	HIS
1	A	792	HIS
1	A	824	ASN
1	D	55	ASN
1	D	104	ASN
1	D	107	GLN
1	D	163	GLN
1	D	574	GLN
1	D	682	GLN
1	D	726	HIS
1	D	824	ASN

### 5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	B	76/83 (91%)	11 (14%)	4 (5%)
2	E	76/83 (91%)	8 (10%)	4 (5%)
All	All	152/166 (91%)	19 (12%)	8 (5%)

All (19) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	B	10	G
2	B	18	G
2	B	19	G
2	B	20	U
2	B	47(B)	A
2	B	47(C)	A
2	B	47(D)	G
2	B	48	U
2	B	73	A
2	B	75	C
2	B	76	A
2	E	10	G
2	E	18	G

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Mol	Chain	Res	Type
2	E	19	G
2	E	20	U
2	E	48	U
2	E	73	A
2	E	75	C
2	E	76	A

All (8) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	B	9	G
2	B	18	G
2	B	74	C
2	B	75	C
2	E	9	G
2	E	18	G
2	E	74	C
2	E	75	C

## 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 23 ligands modelled in this entry, 6 are monoatomic - leaving 17 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
6	SO4	D	1701	-	4,4,4	0.29	0	6,6,6	0.06	0
6	SO4	A	1503	-	4,4,4	0.27	0	6,6,6	0.23	0
6	SO4	A	1510	-	4,4,4	0.27	0	6,6,6	0.07	0
6	SO4	A	1504	-	4,4,4	0.27	0	6,6,6	0.13	0
6	SO4	D	1704	-	4,4,4	0.27	0	6,6,6	0.07	0
6	SO4	A	1509	-	4,4,4	0.26	0	6,6,6	0.09	0
6	SO4	D	1710	-	4,4,4	0.28	0	6,6,6	0.05	0
6	SO4	A	1511	-	4,4,4	0.29	0	6,6,6	0.12	0
6	SO4	A	1505	-	4,4,4	0.27	0	6,6,6	0.10	0
6	SO4	D	1703	-	4,4,4	0.30	0	6,6,6	0.06	0
6	SO4	A	1506	-	4,4,4	0.24	0	6,6,6	0.08	0
6	SO4	D	1702	-	4,4,4	0.24	0	6,6,6	0.11	0
6	SO4	D	1708	-	4,4,4	0.25	0	6,6,6	0.07	0
6	SO4	A	1502	-	4,4,4	0.31	0	6,6,6	0.19	0
6	SO4	A	1501	-	4,4,4	0.29	0	6,6,6	0.09	0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	876/878 (99%)	-0.17	16 (1%) 68 67	10, 65, 121, 159	0
1	D	876/878 (99%)	0.19	55 (6%) 20 20	46, 101, 144, 160	0
2	B	78/83 (93%)	0.27	3 (3%) 40 37	28, 83, 173, 202	0
2	E	78/83 (93%)	0.46	4 (5%) 28 26	51, 95, 187, 202	0
All	All	1908/1922 (99%)	0.04	78 (4%) 37 35	10, 84, 143, 202	0

All (78) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	180	GLU	5.5
1	D	587	GLU	5.0
1	D	172	VAL	4.9
1	D	624	PRO	4.8
1	D	93	PHE	4.7
2	B	32	C	4.5
1	D	797	ASP	4.4
1	D	173	GLU	4.4
1	D	174	GLY	4.0
2	E	17	G	4.0
2	B	17	G	3.9
1	A	180	GLU	3.9
1	A	876	VAL	3.4
1	D	432	THR	3.4
1	A	858	GLY	3.4
1	D	855	HIS	3.3
1	D	490	PRO	3.3
1	D	175	ARG	3.2
1	D	589	GLU	3.2
1	D	626	GLU	3.2
2	B	31	A	3.1

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Mol	Chain	Res	Type	RSRZ
1	D	481	GLU	3.0
1	D	497	THR	2.9
1	D	597	GLU	2.9
1	A	875	VAL	2.9
1	D	591	SER	2.8
1	D	183	PRO	2.8
2	E	30	G	2.8
1	D	467	PRO	2.8
1	D	488	GLY	2.8
1	D	642	LYS	2.8
1	A	173	GLU	2.8
1	A	850	ARG	2.7
1	D	876	VAL	2.7
1	D	599	THR	2.7
1	D	862	VAL	2.7
1	D	850	ARG	2.6
1	D	860	GLU	2.6
1	D	182	THR	2.6
1	D	612	LEU	2.5
1	D	181	ASP	2.5
1	A	443	GLY	2.5
1	A	497	THR	2.5
1	D	829	GLY	2.5
1	D	463	GLU	2.5
1	D	505	SER	2.5
1	A	855	HIS	2.4
1	D	278	GLU	2.4
1	D	466	ARG	2.4
1	D	606	PRO	2.4
1	A	93	PHE	2.4
1	D	830	THR	2.4
1	D	431	GLY	2.3
1	D	605	ILE	2.3
1	D	851	ASN	2.3
1	D	462	VAL	2.3
1	D	31	GLY	2.2
1	D	475	ALA	2.2
1	A	499	ASP	2.2
1	D	864	GLU	2.2
1	D	298	GLU	2.2
1	D	630	LEU	2.2
2	E	31	A	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	621	GLU	2.1
1	A	470	LYS	2.1
1	D	465	ILE	2.1
1	D	285	GLU	2.1
1	A	851	ASN	2.1
1	D	858	GLY	2.1
1	D	83	GLY	2.1
1	D	590	GLY	2.1
1	A	32	ARG	2.1
1	A	83	GLY	2.1
1	D	623	ARG	2.1
1	D	863	LYS	2.0
2	E	73	A	2.0
1	A	826	ARG	2.0
1	D	796	PRO	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	ZN	D	1602	1/1	0.80	0.08	147,147,147,147	0
6	SO4	D	1701	5/5	0.81	0.30	194,194,194,195	0
6	SO4	A	1511	5/5	0.82	0.20	162,162,163,163	0
6	SO4	A	1501	5/5	0.85	0.28	150,150,152,152	0
6	SO4	A	1509	5/5	0.86	0.26	159,159,160,160	0
6	SO4	A	1505	5/5	0.87	0.15	143,143,145,145	0
6	SO4	D	1710	5/5	0.88	0.50	173,173,173,174	0
6	SO4	D	1704	5/5	0.88	0.13	163,165,165,165	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
6	SO4	D	1703	5/5	0.88	0.18	168,168,168,169	0
4	ZN	A	1302	1/1	0.88	0.03	120,120,120,120	0
4	ZN	D	1603	1/1	0.90	0.05	137,137,137,137	0
6	SO4	A	1506	5/5	0.91	0.41	107,109,111,111	0
6	SO4	D	1708	5/5	0.91	0.30	163,163,164,165	0
3	LEU	D	1601	9/9	0.92	0.21	92,95,96,96	0
6	SO4	A	1510	5/5	0.92	0.25	154,155,156,156	0
6	SO4	A	1504	5/5	0.93	0.13	118,119,120,120	0
6	SO4	D	1702	5/5	0.93	0.11	126,127,129,129	0
4	ZN	A	1303	1/1	0.95	0.09	85,85,85,85	0
3	LEU	A	1301	9/9	0.96	0.19	45,50,56,57	0
6	SO4	A	1503	5/5	0.96	0.11	77,78,83,84	0
6	SO4	A	1502	5/5	0.97	0.13	55,57,58,58	0
5	HG	A	1304	1/1	0.99	0.07	86,86,86,86	0
5	HG	D	1604	1/1	0.99	0.05	140,140,140,140	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.