



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 11:09 PM UTC

PDB ID : 2DET / pdb_00002det
Title : Cocrystal structure of an RNA sulfuration enzyme MnmA and tRNA-Glu in the pre-reaction state
Authors : Numata, T.; Ikeuchi, Y.; Fukai, S.; Suzuki, T.; Nureki, O.
Deposited on : 2006-02-17
Resolution : 3.40 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

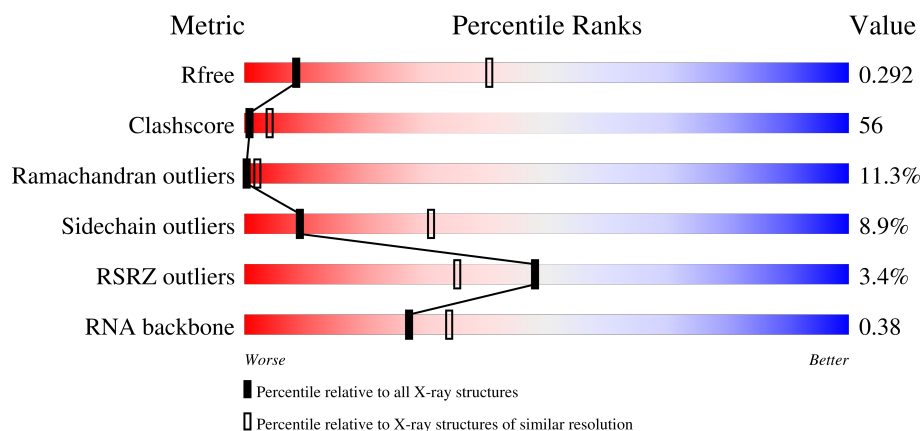
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.40 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1001 (3.44-3.36)
Clashscore	190562	1022 (3.44-3.36)
Ramachandran outliers	187476	1012 (3.44-3.36)
Sidechain outliers	187428	1012 (3.44-3.36)
RSRZ outliers	180081	1001 (3.44-3.36)
RNA backbone	3983	1157 (3.80-3.00)

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

Mol	Chain	Length	Quality of chain
1	C	76	
2	A	380	

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
3	SO4	A	5001	-	-	X	-

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4354 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 RNA chain called tRNA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	70	Total	C	N	O	P	0	0	0
			1488	663	263	492	70			

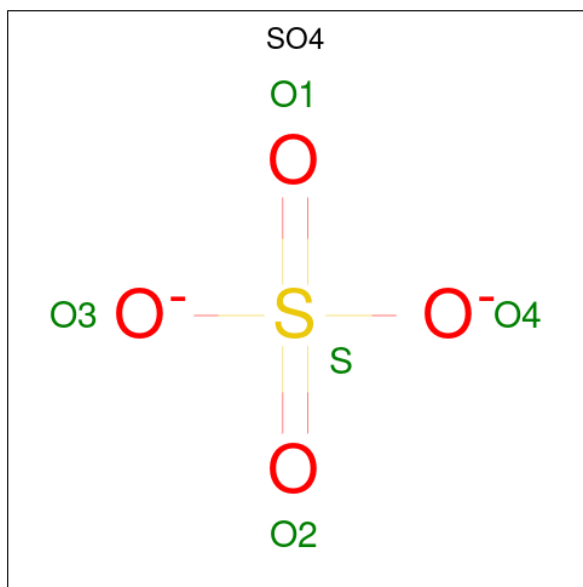
- Molecule 2 is a protein called tRNA-specific 2-thiouridylase mnmA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	365	Total	C	N	O	S	0	0	0
			2861	1814	486	549	12			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-11	MET	-	expression tag	UNP P25745
A	-10	ARG	-	expression tag	UNP P25745
A	-9	GLY	-	expression tag	UNP P25745
A	-8	SER	-	expression tag	UNP P25745
A	-7	HIS	-	expression tag	UNP P25745
A	-6	HIS	-	expression tag	UNP P25745
A	-5	HIS	-	expression tag	UNP P25745
A	-4	HIS	-	expression tag	UNP P25745
A	-3	HIS	-	expression tag	UNP P25745
A	-2	HIS	-	expression tag	UNP P25745
A	-1	GLY	-	expression tag	UNP P25745
A	0	SER	-	expression tag	UNP P25745

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

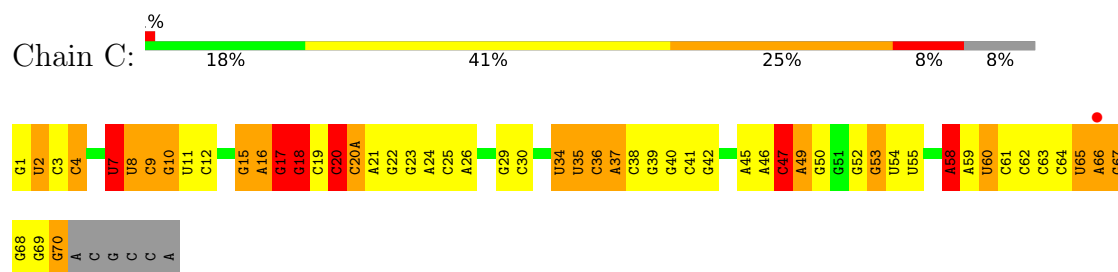


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		

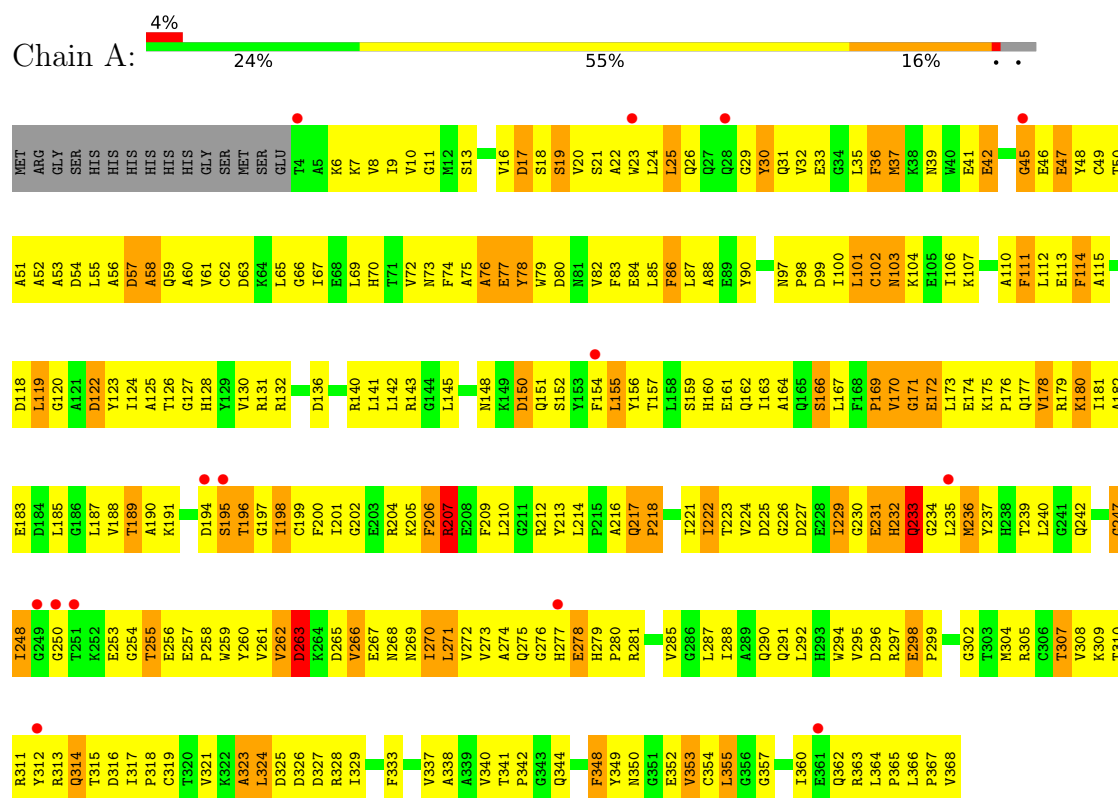
3 Residue-property plots [i](#)

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

• Molecule 1: tRNA



• Molecule 2: tRNA-specific 2-thiouridylase mmA



4 Data and refinement statistics

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	101.54Å 108.02Å 211.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.48 – 3.40 39.48 – 3.40	Depositor EDS
% Data completeness (in resolution range)	96.8 (39.48-3.40) 96.7 (39.48-3.40)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.42 (at 2.81Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.263 , 0.305 0.233 , 0.292	Depositor DCC
R_{free} test set	1097 reflections (3.91%)	wwPDB-VP
Wilson B-factor (Å ²)	63.1	Xtriage
Anisotropy	0.048	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.24 , 75.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	4354	wwPDB-VP
Average B, all atoms (Å ²)	82.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality

5.1 Standard geometry

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

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	C	0.42	0/1660	0.84	7/2583 (0.3%)
2	A	0.53	0/2920	1.07	22/3951 (0.6%)
All	All	0.49	0/4580	0.98	29/6534 (0.4%)

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	C	0	3

There are no bond length outliers.

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	353	VAL	N-CA-C	8.72	120.41	108.89
2	A	170	VAL	N-CA-C	6.46	117.14	110.36
2	A	102	CYS	N-CA-C	-6.34	103.66	111.33
2	A	364	LEU	CA-C-N	6.18	126.19	119.89
2	A	364	LEU	C-N-CA	6.18	126.19	119.89
2	A	217	GLN	CA-C-N	5.97	127.30	119.84
2	A	217	GLN	C-N-CA	5.97	127.30	119.84
2	A	31	GLN	N-CA-C	-5.92	100.62	109.15
2	A	340	VAL	N-CA-C	-5.70	102.18	109.30
1	C	47	C	N1-C1'-C2'	5.61	122.41	114.00
1	C	17	G	N9-C1'-C2'	5.55	120.33	112.00
2	A	127	GLY	N-CA-C	-5.55	108.05	115.32
2	A	195	SER	N-CA-C	5.51	116.15	108.00
1	C	60	U	C2'-C3'-O3'	-5.51	105.44	113.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	298	GLU	CA-C-N	5.41	126.61	119.84
2	A	298	GLU	C-N-CA	5.41	126.61	119.84
2	A	353	VAL	CB-CA-C	-5.40	104.13	111.15
1	C	18	G	N9-C1'-C2'	5.38	122.07	114.00
2	A	11	GLY	N-CA-C	-5.35	104.27	111.54
2	A	338	ALA	N-CA-C	5.33	116.93	108.67
1	C	17	G	C4'-C3'-O3'	-5.30	105.05	113.00
2	A	57	ASP	N-CA-C	-5.25	104.97	111.33
2	A	216	ALA	N-CA-C	5.25	117.29	107.99
1	C	58	A	C4'-C3'-O3'	-5.21	105.19	113.00
2	A	37	MET	N-CA-C	5.13	117.60	109.24
1	C	7	U	C2'-C3'-O3'	5.10	117.15	109.50
2	A	25	LEU	N-CA-C	-5.08	105.63	111.07
2	A	324	LEU	N-CA-C	5.08	116.82	111.28
2	A	172	GLU	N-CA-C	-5.00	107.35	113.50

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	17	G	Sidechain
1	C	20	C	Sidechain
1	C	47	C	Sidechain

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	C	1488	0	758	98	0
2	A	2861	0	2804	348	0
3	A	5	0	0	2	0
All	All	4354	0	3562	442	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 56.

All (442) 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)
2:A:255:THR:HB	2:A:257:GLU:HG2	1.41	1.02
1:C:3:C:H2'	1:C:4:C:H5''	1.45	0.98
1:C:21:A:H61	1:C:46:A:H2'	1.26	0.98
2:A:132:ARG:HE	2:A:164:ALA:HA	1.31	0.94
2:A:198:ILE:HD12	2:A:198:ILE:H	1.31	0.94
2:A:35:LEU:HD23	2:A:36:PHE:N	1.83	0.93
2:A:55:LEU:O	2:A:58:ALA:HB3	1.70	0.91
2:A:363:ARG:O	2:A:365:PRO:HD3	1.72	0.90
2:A:97:ASN:O	2:A:100:ILE:HG22	1.70	0.89
2:A:130:VAL:O	2:A:171:GLY:HA3	1.72	0.89
2:A:222:ILE:HG13	2:A:223:THR:H	1.37	0.88
1:C:69:G:H2'	1:C:70:G:N2	1.89	0.87
2:A:236:MET:HE2	2:A:236:MET:H	1.37	0.87
2:A:6:LYS:HB3	2:A:122:ASP:OD2	1.76	0.84
2:A:267:GLU:HG3	2:A:268:ASN:H	1.41	0.83
2:A:310:THR:HB	2:A:314:GLN:OE1	1.79	0.82
2:A:111:PHE:CD1	2:A:124:ILE:HD11	2.15	0.82
2:A:102:CYS:SG	2:A:107:LYS:HD2	2.20	0.82
2:A:223:THR:HG22	2:A:225:ASP:H	1.43	0.82
2:A:240:LEU:HD12	2:A:341:THR:HG23	1.62	0.81
2:A:202:GLY:HA3	2:A:204:ARG:HH21	1.46	0.80
2:A:103:ASN:N	2:A:103:ASN:HD22	1.80	0.80
1:C:24:A:H2'	1:C:25:C:C6	2.16	0.79
2:A:279:HIS:CD2	2:A:281:ARG:H	2.00	0.79
1:C:50:G:H1	1:C:64:C:H42	1.29	0.79
2:A:221:ILE:HG12	2:A:271:LEU:HD23	1.63	0.79
2:A:130:VAL:HG13	2:A:131:ARG:N	1.99	0.78
2:A:218:PRO:HA	2:A:234:GLY:H	1.50	0.77
2:A:101:LEU:HD12	2:A:104:LYS:HB3	1.67	0.76
2:A:101:LEU:CD1	2:A:104:LYS:HB3	2.16	0.76
2:A:111:PHE:CE1	2:A:124:ILE:HD11	2.21	0.76
2:A:74:PHE:O	2:A:77:GLU:HG2	1.86	0.75
2:A:82:VAL:HG12	2:A:83:PHE:N	1.99	0.75
2:A:107:LYS:NZ	2:A:199:CYS:SG	2.58	0.75
2:A:218:PRO:HB3	2:A:233:GLN:HA	1.70	0.74
2:A:257:GLU:HG3	2:A:275:GLN:HG2	1.68	0.73
1:C:35:U:H6	1:C:35:U:H5'	1.52	0.73
2:A:61:VAL:HG13	2:A:187:LEU:HD22	1.70	0.73
2:A:106:ILE:HG21	2:A:200:PHE:HE1	1.51	0.73
2:A:259:TRP:HE3	2:A:273:VAL:HG12	1.54	0.73
2:A:310:THR:HG22	2:A:310:THR:O	1.89	0.72
2:A:103:ASN:ND2	2:A:107:LYS:HD3	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:115:ALA:HA	2:A:119:LEU:HD12	1.69	0.72
2:A:288:ILE:HG13	2:A:324:LEU:HD22	1.72	0.71
1:C:52:G:C3'	1:C:53:G:H5''	2.19	0.71
2:A:39:ASN:OD1	2:A:74:PHE:HB2	1.91	0.71
2:A:266:VAL:HG13	2:A:267:GLU:H	1.55	0.71
2:A:288:ILE:HA	2:A:329:ILE:O	1.91	0.70
2:A:207:ARG:H	2:A:207:ARG:HD3	1.57	0.70
2:A:42:GLU:CD	2:A:42:GLU:H	2.00	0.70
2:A:236:MET:H	2:A:236:MET:CE	2.05	0.70
1:C:3:C:C2'	1:C:4:C:H5''	2.22	0.69
2:A:83:PHE:O	2:A:86:PHE:HB3	1.91	0.69
2:A:296:ASP:OD2	2:A:298:GLU:HB3	1.91	0.69
2:A:308:VAL:O	2:A:317:ILE:HG12	1.92	0.69
1:C:24:A:H2'	1:C:25:C:H6	1.56	0.68
1:C:35:U:O2'	1:C:36:C:H5'	1.92	0.68
2:A:222:ILE:HG23	2:A:223:THR:N	2.07	0.68
2:A:36:PHE:CD2	2:A:36:PHE:C	2.70	0.68
2:A:210:LEU:HD22	2:A:237:TYR:HE2	1.59	0.68
2:A:141:LEU:C	2:A:142:LEU:HD23	2.19	0.67
2:A:107:LYS:HD2	2:A:199:CYS:SG	2.34	0.67
2:A:270:ILE:HG22	2:A:271:LEU:H	1.58	0.67
1:C:58:A:O2'	1:C:60:U:H5	1.77	0.67
2:A:298:GLU:CG	2:A:299:PRO:HD2	2.24	0.67
1:C:20:C:H1'	1:C:21:A:O4'	1.95	0.67
2:A:255:THR:HB	2:A:257:GLU:CG	2.22	0.67
2:A:36:PHE:C	2:A:36:PHE:HD2	2.03	0.67
2:A:262:VAL:HG21	2:A:281:ARG:HB3	1.75	0.67
1:C:50:G:N2	1:C:65:U:H3	1.93	0.66
2:A:18:SER:O	2:A:21:SER:HB3	1.95	0.66
1:C:11:U:H2'	1:C:12:C:C6	2.31	0.66
2:A:170:VAL:O	2:A:172:GLU:N	2.29	0.65
2:A:240:LEU:HA	2:A:261:VAL:HG12	1.78	0.65
2:A:166:SER:C	2:A:167:LEU:HD12	2.21	0.65
2:A:232:HIS:ND1	2:A:234:GLY:O	2.28	0.65
1:C:49:A:H2'	1:C:50:G:H8	1.62	0.65
2:A:317:ILE:O	2:A:317:ILE:HG13	1.96	0.65
1:C:15:G:H1'	1:C:20:C:H42	1.62	0.65
2:A:106:ILE:HG22	2:A:107:LYS:N	2.09	0.65
2:A:170:VAL:C	2:A:172:GLU:H	2.03	0.64
2:A:298:GLU:HG3	2:A:299:PRO:HD2	1.80	0.64
1:C:49:A:H2'	1:C:50:G:C8	2.31	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:47:GLU:HG3	2:A:204:ARG:HH22	1.61	0.64
1:C:36:C:H2'	1:C:37:A:O5'	1.98	0.64
2:A:114:PHE:CE2	2:A:119:LEU:HD21	2.33	0.64
2:A:174:GLU:CB	2:A:177:GLN:HE21	2.11	0.64
2:A:99:ASP:OD1	2:A:198:ILE:HA	1.98	0.63
2:A:57:ASP:O	2:A:61:VAL:HG23	1.98	0.63
1:C:52:G:H2'	1:C:53:G:H5''	1.79	0.63
2:A:10:VAL:HG21	2:A:22:ALA:HB2	1.80	0.63
2:A:254:GLY:C	2:A:256:GLU:H	2.07	0.63
2:A:267:GLU:HG3	2:A:268:ASN:N	2.13	0.63
2:A:97:ASN:HD22	2:A:97:ASN:C	2.05	0.63
2:A:224:VAL:HG21	2:A:274:ALA:HB2	1.79	0.63
2:A:174:GLU:HB2	2:A:177:GLN:HE21	1.63	0.63
2:A:315:THR:O	2:A:317:ILE:HG23	1.99	0.63
1:C:36:C:H4'	2:A:206:PHE:CE1	2.34	0.62
2:A:262:VAL:HG12	2:A:272:VAL:O	1.99	0.62
1:C:40:G:O2'	1:C:41:C:H5'	1.99	0.62
1:C:52:G:C2'	1:C:53:G:H5''	2.29	0.62
2:A:61:VAL:HG13	2:A:187:LEU:CD2	2.29	0.62
2:A:174:GLU:H	2:A:177:GLN:NE2	1.98	0.62
2:A:348:PHE:N	2:A:348:PHE:CD1	2.67	0.62
2:A:106:ILE:HG21	2:A:200:PHE:CE1	2.34	0.61
1:C:69:G:H2'	1:C:70:G:H21	1.64	0.61
2:A:240:LEU:CD1	2:A:341:THR:HG23	2.30	0.61
2:A:47:GLU:HG3	2:A:204:ARG:NH2	2.16	0.60
2:A:141:LEU:O	2:A:142:LEU:HD23	2.01	0.60
2:A:309:LYS:HE2	2:A:316:ASP:OD2	2.02	0.60
2:A:78:TYR:HA	2:A:106:ILE:HD11	1.84	0.60
2:A:100:ILE:CD1	2:A:154:PHE:HA	2.31	0.60
1:C:20:C:H5'	1:C:20(A):C:OP1	2.01	0.60
2:A:37:MET:HB3	2:A:39:ASN:ND2	2.17	0.60
2:A:10:VAL:HG23	2:A:10:VAL:O	2.02	0.60
2:A:261:VAL:CG1	2:A:262:VAL:N	2.63	0.60
2:A:10:VAL:HG12	2:A:125:ALA:HB3	1.84	0.60
1:C:20:C:H4'	1:C:20(A):C:OP1	2.02	0.59
1:C:11:U:H2'	1:C:12:C:H6	1.65	0.59
2:A:132:ARG:NE	2:A:164:ALA:HA	2.11	0.59
1:C:38:C:H2'	1:C:39:G:C5'	2.32	0.59
1:C:52:G:H3'	1:C:53:G:H5''	1.85	0.59
2:A:17:ASP:O	2:A:18:SER:C	2.46	0.58
2:A:314:GLN:HG2	2:A:315:THR:H	1.68	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:20:C:O2'	1:C:20(A):C:H5''	2.03	0.58
2:A:295:VAL:HG13	2:A:296:ASP:N	2.19	0.58
1:C:53:G:O2'	1:C:54:U:H5'	2.02	0.58
2:A:257:GLU:HB2	2:A:258:PRO:HD2	1.83	0.58
2:A:170:VAL:C	2:A:172:GLU:N	2.61	0.58
1:C:21:A:N6	1:C:46:A:H2'	2.08	0.58
2:A:103:ASN:N	2:A:103:ASN:ND2	2.49	0.58
2:A:262:VAL:HG22	2:A:262:VAL:O	2.03	0.58
1:C:38:C:O2'	1:C:39:G:H5'	2.04	0.58
2:A:132:ARG:HD2	2:A:163:ILE:HG22	1.86	0.58
2:A:206:PHE:O	2:A:209:PHE:N	2.36	0.58
2:A:261:VAL:HG12	2:A:262:VAL:N	2.17	0.58
2:A:324:LEU:HB3	2:A:329:ILE:HA	1.85	0.58
2:A:103:ASN:HA	2:A:107:LYS:HB2	1.85	0.58
2:A:148:ASN:HD21	2:A:313:ARG:NH2	2.01	0.58
2:A:221:ILE:HG13	2:A:231:GLU:O	2.03	0.57
2:A:325:ASP:CG	2:A:326:ASP:H	2.10	0.57
2:A:317:ILE:HD12	2:A:337:VAL:HG21	1.86	0.57
2:A:111:PHE:C	2:A:111:PHE:CD2	2.81	0.57
2:A:207:ARG:HD3	2:A:207:ARG:N	2.19	0.57
2:A:199:CYS:O	2:A:200:PHE:HB2	2.02	0.57
2:A:222:ILE:HG13	2:A:223:THR:N	2.14	0.57
1:C:36:C:C2'	1:C:37:A:O5'	2.53	0.57
2:A:123:TYR:HB3	2:A:167:LEU:HD13	1.85	0.57
1:C:9:C:H5'	1:C:10:G:OP2	2.05	0.57
1:C:37:A:H4'	2:A:242:GLN:HG3	1.87	0.57
2:A:262:VAL:CG1	2:A:272:VAL:HG12	2.34	0.57
1:C:23:G:H2'	1:C:24:A:C8	2.40	0.57
2:A:195:SER:O	2:A:196:THR:CB	2.53	0.57
2:A:229:ILE:HG23	2:A:230:GLY:N	2.20	0.57
1:C:53:G:C2'	1:C:54:U:H5'	2.35	0.56
2:A:29:GLY:O	2:A:30:TYR:C	2.47	0.56
2:A:232:HIS:CE1	2:A:235:LEU:HD13	2.41	0.56
2:A:111:PHE:CG	2:A:124:ILE:HD11	2.40	0.56
2:A:277:HIS:O	2:A:278:GLU:HG2	2.05	0.56
2:A:113:GLU:C	2:A:115:ALA:H	2.14	0.56
2:A:114:PHE:O	2:A:119:LEU:HG	2.06	0.55
2:A:190:ALA:O	2:A:191:LYS:HB3	2.06	0.55
1:C:50:G:H1	1:C:64:C:N4	2.02	0.55
2:A:260:TYR:CZ	2:A:277:HIS:HB2	2.41	0.55
1:C:38:C:C2'	1:C:39:G:H5'	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:62:C:O2'	1:C:63:C:H5'	2.07	0.55
2:A:77:GLU:O	2:A:78:TYR:C	2.50	0.55
2:A:50:THR:O	2:A:51:ALA:C	2.50	0.54
2:A:159:SER:O	2:A:161:GLU:N	2.41	0.54
2:A:240:LEU:HA	2:A:261:VAL:CG1	2.37	0.54
2:A:288:ILE:HB	2:A:362:GLN:HB3	1.89	0.54
2:A:324:LEU:HD23	2:A:328:ARG:HB3	1.89	0.54
2:A:288:ILE:HB	2:A:362:GLN:CB	2.37	0.54
2:A:170:VAL:O	2:A:173:LEU:N	2.35	0.54
2:A:141:LEU:HD12	2:A:142:LEU:N	2.23	0.54
2:A:326:ASP:CG	2:A:327:ASP:H	2.15	0.54
1:C:15:G:H1'	1:C:20:C:N4	2.22	0.54
2:A:198:ILE:HD12	2:A:198:ILE:N	2.13	0.54
2:A:315:THR:O	2:A:316:ASP:C	2.51	0.54
1:C:34:U:H2'	1:C:35:U:H5''	1.89	0.54
2:A:213:TYR:O	2:A:214:LEU:HD23	2.08	0.54
2:A:18:SER:O	2:A:19:SER:C	2.50	0.53
1:C:20:C:C4'	1:C:20(A):C:OP1	2.56	0.53
2:A:29:GLY:O	2:A:30:TYR:O	2.26	0.53
2:A:195:SER:O	2:A:196:THR:HB	2.08	0.53
2:A:279:HIS:HD2	2:A:281:ARG:H	1.55	0.53
2:A:231:GLU:O	2:A:232:HIS:HB2	2.08	0.53
2:A:205:LYS:HE2	2:A:207:ARG:HH21	1.73	0.53
2:A:159:SER:HB3	2:A:297:ARG:HG3	1.91	0.53
2:A:240:LEU:HD12	2:A:341:THR:CG2	2.36	0.53
2:A:248:ILE:HG21	2:A:259:TRP:CD1	2.44	0.53
2:A:33:GLU:HA	2:A:67:ILE:CG2	2.39	0.53
2:A:63:ASP:C	2:A:65:LEU:H	2.15	0.53
2:A:310:THR:O	2:A:310:THR:CG2	2.56	0.53
1:C:67:G:OP1	1:C:67:G:C8	2.62	0.53
2:A:82:VAL:O	2:A:83:PHE:C	2.51	0.53
2:A:178:VAL:O	2:A:179:ARG:C	2.50	0.52
1:C:8:U:H2'	1:C:8:U:O2	2.08	0.52
1:C:67:G:O4'	1:C:67:G:P	2.67	0.52
2:A:17:ASP:HB2	3:A:5001:SO4:O4	2.09	0.52
2:A:87:LEU:O	2:A:88:ALA:C	2.53	0.52
2:A:25:LEU:O	2:A:26:GLN:C	2.52	0.52
2:A:279:HIS:CD2	2:A:281:ARG:N	2.75	0.52
2:A:42:GLU:HG2	2:A:48:TYR:CD1	2.44	0.52
2:A:311:ARG:O	2:A:312:TYR:C	2.52	0.52
2:A:326:ASP:CG	2:A:327:ASP:N	2.68	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:260:TYR:OH	2:A:277:HIS:HB2	2.09	0.52
2:A:270:ILE:O	2:A:271:LEU:HB2	2.10	0.52
2:A:312:TYR:CZ	2:A:313:ARG:HG3	2.45	0.52
2:A:218:PRO:CA	2:A:234:GLY:H	2.22	0.52
2:A:48:TYR:O	2:A:49:CYS:C	2.53	0.52
2:A:314:GLN:HG2	2:A:315:THR:N	2.25	0.52
1:C:29:G:H2'	1:C:30:C:H6	1.75	0.52
2:A:110:ALA:O	2:A:111:PHE:C	2.53	0.52
2:A:232:HIS:HE1	2:A:235:LEU:HD13	1.75	0.52
2:A:288:ILE:HG13	2:A:324:LEU:CD2	2.39	0.52
2:A:97:ASN:O	2:A:98:PRO:C	2.54	0.51
2:A:349:TYR:CE2	2:A:354:CYS:HB2	2.45	0.51
2:A:355:LEU:N	2:A:355:LEU:HD23	2.24	0.51
2:A:202:GLY:CA	2:A:204:ARG:HH21	2.18	0.51
2:A:366:LEU:HG	2:A:367:PRO:HD2	1.92	0.51
2:A:229:ILE:HG23	2:A:230:GLY:H	1.74	0.51
1:C:4:C:H6	1:C:4:C:H5'	1.75	0.51
1:C:20:C:O2	1:C:21:A:H1'	2.11	0.51
2:A:47:GLU:O	2:A:50:THR:N	2.44	0.51
2:A:112:LEU:O	2:A:115:ALA:HB3	2.11	0.51
2:A:79:TRP:CD1	2:A:79:TRP:C	2.89	0.51
2:A:174:GLU:N	2:A:177:GLN:NE2	2.59	0.51
2:A:210:LEU:HD21	2:A:236:MET:SD	2.51	0.51
2:A:353:VAL:HG12	2:A:355:LEU:HD23	1.93	0.51
1:C:53:G:H2'	1:C:54:U:H5'	1.93	0.50
1:C:9:C:O2'	1:C:45:A:C2'	2.59	0.50
1:C:29:G:C4	1:C:42:G:N2	2.79	0.50
2:A:35:LEU:HD23	2:A:35:LEU:C	2.36	0.50
2:A:59:GLN:HG3	2:A:63:ASP:OD1	2.11	0.50
2:A:210:LEU:HD22	2:A:237:TYR:CE2	2.45	0.50
1:C:34:U:O2'	1:C:35:U:OP1	2.26	0.50
2:A:223:THR:HG22	2:A:224:VAL:N	2.25	0.50
2:A:333:PHE:CE1	2:A:337:VAL:HB	2.46	0.50
2:A:50:THR:O	2:A:53:ALA:N	2.44	0.50
2:A:7:LYS:HD3	2:A:120:GLY:O	2.10	0.50
2:A:181:ILE:HG22	2:A:185:LEU:HD12	1.94	0.50
1:C:29:G:H2'	1:C:30:C:C6	2.46	0.50
2:A:16:VAL:O	2:A:17:ASP:C	2.55	0.50
2:A:267:GLU:CG	2:A:268:ASN:H	2.19	0.49
2:A:177:GLN:O	2:A:178:VAL:C	2.55	0.49
2:A:9:ILE:HA	2:A:33:GLU:O	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:224:VAL:CG2	2:A:274:ALA:HB2	2.42	0.49
2:A:189:THR:O	2:A:190:ALA:C	2.55	0.49
2:A:266:VAL:HG13	2:A:267:GLU:N	2.26	0.49
2:A:308:VAL:HG12	2:A:319:CYS:SG	2.52	0.49
2:A:210:LEU:HD23	2:A:210:LEU:O	2.13	0.49
2:A:287:LEU:C	2:A:287:LEU:HD12	2.38	0.49
2:A:290:GLN:O	2:A:291:GLN:C	2.55	0.49
2:A:232:HIS:O	2:A:233:GLN:C	2.56	0.49
1:C:2:U:O5'	1:C:2:U:H6	1.95	0.49
1:C:8:U:H5'	1:C:9:C:OP2	2.12	0.49
2:A:63:ASP:C	2:A:65:LEU:N	2.70	0.48
2:A:100:ILE:CG1	2:A:156:TYR:HE2	2.26	0.48
2:A:279:HIS:HD2	2:A:281:ARG:N	2.11	0.48
2:A:295:VAL:CG1	2:A:296:ASP:N	2.76	0.48
2:A:124:ILE:HG22	2:A:166:SER:HA	1.95	0.48
1:C:58:A:O2'	1:C:60:U:C5	2.59	0.48
2:A:262:VAL:O	2:A:263:ASP:OD1	2.31	0.48
2:A:350:ASN:HB3	2:A:355:LEU:HD21	1.94	0.48
2:A:37:MET:HB3	2:A:39:ASN:HD21	1.76	0.48
2:A:103:ASN:OD1	2:A:155:LEU:CD2	2.62	0.48
2:A:103:ASN:HD22	2:A:107:LYS:HD3	1.78	0.48
2:A:118:ASP:C	2:A:120:GLY:H	2.20	0.48
2:A:126:THR:OG1	2:A:128:HIS:HB2	2.14	0.48
2:A:72:VAL:HG11	2:A:74:PHE:CE2	2.49	0.48
1:C:1:G:H5''	1:C:2:U:OP1	2.14	0.48
1:C:9:C:O2'	1:C:45:A:H1'	2.13	0.48
1:C:53:G:H2'	1:C:54:U:C5'	2.44	0.48
2:A:47:GLU:O	2:A:48:TYR:C	2.57	0.48
2:A:111:PHE:C	2:A:111:PHE:HD2	2.22	0.48
2:A:72:VAL:HG12	2:A:73:ASN:N	2.28	0.48
2:A:114:PHE:O	2:A:114:PHE:CG	2.67	0.48
2:A:255:THR:C	2:A:257:GLU:N	2.72	0.48
1:C:1:G:OP1	1:C:1:G:H3'	2.14	0.47
2:A:19:SER:O	2:A:20:VAL:C	2.56	0.47
2:A:239:THR:O	2:A:242:GLN:HB2	2.14	0.47
2:A:254:GLY:O	2:A:256:GLU:N	2.47	0.47
1:C:35:U:H2'	1:C:36:C:C6	2.49	0.47
2:A:8:VAL:HG12	2:A:123:TYR:HB2	1.95	0.47
2:A:36:PHE:CE1	2:A:55:LEU:HA	2.49	0.47
2:A:132:ARG:HD2	2:A:163:ILE:CG2	2.44	0.47
2:A:254:GLY:C	2:A:256:GLU:N	2.71	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:A:C2'	1:C:38:C:H5'	2.44	0.47
2:A:342:PRO:HA	2:A:360:ILE:HG22	1.95	0.47
1:C:69:G:H2'	1:C:70:G:H22	1.76	0.47
1:C:47:C:C2	1:C:59:A:H1'	2.49	0.47
1:C:68:G:N2	1:C:69:G:H1'	2.29	0.47
2:A:22:ALA:C	2:A:24:LEU:N	2.69	0.47
2:A:83:PHE:O	2:A:84:GLU:C	2.57	0.47
1:C:9:C:HO2'	1:C:45:A:C1'	2.27	0.47
1:C:38:C:H2'	1:C:39:G:O4'	2.15	0.47
2:A:111:PHE:CZ	2:A:124:ILE:HD11	2.50	0.47
2:A:124:ILE:CG2	2:A:166:SER:HB3	2.44	0.47
2:A:227:ASP:OD1	2:A:227:ASP:N	2.48	0.47
2:A:210:LEU:HD23	2:A:210:LEU:C	2.39	0.47
1:C:17:G:N2	1:C:55:U:O2	2.40	0.46
2:A:86:PHE:CE1	2:A:90:TYR:HE1	2.33	0.46
2:A:212:ARG:HB2	2:A:213:TYR:CE1	2.50	0.46
2:A:35:LEU:HD23	2:A:36:PHE:CA	2.45	0.46
1:C:24:A:O2'	2:A:256:GLU:O	2.32	0.46
1:C:38:C:H2'	1:C:39:G:H5'	1.95	0.46
2:A:7:LYS:N	2:A:122:ASP:OD2	2.49	0.46
2:A:255:THR:C	2:A:257:GLU:H	2.24	0.46
1:C:17:G:HO2'	1:C:18:G:P	2.38	0.46
2:A:41:GLU:OE1	2:A:41:GLU:HA	2.16	0.46
1:C:15:G:O2'	1:C:16:A:P	2.74	0.46
2:A:6:LYS:HE2	2:A:122:ASP:OD2	2.16	0.46
1:C:35:U:C2'	1:C:36:C:H5'	2.46	0.46
2:A:156:TYR:HB2	2:A:357:GLY:H	1.81	0.46
2:A:267:GLU:C	2:A:269:ASN:N	2.74	0.46
1:C:9:C:HO2'	1:C:45:A:H1'	1.81	0.46
2:A:307:THR:HG22	2:A:318:PRO:N	2.31	0.46
2:A:16:VAL:O	2:A:19:SER:HB2	2.16	0.45
2:A:198:ILE:H	2:A:198:ILE:CD1	2.09	0.45
2:A:268:ASN:HB3	2:A:270:ILE:HG13	1.98	0.45
2:A:8:VAL:HG23	2:A:32:VAL:HA	1.98	0.45
2:A:99:ASP:C	2:A:101:LEU:H	2.24	0.45
2:A:181:ILE:HG22	2:A:182:ALA:N	2.30	0.45
2:A:240:LEU:CD1	2:A:342:PRO:HD2	2.46	0.45
2:A:10:VAL:O	2:A:10:VAL:CG2	2.65	0.45
2:A:317:ILE:CD1	2:A:337:VAL:HG21	2.46	0.45
2:A:143:ARG:HG3	2:A:352:GLU:O	2.15	0.45
1:C:20:C:C2	1:C:21:A:H1'	2.51	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:42:GLU:CD	2:A:42:GLU:N	2.72	0.45
2:A:206:PHE:O	2:A:207:ARG:C	2.59	0.45
2:A:36:PHE:CD2	2:A:37:MET:N	2.84	0.45
2:A:270:ILE:HG22	2:A:271:LEU:N	2.28	0.45
2:A:197:GLY:O	2:A:198:ILE:C	2.59	0.45
1:C:67:G:OP1	1:C:67:G:H8	2.00	0.45
2:A:20:VAL:O	2:A:21:SER:C	2.59	0.45
2:A:106:ILE:HD12	2:A:106:ILE:N	2.31	0.45
2:A:114:PHE:O	2:A:114:PHE:CD2	2.70	0.45
2:A:188:VAL:HG13	2:A:189:THR:N	2.31	0.45
2:A:235:LEU:C	2:A:237:TYR:H	2.25	0.45
2:A:239:THR:O	2:A:240:LEU:C	2.60	0.45
1:C:17:G:O2'	1:C:18:G:P	2.75	0.44
1:C:20:C:C5'	1:C:20(A):C:OP1	2.64	0.44
1:C:35:U:OP1	2:A:196:THR:HA	2.17	0.44
2:A:69:LEU:HD12	2:A:70:HIS:N	2.33	0.44
2:A:180:LYS:O	2:A:181:ILE:C	2.60	0.44
2:A:33:GLU:HA	2:A:67:ILE:HG23	1.98	0.44
2:A:124:ILE:O	2:A:167:LEU:N	2.46	0.44
2:A:367:PRO:O	2:A:368:VAL:C	2.59	0.44
1:C:3:C:O5'	1:C:3:C:H6	2.01	0.44
1:C:25:C:H2'	1:C:26:A:O4'	2.17	0.44
2:A:18:SER:HB3	3:A:5001:SO4:O1	2.17	0.44
2:A:223:THR:CG2	2:A:224:VAL:N	2.79	0.44
1:C:7:U:O2'	1:C:8:U:P	2.76	0.44
1:C:66:A:N3	1:C:66:A:H2'	2.32	0.44
2:A:97:ASN:HB3	2:A:100:ILE:CG2	2.47	0.44
2:A:118:ASP:C	2:A:120:GLY:N	2.74	0.44
2:A:174:GLU:N	2:A:177:GLN:HE21	2.15	0.44
1:C:69:G:N2	1:C:70:G:H1	2.15	0.44
2:A:45:GLY:O	2:A:46:GLU:C	2.60	0.44
2:A:47:GLU:CG	2:A:204:ARG:HH22	2.29	0.44
2:A:115:ALA:HA	2:A:119:LEU:CD1	2.43	0.44
2:A:74:PHE:O	2:A:75:ALA:C	2.61	0.44
2:A:255:THR:O	2:A:255:THR:HG22	2.17	0.44
2:A:198:ILE:HG21	2:A:201:ILE:HD12	2.00	0.44
2:A:47:GLU:O	2:A:50:THR:HB	2.17	0.43
2:A:119:LEU:HG	2:A:119:LEU:H	1.56	0.43
2:A:221:ILE:O	2:A:229:ILE:HG22	2.18	0.43
1:C:69:G:H2'	1:C:69:G:N3	2.33	0.43
2:A:142:LEU:HD23	2:A:142:LEU:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:155:LEU:N	2:A:155:LEU:HD23	2.32	0.43
2:A:235:LEU:O	2:A:235:LEU:HD12	2.18	0.43
2:A:342:PRO:HA	2:A:360:ILE:CG2	2.48	0.43
2:A:22:ALA:O	2:A:23:TRP:C	2.61	0.43
2:A:52:ALA:O	2:A:55:LEU:HB3	2.19	0.43
2:A:53:ALA:O	2:A:56:ALA:HB3	2.19	0.43
2:A:276:GLY:O	2:A:278:GLU:N	2.48	0.43
2:A:62:CYS:O	2:A:66:GLY:N	2.45	0.43
2:A:113:GLU:O	2:A:115:ALA:N	2.52	0.43
2:A:207:ARG:H	2:A:207:ARG:CD	2.30	0.43
1:C:58:A:HO2'	1:C:60:U:H5	1.54	0.43
2:A:102:CYS:HB3	2:A:103:ASN:HD22	1.82	0.43
2:A:142:LEU:HD21	2:A:353:VAL:HG22	2.00	0.43
2:A:232:HIS:NE2	2:A:271:LEU:HB2	2.33	0.43
1:C:17:G:O2'	1:C:18:G:O5'	2.33	0.43
2:A:85:LEU:O	2:A:87:LEU:N	2.52	0.43
2:A:100:ILE:HD12	2:A:100:ILE:HA	1.82	0.42
2:A:174:GLU:O	2:A:175:LYS:C	2.62	0.42
2:A:217:GLN:CD	2:A:217:GLN:H	2.26	0.42
2:A:292:LEU:HD12	2:A:294:TRP:CE2	2.53	0.42
2:A:53:ALA:O	2:A:54:ASP:C	2.62	0.42
2:A:62:CYS:HB3	2:A:67:ILE:O	2.19	0.42
2:A:85:LEU:C	2:A:87:LEU:N	2.77	0.42
1:C:9:C:O2'	1:C:45:A:Cl'	2.67	0.42
2:A:50:THR:O	2:A:53:ALA:HB3	2.18	0.42
2:A:131:ARG:HE	2:A:131:ARG:HB3	1.47	0.42
2:A:341:THR:O	2:A:344:GLN:HB2	2.19	0.42
1:C:8:U:H5'	1:C:9:C:P	2.59	0.42
2:A:8:VAL:HA	2:A:123:TYR:O	2.19	0.42
2:A:176:PRO:O	2:A:177:GLN:C	2.62	0.42
2:A:240:LEU:HD12	2:A:341:THR:HA	2.00	0.42
2:A:170:VAL:HG23	2:A:171:GLY:N	2.34	0.42
2:A:6:LYS:HB3	2:A:6:LYS:HE2	1.85	0.42
2:A:304:MET:HE3	2:A:321:VAL:HG21	2.02	0.42
1:C:47:C:HO2'	1:C:49:A:P	2.43	0.42
2:A:8:VAL:HG12	2:A:123:TYR:CB	2.49	0.42
2:A:212:ARG:HH11	2:A:212:ARG:HG2	1.85	0.42
2:A:74:PHE:C	2:A:76:ALA:N	2.77	0.42
2:A:100:ILE:HD12	2:A:154:PHE:HA	2.02	0.42
2:A:10:VAL:HA	2:A:125:ALA:O	2.20	0.42
2:A:6:LYS:HE2	2:A:122:ASP:CG	2.45	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:107:LYS:O	2:A:111:PHE:HB3	2.20	0.41
2:A:317:ILE:O	2:A:318:PRO:C	2.63	0.41
2:A:132:ARG:HE	2:A:164:ALA:CA	2.15	0.41
2:A:142:LEU:CD2	2:A:353:VAL:HG22	2.50	0.41
2:A:180:LYS:O	2:A:183:GLU:HB2	2.21	0.41
2:A:130:VAL:HG22	2:A:142:LEU:O	2.21	0.41
2:A:217:GLN:HA	2:A:218:PRO:HD2	1.83	0.41
2:A:97:ASN:C	2:A:97:ASN:ND2	2.73	0.41
2:A:150:ASP:CG	2:A:151:GLN:N	2.79	0.41
2:A:247:GLY:O	2:A:248:ILE:C	2.63	0.41
1:C:30:C:H42	1:C:40:G:H1	1.67	0.41
2:A:151:GLN:O	2:A:152:SER:C	2.64	0.41
2:A:221:ILE:HA	2:A:271:LEU:HB3	2.02	0.41
1:C:9:C:H4'	1:C:46:A:O4'	2.21	0.41
1:C:22:G:O6	1:C:46:A:N1	2.54	0.41
1:C:60:U:H5''	1:C:61:C:OP2	2.21	0.41
2:A:141:LEU:HD12	2:A:142:LEU:H	1.86	0.41
2:A:265:ASP:OD2	2:A:270:ILE:HD12	2.19	0.41
1:C:58:A:N6	1:C:61:C:C2	2.89	0.41
2:A:21:SER:O	2:A:169:PRO:HG2	2.21	0.41
2:A:98:PRO:HB2	2:A:198:ILE:HG23	2.03	0.41
2:A:259:TRP:CE3	2:A:273:VAL:HG12	2.44	0.40
1:C:10:G:N2	1:C:26:A:H1'	2.36	0.40
2:A:236:MET:CE	2:A:236:MET:N	2.79	0.40
2:A:99:ASP:C	2:A:101:LEU:N	2.79	0.40
2:A:150:ASP:OD1	2:A:150:ASP:C	2.64	0.40
2:A:59:GLN:O	2:A:62:CYS:N	2.55	0.40
1:C:49:A:H61	1:C:66:A:N6	2.19	0.40
2:A:159:SER:O	2:A:162:GLN:N	2.47	0.40
2:A:279:HIS:HA	2:A:280:PRO:HD3	1.96	0.40
2:A:302:GLY:O	2:A:323:ALA:N	2.47	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
2	A	363/380 (96%)	232 (64%)	90 (25%)	41 (11%)	0 2

All (41) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	19	SER
2	A	30	TYR
2	A	160	HIS
2	A	178	VAL
2	A	194	ASP
2	A	196	THR
2	A	231	GLU
2	A	232	HIS
2	A	262	VAL
2	A	278	GLU
2	A	114	PHE
2	A	145	LEU
2	A	171	GLY
2	A	207	ARG
2	A	229	ILE
2	A	233	GLN
2	A	255	THR
2	A	263	ASP
2	A	266	VAL
2	A	271	LEU
2	A	314	GLN
2	A	42	GLU
2	A	60	ALA
2	A	78	TYR
2	A	86	PHE
2	A	198	ILE
2	A	206	PHE
2	A	17	ASP
2	A	58	ALA
2	A	76	ALA
2	A	248	ILE
2	A	45	GLY
2	A	111	PHE
2	A	226	GLY
2	A	323	ALA

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Mol	Chain	Res	Type
2	A	169	PRO
2	A	222	ILE
2	A	270	ILE
2	A	218	PRO
2	A	247	GLY
2	A	250	GLY

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	
2	A	302/315 (96%)	275 (91%)	27 (9%)	9	31

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	13	SER
2	A	36	PHE
2	A	47	GLU
2	A	77	GLU
2	A	80	ASP
2	A	101	LEU
2	A	103	ASN
2	A	119	LEU
2	A	122	ASP
2	A	136	ASP
2	A	140	ARG
2	A	150	ASP
2	A	155	LEU
2	A	157	THR
2	A	166	SER
2	A	180	LYS
2	A	189	THR
2	A	207	ARG
2	A	233	GLN
2	A	236	MET

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Mol	Chain	Res	Type
2	A	253	GLU
2	A	263	ASP
2	A	285	VAL
2	A	305	ARG
2	A	307	THR
2	A	348	PHE
2	A	355	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	31	GLN
2	A	97	ASN
2	A	103	ASN
2	A	128	HIS
2	A	148	ASN
2	A	160	HIS
2	A	177	GLN
2	A	233	GLN
2	A	242	GLN
2	A	279	HIS

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	69/76 (90%)	22 (31%)	9 (13%)

All (22) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	2	U
1	C	4	C
1	C	8	U
1	C	9	C
1	C	10	G
1	C	16	A
1	C	17	G
1	C	18	G
1	C	19	C
1	C	20	C

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Mol	Chain	Res	Type
1	C	20(A)	C
1	C	34	U
1	C	35	U
1	C	37	A
1	C	47	C
1	C	49	A
1	C	53	G
1	C	58	A
1	C	65	U
1	C	66	A
1	C	67	G
1	C	70	G

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C	7	U
1	C	9	C
1	C	15	G
1	C	17	G
1	C	18	G
1	C	20	C
1	C	34	U
1	C	36	C
1	C	47	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	SO4	A	5001	-	4,4,4	1.05	0	6,6,6	0.28	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.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	5001	SO4	2	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	C	70/76 (92%)	-0.24	1 (1%) 73 59	44, 77, 183, 200	0
2	A	365/380 (96%)	-0.01	14 (3%) 44 31	28, 74, 130, 154	0
All	All	435/456 (95%)	-0.05	15 (3%) 48 35	28, 74, 135, 200	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	250	GLY	5.1
2	A	312	TYR	4.1
2	A	361	GLU	3.5
2	A	4	THR	3.3
2	A	251	THR	3.1
2	A	45	GLY	2.8
2	A	194	ASP	2.7
2	A	154	PHE	2.6
2	A	249	GLY	2.5
1	C	66	A	2.5
2	A	195	SER	2.4
2	A	23	TRP	2.2
2	A	235	LEU	2.2
2	A	277	HIS	2.1
2	A	28	GLN	2.1

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	SO4	A	5001	5/5	0.98	0.04	42,50,55,58	0

6.5 Other polymers

There are no such residues in this entry.