Full wwPDB X-ray Structure Validation Report ⓘ

Jun 19, 2020 – 08:23 pm BST

PDB ID	:	2AZX
Title	:	Charged and uncharged tRNAs adopt distinct conformations when complexed with human tryptophanyl-tRNA synthetase
Authors	:	Yang, X.L.; Otero, F.J.; Ewalt, K.L.; Liu, J.; Swairjo, M.A.; Kohrer, C.; RajBhandary, U.L.; Skene, R.J.; McRee, D.E.; Schimmel, P.
Deposited on	:	2005-09-12
Resolution	:	2.80 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

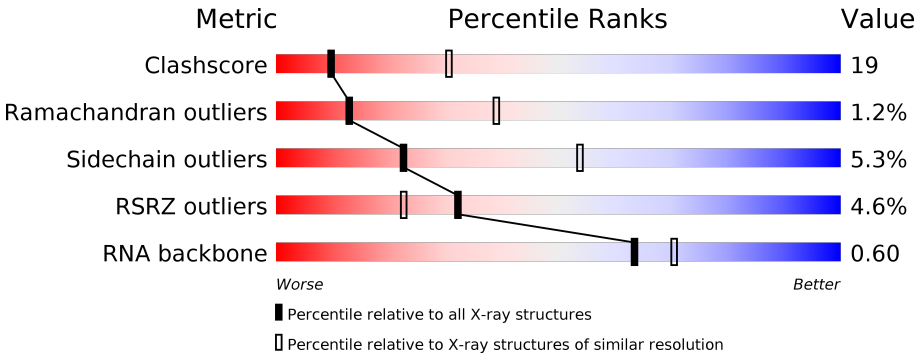
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA,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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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))
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)
RNA backbone	3102	1227 (3.10-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	75	32% 37% 43% 16%
1	D	75	23% 36% 39% 20%
2	A	477	51% 27% 19%
2	B	477	51% 27% 19%

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 9445 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 72-MER.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	72	Total	C	N	O	P	0	0	0
			1541	686	276	507	72			
1	D	72	Total	C	N	O	P	0	0	0
			1541	686	276	507	72			

- Molecule 2 is a protein called Tryptophanyl-tRNA synthetase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	A	387	Total	C	N	O	S	Se	0	0	0
			3114	1994	527	578	5	10			
2	B	388	Total	C	N	O	S	Se	0	0	0
			3119	1997	528	579	5	10			

There are 42 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P23381
A	42	MSE	MET	MODIFIED RESIDUE	UNP P23381
A	48	MSE	MET	MODIFIED RESIDUE	UNP P23381
A	143	MSE	MET	MODIFIED RESIDUE	UNP P23381
A	169	MSE	MET	MODIFIED RESIDUE	UNP P23381
A	195	MSE	MET	MODIFIED RESIDUE	UNP P23381
A	213	GLY	SER	VARIANT	UNP P23381
A	214	ASP	TYR	VARIANT	UNP P23381
A	241	MSE	MET	MODIFIED RESIDUE	UNP P23381
A	243	MSE	MET	MODIFIED RESIDUE	UNP P23381
A	319	MSE	MET	MODIFIED RESIDUE	UNP P23381
A	350	MSE	MET	MODIFIED RESIDUE	UNP P23381
A	401	MSE	MET	MODIFIED RESIDUE	UNP P23381
A	425	MSE	MET	MODIFIED RESIDUE	UNP P23381
A	461	MSE	MET	MODIFIED RESIDUE	UNP P23381
A	472	HIS	-	EXPRESSION TAG	UNP P23381
A	473	HIS	-	EXPRESSION TAG	UNP P23381

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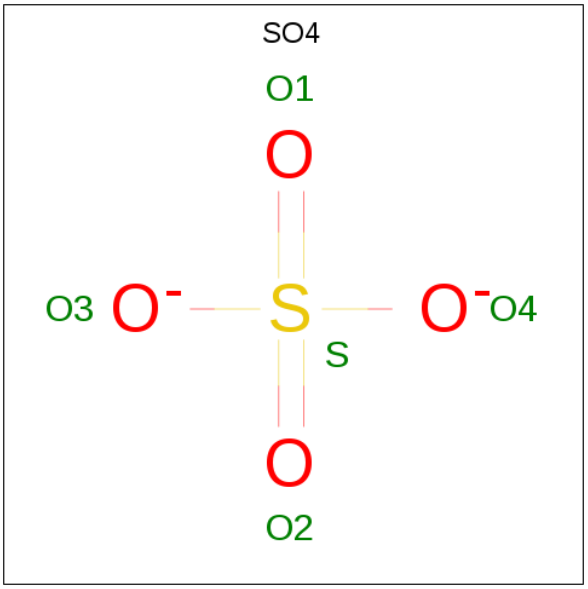
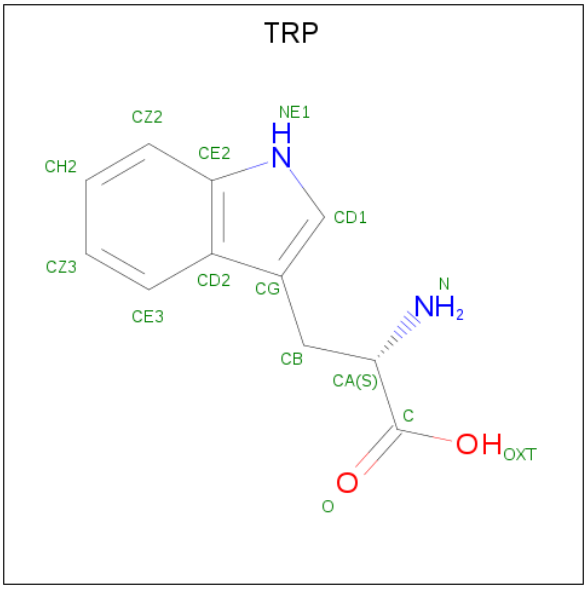
Chain	Residue	Modelled	Actual	Comment	Reference
A	474	HIS	-	EXPRESSION TAG	UNP P23381
A	475	HIS	-	EXPRESSION TAG	UNP P23381
A	476	HIS	-	EXPRESSION TAG	UNP P23381
A	477	HIS	-	EXPRESSION TAG	UNP P23381
B	1	MSE	MET	MODIFIED RESIDUE	UNP P23381
B	42	MSE	MET	MODIFIED RESIDUE	UNP P23381
B	48	MSE	MET	MODIFIED RESIDUE	UNP P23381
B	143	MSE	MET	MODIFIED RESIDUE	UNP P23381
B	169	MSE	MET	MODIFIED RESIDUE	UNP P23381
B	195	MSE	MET	MODIFIED RESIDUE	UNP P23381
B	213	GLY	SER	VARIANT	UNP P23381
B	214	ASP	TYR	VARIANT	UNP P23381
B	241	MSE	MET	MODIFIED RESIDUE	UNP P23381
B	243	MSE	MET	MODIFIED RESIDUE	UNP P23381
B	319	MSE	MET	MODIFIED RESIDUE	UNP P23381
B	350	MSE	MET	MODIFIED RESIDUE	UNP P23381
B	401	MSE	MET	MODIFIED RESIDUE	UNP P23381
B	425	MSE	MET	MODIFIED RESIDUE	UNP P23381
B	461	MSE	MET	MODIFIED RESIDUE	UNP P23381
B	472	HIS	-	EXPRESSION TAG	UNP P23381
B	473	HIS	-	EXPRESSION TAG	UNP P23381
B	474	HIS	-	EXPRESSION TAG	UNP P23381
B	475	HIS	-	EXPRESSION TAG	UNP P23381
B	476	HIS	-	EXPRESSION TAG	UNP P23381
B	477	HIS	-	EXPRESSION TAG	UNP P23381

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

- Molecule 4 is TRYPTOPHAN (three-letter code: TRP) (formula: $C_{11}H_{12}N_2O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 15 11 2 2	0	0
4	A	1	Total C N O 15 11 2 2	0	0

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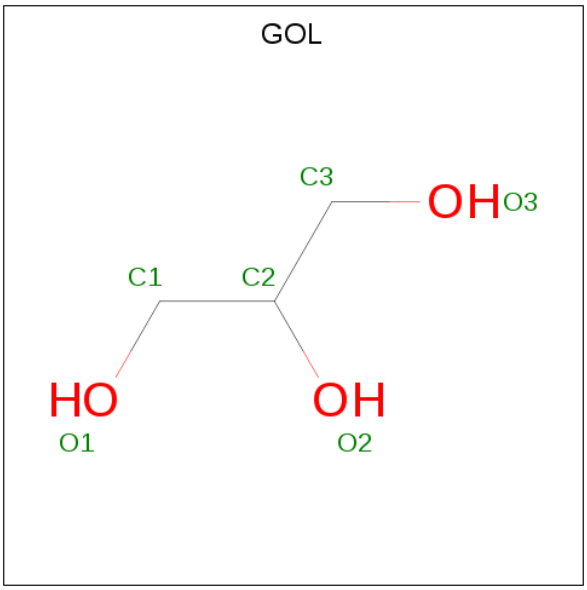
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C N O 15 11 2 2	0	0

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

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

- Molecule 6 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	B	1	Total C O 6 3 3	0	0
6	B	1	Total C O 6 3 3	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	C	2	Total O 2 2	0	0
7	D	2	Total O 2 2	0	0
7	A	9	Total O 9 9	0	0

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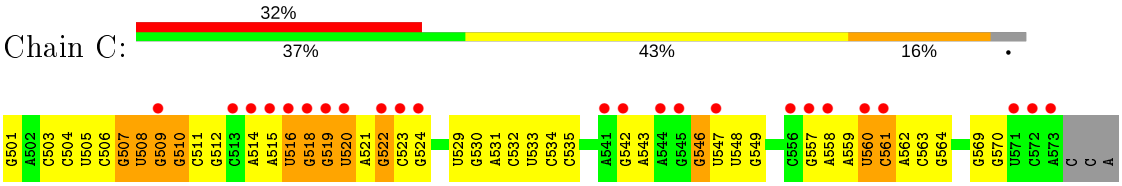
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	B	9	Total O 9 9	0	0

3 Residue-property plots

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

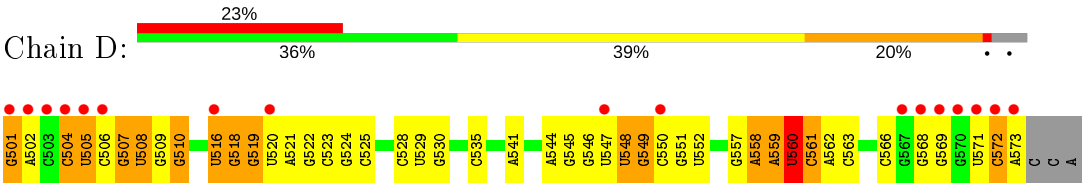
- Molecule 1: 72-MER

Chain C:



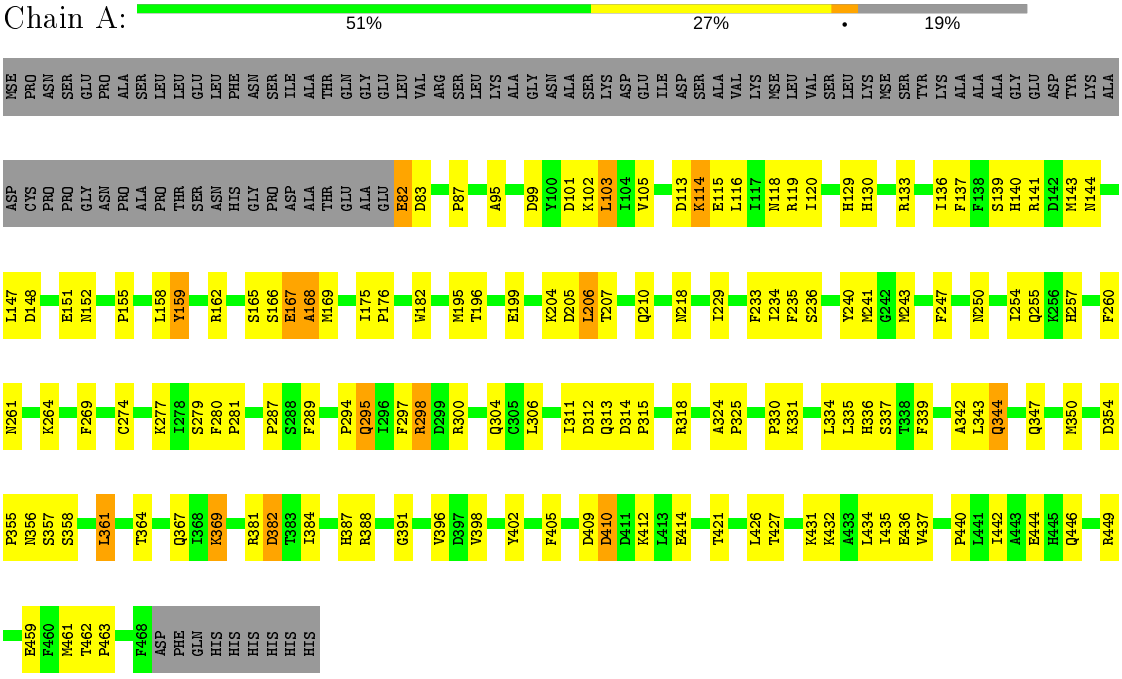
- Molecule 1: 72-MER

Chain D:



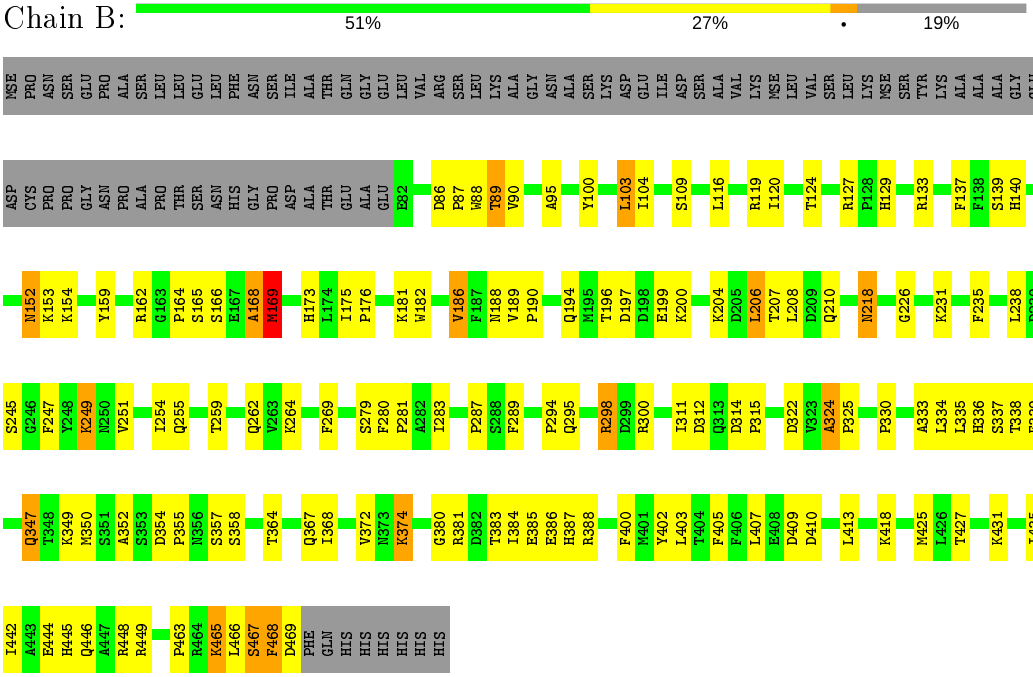
- Molecule 2: Tryptophanyl-tRNA synthetase

Chain A:



- Molecule 2: Tryptophanyl-tRNA synthetase

Chain B:


51%
27%
19%
MSE PRO ASN SER GLU PRO ALA SER LEU LEU GLU GLU LEU PHE ASN SER ILE ALA THR GLN GLY GLU LEU VAL ARG SER LEU LYS ALA GLY ASN ALA SER LYS ASP GLU ILE ASP SER ALA VAL LYS MSE LEU VAL SER LEU LYS MSE SER TYR LYS ALA ALA ALA GLY GLU ASP TYR LYS ALA
ASP CYS PRO PRO GLY ASN PRO ALA PRO THR SER ASN HIS GLY PRO ASP ALA THR GLU ALA GLU B82 D86 P87 W88 T89 V90 A95 Y100 L103 I104 S109 L116 R119 I120 T124 R127 P128 H129 R133 F137 F138 S139 H140 M143 N144 L147
N152 K153 K154 Y159 R162 G163 P164 S165 S166 E167 A168 K169 H173 L174 I175 P176 K181 W182 V186 F187 N188 V189 P190 Q194 M195 T196 D197 D198 E199 K200 K204 D205 L206 T207 L208 D209 Q210 N218 G226 K231 F235 L238 D239 Y240 M241 S244
S245 G246 F247 Y248 K249 N250 V251 I254 Q255 T259 Q262 Y263 K264 F269 S279 F280 P281 A282 I283 P287 S288 F289 P294 Q295 R298 D299 R300 I311 D312 Q313 D314 P315 D322 V323 A324 P325 P330 A333 L334 L335 H336 S337 T338 F339 F340 P341 Q344
Q347 T348 K349 M350 S351 A352 S353 D354 P355 N356 S357 S358 T364 Q367 I368 V372 N373 K374 G380 R381 D382 T383 I384 E385 E386 H387 R388 F400 N401 Y402 L403 T404 F405 F406 L407 E408 D409 D410 L413 K418 M425 L426 T427 K431 I435 Q439 P440 L441
T442 A443 E444 H445 Q446 A447 R448 R449 P463 R464 K465 L466 S467 F468 D469 PHE GLN HIS HIS HIS HIS HIS HIS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	114.06Å 132.62Å 246.63Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.80 45.27 – 2.79	Depositor EDS
% Data completeness (in resolution range)	89.0 (50.00-2.80) 91.9 (45.27-2.79)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.11 (at 2.77Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.205 , 0.252 0.205 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	67.1	Xtriage
Anisotropy	0.295	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 49.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	9445	wwPDB-VP
Average B, all atoms (Å^2)	78.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.26% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: GOL, MG, 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	0.36	1/1722 (0.1%)	0.70	0/2682
1	D	0.40	1/1722 (0.1%)	0.71	1/2682 (0.0%)
2	A	0.41	0/3179	0.65	0/4276
2	B	0.44	0/3184	0.67	0/4283
All	All	0.41	2/9807 (0.0%)	0.68	1/13923 (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	C	0	1
1	D	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	501	G	OP3-P	-7.40	1.52	1.61
1	D	501	G	OP3-P	-7.17	1.52	1.61

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	560	U	N1-C1'-C2'	5.06	120.58	114.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	560	U	Sidechain
1	D	560	U	Sidechain

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	C	1541	0	777	48	0
1	D	1541	0	777	43	0
2	A	3114	0	3061	138	0
2	B	3119	0	3063	116	0
3	A	20	0	0	1	0
3	B	30	0	0	2	0
4	A	30	0	18	1	0
4	B	15	0	9	0	0
5	B	1	0	0	0	0
6	B	12	0	16	2	0
7	A	9	0	0	1	0
7	B	9	0	0	0	0
7	C	2	0	0	0	0
7	D	2	0	0	0	0
All	All	9445	0	7721	328	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 19.

All (328) 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:B:465:LYS:HD3	2:B:465:LYS:H	1.02	1.16
2:A:364:THR:H	2:A:367:GLN:NE2	1.53	1.07
1:D:518:G:H2'	1:D:557:G:N2	1.75	1.01
1:D:558:A:H4'	1:D:559:A:OP1	1.57	0.99
2:A:143:MSE:HE1	2:A:306:LEU:HD11	1.42	0.99
2:A:331:LYS:H	2:B:152:ASN:HD21	0.96	0.94
1:C:558:A:H1'	1:C:560:U:H5	1.35	0.92
2:B:465:LYS:HD3	2:B:465:LYS:N	1.87	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:165:SER:H	2:A:218:ASN:ND2	1.77	0.82
2:A:364:THR:H	2:A:367:GLN:HE21	1.28	0.81
2:A:165:SER:H	2:A:218:ASN:HD21	1.28	0.80
2:A:331:LYS:N	2:B:152:ASN:HD21	1.78	0.79
2:B:181:LYS:HE2	2:B:226:GLY:O	1.81	0.79
2:A:295:GLN:HG3	2:A:463:PRO:HB2	1.65	0.79
1:C:558:A:H1'	1:C:560:U:C5	2.19	0.78
1:D:504:C:C3'	1:D:505:U:H5"	2.13	0.78
2:A:255:GLN:HE21	2:A:279:SER:HB2	1.48	0.78
2:A:95:ALA:HA	2:A:347:GLN:HE21	1.48	0.77
2:B:188:ASN:OD1	2:B:231:LYS:HE2	1.86	0.76
1:D:504:C:H3'	1:D:505:U:H5"	1.67	0.75
2:A:331:LYS:H	2:B:152:ASN:ND2	1.81	0.75
2:B:255:GLN:HE21	2:B:279:SER:HB2	1.50	0.75
2:B:442:ILE:O	2:B:446:GLN:HG3	1.87	0.73
2:B:465:LYS:H	2:B:465:LYS:CD	1.80	0.72
2:B:169:MSE:HG3	2:B:218:ASN:HD21	1.55	0.71
1:C:535:C:C2	2:A:427:THR:HG21	2.26	0.71
2:A:207:THR:OG1	2:A:210:GLN:HG3	1.91	0.71
2:A:434:LEU:O	2:A:437:VAL:HG22	1.90	0.70
2:B:124:THR:HG21	2:B:186:VAL:HG13	1.74	0.70
1:C:509:G:H4'	1:C:510:G:OP2	1.90	0.70
1:C:519:G:O2'	1:C:520:U:OP2	2.09	0.70
2:B:383:THR:OG1	2:B:386:GLU:HG3	1.91	0.70
2:B:435:ILE:O	2:B:439:GLN:HG3	1.92	0.70
2:B:140:HIS:HD2	2:B:143:MSE:H	1.38	0.69
2:B:175:ILE:HB	2:B:176:PRO:HD3	1.73	0.69
1:C:534:C:H5'	2:A:384:ILE:HD11	1.75	0.69
1:C:505:U:H2'	1:C:506:C:C6	2.29	0.68
2:A:147:LEU:O	2:A:151:GLU:HG3	1.93	0.68
2:A:442:ILE:O	2:A:446:GLN:HG3	1.94	0.67
2:B:241:MSE:HE1	2:B:283:ILE:HD12	1.76	0.67
2:A:364:THR:HG23	2:A:367:GLN:NE2	2.09	0.67
1:D:528:C:H2'	1:D:529:U:H6	1.60	0.67
2:B:350:MSE:CG	2:B:358:SER:HB3	2.25	0.67
2:A:137:PHE:CZ	2:A:337:SER:HB3	2.29	0.66
2:A:99:ASP:OD2	2:A:102:LYS:HE3	1.95	0.66
1:D:560:U:H5"	1:D:561:C:H5	1.60	0.66
2:A:165:SER:HB2	2:A:168:ALA:HB3	1.78	0.65
2:B:124:THR:HG21	2:B:186:VAL:CG1	2.25	0.65
1:C:516:U:H4'	1:C:560:U:O2	1.95	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:143:MSE:HE3	2:A:335:LEU:HG	1.77	0.65
2:A:99:ASP:OD1	2:A:102:LYS:HD3	1.96	0.65
1:C:534:C:OP1	2:A:384:ILE:HG13	1.97	0.64
2:A:364:THR:N	2:A:367:GLN:NE2	2.37	0.64
2:A:431:LYS:O	2:A:435:ILE:HG13	1.96	0.64
2:B:449:ARG:HH11	2:B:449:ARG:HG2	1.62	0.64
2:A:143:MSE:HE3	2:A:335:LEU:CD2	2.27	0.64
1:C:558:A:HO2'	1:C:560:U:H5	1.45	0.64
1:D:548:U:O2'	1:D:549:G:P	2.56	0.63
1:D:528:C:H2'	1:D:529:U:C6	2.32	0.63
2:A:264:LYS:HG3	2:A:269:PHE:O	1.98	0.63
2:B:208:LEU:H	6:B:801:GOL:H12	1.64	0.62
2:B:341:PRO:HG2	2:B:402:TYR:HE1	1.64	0.62
2:B:166:SER:HA	2:B:218:ASN:ND2	2.14	0.62
2:A:143:MSE:HE1	2:A:306:LEU:CD1	2.24	0.62
2:B:255:GLN:NE2	2:B:279:SER:HB2	2.14	0.62
2:B:241:MSE:SE	2:B:247:PHE:HD2	2.33	0.62
1:D:518:G:H2'	1:D:557:G:H22	1.63	0.61
2:A:116:LEU:O	2:A:120:ILE:HG13	2.01	0.61
2:A:294:PRO:HA	2:A:298:ARG:O	2.00	0.60
2:A:119:ARG:HG3	2:A:147:LEU:HD13	1.82	0.60
1:C:518:G:H2'	1:C:557:G:N2	2.17	0.60
1:D:518:G:C2'	1:D:557:G:N2	2.61	0.60
2:A:364:THR:N	2:A:367:GLN:HE21	1.96	0.60
2:A:144:ASN:HB2	3:A:704:SO4:O1	2.02	0.60
2:A:143:MSE:HE3	2:A:335:LEU:HD21	1.84	0.60
2:A:143:MSE:HE3	2:A:335:LEU:CG	2.32	0.59
2:A:381:ARG:H	2:A:387:HIS:HD2	1.49	0.59
1:D:504:C:C2'	1:D:505:U:H5"	2.33	0.59
2:A:136:ILE:HD12	2:A:405:PHE:CE1	2.37	0.59
2:A:143:MSE:CE	2:A:335:LEU:HG	2.33	0.59
2:A:140:HIS:HD2	2:A:143:MSE:H	1.51	0.59
1:C:529:U:H2'	1:C:530:G:C8	2.38	0.59
2:B:137:PHE:CZ	2:B:337:SER:HB3	2.38	0.59
2:B:207:THR:OG1	2:B:210:GLN:HG3	2.02	0.59
1:C:558:A:H2'	1:C:560:U:OP2	2.03	0.58
2:B:139:SER:HB3	2:B:336:HIS:HB2	1.85	0.58
1:D:504:C:H2'	1:D:505:U:H5"	1.85	0.58
2:A:312:ASP:HB3	2:A:339:PHE:CE1	2.37	0.58
1:D:501:G:OP2	1:D:501:G:H3'	2.03	0.58
2:A:254:ILE:HD11	2:A:289:PHE:HE2	1.69	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:333:ALA:C	2:B:334:LEU:HD12	2.24	0.58
1:D:520:U:H5'	1:D:521:A:H5'	1.85	0.57
2:A:364:THR:H	2:A:367:GLN:HE22	1.49	0.57
2:A:384:ILE:O	2:A:388:ARG:HG2	2.05	0.57
2:B:119:ARG:HG3	2:B:147:LEU:HD13	1.85	0.57
2:B:133:ARG:NH1	2:B:410:ASP:OD1	2.38	0.56
2:A:414:GLU:HA	2:A:414:GLU:OE2	2.04	0.56
2:A:103:LEU:HD13	2:A:311:ILE:HG12	1.87	0.56
2:A:119:ARG:HG2	2:A:119:ARG:HH11	1.68	0.56
2:A:158:LEU:HD23	2:A:306:LEU:HB3	1.87	0.56
2:A:304:GLN:HE21	2:B:154:LYS:NZ	2.03	0.56
2:B:153:LYS:HD2	2:B:153:LYS:N	2.21	0.56
2:B:162:ARG:NH2	2:B:169:MSE:HG2	2.21	0.56
2:A:119:ARG:NH2	2:A:148:ASP:OD2	2.39	0.55
2:B:241:MSE:CE	2:B:283:ILE:HD12	2.37	0.55
1:C:503:C:H2'	1:C:504:C:H6	1.71	0.55
2:B:140:HIS:CD2	2:B:143:MSE:HB2	2.42	0.55
2:B:344:GLN:HE22	2:B:357:SER:HA	1.72	0.55
2:A:342:ALA:HB1	2:A:357:SER:HB2	1.88	0.55
2:B:381:ARG:N	2:B:381:ARG:HD3	2.22	0.55
2:A:204:LYS:HB2	2:A:206:LEU:HD21	1.89	0.55
2:A:169:MSE:HG3	2:A:361:LEU:HD22	1.89	0.54
2:B:445:HIS:HA	2:B:448:ARG:HH21	1.72	0.54
1:C:511:C:H2'	1:C:512:G:C8	2.42	0.54
2:B:124:THR:CG2	2:B:186:VAL:HG13	2.37	0.54
1:D:551:G:H2'	1:D:552:U:C6	2.43	0.54
2:A:175:ILE:HB	2:A:176:PRO:HD3	1.89	0.54
2:A:412:LYS:HB3	2:A:412:LYS:NZ	2.22	0.53
2:B:407:LEU:HD23	2:B:413:LEU:HB2	1.88	0.53
1:C:557:G:C2'	1:C:558:A:H5'	2.38	0.53
1:C:512:G:H1	1:C:523:C:H42	1.57	0.53
2:B:199:GLU:HB2	2:B:280:PHE:CZ	2.44	0.53
2:A:312:ASP:HB3	2:A:339:PHE:HE1	1.75	0.52
2:B:294:PRO:HA	2:B:298:ARG:O	2.08	0.52
2:B:384:ILE:O	2:B:388:ARG:HG2	2.09	0.52
1:D:544:A:H2'	1:D:545:G:O4'	2.09	0.52
2:A:297:PHE:C	2:A:298:ARG:HD2	2.29	0.52
2:A:350:MSE:CG	2:A:358:SER:HB3	2.39	0.52
2:B:162:ARG:O	2:B:164:PRO:HD3	2.08	0.52
2:B:364:THR:O	2:B:368:ILE:HG13	2.09	0.52
2:A:82:GLU:HG2	2:A:82:GLU:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:387:HIS:HE1	2:B:425:MSE:O	1.92	0.52
1:C:518:G:H2'	1:C:557:G:H22	1.75	0.52
2:B:140:HIS:CD2	2:B:143:MSE:H	2.23	0.52
2:B:208:LEU:HB2	6:B:801:GOL:H12	1.92	0.51
2:A:140:HIS:CD2	2:A:143:MSE:H	2.28	0.51
1:D:518:G:H2'	1:D:557:G:C2	2.43	0.51
1:D:548:U:O2'	1:D:549:G:OP2	2.27	0.51
2:B:127:ARG:HG3	2:B:127:ARG:HH11	1.74	0.51
2:B:95:ALA:HA	2:B:347:GLN:HE22	1.75	0.51
1:C:523:C:H2'	1:C:524:G:C8	2.46	0.51
2:B:368:ILE:CD1	2:B:442:ILE:HD12	2.41	0.51
1:C:519:G:O2'	1:C:520:U:P	2.69	0.51
1:D:506:C:H1'	1:D:568:G:H22	1.75	0.51
2:A:369:LYS:HA	2:A:435:ILE:HD13	1.92	0.51
1:C:559:A:H2'	1:C:560:U:O4'	2.11	0.51
1:D:506:C:O2'	1:D:507:G:H5'	2.11	0.51
2:B:400:PHE:O	2:B:403:LEU:HB2	2.11	0.51
2:B:468:PHE:O	2:B:469:ASP:CB	2.59	0.51
2:B:350:MSE:HG2	2:B:358:SER:HB3	1.93	0.51
2:A:139:SER:HB3	2:A:336:HIS:HB2	1.93	0.50
2:A:162:ARG:HH11	2:A:162:ARG:HG3	1.76	0.50
2:B:449:ARG:HG2	2:B:449:ARG:NH1	2.25	0.50
2:B:175:ILE:HD12	2:B:405:PHE:CD1	2.46	0.50
2:A:257:HIS:NE2	7:A:1001:HOH:O	2.35	0.50
2:A:304:GLN:HE21	2:B:154:LYS:HZ1	1.59	0.50
2:B:144:ASN:HB2	3:B:703:SO4:O3	2.12	0.50
2:B:259:THR:OG1	2:B:262:GLN:HG3	2.11	0.50
2:A:168:ALA:O	2:A:169:MSE:HB3	2.11	0.50
2:A:260:PHE:CE2	2:A:264:LYS:HD3	2.46	0.50
1:C:534:C:O2	2:A:426:LEU:HB3	2.12	0.50
1:D:523:C:H2'	1:D:524:G:H8	1.76	0.50
1:D:568:G:O2'	1:D:569:G:H5'	2.11	0.50
2:A:274:CYS:SG	2:A:277:LYS:HG3	2.52	0.50
2:A:133:ARG:NH1	2:A:410:ASP:OD1	2.45	0.49
2:A:344:GLN:HE22	2:A:357:SER:CB	2.24	0.49
2:B:341:PRO:HG2	2:B:402:TYR:CE1	2.46	0.49
2:A:167:GLU:O	2:A:168:ALA:O	2.31	0.49
1:D:507:G:C2'	1:D:508:U:OP1	2.60	0.49
2:B:95:ALA:HA	2:B:347:GLN:NE2	2.27	0.49
2:A:396:VAL:O	2:A:396:VAL:HG22	2.12	0.49
1:C:563:C:H2'	1:C:564:G:O4'	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:509:G:H4'	1:D:509:G:OP1	2.12	0.49
2:A:381:ARG:H	2:A:387:HIS:CD2	2.30	0.49
2:A:229:ILE:HD11	2:A:459:GLU:HB3	1.94	0.49
2:B:104:ILE:HG23	2:B:109:SER:OG	2.13	0.49
2:B:240:TYR:CZ	2:B:244:SER:HB2	2.48	0.49
1:C:522:G:O2'	1:C:523:C:H5'	2.12	0.49
2:A:314:ASP:N	2:A:315:PRO:CD	2.76	0.48
1:C:520:U:H2'	1:C:521:A:OP1	2.14	0.48
1:C:557:G:O2'	1:C:558:A:H5'	2.13	0.48
2:A:432:LYS:O	2:A:436:GLU:HG3	2.13	0.48
1:D:571:U:H5"	1:D:572:C:OP1	2.12	0.48
2:B:295:GLN:NE2	2:B:463:PRO:HB2	2.29	0.48
2:A:159:TYR:CZ	2:A:287:PRO:HB2	2.49	0.48
2:B:364:THR:HG23	2:B:367:GLN:OE1	2.14	0.48
2:A:114:LYS:HD2	2:A:118:ASN:HD21	1.78	0.48
2:B:381:ARG:HG2	2:B:387:HIS:HA	1.95	0.48
2:A:113:ASP:OD2	2:A:115:GLU:HB2	2.14	0.48
2:A:324:ALA:HB3	2:A:325:PRO:CD	2.44	0.48
2:A:206:LEU:HD23	2:A:206:LEU:N	2.28	0.48
2:A:241:MSE:SE	2:A:247:PHE:HD1	2.47	0.48
1:C:518:G:O2'	1:C:519:G:P	2.72	0.48
2:A:140:HIS:HA	2:A:334:LEU:O	2.14	0.47
1:D:519:G:O3'	1:D:520:U:O4'	2.31	0.47
1:D:509:G:O2'	1:D:546:G:H5'	2.14	0.47
2:A:254:ILE:HD11	2:A:289:PHE:CE2	2.47	0.47
1:C:514:A:O2'	1:C:515:A:H5'	2.14	0.47
1:D:562:A:H2'	1:D:563:C:C6	2.49	0.47
2:A:162:ARG:NH1	2:A:162:ARG:HG3	2.29	0.47
2:A:175:ILE:H	2:A:175:ILE:HD12	1.79	0.47
2:A:391:GLY:HA3	2:A:421:THR:O	2.15	0.47
2:B:467:SER:O	2:B:468:PHE:CB	2.62	0.47
1:C:509:G:C4'	1:C:510:G:OP2	2.63	0.47
2:A:234:ILE:O	2:A:461:MSE:HA	2.14	0.47
2:B:204:LYS:HB3	2:B:206:LEU:HD11	1.97	0.47
2:B:87:PRO:HB2	2:B:88:TRP:CE3	2.50	0.47
1:D:501:G:H2'	1:D:501:G:N3	2.30	0.46
1:D:523:C:H2'	1:D:524:G:C8	2.50	0.46
2:A:364:THR:HG23	2:A:367:GLN:HE22	1.78	0.46
1:C:529:U:H2'	1:C:530:G:H8	1.80	0.46
1:C:530:G:O2'	1:C:531:A:H5'	2.14	0.46
2:B:245:SER:O	2:B:249:LYS:HE2	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:199:GLU:HB2	2:B:280:PHE:CE1	2.50	0.46
1:C:557:G:H2'	1:C:558:A:H5'	1.96	0.46
2:A:119:ARG:HG2	2:A:119:ARG:NH1	2.30	0.46
2:A:129:HIS:HB2	2:A:182:TRP:CE2	2.50	0.46
2:B:350:MSE:HG3	2:B:358:SER:HB3	1.96	0.46
1:C:561:C:H2'	1:C:562:A:C8	2.50	0.46
2:A:398:VAL:HG13	2:A:402:TYR:CE1	2.51	0.46
2:B:314:ASP:N	2:B:315:PRO:CD	2.79	0.46
2:B:427:THR:O	2:B:431:LYS:HG3	2.16	0.45
2:A:462:THR:O	2:A:463:PRO:C	2.54	0.45
2:B:100:TYR:CZ	2:B:338:THR:HB	2.51	0.45
2:B:218:ASN:HD22	2:B:218:ASN:HA	1.55	0.45
2:A:136:ILE:HG23	2:A:405:PHE:CE1	2.51	0.45
1:C:560:U:P	1:C:561:C:H41	2.40	0.45
2:A:354:ASP:HA	2:A:355:PRO:HD3	1.68	0.45
2:B:431:LYS:O	2:B:435:ILE:HG13	2.17	0.45
2:A:350:MSE:HG2	2:A:358:SER:HB3	1.98	0.45
2:B:324:ALA:HB3	2:B:325:PRO:CD	2.46	0.45
1:C:503:C:H2'	1:C:504:C:C6	2.51	0.45
2:A:313:GLN:OE1	4:A:601:TRP:HA	2.16	0.45
2:B:354:ASP:HA	2:B:355:PRO:HD3	1.83	0.45
1:D:549:G:N2	1:D:550:C:H1'	2.32	0.45
2:B:355:PRO:HA	3:B:705:SO4:O1	2.16	0.44
2:A:136:ILE:HG23	2:A:405:PHE:HE1	1.82	0.44
1:D:516:U:HO2'	1:D:518:G:P	2.39	0.44
2:A:294:PRO:HG2	2:A:295:GLN:NE2	2.31	0.44
2:A:137:PHE:CE1	2:A:337:SER:HB3	2.52	0.44
1:C:534:C:H5'	2:A:384:ILE:CD1	2.43	0.44
2:B:368:ILE:HD13	2:B:442:ILE:HD12	1.98	0.44
1:C:516:U:H1'	1:C:560:U:HO2'	1.83	0.44
2:A:381:ARG:HG2	2:A:387:HIS:HA	2.00	0.44
2:A:330:PRO:HB3	2:B:152:ASN:O	2.17	0.44
2:A:175:ILE:N	2:A:175:ILE:HD12	2.33	0.44
1:C:542:G:O2'	1:C:543:A:H5'	2.17	0.44
1:D:516:U:O2'	1:D:518:G:OP1	2.35	0.44
2:B:208:LEU:HD22	2:B:238:LEU:CD1	2.48	0.44
2:B:466:LEU:O	2:B:467:SER:C	2.57	0.44
2:A:300:ARG:NH2	2:B:300:ARG:NH2	2.66	0.43
2:A:440:PRO:O	2:A:444:GLU:HG3	2.18	0.43
1:C:523:C:H2'	1:C:524:G:H8	1.83	0.43
1:D:528:C:C2	1:D:529:U:C5	3.06	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:137:PHE:CE2	2:A:337:SER:HB3	2.53	0.43
2:A:195:MSE:HE1	2:A:218:ASN:HB3	2.01	0.43
2:B:168:ALA:HB1	2:B:352:ALA:HB2	2.01	0.43
2:A:140:HIS:HB2	2:A:334:LEU:O	2.18	0.43
2:B:189:VAL:HB	2:B:190:PRO:HD2	1.99	0.43
2:A:240:TYR:HA	2:A:243:MSE:HG2	2.00	0.43
2:B:312:ASP:HB3	2:B:339:PHE:CE1	2.53	0.43
2:A:295:GLN:HG3	2:A:463:PRO:CB	2.40	0.43
2:B:194:GLN:HB2	2:B:235:PHE:CZ	2.54	0.43
2:A:152:ASN:O	2:B:330:PRO:HB3	2.18	0.43
2:B:335:LEU:HA	2:B:335:LEU:HD23	1.88	0.43
2:A:233:PHE:CZ	2:A:235:PHE:HB3	2.52	0.43
2:A:165:SER:CB	2:A:168:ALA:HB3	2.47	0.43
1:C:533:U:O2'	2:A:382:ASP:O	2.14	0.43
2:A:343:LEU:HD12	2:A:356:ASN:O	2.19	0.43
2:A:99:ASP:CG	2:A:102:LYS:HD3	2.39	0.43
1:C:558:A:N6	1:C:561:C:C2	2.87	0.43
2:A:103:LEU:HD23	2:A:103:LEU:HA	1.83	0.43
1:C:507:G:O2'	1:C:508:U:OP1	2.30	0.43
1:C:531:A:O2'	1:C:532:C:H5'	2.19	0.43
1:C:518:G:HO2'	1:C:519:G:P	2.42	0.42
2:B:196:THR:HB	2:B:199:GLU:HB3	2.00	0.42
2:A:129:HIS:CE1	2:A:130:HIS:CE1	3.08	0.42
2:A:330:PRO:HA	2:B:152:ASN:ND2	2.34	0.42
1:C:508:U:O4'	1:C:548:U:O2'	2.37	0.42
2:A:166:SER:C	2:A:168:ALA:H	2.22	0.42
1:D:505:U:H3	1:D:568:G:H1	1.68	0.42
2:A:294:PRO:O	2:A:298:ARG:N	2.52	0.42
2:A:409:ASP:OD1	2:A:412:LYS:HG3	2.19	0.42
2:B:280:PHE:N	2:B:281:PRO:CD	2.83	0.42
2:B:372:VAL:HG12	2:B:431:LYS:HD3	2.00	0.42
2:A:344:GLN:NE2	2:A:344:GLN:H	2.17	0.42
2:B:90:VAL:HB	2:B:349:LYS:HG2	2.01	0.42
2:A:381:ARG:N	2:A:387:HIS:HD2	2.14	0.42
2:B:254:ILE:HD11	2:B:289:PHE:HE2	1.85	0.41
2:B:418:LYS:HB2	2:B:418:LYS:HE3	1.85	0.41
1:C:521:A:N6	1:C:546:G:H2'	2.35	0.41
1:D:524:G:C6	1:D:525:C:C4	3.08	0.41
2:A:280:PHE:N	2:A:281:PRO:CD	2.83	0.41
2:A:159:TYR:CE2	2:A:287:PRO:HB2	2.55	0.41
2:A:204:LYS:HB2	2:A:206:LEU:CD2	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:206:LEU:HD12	2:B:206:LEU:N	2.35	0.41
2:A:141:ARG:NH2	2:A:318:ARG:HD3	2.35	0.41
2:B:116:LEU:O	2:B:120:ILE:HG13	2.19	0.41
1:D:505:U:O4	1:D:568:G:O6	2.37	0.41
2:B:103:LEU:HD13	2:B:311:ILE:HG12	2.01	0.41
1:C:569:G:O2'	1:C:570:G:H5'	2.20	0.41
2:A:101:ASP:O	2:A:105:VAL:HG23	2.20	0.41
2:A:250:ASN:HA	2:A:250:ASN:HD22	1.60	0.41
2:B:153:LYS:CD	2:B:153:LYS:N	2.82	0.41
2:B:380:GLY:C	2:B:381:ARG:HD3	2.40	0.41
2:B:441:LEU:O	2:B:441:LEU:HD12	2.20	0.41
2:B:169:MSE:HE2	2:B:173:HIS:HB3	2.02	0.41
2:B:208:LEU:HA	2:B:208:LEU:HD23	1.93	0.41
1:D:535:C:C2	2:B:427:THR:HG21	2.56	0.41
2:B:88:TRP:O	2:B:89:THR:HG23	2.21	0.41
2:A:449:ARG:HG2	2:A:449:ARG:HH11	1.86	0.41
2:B:264:LYS:HG3	2:B:269:PHE:O	2.21	0.41
1:C:560:U:O2'	1:C:561:C:OP1	2.29	0.41
1:D:507:G:H2'	1:D:508:U:OP1	2.20	0.41
1:D:530:G:C2	1:D:541:A:C2	3.09	0.41
1:D:518:G:H5'	1:D:519:G:OP2	2.20	0.41
2:A:129:HIS:HB2	2:A:182:TRP:CD2	2.56	0.40
2:A:412:LYS:HB3	2:A:412:LYS:HZ2	1.84	0.40
2:B:374:LYS:N	2:B:374:LYS:HD2	2.36	0.40
2:A:300:ARG:HH21	2:B:300:ARG:NH2	2.18	0.40
1:D:510:G:OP1	1:D:510:G:C8	2.75	0.40
1:D:560:U:C2'	1:D:561:C:OP1	2.70	0.40
2:A:344:GLN:HB2	2:A:344:GLN:HE21	1.71	0.40
2:B:129:HIS:HB2	2:B:182:TRP:CD2	2.56	0.40
2:A:196:THR:HB	2:A:199:GLU:HB2	2.03	0.40
2:B:159:TYR:CZ	2:B:287:PRO:HB2	2.57	0.40
2:B:197:ASP:OD2	2:B:238:LEU:HD12	2.21	0.40
2:B:251:VAL:O	2:B:255:GLN:HG3	2.22	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
2	A	385/477 (81%)	358 (93%)	25 (6%)	2 (0%)	29 61
2	B	386/477 (81%)	358 (93%)	21 (5%)	7 (2%)	8 28
All	All	771/954 (81%)	716 (93%)	46 (6%)	9 (1%)	13 39

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	A	168	ALA
2	B	165	SER
2	B	168	ALA
2	B	467	SER
2	B	468	PHE
2	B	409	ASP
2	B	169	MSE
2	B	324	ALA
2	A	87	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
2	A	340/402 (85%)	322 (95%)	18 (5%)	22 54
2	B	340/402 (85%)	322 (95%)	18 (5%)	22 54
All	All	680/804 (85%)	644 (95%)	36 (5%)	22 54

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	82	GLU
2	A	83	ASP
2	A	103	LEU
2	A	114	LYS
2	A	155	PRO
2	A	159	TYR
2	A	167	GLU
2	A	205	ASP
2	A	206	LEU
2	A	236	SER
2	A	261	ASN
2	A	295	GLN
2	A	298	ARG
2	A	344	GLN
2	A	361	LEU
2	A	369	LYS
2	A	382	ASP
2	A	410	ASP
2	B	86	ASP
2	B	89	THR
2	B	103	LEU
2	B	143	MSE
2	B	152	ASN
2	B	169	MSE
2	B	186	VAL
2	B	200	LYS
2	B	206	LEU
2	B	218	ASN
2	B	249	LYS
2	B	298	ARG
2	B	322	ASP
2	B	347	GLN
2	B	374	LYS
2	B	385	GLU
2	B	444	GLU
2	B	465	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	91	GLN

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Mol	Chain	Res	Type
2	A	140	HIS
2	A	144	ASN
2	A	218	ASN
2	A	250	ASN
2	A	255	GLN
2	A	261	ASN
2	A	295	GLN
2	A	304	GLN
2	A	344	GLN
2	A	347	GLN
2	A	367	GLN
2	A	387	HIS
2	A	389	GLN
2	B	118	ASN
2	B	126	GLN
2	B	140	HIS
2	B	145	GLN
2	B	152	ASN
2	B	255	GLN
2	B	262	GLN
2	B	344	GLN
2	B	347	GLN
2	B	387	HIS
2	B	389	GLN

5.3.3 RNA

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	71/75 (94%)	12 (16%)	4 (5%)
1	D	71/75 (94%)	19 (26%)	5 (7%)
All	All	142/150 (94%)	31 (21%)	9 (6%)

All (31) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	508	U
1	C	509	G
1	C	510	G
1	C	516	U
1	C	518	G
1	C	519	G

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Mol	Chain	Res	Type
1	C	520	U
1	C	522	G
1	C	546	G
1	C	547	U
1	C	549	G
1	C	561	C
1	D	502	A
1	D	504	C
1	D	505	U
1	D	508	U
1	D	510	G
1	D	516	U
1	D	518	G
1	D	519	G
1	D	522	G
1	D	547	U
1	D	548	U
1	D	549	G
1	D	558	A
1	D	559	A
1	D	560	U
1	D	561	C
1	D	566	C
1	D	572	C
1	D	573	A

All (9) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C	507	G
1	C	509	G
1	C	518	G
1	C	519	G
1	D	507	G
1	D	516	U
1	D	518	G
1	D	548	U
1	D	558	A

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 16 ligands modelled in this entry, 1 is monoatomic - leaving 15 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	$\#\|Z\| > 2$
3	SO4	B	703	-	4,4,4	0.28	0	6,6,6	0.18	0
3	SO4	A	704	-	4,4,4	0.26	0	6,6,6	0.18	0
3	SO4	A	708	-	4,4,4	0.29	0	6,6,6	0.10	0
3	SO4	B	706	-	4,4,4	0.26	0	6,6,6	0.15	0
3	SO4	A	707	-	4,4,4	0.29	0	6,6,6	0.07	0
3	SO4	B	710	-	4,4,4	0.26	0	6,6,6	0.07	0
6	GOL	B	801	-	5,5,5	0.39	0	5,5,5	0.35	0
3	SO4	B	705	-	4,4,4	0.28	0	6,6,6	0.14	0
3	SO4	B	701	-	4,4,4	0.29	0	6,6,6	0.07	0
3	SO4	B	709	-	4,4,4	0.28	0	6,6,6	0.06	0
6	GOL	B	802	-	5,5,5	0.38	0	5,5,5	0.30	0
3	SO4	A	702	-	4,4,4	0.26	0	6,6,6	0.15	0

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
6	GOL	B	802	-	-	0/4/4/4	-
6	GOL	B	801	-	-	0/4/4/4	-

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.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	703	SO4	1	0
3	A	704	SO4	1	0
6	B	801	GOL	2	0
3	B	705	SO4	1	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

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^{th} 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	72/75 (96%)	1.49	24 (33%) 0 0	81, 127, 155, 167	0
1	D	72/75 (96%)	0.91	17 (23%) 0 0	57, 107, 188, 200	0
2	A	377/477 (79%)	-0.07	0 100 100	39, 60, 84, 97	0
2	B	378/477 (79%)	0.01	0 100 100	39, 54, 72, 98	1 (0%)
All	All	899/1104 (81%)	0.17	41 (4%) 32 22	39, 59, 134, 200	1 (0%)

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	570	G	5.9
1	D	502	A	5.7
1	C	520	U	5.3
1	C	516	U	5.1
1	D	572	C	4.7
1	D	571	U	4.7
1	C	518	G	4.5
1	C	573	A	4.3
1	C	545	G	4.0
1	D	501	G	4.0
1	C	519	G	3.7
1	D	573	A	3.6
1	C	544	A	3.3
1	C	557	G	3.0
1	C	542	G	2.9
1	C	547	U	2.8
1	C	515	A	2.8
1	D	568	G	2.8
1	C	541	A	2.7
1	C	556	C	2.7
1	C	572	C	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	522	G	2.6
1	D	567	G	2.4
1	C	509	G	2.4
1	D	503	C	2.4
1	C	558	A	2.4
1	D	547	U	2.3
1	D	516	U	2.3
1	D	569	G	2.3
1	D	504	C	2.3
1	C	523	C	2.2
1	C	561	C	2.2
1	C	524	G	2.2
1	D	505	U	2.2
1	C	560	U	2.1
1	D	506	C	2.1
1	C	513	C	2.1
1	D	550	C	2.1
1	C	571	U	2.1
1	C	514	A	2.0
1	D	520	U	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^{th} 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(Å^2)	Q<0.9
3	SO4	B	710	5/5	0.74	0.30	155,155,156,156	0
5	MG	B	901	1/1	0.74	0.28	82,82,82,82	0
6	GOL	B	802	6/6	0.83	0.44	93,94,95,96	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
4	TRP	A	602	15/15	0.84	0.41	103,106,112,113	0
3	SO4	B	709	5/5	0.90	0.16	131,131,131,132	0
3	SO4	A	708	5/5	0.90	0.22	122,123,124,124	0
6	GOL	B	801	6/6	0.90	0.27	64,67,67,71	0
3	SO4	B	706	5/5	0.93	0.14	112,114,114,114	0
3	SO4	A	707	5/5	0.93	0.18	125,125,126,126	0
3	SO4	A	702	5/5	0.94	0.19	100,102,103,103	0
3	SO4	B	705	5/5	0.95	0.17	103,104,104,105	0
4	TRP	A	601	15/15	0.96	0.23	51,53,61,62	0
3	SO4	A	704	5/5	0.96	0.23	76,78,79,80	0
4	TRP	B	603	15/15	0.96	0.28	43,45,55,55	0
3	SO4	B	701	5/5	0.97	0.23	77,79,80,80	0
3	SO4	B	703	5/5	0.98	0.12	72,73,74,75	0

6.5 Other polymers

There are no such residues in this entry.