



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 30, 2026 – 12:21 AM UTC

PDB ID : 1ZE2 / pdb_00001ze2
Title : Conformational change of pseudouridine 55 synthase upon its association with RNA substrate
Authors : Phannachet, K.; Huang, R.H.
Deposited on : 2005-04-16
Resolution : 3.00 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

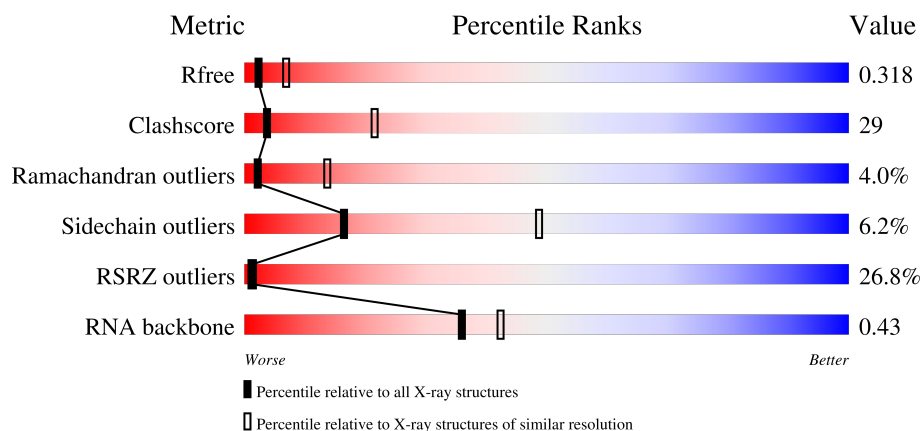
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)
RNA backbone	3983	1109 (3.20-2.80)

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	22	23% 36% 32% 23% 9%
1	D	22	36% 18% 50% 5% 27%
2	A	309	6% 48% 45% 5%
2	B	309	38% 27% 38% 6% 29%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5302 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 5'-R(*GP*GP*CP*CP*AP*CP*GP*GP*UP*(FHU)P*C P*GP*AP*AP*UP*CP*CP*GP*UP*GP*GP*C)-3'.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	C	22	Total	C	F	N	O	P	0	0	0
			469	209	1	84	154	21			
1	D	22	Total	C	F	N	O	P	0	0	0
			469	209	1	84	154	21			

- Molecule 2 is a protein called tRNA pseudouridine synthase B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	300	Total	C	N	O	S	0	0	0
			2416	1546	420	440	10			
2	B	218	Total	C	N	O	S	0	0	0
			1760	1131	313	311	5			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	296	GLN	ASN	SEE REMARK 999	UNP Q9WZW0
A	307	GLN	ASN	SEE REMARK 999	UNP Q9WZW0
B	296	GLN	ASN	SEE REMARK 999	UNP Q9WZW0
B	307	GLN	ASN	SEE REMARK 999	UNP Q9WZW0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	C	29	Total	O	0	0
			29	29		
3	D	20	Total	O	0	0
			20	20		
3	A	81	Total	O	0	0
			81	81		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	58	Total	O	0	0
			58	58		

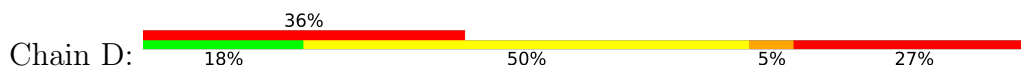
3 Residue-property plots [i](#)

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.

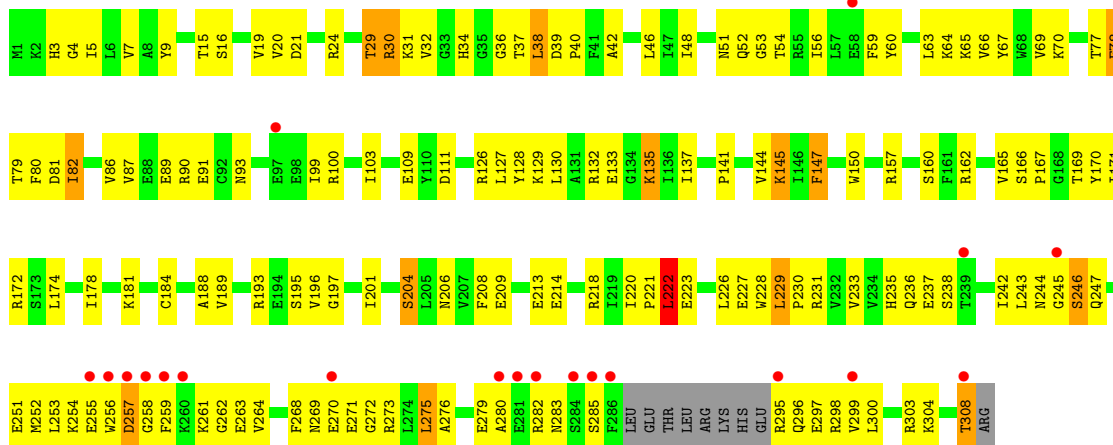
- Molecule 1: 5'-R(*GP*GP*CP*CP*AP*CP*GP*GP*UP*(FHU)P*CP*GP*AP*AP*UP*CP*CP*GP*UP*GP*GP*C)-3'



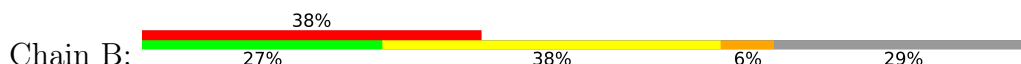
- Molecule 1: 5'-R(*GP*GP*CP*CP*AP*CP*GP*GP*UP*(FHU)P*CP*GP*AP*AP*UP*CP*CP*GP*UP*GP*GP*C)-3'

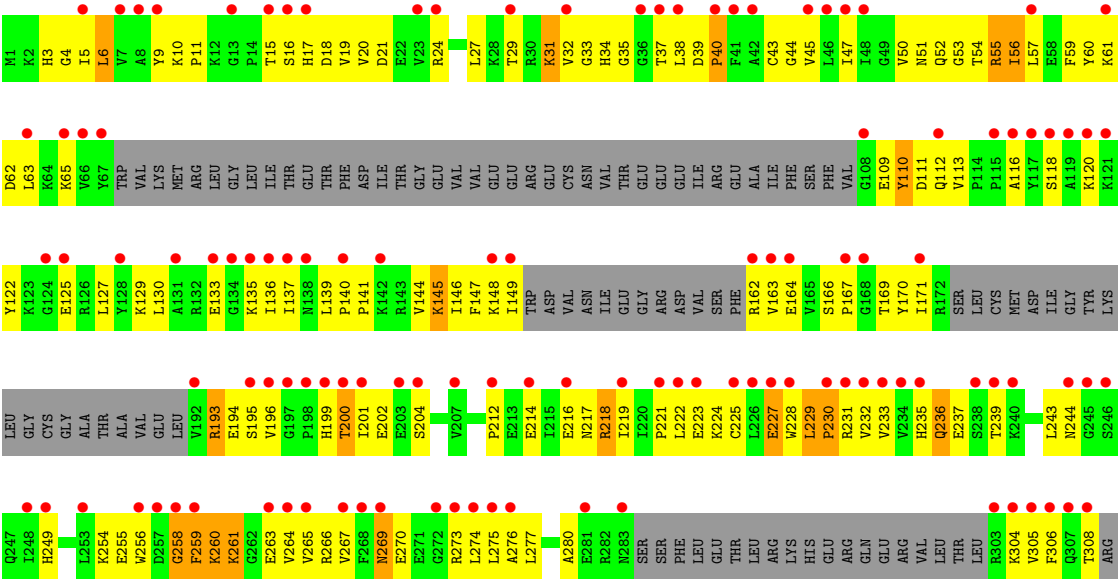


- Molecule 2: tRNA pseudouridine synthase B



- Molecule 2: tRNA pseudouridine synthase B





4 Data and refinement statistics

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α , β , γ	134.97Å 134.97Å 139.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 50.00 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.00) 97.7 (50.00-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	5.98 (at 2.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.261 , 0.318 0.264 , 0.318	Depositor DCC
R_{free} test set	2327 reflections (8.01%)	wwPDB-VP
Wilson B-factor (Å ²)	61.3	Xtriage
Anisotropy	0.061	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 67.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.016 for -h,l,k 0.008 for -l,-k,-h	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	5302	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.43% 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 [i](#)

5.1 Standard geometry [i](#)

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

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	0.51	0/499	1.26	13/777 (1.7%)
1	D	0.49	1/499 (0.2%)	1.24	9/777 (1.2%)
2	A	0.63	0/2461	0.96	5/3314 (0.2%)
2	B	0.44	0/1792	0.90	2/2405 (0.1%)
All	All	0.55	1/5251 (0.0%)	1.01	29/7273 (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	D	1	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	10	FHU	O3'-P	5.33	1.61	1.56

All (29) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	14	A	C2'-C3'-O3'	10.29	129.14	113.70
1	D	12	G	C2'-C3'-O3'	9.36	123.54	109.50
1	C	14	A	C4'-C3'-O3'	8.23	125.34	113.00
1	D	9	U	C2'-C3'-O3'	7.74	121.11	109.50
1	C	12	G	C2'-C3'-O3'	7.58	120.87	109.50
1	C	9	U	C1'-C2'-O2'	-7.08	101.17	111.80
2	A	30	ARG	N-CA-C	-6.83	105.89	114.56
1	C	14	A	C4'-C3'-C2'	6.57	109.17	102.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	12	G	C4'-C3'-O3'	6.55	119.22	109.40
1	D	13	A	C2'-C3'-O3'	6.55	123.52	113.70
1	D	14	A	C4'-C3'-O3'	6.49	122.73	113.00
1	D	13	A	C4'-C3'-C2'	6.36	108.96	102.60
1	C	13	A	C4'-C3'-C2'	6.21	108.81	102.60
1	C	15	U	C5'-C4'-C3'	-6.17	105.94	115.20
1	C	13	A	C2'-C3'-O3'	6.12	122.88	113.70
1	C	14	A	C2'-C3'-O3'	5.86	122.49	113.70
2	A	196	VAL	N-CA-C	-5.61	99.47	107.77
1	C	12	G	N9-C1'-C2'	5.54	122.31	114.00
1	D	14	A	C4'-C3'-C2'	5.53	108.13	102.60
1	C	9	U	C2'-C3'-O3'	5.49	117.74	109.50
1	C	11	C	C2'-C3'-O3'	5.47	117.70	109.50
2	B	269	ASN	N-CA-C	-5.45	102.12	110.14
1	C	15	U	C2'-C3'-O3'	5.37	117.55	109.50
1	D	11	C	C2'-C3'-O3'	5.29	117.43	109.50
1	C	9	U	N1-C1'-C2'	5.21	121.81	114.00
2	A	201	ILE	N-CA-C	-5.19	106.01	113.07
2	A	303	ARG	N-CA-C	-5.18	107.97	114.56
2	B	227	GLU	N-CA-C	-5.03	105.70	111.14
2	A	147	PHE	N-CA-C	5.03	116.84	111.36

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	14	A	C3'

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	9	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	469	0	241	16	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	469	0	241	26	0
2	A	2416	0	2477	119	0
2	B	1760	0	1831	148	0
3	A	81	0	0	10	0
3	B	58	0	0	11	0
3	C	29	0	0	2	0
3	D	20	0	0	3	0
All	All	5302	0	4790	286	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 29.

All (286) 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:269:ASN:HD21	2:B:273:ARG:HB3	1.23	0.98
2:B:65:LYS:HG2	2:B:193:ARG:HH11	1.35	0.91
2:A:165:VAL:HG21	2:A:169:THR:HG21	1.54	0.89
2:B:65:LYS:HE3	2:B:196:VAL:HG13	1.55	0.87
2:A:233:VAL:HG12	2:A:255:GLU:HB2	1.59	0.83
2:A:109:GLU:HG2	2:A:145:LYS:HB3	1.59	0.82
2:A:82:ILE:HD11	2:A:189:VAL:O	1.79	0.82
2:B:239:THR:HA	2:B:275:LEU:HD21	1.62	0.82
2:B:47:ILE:HD12	2:B:47:ILE:H	1.44	0.81
2:B:139:LEU:HB3	2:B:140:PRO:HD2	1.62	0.80
2:B:239:THR:HG23	2:B:275:LEU:HD11	1.62	0.80
2:B:269:ASN:ND2	2:B:273:ARG:HB3	1.98	0.78
2:A:63:LEU:HD13	2:A:197:GLY:HA3	1.67	0.77
2:B:47:ILE:HD11	2:B:196:VAL:HG11	1.67	0.77
2:B:229:LEU:HD22	2:B:264:VAL:HB	1.69	0.74
2:A:145:LYS:HG2	2:A:166:SER:HB3	1.70	0.74
2:B:145:LYS:HD3	2:B:145:LYS:H	1.52	0.73
2:A:233:VAL:HG13	2:A:254:LYS:HB3	1.68	0.73
2:B:135:LYS:HD2	2:B:135:LYS:H	1.52	0.73
2:B:120:LYS:HB2	2:B:127:LEU:HD12	1.71	0.72
2:A:157:ARG:HG2	3:A:346:HOH:O	1.89	0.71
2:B:147:PHE:HD2	2:B:164:GLU:HG2	1.55	0.71
2:A:276:ALA:HB1	2:A:304:LYS:O	1.89	0.71
2:A:231:ARG:HG3	2:A:231:ARG:O	1.90	0.71
1:D:10:FHU:HN1	2:B:171:ILE:H	1.38	0.69
2:A:82:ILE:HG12	2:A:189:VAL:HA	1.72	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:82:ILE:HD13	2:A:189:VAL:HG13	1.74	0.69
2:B:193:ARG:HD2	2:B:196:VAL:HG22	1.74	0.69
2:A:251:GLU:HB2	2:A:296:GLN:NE2	2.08	0.69
2:B:243:LEU:HD13	2:B:275:LEU:HG	1.76	0.68
2:A:247:GLN:HG3	2:A:298:ARG:CZ	2.23	0.68
1:C:10:FHU:HN1	2:A:171:ILE:H	1.40	0.68
1:D:12:G:N2	2:B:40:PRO:HG2	2.09	0.68
2:A:29:THR:HG22	2:A:30:ARG:H	1.56	0.67
2:B:111:ASP:HB3	2:B:141:PRO:HB2	1.75	0.67
2:B:20:VAL:HG12	2:B:24:ARG:HD2	1.76	0.67
2:A:261:LYS:O	2:A:280:ALA:HB3	1.94	0.66
1:D:1:G:H2'	1:D:2:G:H5'	1.78	0.66
2:B:231:ARG:HB3	2:B:266:ARG:NH2	2.11	0.66
1:D:16:C:O2'	2:B:54:THR:OG1	2.14	0.65
1:D:10:FHU:HN1	2:B:171:ILE:N	1.95	0.64
2:A:214:GLU:O	2:A:218:ARG:HG2	1.98	0.64
2:A:299:VAL:HG23	2:A:300:LEU:HG	1.78	0.64
1:C:21:G:H5'	2:B:305:VAL:HB	1.78	0.64
1:C:10:FHU:HN1	2:A:170:TYR:HA	1.63	0.64
2:B:29:THR:HG22	2:B:31:LYS:H	1.63	0.63
2:A:127:LEU:HD22	2:A:137:ILE:HB	1.81	0.63
2:B:3:HIS:HB3	2:B:52:GLN:HB2	1.81	0.62
2:A:15:THR:HG22	2:A:40:PRO:HG3	1.79	0.62
2:B:29:THR:HG21	2:B:51:ASN:OD1	1.99	0.62
2:B:216:GLU:O	2:B:219:ILE:HG22	1.99	0.62
2:A:91:GLU:HG3	3:A:342:HOH:O	2.00	0.62
2:B:65:LYS:HG2	2:B:193:ARG:NH1	2.12	0.61
2:B:6:LEU:HD23	2:B:218:ARG:O	2.00	0.61
2:B:11:PRO:HB3	3:B:340:HOH:O	2.00	0.61
2:B:31:LYS:HB3	2:B:51:ASN:HA	1.81	0.61
2:B:231:ARG:HB3	2:B:266:ARG:CZ	2.31	0.61
2:B:118:SER:HB2	2:B:127:LEU:HD12	1.82	0.61
2:B:227:GLU:HB3	3:B:356:HOH:O	1.99	0.61
1:D:16:C:H2'	1:D:17:C:O4'	2.00	0.61
2:B:228:TRP:CD1	2:B:229:LEU:HG	2.36	0.61
2:A:218:ARG:HA	2:A:218:ARG:HH11	1.66	0.60
2:B:149:ILE:HA	2:B:163:VAL:HG12	1.83	0.60
2:B:5:ILE:HD13	2:B:56:ILE:HD11	1.83	0.60
2:B:230:PRO:HB2	2:B:265:VAL:HG12	1.85	0.59
1:C:11:C:N4	2:A:79:THR:HB	2.18	0.59
2:A:34:HIS:HD2	2:A:36:GLY:H	1.50	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:233:VAL:HG12	2:B:255:GLU:HB3	1.84	0.59
2:B:223:GLU:CD	2:B:273:ARG:HA	2.29	0.57
1:D:11:C:H5'	2:B:39:ASP:OD1	2.05	0.57
2:B:221:PRO:HG2	2:B:224:LYS:HB2	1.86	0.57
1:D:4:C:H2'	1:D:5:A:H8	1.70	0.57
2:A:253:LEU:HD11	2:A:299:VAL:HG21	1.87	0.57
2:B:116:ALA:HB2	2:B:136:ILE:HG23	1.88	0.56
2:B:304:LYS:HG3	2:B:305:VAL:N	2.20	0.56
2:B:45:VAL:HG21	2:B:200:THR:O	2.05	0.56
1:D:11:C:H5''	3:B:362:HOH:O	2.05	0.56
2:B:120:LYS:HB2	2:B:127:LEU:CD1	2.35	0.56
2:B:239:THR:HG21	3:B:328:HOH:O	2.06	0.56
2:A:99:ILE:O	2:A:103:ILE:HG12	2.06	0.56
2:B:118:SER:O	2:B:127:LEU:HB2	2.04	0.56
2:A:233:VAL:HA	2:A:268:PHE:O	2.05	0.55
2:A:5:ILE:HD11	2:A:56:ILE:HG13	1.87	0.55
2:B:261:LYS:C	2:B:263:GLU:H	2.14	0.55
2:B:55:ARG:NH1	2:B:304:LYS:HD2	2.21	0.55
1:D:10:FHU:HN1	2:B:170:TYR:HA	1.72	0.55
2:B:50:VAL:HG12	2:B:51:ASN:ND2	2.22	0.55
2:B:62:ASP:HB2	3:B:332:HOH:O	2.06	0.55
2:B:10:LYS:HD2	2:B:16:SER:HA	1.87	0.55
2:B:232:VAL:HG11	2:B:259:PHE:CE1	2.42	0.55
1:D:16:C:H5'	3:D:26:HOH:O	2.07	0.55
2:B:222:LEU:HG	2:B:274:LEU:HD23	1.88	0.55
2:B:10:LYS:O	2:B:43:CYS:HA	2.06	0.55
2:A:31:LYS:HB3	2:A:51:ASN:HA	1.88	0.54
1:D:13:A:N6	2:B:34:HIS:O	2.33	0.54
1:D:9:U:O4'	2:B:61:LYS:HE3	2.08	0.54
2:A:226:LEU:HB3	2:A:229:LEU:HD12	1.89	0.54
2:B:6:LEU:HD13	2:B:6:LEU:O	2.08	0.53
2:B:52:GLN:HG3	2:B:308:THR:HG22	1.90	0.53
2:B:10:LYS:HG3	2:B:19:VAL:CG2	2.38	0.53
1:C:16:C:H2'	1:C:17:C:H6	1.74	0.53
2:A:66:VAL:HB	2:A:195:SER:OG	2.09	0.53
2:A:5:ILE:HG13	2:A:60:TYR:OH	2.09	0.53
3:D:27:HOH:O	2:B:39:ASP:HA	2.09	0.53
2:A:82:ILE:CD1	2:A:189:VAL:HG13	2.40	0.52
2:B:125:GLU:CD	2:B:130:LEU:HD21	2.34	0.52
2:B:116:ALA:CB	2:B:136:ILE:HG23	2.39	0.52
2:B:145:LYS:C	2:B:146:ILE:HD12	2.35	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:269:ASN:HD21	2:A:271:GLU:HG2	1.73	0.52
2:B:21:ASP:HA	2:B:24:ARG:HD3	1.91	0.52
2:A:31:LYS:HG2	3:A:331:HOH:O	2.10	0.51
2:B:47:ILE:HD12	2:B:47:ILE:N	2.18	0.51
2:B:63:LEU:HD11	2:B:228:TRP:CH2	2.45	0.51
2:A:228:TRP:O	2:A:229:LEU:HB2	2.10	0.51
2:A:251:GLU:H	2:A:296:GLN:HE22	1.56	0.51
2:B:222:LEU:HD21	2:B:306:PHE:CG	2.44	0.51
2:B:228:TRP:O	2:B:229:LEU:HB2	2.11	0.51
1:D:17:C:H2'	1:D:18:G:H8	1.75	0.51
2:A:145:LYS:HG2	2:A:166:SER:CB	2.39	0.51
2:A:245:GLY:O	2:A:246:SER:HB3	2.10	0.51
2:A:59:PHE:HE2	2:A:264:VAL:HG21	1.76	0.51
2:A:51:ASN:O	2:A:54:THR:HG23	2.11	0.51
2:B:5:ILE:HB	2:B:225:CYS:SG	2.51	0.50
1:D:15:U:C2	2:B:17:HIS:HE1	2.30	0.50
2:A:269:ASN:ND2	2:A:271:GLU:HG2	2.27	0.50
1:C:22:C:H2'	1:D:1:G:H1'	1.94	0.50
1:D:12:G:H22	2:B:40:PRO:HG2	1.77	0.50
2:A:261:LYS:C	2:A:263:GLU:H	2.20	0.50
2:A:243:LEU:HD21	2:A:273:ARG:NH2	2.27	0.50
2:B:47:ILE:H	2:B:47:ILE:CD1	2.21	0.50
2:B:277:LEU:HG	2:B:306:PHE:CE1	2.47	0.50
2:A:21:ASP:HA	2:A:24:ARG:HD2	1.93	0.49
2:B:5:ILE:HG12	2:B:60:TYR:OH	2.11	0.49
2:B:29:THR:HG22	2:B:31:LYS:N	2.25	0.49
2:B:276:ALA:HB1	2:B:304:LYS:O	2.11	0.49
1:C:10:FHU:HN1	2:A:171:ILE:N	2.06	0.49
1:C:13:A:O2'	1:C:15:U:OP2	2.30	0.49
2:A:78:GLU:H	2:A:78:GLU:CD	2.16	0.49
2:B:29:THR:CG2	2:B:31:LYS:HB2	2.42	0.49
1:D:8:G:H2'	1:D:9:U:C6	2.47	0.49
2:B:3:HIS:CD2	2:B:308:THR:HB	2.47	0.49
2:A:4:GLY:HA3	2:A:220:ILE:O	2.13	0.49
2:B:233:VAL:O	2:B:254:LYS:HB3	2.13	0.49
2:B:47:ILE:HG21	2:B:60:TYR:CD1	2.47	0.49
2:B:221:PRO:HG3	3:B:335:HOH:O	2.12	0.49
2:A:150:TRP:NE1	2:A:162:ARG:HD2	2.28	0.48
2:B:20:VAL:HG13	2:B:32:VAL:HG12	1.95	0.48
2:A:51:ASN:O	2:A:53:GLY:N	2.46	0.48
2:A:109:GLU:CG	2:A:145:LYS:HB3	2.38	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:113:VAL:HG13	2:B:139:LEU:O	2.14	0.48
2:A:90:ARG:HD2	2:A:184:CYS:O	2.13	0.48
2:B:55:ARG:HH12	2:B:304:LYS:HD2	1.78	0.48
2:A:19:VAL:HG11	2:A:46:LEU:HD23	1.95	0.48
2:A:282:ARG:HG3	2:A:282:ARG:HH11	1.79	0.48
2:B:29:THR:HG22	2:B:31:LYS:HB2	1.94	0.48
2:A:280:ALA:HA	2:A:300:LEU:HD23	1.94	0.47
2:A:251:GLU:N	2:A:296:GLN:HE22	2.12	0.47
2:A:16:SER:HB2	2:A:37:THR:HG23	1.95	0.47
2:A:221:PRO:O	2:A:222:LEU:C	2.58	0.47
2:B:256:TRP:C	2:B:258:GLY:H	2.21	0.47
2:A:81:ASP:HA	2:A:188:ALA:O	2.14	0.47
2:A:126:ARG:HD3	2:A:128:TYR:CZ	2.49	0.47
2:A:256:TRP:O	2:A:257:ASP:HB2	2.14	0.47
2:B:9:TYR:HA	2:B:44:GLY:O	2.13	0.47
1:D:10:FHU:N1	2:B:170:TYR:HA	2.28	0.47
2:A:20:VAL:HG13	2:A:32:VAL:HG12	1.96	0.47
2:A:79:THR:O	2:A:80:PHE:HB2	2.15	0.47
2:B:147:PHE:CD2	2:B:164:GLU:HG2	2.43	0.47
1:C:16:C:H2'	1:C:17:C:C6	2.50	0.47
2:B:261:LYS:O	2:B:280:ALA:HB3	2.13	0.47
2:A:67:TYR:CE2	2:A:193:ARG:HD3	2.50	0.47
1:D:14:A:H5'	1:D:15:U:OP2	2.16	0.46
1:D:17:C:H2'	1:D:18:G:C8	2.50	0.46
2:A:77:THR:HG22	2:A:87:VAL:HG12	1.96	0.46
2:A:135:LYS:HE3	3:A:356:HOH:O	2.15	0.46
2:A:165:VAL:HG21	2:A:169:THR:CG2	2.36	0.46
2:A:165:VAL:HG22	2:A:166:SER:N	2.30	0.46
2:B:51:ASN:O	2:B:54:THR:HG22	2.15	0.46
2:A:282:ARG:HB3	2:A:283:ASN:H	1.55	0.46
2:A:37:THR:HG22	2:A:38:LEU:N	2.30	0.46
2:A:251:GLU:HB2	2:A:296:GLN:HE22	1.77	0.46
2:B:214:GLU:HA	2:B:217:ASN:HD22	1.79	0.46
2:A:206:ASN:OD1	2:A:208:PHE:HB2	2.15	0.46
2:B:15:THR:O	2:B:18:ASP:HB2	2.16	0.46
2:B:50:VAL:HG12	2:B:51:ASN:HD22	1.80	0.46
2:A:166:SER:HB2	2:A:167:PRO:HD2	1.98	0.46
1:C:18:G:H4'	3:C:27:HOH:O	2.16	0.46
2:A:100:ARG:HD2	3:A:313:HOH:O	2.16	0.46
2:A:229:LEU:HA	2:A:230:PRO:HD3	1.83	0.46
2:B:4:GLY:O	2:B:53:GLY:HA3	2.16	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:125:GLU:OE1	2:B:130:LEU:HD11	2.15	0.46
2:A:51:ASN:C	2:A:53:GLY:N	2.74	0.46
2:A:130:LEU:HD13	2:A:137:ILE:HD11	1.97	0.46
2:A:262:GLY:HA2	2:A:279:GLU:CG	2.46	0.46
2:A:221:PRO:O	2:A:223:GLU:N	2.50	0.46
1:D:4:C:H2'	1:D:5:A:C8	2.49	0.45
2:A:103:ILE:HD13	2:A:178:ILE:HG21	1.98	0.45
2:B:122:TYR:CD2	2:B:137:ILE:HD13	2.51	0.45
2:B:35:GLY:HA2	2:B:57:LEU:HG	1.99	0.45
2:B:212:PRO:O	2:B:216:GLU:HG3	2.16	0.45
2:A:242:ILE:C	2:A:244:ASN:H	2.25	0.45
1:D:16:C:C1'	2:B:33:GLY:HA3	2.46	0.45
2:B:277:LEU:HG	2:B:306:PHE:HE1	1.80	0.45
1:D:19:U:H2'	1:D:20:G:O4'	2.17	0.45
2:B:129:LYS:HE2	2:B:133:GLU:OE2	2.16	0.45
2:B:162:ARG:HB3	3:B:360:HOH:O	2.16	0.45
2:A:213:GLU:H	2:A:213:GLU:CD	2.20	0.45
2:B:63:LEU:HD11	2:B:228:TRP:CZ2	2.51	0.45
2:B:147:PHE:O	2:B:148:LYS:HB3	2.17	0.45
2:A:295:ARG:HB2	2:A:297:GLU:OE1	2.15	0.45
2:A:21:ASP:HA	2:A:24:ARG:CD	2.46	0.44
2:B:45:VAL:H	2:B:193:ARG:HB3	1.81	0.44
2:B:146:ILE:HD12	2:B:146:ILE:N	2.33	0.44
1:D:3:C:N4	1:D:4:C:N4	2.65	0.44
2:B:144:VAL:HB	2:B:169:THR:HG23	1.98	0.44
2:B:236:GLN:HG2	2:B:270:GLU:HB2	1.99	0.44
2:B:256:TRP:C	2:B:258:GLY:N	2.75	0.44
1:C:20:G:O2'	2:B:305:VAL:HG21	2.17	0.44
2:A:243:LEU:HD11	2:A:275:LEU:HG	1.98	0.44
2:A:111:ASP:HB3	2:A:141:PRO:HB2	1.98	0.44
2:A:128:TYR:O	2:A:132:ARG:HG3	2.18	0.44
2:B:214:GLU:HA	2:B:217:ASN:ND2	2.33	0.44
2:B:163:VAL:HG13	3:B:347:HOH:O	2.17	0.43
2:A:80:PHE:HB2	2:A:172:ARG:HD2	2.00	0.43
2:B:27:LEU:HD13	2:B:50:VAL:HG11	2.00	0.43
2:A:7:VAL:HB	3:A:315:HOH:O	2.17	0.43
2:A:15:THR:O	2:A:19:VAL:HG23	2.17	0.43
2:A:257:ASP:O	2:A:259:PHE:HD1	2.02	0.43
2:B:166:SER:HB2	2:B:167:PRO:HD2	2.00	0.43
2:B:232:VAL:HG12	2:B:256:TRP:O	2.19	0.43
2:A:90:ARG:HG3	3:A:368:HOH:O	2.18	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:U:O2'	1:C:20:G:H5'	2.19	0.43
2:B:6:LEU:C	2:B:6:LEU:HD22	2.44	0.43
2:B:304:LYS:HG3	2:B:305:VAL:H	1.84	0.43
2:B:308:THR:HG23	3:B:329:HOH:O	2.18	0.43
2:B:16:SER:HB2	2:B:38:LEU:O	2.19	0.43
2:B:63:LEU:HG	3:B:332:HOH:O	2.19	0.43
2:B:139:LEU:HB3	2:B:140:PRO:CD	2.41	0.43
2:A:78:GLU:CG	2:A:86:VAL:HB	2.49	0.43
2:A:247:GLN:HG3	2:A:298:ARG:NE	2.34	0.43
2:B:59:PHE:HE2	2:B:264:VAL:HG11	1.84	0.42
2:B:227:GLU:HG3	3:B:311:HOH:O	2.17	0.42
2:B:260:LYS:HB2	2:B:263:GLU:OE1	2.18	0.42
2:A:238:SER:HB2	2:A:252:MET:HE2	2.02	0.42
2:A:262:GLY:HA2	2:A:279:GLU:HG3	2.01	0.42
2:B:231:ARG:HG3	2:B:231:ARG:HH11	1.84	0.42
2:B:236:GLN:HB2	2:B:270:GLU:OE1	2.19	0.42
2:B:110:TYR:CE1	2:B:112:GLN:HB2	2.54	0.42
2:B:243:LEU:CD1	2:B:275:LEU:HG	2.47	0.42
3:D:25:HOH:O	2:B:34:HIS:HE1	2.02	0.42
2:A:256:TRP:HB2	3:A:326:HOH:O	2.19	0.42
2:B:47:ILE:HD11	2:B:196:VAL:HG21	2.02	0.42
2:B:21:ASP:HA	2:B:24:ARG:CD	2.50	0.42
2:B:38:LEU:HD23	2:B:39:ASP:N	2.34	0.42
2:A:235:HIS:O	2:A:237:GLU:N	2.53	0.42
2:A:251:GLU:HB2	2:A:296:GLN:CD	2.44	0.42
2:B:110:TYR:CE2	2:B:146:ILE:HD11	2.55	0.42
2:B:223:GLU:OE2	2:B:273:ARG:HA	2.20	0.42
2:B:267:VAL:O	2:B:275:LEU:HB2	2.19	0.42
2:A:3:HIS:CD2	2:A:308:THR:HG22	2.55	0.42
2:A:226:LEU:O	2:A:228:TRP:O	2.38	0.42
1:D:13:A:N1	2:B:34:HIS:N	2.67	0.42
2:A:29:THR:HG22	2:A:30:ARG:N	2.30	0.42
2:A:34:HIS:HB3	2:A:48:ILE:HD13	2.01	0.42
2:A:51:ASN:C	2:A:53:GLY:H	2.28	0.42
1:C:21:G:C5'	2:B:305:VAL:HB	2.46	0.41
2:A:64:LYS:HE2	2:A:147:PHE:CE2	2.54	0.41
2:A:69:VAL:HG22	2:A:70:LYS:N	2.35	0.41
2:B:135:LYS:HD2	2:B:135:LYS:N	2.28	0.41
2:A:285:SER:HA	3:A:327:HOH:O	2.19	0.41
2:B:232:VAL:HG11	2:B:259:PHE:CZ	2.55	0.41
2:A:9:TYR:HB2	2:A:204:SER:OG	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:145:LYS:H	2:B:145:LYS:CD	2.24	0.41
1:C:10:FHU:N3	2:A:39:ASP:OD2	2.51	0.41
1:C:16:C:H5'	2:A:32:VAL:O	2.21	0.41
2:A:65:LYS:HE3	3:A:384:HOH:O	2.21	0.41
2:A:80:PHE:N	2:A:80:PHE:CD1	2.89	0.41
2:A:20:VAL:HG13	2:A:32:VAL:CG1	2.50	0.41
2:A:270:GLU:C	2:A:272:GLY:H	2.28	0.41
2:A:129:LYS:HE2	2:A:133:GLU:OE2	2.21	0.41
2:B:235:HIS:C	2:B:237:GLU:H	2.29	0.40
2:A:299:VAL:O	2:A:300:LEU:HD23	2.22	0.40
2:B:194:GLU:HA	2:B:201:ILE:HB	2.02	0.40
2:B:195:SER:HA	2:B:199:HIS:O	2.20	0.40
1:C:9:U:H5''	3:C:35:HOH:O	2.20	0.40
2:A:38:LEU:HD22	2:A:42:ALA:HB3	2.02	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	296/309 (96%)	251 (85%)	39 (13%)	6 (2%)	6	28
2	B	208/309 (67%)	155 (74%)	39 (19%)	14 (7%)	1	5
All	All	504/618 (82%)	406 (81%)	78 (16%)	20 (4%)	2	14

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	200	THR
2	A	236	GLN
2	A	258	GLY
2	B	193	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	204	SER
2	B	258	GLY
2	B	261	LYS
2	A	222	LEU
2	B	40	PRO
2	B	109	GLU
2	B	244	ASN
2	B	259	PHE
2	B	229	LEU
2	B	260	LYS
2	A	246	SER
2	A	52	GLN
2	A	229	LEU
2	B	31	LYS
2	B	230	PRO
2	B	56	ILE

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	264/273 (97%)	245 (93%)	19 (7%)	13	43
2	B	191/273 (70%)	182 (95%)	9 (5%)	23	58
All	All	455/546 (83%)	427 (94%)	28 (6%)	16	49

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	A	29	THR
2	A	38	LEU
2	A	78	GLU
2	A	82	ILE
2	A	89	GLU
2	A	93	ASN
2	A	135	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	A	144	VAL
2	A	145	LYS
2	A	160	SER
2	A	174	LEU
2	A	181	LYS
2	A	204	SER
2	A	209	GLU
2	A	222	LEU
2	A	227	GLU
2	A	257	ASP
2	A	275	LEU
2	A	308	THR
2	B	6	LEU
2	B	37	THR
2	B	55	ARG
2	B	110	TYR
2	B	145	LYS
2	B	202	GLU
2	B	218	ARG
2	B	236	GLN
2	B	249	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
2	A	34	HIS
2	A	93	ASN
2	A	296	GLN
2	B	112	GLN
2	B	199	HIS
2	B	206	ASN
2	B	217	ASN
2	B	307	GLN

5.3.3 RNA ⓘ

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	21/22 (95%)	4 (19%)	2 (9%)
1	D	21/22 (95%)	7 (33%)	3 (14%)
All	All	42/44 (95%)	11 (26%)	5 (11%)

All (11) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
1	C	10	FHU
1	C	12	G
1	C	13	A
1	C	14	A
1	D	9	U
1	D	10	FHU
1	D	11	C
1	D	12	G
1	D	13	A
1	D	14	A
1	D	15	U

All (5) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
1	C	12	G
1	C	13	A
1	D	11	C
1	D	12	G
1	D	13	A

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

2 non-standard protein/DNA/RNA residues are 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	$\# Z > 2$
1	FHU	C	10	1	16,23,24	3.58	4 (25%)	18,35,38	2.67	5 (27%)
1	FHU	D	10	1	16,23,24	3.62	4 (25%)	18,35,38	2.68	4 (22%)

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
1	FHU	C	10	1	-	0/3/47/48	0/2/2/2
1	FHU	D	10	1	-	2/3/47/48	0/2/2/2

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	10	FHU	O4-C4	11.67	1.43	1.22
1	C	10	FHU	O4-C4	11.56	1.43	1.22
1	D	10	FHU	C4-N3	6.71	1.48	1.37
1	C	10	FHU	C4-N3	6.49	1.47	1.37
1	D	10	FHU	F5-C5	-3.65	1.33	1.39
1	C	10	FHU	F5-C5	-3.53	1.33	1.39
1	C	10	FHU	C2-N1	3.15	1.40	1.34
1	D	10	FHU	C2-N1	2.92	1.40	1.34

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	10	FHU	O4-C4-N3	-7.10	109.09	120.59
1	D	10	FHU	O4-C4-N3	-6.96	109.31	120.59
1	D	10	FHU	C5-C4-N3	-5.98	110.51	116.74
1	C	10	FHU	C5-C4-N3	-5.65	110.85	116.74
1	D	10	FHU	N3-C2-N1	4.56	120.64	116.06
1	C	10	FHU	N3-C2-N1	4.42	120.50	116.06
1	D	10	FHU	C4-N3-C2	-3.44	120.90	126.04
1	C	10	FHU	C4-N3-C2	-3.40	120.96	126.04
1	C	10	FHU	O2'-C2'-C1'	-2.24	107.31	112.78

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	D	10	FHU	O4'-C4'-C5'-O5'
1	D	10	FHU	C3'-C4'-C5'-O5'

There are no ring outliers.

2 monomers are involved in 8 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	10	FHU	4	0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	10	FHU	4	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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, 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	21/22 (95%)	0.95	5 (23%) 2 1	25, 35, 81, 98	0
1	D	21/22 (95%)	2.00	8 (38%) 1 1	45, 61, 99, 99	0
2	A	300/309 (97%)	0.33	20 (6%) 24 12	13, 39, 88, 100	1 (0%)
2	B	218/309 (70%)	2.18	117 (53%) 0 0	36, 92, 100, 100	0
All	All	560/662 (84%)	1.14	150 (26%) 1 1	13, 57, 100, 100	1 (0%)

All (150) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	269	ASN	6.9
2	A	299	VAL	6.4
1	D	1	G	6.0
2	B	67	TYR	4.4
2	B	65	LYS	4.3
1	D	2	G	4.3
2	B	225	CYS	4.2
2	B	268	PHE	4.1
2	B	38	LEU	4.1
2	B	226	LEU	4.1
2	B	198	PRO	4.0
2	B	257	ASP	4.0
2	B	304	LYS	3.9
2	B	275	LEU	3.9
2	B	201	ILE	3.9
2	B	196	VAL	3.8
2	B	195	SER	3.8
2	B	66	VAL	3.8
2	B	234	VAL	3.7
2	B	37	THR	3.7
2	B	116	ALA	3.6

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	259	PHE	3.5
2	B	235	HIS	3.5
2	A	282	ARG	3.5
2	B	36	GLY	3.5
2	B	61	LYS	3.5
2	B	119	ALA	3.5
2	B	276	ALA	3.4
2	A	260	LYS	3.4
2	B	244	ASN	3.3
2	B	57	LEU	3.3
2	B	222	LEU	3.3
2	B	168	GLY	3.3
2	B	140	PRO	3.3
2	B	230	PRO	3.3
2	B	264	VAL	3.3
2	B	253	LEU	3.2
2	B	32	VAL	3.2
1	D	3	C	3.2
2	A	256	TRP	3.2
2	B	227	GLU	3.1
2	B	167	PRO	3.1
2	B	16	SER	3.1
2	B	273	ARG	3.1
2	B	274	LEU	3.1
2	A	259	PHE	3.1
2	B	149	ILE	3.1
2	B	246	SER	3.0
2	B	228	TRP	3.0
1	C	1	G	3.0
2	A	245	GLY	3.0
2	B	308	THR	3.0
1	D	13	A	3.0
2	B	42	ALA	3.0
2	B	238	SER	3.0
2	B	13	GLY	3.0
2	B	267	VAL	3.0
2	B	306	PHE	3.0
2	B	200	THR	3.0
2	B	272	GLY	2.9
2	B	47	ILE	2.9
2	B	41	PHE	2.9
2	B	8	ALA	2.9

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	5	ILE	2.9
2	B	131	ALA	2.9
2	B	223	GLU	2.9
2	B	203	GLU	2.8
2	B	118	SER	2.8
2	B	163	VAL	2.8
2	B	232	VAL	2.8
2	A	286	PHE	2.8
2	B	307	GLN	2.8
2	B	15	THR	2.8
2	A	308	THR	2.8
2	B	164	GLU	2.8
2	A	239	THR	2.7
2	B	7	VAL	2.7
2	B	248	ILE	2.6
2	B	214	GLU	2.6
2	B	197	GLY	2.6
2	B	216	GLU	2.6
2	B	29	THR	2.6
2	B	23	VAL	2.6
2	B	233	VAL	2.6
2	B	108	GLY	2.6
2	A	281	GLU	2.6
2	B	239	THR	2.6
2	B	63	LEU	2.6
2	B	263	GLU	2.6
2	B	258	GLY	2.5
2	B	138	ASN	2.5
2	B	219	ILE	2.5
1	D	11	C	2.5
2	B	283	ASN	2.5
2	B	128	TYR	2.5
2	B	125	GLU	2.5
2	B	46	LEU	2.5
2	A	258	GLY	2.5
2	B	124	GLY	2.4
2	B	24	ARG	2.4
1	C	22	C	2.4
2	B	45	VAL	2.4
2	A	58	GLU	2.4
1	C	6	C	2.3
2	B	9	TYR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	A	280	ALA	2.3
2	B	48	ILE	2.3
2	B	249	HIS	2.3
2	B	112	GLN	2.3
2	B	134	GLY	2.3
2	B	305	VAL	2.3
2	B	221	PRO	2.3
2	B	204	SER	2.3
1	C	21	G	2.3
2	B	192	VAL	2.3
1	D	19	U	2.3
2	B	265	VAL	2.3
2	B	133	GLU	2.2
2	B	199	HIS	2.2
2	B	121	LYS	2.2
2	B	135	LYS	2.2
2	A	257	ASP	2.2
1	C	2	G	2.2
2	B	117	TYR	2.2
2	B	303	ARG	2.2
2	B	115	PRO	2.2
2	A	285	SER	2.2
2	B	136	ILE	2.2
2	B	212	PRO	2.2
2	B	256	TRP	2.2
1	D	4	C	2.1
2	B	148	LYS	2.1
2	A	97	GLU	2.1
2	A	295	ARG	2.1
2	B	142	LYS	2.1
2	B	231	ARG	2.1
1	D	22	C	2.1
2	A	255	GLU	2.1
2	A	270	GLU	2.1
2	B	245	GLY	2.1
2	B	17	HIS	2.1
2	B	240	LYS	2.1
2	B	120	LYS	2.1
2	B	171	ILE	2.1
2	B	207	VAL	2.0
2	B	162	ARG	2.0
2	A	284	SER	2.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	40	PRO	2.0
2	B	281	GLU	2.0
2	B	137	ILE	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	FHU	D	10	22/23	0.82	0.18	67,82,85,85	0
1	FHU	C	10	22/23	0.92	0.12	28,34,38,40	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.