W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:04 AM GMT

|		
PDB ID	:	1ZE2
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)

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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 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.
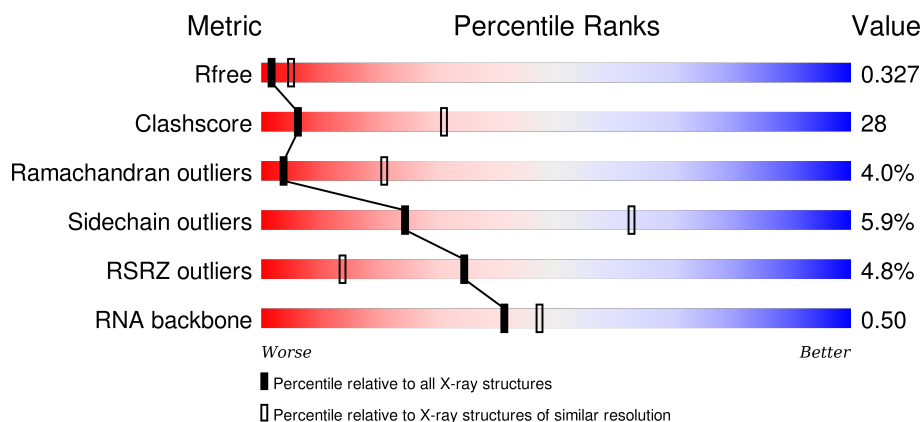
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)
RNA backbone	2183	1036 (3.40-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	
1	D	22	
2	A	309	
2	B	309	

2 Entry composition (i)

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*CP*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	A	81	Total	O	0	0
			81	81		
3	B	58	Total	O	0	0
			58	58		
3	C	29	Total	O	0	0
			29	29		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	D	20	Total 20	O 20	0	0

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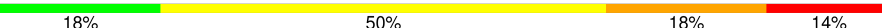
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according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

• Molecule 1: 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'

Chain C:

• 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'

Chain D:

• Molecule 2: tRNA pseudouridine synthase B

Chain A:

• Molecule 2: tRNA pseudouridine synthase B

Chain B:
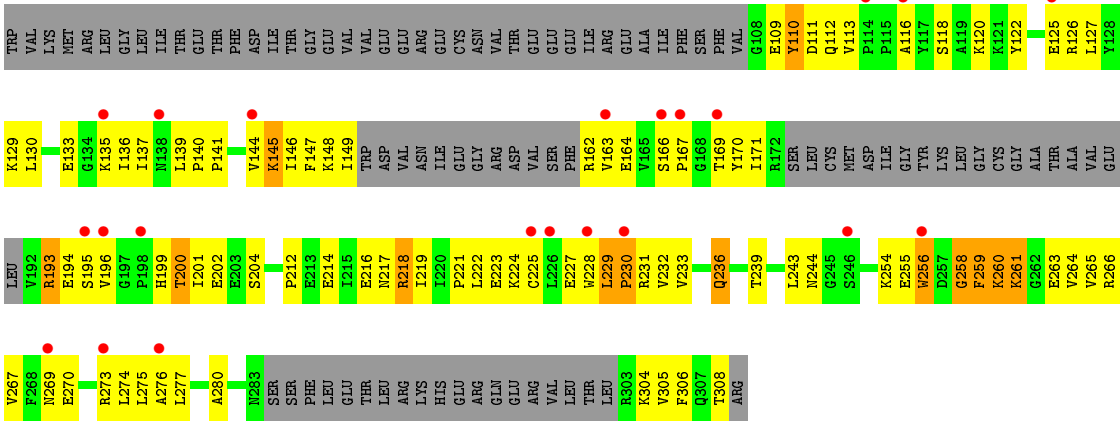
4 Data and refinement statistics (i)

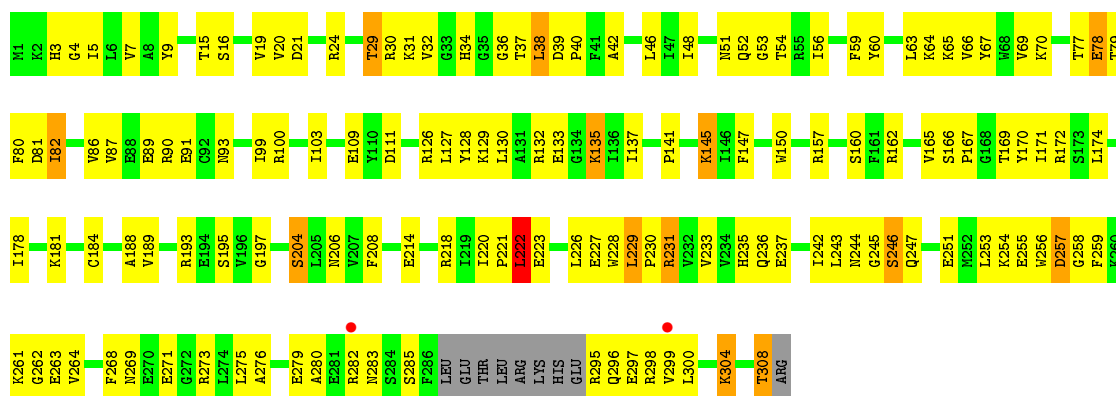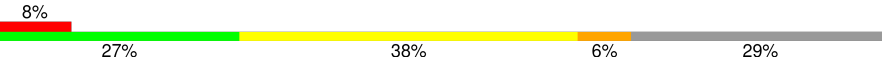| Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, α, β, γ	134.97Å 134.97Å 139.54Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 3.00 47.72 – 2.90	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-3.00) 97.3 (47.72-2.90)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	5.98 (at 2.91Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.261 , 0.318 0.267 , 0.327	Depositor DCC
R_{free} test set	2110 reflections (8.89%)	DCC
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 , 66.3	EDS
Estimated twinning fraction	0.016 for -h,l,k 0.008 for -l,-k,-h	Xtriage
L-test for twinning [2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Outliers	3 of 29041 reflections (0.010%)	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.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.62	0/499	1.16	8/777 (1.0%)
1	D	0.56	0/499	1.12	5/777 (0.6%)
2	A	0.50	0/2461	0.68	0/3314
2	B	0.36	0/1792	0.58	0/2405
All	All	0.48	0/5251	0.77	13/7273 (0.2%)

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

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	14	A	C2'-C3'-O3'	8.93	129.14	109.50
1	C	14	A	C4'-C3'-C2'	6.57	109.17	102.60
1	C	12	G	N9-C1'-C2'	6.40	122.31	114.00
1	D	13	A	C4'-C3'-C2'	6.36	108.96	102.60
1	C	15	U	C5'-C4'-C3'	-6.29	105.94	116.00
1	C	13	A	C4'-C3'-C2'	6.21	108.81	102.60
1	C	14	A	C4'-C3'-O3'	6.17	125.34	113.00
1	D	12	G	C2'-C3'-O3'	6.15	123.54	113.70
1	D	13	A	C2'-C3'-O3'	6.14	123.52	113.70
1	C	9	U	N1-C1'-C2'	6.01	121.81	114.00
1	C	13	A	C2'-C3'-O3'	5.73	122.88	113.70
1	D	14	A	C4'-C3'-C2'	5.53	108.13	102.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	14	A	C2'-C3'-O3'	5.49	122.49	113.70

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
1	D	469	0	241	26	0
2	A	2416	0	2477	114	0
2	B	1760	0	1831	145	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	278	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 28.

All (278) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:B:193:ARG:HD2	2:B:196:VAL:HG22	1.74	0.69
2:A:82:ILE:HD13	2:A:189:VAL:HG13	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:299:VAL:HG23	2:A:300:LEU:HG	1.78	0.64
2:A:214:GLU:O	2:A:218:ARG:HG2	1.98	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:29:THR:HG21	2:B:51:ASN:OD1	1.99	0.62
2:A:15:THR:HG22	2:A:40:PRO:HG3	1.79	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:231:ARG:HB3	2:B:266:ARG:CZ	2.31	0.61
2:B:31:LYS:HB3	2:B:51:ASN:HA	1.81	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: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
2:B:228:TRP:CD1	2:B:229:LEU:HG	2.36	0.61
1:D:16:C:H2'	1:D:17:C:O4'	2.00	0.61
2:A:218:ARG:HH11	2:A:218:ARG:HA	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
2:B:233:VAL:HG12	2:B:255:GLU:HB3	1.84	0.59
2:B:304:LYS:HG3	2:B:305:VAL:N	2.20	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
2:A:253:LEU:HD11	2:A:299:VAL:HG21	1.87	0.57
1:D:4:C:H2'	1:D:5:A:H8	1.70	0.57
2:B:116:ALA:HB2	2:B:136:ILE:HG23	1.88	0.56
2:B:45:VAL:HG21	2:B:200:THR:O	2.05	0.56
2:B:120:LYS:HB2	2:B:127:LEU:CD1	2.35	0.56
1:D:11:C:H5"	3:B:362:HOH:O	2.05	0.56
2:B:239:THR:HG21	3:B:328:HOH:O	2.06	0.56
2:B:118:SER:O	2:B:127:LEU:HB2	2.04	0.56
2:A:99:ILE:O	2:A:103:ILE:HG12	2.06	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:55:ARG:NH1	2:B:304:LYS:HD2	2.21	0.55
2:B:62:ASP:HB2	3:B:332:HOH:O	2.06	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:A:226:LEU:HB3	2:A:229:LEU:HD12	1.89	0.54
1:D:9:U:O4'	2:B:61:LYS:HE3	2.08	0.54
2:B:6:LEU:O	2:B:6:LEU:HD13	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
2:A:66:VAL:HB	2:A:195:SER:OG	2.09	0.53
1:C:16:C:H2'	1:C:17:C:H6	1.74	0.53
2:B:223:GLU:CD	2:B:273:ARG:HA	2.29	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:116:ALA:CB	2:B:136:ILE:HG23	2.39	0.52
2:B:21:ASP:HA	2:B:24:ARG:HD3	1.91	0.52
2:A:269:ASN:HD21	2:A:271:GLU:HG2	1.73	0.52
2:B:47:ILE:N	2:B:47:ILE:HD12	2.18	0.51
2:B:63:LEU:HD11	2:B:228:TRP:CH2	2.45	0.51
2:A:31:LYS:HG2	3:A:331:HOH:O	2.10	0.51
2:B:228:TRP:O	2:B:229:LEU:HB2	2.11	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:A:228:TRP:O	2:A:229:LEU:HB2	2.10	0.51
2:A:145:LYS:HG2	2:A:166:SER:CB	2.39	0.51
1:D:17:C:H2'	1:D:18:G:H8	1.75	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
2:B:261:LYS:C	2:B:263:GLU:H	2.14	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:D:12:G:H22	2:B:40:PRO:HG2	1.77	0.50
1:C:22:C:H2'	1:D:1:G:H1'	1.94	0.50
2:B:47:ILE:H	2:B:47:ILE:CD1	2.21	0.50
2:A:243:LEU:HD21	2:A:273:ARG:NH2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:277:LEU:HG	2:B:306:PHE:CE1	2.47	0.50
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
2:A:21:ASP:HA	2:A:24:ARG:HD2	1.93	0.49
1:C:10:FHU:HN1	2:A:171:ILE:N	2.06	0.49
2:B:29:THR:CG2	2:B:31:LYS:HB2	2.42	0.49
1:C:13:A:O2'	1:C:15:U:OP2	2.30	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:B:233:VAL:O	2:B:254:LYS:HB3	2.13	0.49
2:A:4:GLY:HA3	2:A:220:ILE:O	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:B:20:VAL:HG13	2:B:32:VAL:HG12	1.95	0.48
2:A:150:TRP:NE1	2:A:162:ARG:HD2	2.28	0.48
2:A:109:GLU:CG	2:A:145:LYS:HB3	2.38	0.48
2:A:51:ASN:O	2:A:53:GLY:N	2.46	0.48
2:B:113:VAL:HG13	2:B:139:LEU:O	2.14	0.48
2:B:55:ARG:HH12	2:B:304:LYS:HD2	1.78	0.48
2:A:90:ARG:HD2	2:A:184:CYS:O	2.13	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:B:125:GLU:CD	2:B:130:LEU:HD21	2.34	0.47
2:A:16:SER:HB2	2:A:37:THR:HG23	1.95	0.47
2:B:145:LYS:C	2:B:146:ILE:HD12	2.35	0.47
2:B:9:TYR:HA	2:B:44:GLY:O	2.13	0.47
2:A:256:TRP:O	2:A:257:ASP:HB2	2.14	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:B:147:PHE:CD2	2:B:164:GLU:HG2	2.43	0.47
1:D:10:FHU:N1	2:B:170:TYR:HA	2.28	0.47
2:A:79:THR:O	2:A:80:PHE:HB2	2.15	0.47
2:A:20:VAL:HG13	2:A:32:VAL:HG12	1.96	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
2:A:165:VAL:HG21	2:A:169:THR:CG2	2.36	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:D:17:C:H2'	1:D:18:G:C8	2.50	0.46
1:D:14:A:H5'	1:D:15:U:OP2	2.16	0.46
2:A:135:LYS:HE3	3:A:356:HOH:O	2.15	0.46
2:A:77:THR:HG22	2:A:87:VAL:HG12	1.96	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:B:50:VAL:HG12	2:B:51:ASN:HD22	1.80	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:A:166:SER:HB2	2:A:167:PRO:HD2	1.98	0.46
2:A:229:LEU:HA	2:A:230:PRO:HD3	1.83	0.46
2:B:125:GLU:OE1	2:B:130:LEU:HD11	2.15	0.46
2:B:4:GLY:O	2:B:53:GLY:HA3	2.16	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: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:A:78:GLU:CD	2:A:78:GLU:H	2.16	0.45
2:B:122:TYR:CD2	2:B:137:ILE:HD13	2.51	0.45
2:B:212:PRO:O	2:B:216:GLU:HG3	2.16	0.45
2:B:35:GLY:HA2	2:B:57:LEU:HG	1.99	0.45
2:A:261:LYS:C	2:A:263:GLU:H	2.20	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
2:B:129:LYS:HE2	2:B:133:GLU:OE2	2.16	0.45
1:D:19:U:H2'	1:D:20:G:O4'	2.17	0.45
2:B:162:ARG:HB3	3:B:360:HOH:O	2.16	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:B:45:VAL:H	2:B:193:ARG:HB3	1.81	0.44
2:B:146:ILE:N	2:B:146:ILE:HD12	2.33	0.44
2:A:21:ASP:HA	2:A:24:ARG:CD	2.46	0.44
1:D:3:C:N4	1:D:4:C:N4	2.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:236:GLN:HG2	2:B:270:GLU:HB2	1.99	0.44
2:B:144:VAL:HB	2:B:169:THR:HG23	1.98	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:B:256:TRP:C	2:B:258:GLY:H	2.21	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:15:THR:O	2:A:19:VAL:HG23	2.17	0.43
2:B:232:VAL:HG12	2:B:256:TRP:O	2.19	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:A:7:VAL:HB	3:A:315:HOH:O	2.17	0.43
2:A:90:ARG:HG3	3:A:368:HOH:O	2.18	0.43
1:C:19:U:O2'	1:C:20:G:H5'	2.19	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:139:LEU:HB3	2:B:140:PRO:CD	2.41	0.43
2:B:63:LEU:HG	3:B:332:HOH:O	2.19	0.43
2:B:16:SER:HB2	2:B:38:LEU:O	2.19	0.43
2:A:247:GLN:HG3	2:A:298:ARG:NE	2.34	0.43
2:A:78:GLU:CG	2:A:86:VAL:HB	2.49	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:221:PRO:O	2:A:222:LEU:C	2.58	0.42
2:A:262:GLY:HA2	2:A:279:GLU:HG3	2.01	0.42
2:B:231:ARG:HH11	2:B:231:ARG:HG3	1.84	0.42
2:B:236:GLN:HB2	2:B:270:GLU:OE1	2.19	0.42
2:B:243:LEU:CD1	2:B:275:LEU:HG	2.47	0.42
2:B:110:TYR:CE1	2:B:112:GLN:HB2	2.54	0.42
2:B:47:ILE:HD11	2:B:196:VAL:HG21	2.02	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:110:TYR:CE2	2:B:146:ILE:HD11	2.55	0.42
2:A:235:HIS:O	2:A:237:GLU:N	2.53	0.42
2:A:226:LEU:O	2:A:228:TRP:O	2.38	0.42
2:A:3:HIS:CD2	2:A:308:THR:HG22	2.55	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
1:D:13:A:N1	2:B:34:HIS:N	2.67	0.42
1:C:21:G:C5'	2:B:305:VAL:HB	2.46	0.41
2:B:135:LYS:N	2:B:135:LYS:HD2	2.28	0.41
2:A:69:VAL:HG22	2:A:70:LYS:N	2.35	0.41
2:A:64:LYS:HE2	2:A:147:PHE:CE2	2.54	0.41
2:B:232:VAL:HG11	2:B:259:PHE:CZ	2.55	0.41
2:A:285:SER:HA	3:A:327:HOH:O	2.19	0.41
2:B:145:LYS:H	2:B:145:LYS:CD	2.24	0.41
2:A:9:TYR:HB2	2:A:204:SER:OG	2.20	0.41
1:C:10:FHU:N3	2:A:39:ASP:OD2	2.51	0.41
2:A:51:ASN:C	2:A:53:GLY:N	2.74	0.41
1:C:16:C:H5'	2:A:32:VAL:O	2.21	0.41
2:A:80:PHE:CD1	2:A:80:PHE:N	2.89	0.41
2:A:65:LYS:HE3	3:A:384:HOH:O	2.21	0.41
2:A:20:VAL:HG13	2:A:32:VAL:CG1	2.50	0.41
2:A:129:LYS:HE2	2:A:133:GLU:OE2	2.21	0.41
2:A:242:ILE:C	2:A:244:ASN:H	2.25	0.41
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
2:A:38:LEU:HD22	2:A:42:ALA:HB3	2.02	0.40
1:C:9:U:H5"	3:C:35:HOH:O	2.20	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	296/309 (96%)	251 (85%)	39 (13%)	6 (2%)	9	41
2	B	208/309 (67%)	155 (74%)	39 (19%)	14 (7%)	1	8
All	All	504/618 (82%)	406 (81%)	78 (16%)	20 (4%)	4	21

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
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 (i)

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%)	246 (93%)	18 (7%)	20	56
2	B	191/273 (70%)	182 (95%)	9 (5%)	32	72
All	All	455/546 (83%)	428 (94%)	27 (6%)	24	63

All (27) 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
2	A	145	LYS
2	A	160	SER
2	A	174	LEU
2	A	181	LYS
2	A	204	SER
2	A	222	LEU
2	A	227	GLU
2	A	231	ARG
2	A	257	ASP
2	A	304	LYS
2	A	308	THR
2	B	6	LEU
2	B	37	THR
2	B	110	TYR
2	B	126	ARG
2	B	145	LYS
2	B	202	GLU
2	B	218	ARG
2	B	236	GLN
2	B	256	TRP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

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

5.3.3 RNA (i)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
1	C	21/22 (95%)	4 (19%)	2 (9%)
1	D	21/22 (95%)	6 (28%)	3 (14%)
All	All	42/44 (95%)	10 (23%)	5 (11%)

All (10) 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	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	15,23,24	3.42	3 (20%)	17,35,38	2.55	5 (29%)
1	FHU	D	10	1	15,23,24	3.46	3 (20%)	17,35,38	2.53	4 (23%)

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	-	0/3/47/48	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	10	FHU	C2-N1	2.36	1.40	1.34
1	C	10	FHU	C2-N1	2.55	1.40	1.34
1	C	10	FHU	C4-N3	6.14	1.47	1.37
1	D	10	FHU	C4-N3	6.36	1.48	1.37
1	C	10	FHU	O4-C4	11.07	1.43	1.22
1	D	10	FHU	O4-C4	11.18	1.43	1.22

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	10	FHU	O4-C4-N3	-6.76	109.09	120.50
1	D	10	FHU	O4-C4-N3	-6.63	109.31	120.50
1	D	10	FHU	C4-N3-C2	-3.40	120.90	126.00
1	C	10	FHU	C4-N3-C2	-3.36	120.96	126.00
1	C	10	FHU	O2'-C2'-C1'	-2.16	107.31	112.90
1	C	10	FHU	N3-C2-N1	3.98	120.50	116.14
1	D	10	FHU	N3-C2-N1	4.11	120.64	116.14
1	D	10	FHU	F5-C5-C6	4.90	109.69	102.84
1	C	10	FHU	F5-C5-C6	5.11	109.98	102.84

There are no chirality outliers.

There are no torsion outliers.

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
1	D	10	FHU	4	0

5.5 Carbohydrates (i)

There are no carbohydrates 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 (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	21/22 (95%)	0.10	0	100	100	25, 35, 81, 98	0
1	D	21/22 (95%)	0.43	0	100	100	45, 61, 99, 99	0
2	A	300/309 (97%)	-0.29	2 (0%)	89	70	13, 39, 88, 100	1 (0%)
2	B	218/309 (70%)	0.75	25 (11%)	6	2	36, 92, 100, 100	0
All	All	560/662 (84%)	0.16	27 (4%)	34	14	13, 57, 100, 100	1 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	269	ASN	5.1
2	B	65	LYS	3.9
2	B	116	ALA	3.9
2	B	163	VAL	3.6
2	B	167	PRO	3.4
2	B	125	GLU	3.2
2	B	225	CYS	3.0
2	B	246	SER	2.8
2	B	45	VAL	2.8
2	B	195	SER	2.8
2	A	282	ARG	2.8
2	B	138	ASN	2.7
2	B	166	SER	2.6
2	B	67	TYR	2.5
2	B	114	PRO	2.5
2	B	144	VAL	2.5
2	B	196	VAL	2.4
2	B	228	TRP	2.4
2	B	273	ARG	2.3
2	B	198	PRO	2.3
2	B	256	TRP	2.3

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Mol	Chain	Res	Type	RSRZ
2	A	299	VAL	2.3
2	B	230	PRO	2.3
2	B	276	ALA	2.1
2	B	169	THR	2.1
2	B	226	LEU	2.0
2	B	135	LYS	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors($Å^2$)	Q<0.9
1	FHU	D	10	22/23	0.86	0.21	-	67,82,85,85	0
1	FHU	C	10	22/23	0.95	0.20	-	28,34,38,40	0

6.3 Carbohydrates (i)

There are no carbohydrates 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.