



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 16, 2024 – 08:33 PM EDT

PDB ID : 2XO4  
Title : RIBONUCLEOTIDE REDUCTASE Y730NH2Y MODIFIED R1 SUBUNIT OF E. COLI  
Authors : Minnihan, E.C.; Seyedsayamdost, M.R.; Uhlin, U.; Stubbe, J.  
Deposited on : 2010-08-09  
Resolution : 2.50 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 2.37.1  
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) : 2.37.1

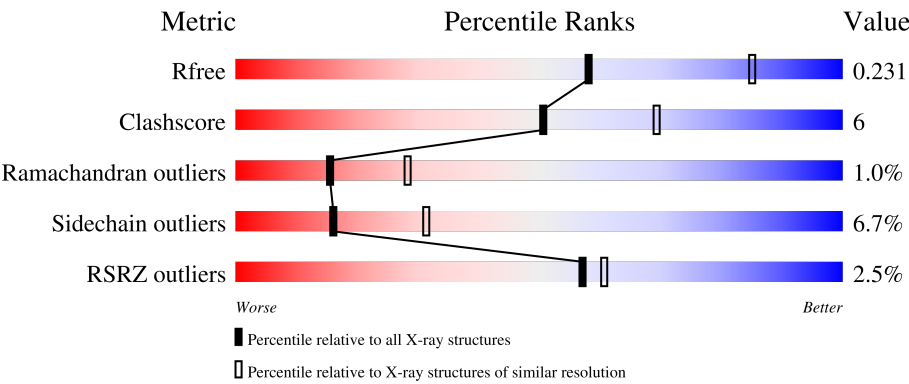
# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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 <sub>free</sub>	130704	4661 (2.50-2.50)
Clashscore	141614	5346 (2.50-2.50)
Ramachandran outliers	138981	5231 (2.50-2.50)
Sidechain outliers	138945	5233 (2.50-2.50)
RSRZ outliers	127900	4559 (2.50-2.50)

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

Mol	Chain	Length	Quality of chain
1	A	761	<div><div>3%</div><div><div></div><div>82%</div><div>11%</div><div>• •</div></div></div>
1	B	761	<div><div>2%</div><div><div></div><div>81%</div><div>14%</div><div>• •</div></div></div>
1	C	761	<div><div>%</div><div><div></div><div>82%</div><div>13%</div><div>• •</div></div></div>
2	D	20	<div><div>15%</div><div><div></div><div>60%</div><div>15%</div><div>5%</div><div>20%</div></div></div>
2	E	20	<div><div>10%</div><div><div></div><div>55%</div><div>20%</div><div>5%</div><div>20%</div></div></div>

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Mol	Chain	Length	Quality of chain
2	F	20	 10% 60% 20%
2	P	20	 5% 10% 85%

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18959 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	734	Total	C	N	O	S	0	0	0
			5846	3712	1005	1105	24			
1	B	734	Total	C	N	O	S	0	0	0
			5846	3712	1005	1105	24			
1	C	734	Total	C	N	O	S	0	0	0
			5846	3712	1005	1105	24			

- Molecule 2 is a protein called RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	16	Total	C	N	O	0	0	0
			129	77	19	33			
2	E	16	Total	C	N	O	0	0	0
			129	77	19	33			
2	F	16	Total	C	N	O	0	0	0
			129	77	19	33			
2	P	3	Total	C	N	O	0	0	0
			27	20	3	4			

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	287	Total	O	0	0
			287	287		
3	B	306	Total	O	0	0
			306	306		
3	C	400	Total	O	0	0
			400	400		
3	D	4	Total	O	0	0
			4	4		

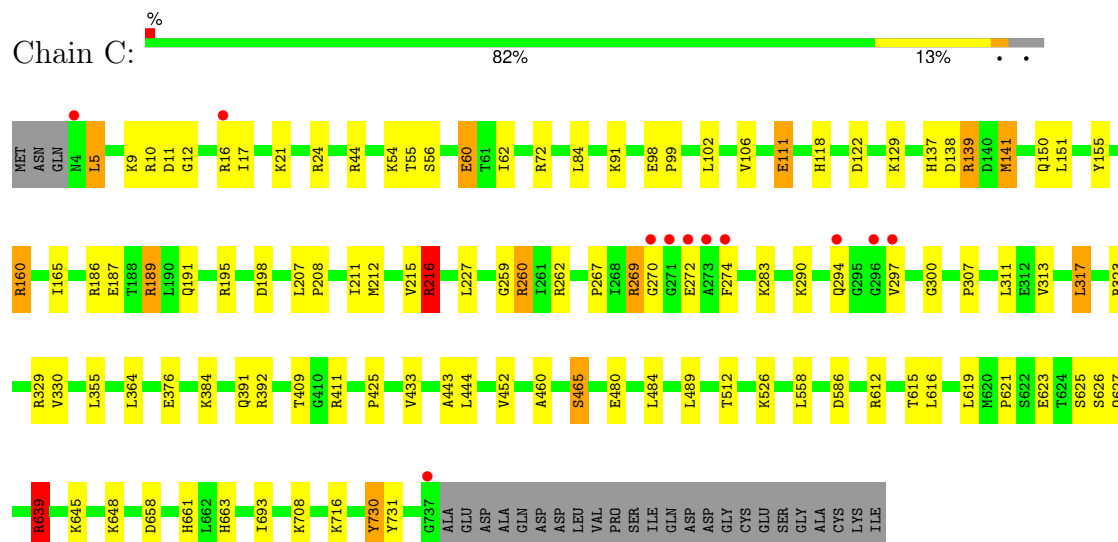
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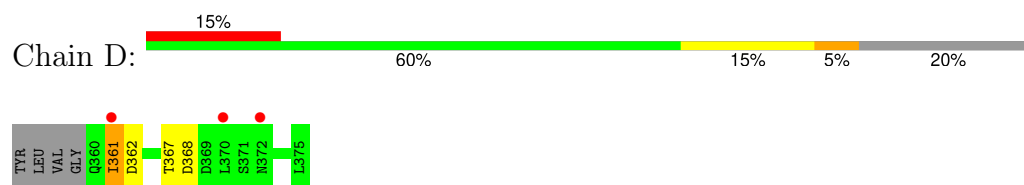
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	3	Total 3	O 3	0	0
3	F	4	Total 4	O 4	0	0
3	P	3	Total 3	O 3	0	0



- Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT ALPHA



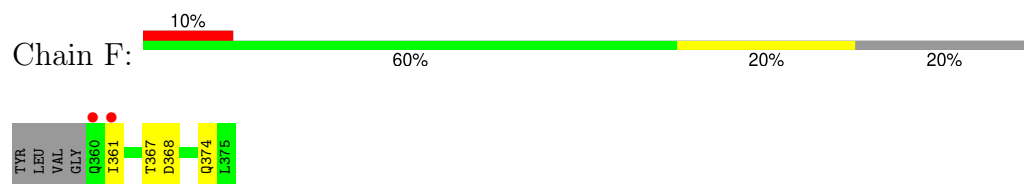
- Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA



- Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA



- Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA



- Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	224.59Å 224.59Å 336.72Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	169.03 – 2.50 84.21 – 2.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (169.03-2.50) 98.7 (84.21-2.50)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.15 (at 2.51Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.188 , 0.233 0.187 , 0.231	Depositor DCC
$R_{free}$ test set	5539 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.4	Xtriage
Anisotropy	0.083	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 45.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	18959	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.21% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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



## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TY2

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
1	A	0.43	0/5959	0.57	0/8069
1	B	0.43	0/5959	0.56	0/8069
1	C	0.49	0/5959	0.60	2/8069 (0.0%)
2	D	0.42	0/129	0.56	0/173
2	E	0.41	0/129	0.61	0/173
2	F	0.44	0/129	0.61	0/173
2	P	0.58	0/27	0.63	0/36
All	All	0.45	0/18291	0.58	2/24762 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	216	ARG	NE-CZ-NH2	-5.91	117.35	120.30
1	C	639	ARG	NE-CZ-NH1	5.01	122.80	120.30

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5846	0	5769	76	0
1	B	5846	0	5769	63	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	5846	0	5769	60	0
2	D	129	0	111	3	0
2	E	129	0	111	3	0
2	F	129	0	111	1	0
2	P	27	0	31	2	0
3	A	287	0	0	17	0
3	B	306	0	0	17	0
3	C	400	0	0	21	0
3	D	4	0	0	0	0
3	E	3	0	0	0	0
3	F	4	0	0	1	0
3	P	3	0	0	2	0
All	All	18959	0	17671	202	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 6.

All (202) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:623:GLU:HG2	3:B:2088:HOH:O	1.53	1.07
1:A:10:ARG:HH11	1:A:10:ARG:HG3	1.28	0.98
1:C:639:ARG:HH11	1:C:639:ARG:HG3	1.34	0.92
1:A:294:GLN:HG3	1:A:295:GLY:N	1.85	0.90
1:B:450:ASN:HB2	3:B:2187:HOH:O	1.74	0.86
1:A:221:GLN:HE22	1:B:271:GLY:HA3	1.42	0.85
1:B:733:ASN:HB3	3:B:2301:HOH:O	1.78	0.81
1:B:212:MET:O	1:B:216:ARG:NH2	2.13	0.81
1:C:480:GLU:HB3	3:C:2121:HOH:O	1.82	0.79
1:B:209:THR:HG23	3:B:2061:HOH:O	1.82	0.79
1:B:215:VAL:O	1:B:216:ARG:HB3	1.82	0.79
1:B:262:ARG:HD2	1:B:274:PHE:HB3	1.65	0.79
1:A:24:ARG:CG	1:A:24:ARG:HH11	1.95	0.78
1:C:10:ARG:HG2	3:C:2009:HOH:O	1.81	0.78
1:A:24:ARG:HH11	1:A:24:ARG:HG2	1.52	0.74
1:A:294:GLN:HG3	1:A:295:GLY:H	1.51	0.73
1:C:212:MET:O	1:C:216:ARG:NH2	2.20	0.73
1:C:272:GLU:OE2	3:C:2167:HOH:O	2.07	0.72
1:B:272:GLU:OE2	3:B:2117:HOH:O	2.08	0.71
1:A:212:MET:O	1:A:216:ARG:NH2	2.23	0.71
1:A:215:VAL:O	1:A:216:ARG:HB3	1.91	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:PRO:O	1:A:78:GLN:HB2	1.91	0.71
1:A:79:TYR:OH	3:A:2037:HOH:O	2.09	0.70
1:A:708:LYS:HD3	2:D:362:ASP:HB2	1.74	0.68
1:A:268:ILE:HG23	1:A:275:HIS:CD2	2.31	0.66
1:B:151:LEU:HA	1:B:155:TYR:HB2	1.78	0.66
1:B:122:ASP:O	1:B:189:ARG:NH2	2.29	0.65
1:C:269:ARG:HH11	1:C:269:ARG:HA	1.62	0.65
1:C:215:VAL:O	1:C:216:ARG:HB3	1.97	0.64
1:A:122:ASP:O	1:A:189:ARG:NH2	2.31	0.64
1:B:10:ARG:HD2	1:B:55:THR:HG21	1.80	0.64
1:B:5:LEU:O	1:B:17:ILE:HB	1.99	0.63
1:A:10:ARG:HH11	1:A:10:ARG:CG	2.06	0.63
1:B:299:GLY:HA2	3:B:2133:HOH:O	1.98	0.63
1:C:207:LEU:HD13	1:C:212:MET:CE	2.28	0.63
1:C:44:ARG:HG3	3:C:2030:HOH:O	1.99	0.62
1:C:392:ARG:HG3	3:C:2231:HOH:O	1.99	0.61
1:A:151:LEU:HA	1:A:155:TYR:HB2	1.82	0.61
1:B:386:ASP:HA	1:B:390:LYS:HZ1	1.66	0.60
1:B:160:ARG:HA	1:B:160:ARG:HE	1.64	0.60
1:C:111:GLU:HG3	2:P:2:LEU:HB2	1.85	0.59
1:C:716:LYS:HE3	3:C:2384:HOH:O	2.03	0.59
1:C:91:LYS:NZ	3:C:2057:HOH:O	2.34	0.59
2:P:3:VAL:HB	3:P:2002:HOH:O	2.03	0.59
1:A:268:ILE:HG23	1:A:275:HIS:HD2	1.68	0.58
1:B:117:ASN:HB2	3:B:2044:HOH:O	2.03	0.58
1:C:208:PRO:HD2	1:C:211:ILE:HD12	1.85	0.58
1:A:290:LYS:HE2	1:A:332:HIS:HB3	1.86	0.57
1:A:648:LYS:N	1:A:648:LYS:HD2	2.18	0.57
1:C:639:ARG:HG3	1:C:639:ARG:NH1	2.13	0.57
1:A:392:ARG:HH11	1:A:392:ARG:HG2	1.69	0.57
1:C:160:ARG:HA	3:C:2096:HOH:O	2.05	0.57
1:A:269:ARG:HE	1:A:269:ARG:HA	1.70	0.56
1:C:313:VAL:HG22	1:C:317:LEU:HD22	1.88	0.56
1:C:329:ARG:HG3	3:C:2191:HOH:O	2.04	0.56
1:C:272:GLU:HG2	3:C:2168:HOH:O	2.05	0.56
1:C:283:LYS:HG3	1:C:330:VAL:HG22	1.88	0.55
1:A:293:SER:HB2	1:A:298:ARG:O	2.06	0.55
1:B:394:LYS:HE3	1:B:397:GLU:OE1	2.06	0.55
1:A:24:ARG:CG	1:A:24:ARG:NH1	2.62	0.54
1:A:480:GLU:HB3	3:A:2079:HOH:O	2.07	0.54
1:A:10:ARG:HB3	3:A:2005:HOH:O	2.06	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:189:ARG:NH1	3:C:2113:HOH:O	2.40	0.54
1:A:314:GLU:HB2	3:A:2124:HOH:O	2.07	0.53
1:C:558:LEU:HD23	1:C:612:ARG:HG2	1.90	0.53
1:B:135:ILE:HD11	1:B:174:ILE:HG21	1.89	0.53
1:B:227:LEU:HB2	1:B:460:ALA:HB3	1.90	0.53
1:A:10:ARG:CG	1:A:10:ARG:NH1	2.70	0.53
1:A:148:VAL:HA	1:A:151:LEU:HD12	1.91	0.53
1:A:710:PRO:HA	2:D:362:ASP:HB3	1.90	0.53
1:B:520:PHE:HB3	1:B:635:ILE:HA	1.91	0.52
1:C:195:ARG:HD3	3:C:2117:HOH:O	2.09	0.52
1:A:141:MET:HG2	3:A:2009:HOH:O	2.09	0.52
1:A:136:ASP:HB3	1:A:139:ARG:HG3	1.92	0.52
1:C:207:LEU:HD13	1:C:212:MET:HE3	1.90	0.52
1:A:433:VAL:HG11	1:A:443:ALA:HB1	1.91	0.51
1:B:208:PRO:HD2	1:B:211:ILE:HD12	1.92	0.51
1:C:138:ASP:O	1:C:141:MET:HB2	2.11	0.51
1:B:126:GLU:HG3	3:B:2051:HOH:O	2.10	0.51
1:B:160:ARG:HA	1:B:160:ARG:NE	2.25	0.51
1:B:56:SER:O	1:B:60:GLU:HG2	2.11	0.51
1:C:9:LYS:HD3	3:C:2009:HOH:O	2.11	0.51
1:C:151:LEU:HA	1:C:155:TYR:HB2	1.93	0.50
1:C:639:ARG:HH11	1:C:639:ARG:CG	2.15	0.50
1:B:91:LYS:NZ	3:B:2035:HOH:O	2.44	0.50
1:A:227:LEU:HB2	1:A:460:ALA:HB3	1.94	0.50
1:B:373:GLU:HG2	3:B:2161:HOH:O	2.11	0.50
1:C:122:ASP:O	1:C:189:ARG:NH2	2.44	0.50
1:C:465:SER:HB2	1:C:489:LEU:HD11	1.92	0.50
1:A:10:ARG:HG3	1:A:10:ARG:NH1	2.08	0.50
1:B:386:ASP:HA	1:B:390:LYS:NZ	2.27	0.50
1:C:207:LEU:HD13	1:C:212:MET:HE1	1.94	0.49
1:C:227:LEU:HB2	1:C:460:ALA:HB3	1.93	0.49
1:C:425:PRO:HG2	1:C:615:THR:HG22	1.95	0.49
1:B:260:ARG:HH21	1:B:448:PRO:HG2	1.77	0.49
1:B:262:ARG:HD2	1:B:274:PHE:CB	2.38	0.49
1:A:283:LYS:HD3	3:A:2133:HOH:O	2.12	0.49
1:C:111:GLU:HG2	3:C:2067:HOH:O	2.10	0.49
1:C:300:GLY:HA2	3:C:2183:HOH:O	2.11	0.49
1:A:328:ASN:HB2	1:A:329:ARG:NH1	2.27	0.49
1:A:510:ARG:NH2	1:A:570:GLU:OE1	2.45	0.49
1:C:376:GLU:HG2	3:C:2224:HOH:O	2.11	0.48
2:E:361:ILE:H	2:E:361:ILE:HD13	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:658:ASP:OD1	1:C:661:HIS:HD2	1.96	0.48
1:B:621:PRO:HD3	1:B:694:SER:OG	2.14	0.48
1:C:433:VAL:HG11	1:C:443:ALA:HB1	1.95	0.48
3:B:2149:HOH:O	2:E:371:SER:HB2	2.14	0.48
1:A:207:LEU:HD13	1:A:212:MET:CE	2.44	0.48
1:A:520:PHE:HB3	1:A:635:ILE:HA	1.95	0.48
1:B:558:LEU:HD23	1:B:612:ARG:HG2	1.96	0.48
1:B:619:LEU:HD12	1:B:693:ILE:HG12	1.95	0.48
1:B:701:PRO:O	1:B:707:GLY:HA2	2.13	0.48
1:B:212:MET:HA	1:B:212:MET:HE2	1.96	0.47
1:B:83:ARG:HG2	1:B:141:MET:HG3	1.96	0.47
1:A:294:GLN:HB3	1:A:298:ARG:NH1	2.30	0.47
1:B:207:LEU:HD13	1:B:212:MET:HE1	1.96	0.47
1:B:443:ALA:O	1:B:444:LEU:HD23	2.15	0.46
1:A:44:ARG:HD3	3:A:2017:HOH:O	2.16	0.46
1:A:40:GLN:NE2	3:A:2014:HOH:O	2.48	0.46
1:A:242:SER:HB2	1:A:452:VAL:HG13	1.98	0.46
1:B:215:VAL:O	1:B:216:ARG:CB	2.60	0.46
1:B:264:LEU:O	1:B:389:ARG:NH2	2.47	0.46
1:B:510:ARG:HB2	1:B:512:THR:HG23	1.98	0.46
1:A:126:GLU:HG3	3:A:2049:HOH:O	2.15	0.46
1:A:268:ILE:HA	3:A:2110:HOH:O	2.15	0.46
1:A:450:ASN:HB2	3:A:2175:HOH:O	2.16	0.46
1:A:392:ARG:HH11	1:A:392:ARG:CG	2.29	0.45
2:D:361:ILE:H	2:D:361:ILE:HD13	1.81	0.45
1:B:217:THR:OG1	1:B:219:THR:HG22	2.16	0.45
1:C:730:TY2:CG	1:C:731:TYR:H	2.30	0.45
1:A:609:HIS:HD2	3:P:2001:HOH:O	2.00	0.45
1:A:58:ILE:O	1:A:62:ILE:HG23	2.17	0.45
1:A:313:VAL:HG22	1:A:317:LEU:HD22	1.99	0.45
1:A:648:LYS:HD2	1:A:648:LYS:H	1.82	0.45
1:C:526:LYS:HE2	3:C:2268:HOH:O	2.15	0.45
1:A:9:LYS:HE3	1:A:10:ARG:N	2.32	0.44
1:A:271:GLY:HA2	1:B:221:GLN:HE22	1.82	0.44
1:B:437:ASN:HB2	3:B:2104:HOH:O	2.17	0.44
1:B:298:ARG:HB2	3:B:2126:HOH:O	2.17	0.44
1:A:9:LYS:HE3	1:A:10:ARG:H	1.82	0.44
1:A:733:ASN:HB3	3:A:2250:HOH:O	2.16	0.44
1:B:172:LEU:O	1:B:176:VAL:HG23	2.18	0.44
1:A:658:ASP:OD1	1:A:661:HIS:HD2	2.00	0.44
1:C:56:SER:O	1:C:60:GLU:HG2	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:ARG:HB2	3:C:2144:HOH:O	2.16	0.44
1:C:262:ARG:HD2	1:C:274:PHE:HB2	1.98	0.44
1:C:444:LEU:HD22	1:C:512:THR:HG21	2.00	0.44
1:A:480:GLU:HG3	3:A:2185:HOH:O	2.17	0.44
1:A:189:ARG:NH1	3:A:2073:HOH:O	2.51	0.44
1:A:696:ASN:N	1:A:696:ASN:HD22	2.16	0.44
1:C:259:GLY:HA3	1:C:307:PRO:HD3	1.99	0.44
1:A:386:ASP:HB2	3:A:2152:HOH:O	2.18	0.43
1:B:434:ARG:CZ	3:B:2108:HOH:O	2.66	0.43
1:A:262:ARG:HH12	1:A:269:ARG:HB2	1.84	0.43
1:A:311:LEU:HA	1:A:355:LEU:HB3	2.01	0.43
1:B:191:GLN:HE21	1:B:191:GLN:HB2	1.56	0.43
1:B:698:ASN:OD1	1:B:733:ASN:HB2	2.18	0.43
1:B:155:TYR:HD1	3:B:2061:HOH:O	2.01	0.43
1:B:298:ARG:NH1	3:B:2128:HOH:O	2.51	0.43
1:B:708:LYS:HD3	2:E:362:ASP:HB2	2.00	0.43
1:A:321:ASN:HA	3:A:2156:HOH:O	2.19	0.43
1:C:62:ILE:HD12	1:C:84:LEU:HD22	2.01	0.43
1:A:444:LEU:HD22	1:A:512:THR:HG21	2.00	0.42
1:B:157:VAL:HG23	1:B:216:ARG:NH1	2.34	0.42
1:A:24:ARG:HH11	1:A:24:ARG:HG3	1.81	0.42
1:A:233:SER:CA	1:A:274:PHE:HZ	2.32	0.42
1:A:233:SER:HA	1:A:274:PHE:CZ	2.54	0.42
1:C:311:LEU:HA	1:C:355:LEU:HB3	2.02	0.42
1:B:479:GLU:HB2	1:B:550:TYR:CE1	2.54	0.42
1:B:510:ARG:NH2	1:B:570:GLU:OE2	2.53	0.42
1:B:258:ALA:HB3	1:B:304:LEU:HD21	2.02	0.42
1:B:286:GLN:HE22	1:B:331:ARG:HH12	1.68	0.42
2:F:368:ASP:HB2	3:F:2003:HOH:O	2.19	0.42
1:A:215:VAL:O	1:A:216:ARG:CB	2.65	0.42
1:C:212:MET:HE2	1:C:212:MET:HA	2.01	0.42
1:A:225:CYS:SG	1:A:442:ILE:HG13	2.59	0.41
1:B:45:SER:HB2	1:B:61:THR:HG22	2.01	0.41
1:B:568:PHE:CZ	1:B:610:GLY:HA2	2.55	0.41
1:A:208:PRO:HD2	1:A:211:ILE:HD12	2.02	0.41
1:A:176:VAL:HG21	1:A:212:MET:HE2	2.02	0.41
1:A:131:MET:HA	1:A:134:PHE:CD2	2.55	0.41
1:C:99:PRO:HG2	1:C:137:HIS:CG	2.56	0.41
1:C:409:THR:O	1:C:411:ARG:HG2	2.21	0.41
1:A:207:LEU:HD13	1:A:212:MET:HE1	2.02	0.41
1:A:212:MET:HE2	1:A:212:MET:HA	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:HIS:CE1	3:B:2023:HOH:O	2.74	0.41
1:C:98:GLU:HG2	3:C:2061:HOH:O	2.21	0.41
1:C:139:ARG:NH2	1:C:198:ASP:OD1	2.50	0.41
1:C:150:GLN:NE2	1:C:627:GLN:OE1	2.49	0.41
1:C:619:LEU:HD12	1:C:693:ILE:HG12	2.03	0.41
1:B:420:CYS:O	1:B:424:SER:HB2	2.21	0.41
1:B:555:SER:HB2	1:B:616:LEU:HD21	2.02	0.40
1:C:102:LEU:O	1:C:106:VAL:HG23	2.20	0.40
1:C:663:HIS:HD2	3:C:2349:HOH:O	2.04	0.40
1:A:322:ASN:HB2	3:A:2130:HOH:O	2.22	0.40
1:C:72:ARG:H	1:C:72:ARG:HG2	1.61	0.40
1:C:44:ARG:HD3	3:C:2034:HOH:O	2.21	0.40
1:C:262:ARG:CG	1:C:274:PHE:HB3	2.50	0.40
1:A:208:PRO:HB2	1:A:210:PRO:HD2	2.04	0.40
1:A:427:ASP:OD2	1:A:575:LYS:NZ	2.55	0.40
1:B:207:LEU:HD13	1:B:212:MET:CE	2.51	0.40
1:C:558:LEU:CD2	1:C:612:ARG:HG2	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	731/761 (96%)	698 (96%)	25 (3%)	8 (1%)	14	26
1	B	731/761 (96%)	699 (96%)	23 (3%)	9 (1%)	13	24
1	C	731/761 (96%)	701 (96%)	24 (3%)	6 (1%)	19	35
2	D	14/20 (70%)	13 (93%)	1 (7%)	0	100	100
2	E	14/20 (70%)	11 (79%)	3 (21%)	0	100	100
2	F	14/20 (70%)	14 (100%)	0	0	100	100
2	P	1/20 (5%)	1 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	2236/2363 (95%)	2137 (96%)	76 (3%)	23 (1%)	15 28

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	GLN
1	B	216	ARG
1	B	268	ILE
1	A	216	ARG
1	A	269	ARG
1	B	12	GLY
1	B	300	GLY
1	C	216	ARG
1	C	270	GLY
1	A	271	GLY
1	B	267	PRO
1	B	294	GLN
1	C	267	PRO
1	B	5	LEU
1	B	270	GLY
1	A	11	ASP
1	C	5	LEU
1	C	294	GLN
1	A	5	LEU
1	C	12	GLY
1	A	268	ILE
1	A	270	GLY
1	B	271	GLY

### 5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	628/650 (97%)	586 (93%)	42 (7%)	16 31
1	B	628/650 (97%)	591 (94%)	37 (6%)	19 37

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	628/650 (97%)	586 (93%)	42 (7%)	16	31
2	D	16/19 (84%)	13 (81%)	3 (19%)	1	2
2	E	16/19 (84%)	13 (81%)	3 (19%)	1	2
2	F	16/19 (84%)	13 (81%)	3 (19%)	1	2
2	P	3/19 (16%)	3 (100%)	0	100	100
All	All	1935/2026 (96%)	1805 (93%)	130 (7%)	16	31

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	9	LYS
1	A	10	ARG
1	A	14	THR
1	A	17	ILE
1	A	21	LYS
1	A	24	ARG
1	A	27	ASP
1	A	54	LYS
1	A	62	ILE
1	A	72	ARG
1	A	78	GLN
1	A	96	GLN
1	A	118	HIS
1	A	149	LYS
1	A	268	ILE
1	A	269	ARG
1	A	290	LYS
1	A	294	GLN
1	A	297	VAL
1	A	298	ARG
1	A	314	GLU
1	A	317	LEU
1	A	320	LYS
1	A	323	ARG
1	A	325	VAL
1	A	328	ASN
1	A	364	LEU
1	A	384	LYS
1	A	392	ARG

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Mol	Chain	Res	Type
1	A	394	LYS
1	A	408	SER
1	A	452	VAL
1	A	484	LEU
1	A	623	GLU
1	A	625	SER
1	A	626	SER
1	A	643	SER
1	A	648	LYS
1	A	696	ASN
1	A	706	SER
1	A	708	LYS
1	B	16	ARG
1	B	17	ILE
1	B	20	ASP
1	B	35	ASN
1	B	96	GLN
1	B	98	GLU
1	B	126	GLU
1	B	139	ARG
1	B	149	LYS
1	B	160	ARG
1	B	161	VAL
1	B	189	ARG
1	B	191	GLN
1	B	206	SER
1	B	226	VAL
1	B	260	ARG
1	B	268	ILE
1	B	269	ARG
1	B	297	VAL
1	B	317	LEU
1	B	320	LYS
1	B	323	ARG
1	B	331	ARG
1	B	341	LYS
1	B	364	LEU
1	B	376	GLU
1	B	389	ARG
1	B	394	LYS
1	B	411	ARG
1	B	452	VAL

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Mol	Chain	Res	Type
1	B	455	GLU
1	B	484	LEU
1	B	510	ARG
1	B	542	LYS
1	B	616	LEU
1	B	651	ILE
1	B	706	SER
1	C	5	LEU
1	C	11	ASP
1	C	16	ARG
1	C	17	ILE
1	C	21	LYS
1	C	24	ARG
1	C	54	LYS
1	C	55	THR
1	C	60	GLU
1	C	111	GLU
1	C	118	HIS
1	C	129	LYS
1	C	139	ARG
1	C	141	MET
1	C	160	ARG
1	C	165	ILE
1	C	186	ARG
1	C	187	GLU
1	C	189	ARG
1	C	191	GLN
1	C	260	ARG
1	C	269	ARG
1	C	290	LYS
1	C	297	VAL
1	C	317	LEU
1	C	323	ARG
1	C	364	LEU
1	C	384	LYS
1	C	391	GLN
1	C	452	VAL
1	C	465	SER
1	C	484	LEU
1	C	586	ASP
1	C	616	LEU
1	C	621	PRO

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Mol	Chain	Res	Type
1	C	623	GLU
1	C	625	SER
1	C	626	SER
1	C	639	ARG
1	C	645	LYS
1	C	648	LYS
1	C	708	LYS
2	D	361	ILE
2	D	367	THR
2	D	368	ASP
2	E	360	GLN
2	E	361	ILE
2	E	364	GLU
2	F	361	ILE
2	F	367	THR
2	F	374	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	117	ASN
1	A	183	ASN
1	A	221	GLN
1	A	250	GLN
1	A	275	HIS
1	A	527	HIS
1	A	609	HIS
1	A	627	GLN
1	A	630	ASN
1	A	661	HIS
1	B	46	HIS
1	B	150	GLN
1	B	183	ASN
1	B	191	GLN
1	B	221	GLN
1	B	250	GLN
1	B	328	ASN
1	B	627	GLN
1	B	630	ASN
1	B	661	HIS
1	B	663	HIS

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Mol	Chain	Res	Type
1	B	696	ASN
1	C	46	HIS
1	C	59	HIS
1	C	183	ASN
1	C	250	GLN
1	C	322	ASN
1	C	328	ASN
1	C	630	ASN
1	C	661	HIS
1	C	663	HIS
1	C	696	ASN
2	E	360	GLN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

3 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	TY2	A	730	1	12,13,14	3.06	3 (25%)	12,17,19	1.45	2 (16%)
1	TY2	C	730	1	12,13,14	3.05	3 (25%)	12,17,19	1.50	1 (8%)
1	TY2	B	730	1	12,13,14	3.20	3 (25%)	12,17,19	1.54	3 (25%)

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	TY2	A	730	1	-	3/5/6/8	0/1/1/1
1	TY2	C	730	1	-	3/5/6/8	0/1/1/1
1	TY2	B	730	1	-	3/5/6/8	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	730	TY2	CE2-CZ	7.16	1.49	1.40
1	C	730	TY2	CD2-CE2	-6.68	1.29	1.40
1	A	730	TY2	CD2-CE2	-6.62	1.29	1.40
1	B	730	TY2	CD2-CE2	-6.22	1.30	1.40
1	A	730	TY2	CE2-CZ	5.78	1.47	1.40
1	C	730	TY2	CE2-CZ	5.71	1.47	1.40
1	A	730	TY2	CD2-CG	-5.66	1.29	1.39
1	C	730	TY2	CD2-CG	-5.46	1.30	1.39
1	B	730	TY2	CD2-CG	-5.40	1.30	1.39

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	730	TY2	CD1-CE1-CZ	-3.53	116.97	120.50
1	A	730	TY2	CD1-CE1-CZ	-3.19	117.31	120.50
1	B	730	TY2	CD1-CE1-CZ	-3.11	117.39	120.50
1	B	730	TY2	CD1-CG-CD2	2.54	122.05	118.55
1	B	730	TY2	OH-CZ-CE2	2.46	120.53	116.50
1	A	730	TY2	CD1-CG-CD2	2.44	121.92	118.55

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	730	TY2	O-C-CA-CB
1	B	730	TY2	O-C-CA-CB
1	C	730	TY2	O-C-CA-CB
1	B	730	TY2	CA-CB-CG-CD1
1	B	730	TY2	CA-CB-CG-CD2
1	C	730	TY2	CA-CB-CG-CD1
1	C	730	TY2	CA-CB-CG-CD2
1	A	730	TY2	CA-CB-CG-CD1
1	A	730	TY2	CA-CB-CG-CD2

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	C	730	TY2	1	0

## 5.5 Carbohydrates [i](#)

There are no monosaccharides 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, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	733/761 (96%)	0.04	23 (3%) 49 52	22, 38, 64, 84	0
1	B	733/761 (96%)	0.06	16 (2%) 62 65	27, 38, 60, 82	0
1	C	733/761 (96%)	-0.06	11 (1%) 73 75	17, 29, 52, 75	0
2	D	16/20 (80%)	1.35	3 (18%) 1 1	71, 83, 90, 90	0
2	E	16/20 (80%)	1.13	2 (12%) 3 3	71, 82, 87, 87	0
2	F	16/20 (80%)	1.13	2 (12%) 3 3	62, 76, 81, 82	0
2	P	3/20 (15%)	0.73	0 100 100	29, 29, 35, 40	0
All	All	2250/2363 (95%)	0.04	57 (2%) 57 61	17, 36, 66, 90	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	273	ALA	7.8
1	A	296	GLY	7.5
1	C	271	GLY	7.5
1	B	296	GLY	7.1
1	A	737	GLY	6.8
1	B	270	GLY	6.3
1	B	271	GLY	6.3
1	A	274	PHE	6.1
1	A	271	GLY	5.8
1	B	273	ALA	5.4
1	B	294	GLN	5.4
1	B	274	PHE	5.3
1	C	273	ALA	5.1
1	C	270	GLY	4.9
1	B	737	GLY	4.5
1	A	6	LEU	4.3
1	C	274	PHE	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	297	VAL	4.0
1	A	297	VAL	3.9
1	C	296	GLY	3.9
1	A	323	ARG	3.8
1	A	270	GLY	3.7
2	D	361	ILE	3.6
1	A	272	GLU	3.4
1	A	4	ASN	3.4
2	F	361	ILE	3.2
1	C	272	GLU	3.1
1	A	17	ILE	3.1
1	B	272	GLU	3.1
2	D	372	ASN	3.0
2	F	360	GLN	3.0
1	A	160	ARG	3.0
1	B	161	VAL	3.0
1	A	268	ILE	3.0
1	A	295	GLY	2.9
1	B	12	GLY	2.9
1	B	295	GLY	2.9
1	A	13	SER	2.9
1	B	6	LEU	2.8
1	C	737	GLY	2.7
1	C	294	GLN	2.7
1	A	14	THR	2.7
1	A	50	TYR	2.6
1	C	16	ARG	2.6
1	C	297	VAL	2.5
1	A	161	VAL	2.5
2	E	364	GLU	2.5
1	B	392	ARG	2.4
2	D	370	LEU	2.3
1	A	298	ARG	2.2
1	A	11	ASP	2.2
1	C	4	ASN	2.2
1	A	118	HIS	2.2
1	B	13	SER	2.2
2	E	372	ASN	2.1
1	A	299	GLY	2.1
1	B	268	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, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	TY2	B	730	13/14	0.97	0.15	31,32,32,32	0
1	TY2	C	730	13/14	0.97	0.16	21,22,23,24	0
1	TY2	A	730	13/14	0.98	0.13	30,31,32,32	0

## 6.3 Carbohydrates [i](#)

There are no monosaccharides 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.