



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:29 PM GMT

PDB ID : 2XAP  
Title : RIBONUCLEOTIDE REDUCTASE Y731NO2Y MODIFIED R1 SUBUNIT  
OF E. COLI TO 2.1 Å RESOLUTION  
Authors : Yokoyama, K.; Uhlin, U.; Stubbe, J.  
Deposited on : 2010-03-31  
Resolution : 2.10 Å(reported)

This is a full wwPDB 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 <http://wwpdb.org/ValidationPDFNotes.html>

---

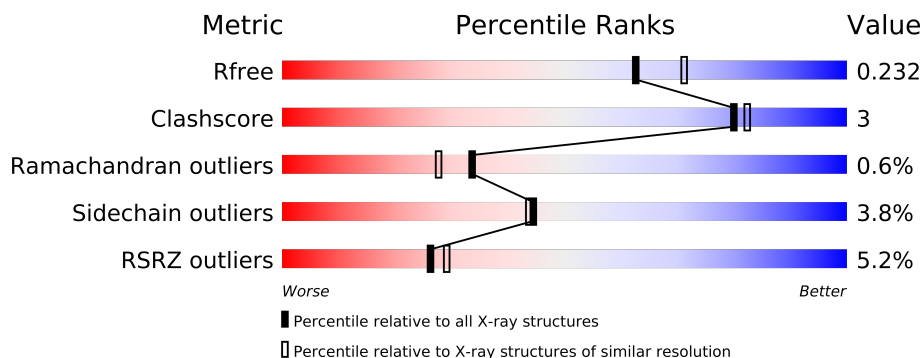
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)  
Validation Pipeline (wwPDB-VP) : stable22683

# 1 Overall quality at a glance

The reported resolution of this entry is 2.10 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))
$R_{free}$	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	761	
1	B	761	
1	C	761	
2	D	20	
2	E	20	
2	F	20	
2	P	20	

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19192 atoms, of which 0 are hydrogen and 0 are deuterium.

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-DIPHOSPHATEREDUCTASE 1 SUBUNIT ALPHA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	728	Total	C	N	O	S	0	0	0
			5807	3688	996	1099	24			
1	B	728	Total	C	N	O	S	0	0	0
			5807	3688	996	1099	24			
1	C	728	Total	C	N	O	S	0	0	0
			5807	3688	996	1099	24			

- Molecule 2 is a protein called RIBONUCLEOSIDE-DIPHOSPHATEREDUCTASE 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	408	Total	O	0	0
			408	408		
3	B	394	Total	O	0	0
			394	394		
3	C	544	Total	O	0	0
			544	544		
3	D	3	Total	O	0	0
			3	3		

*Continued on next page...*

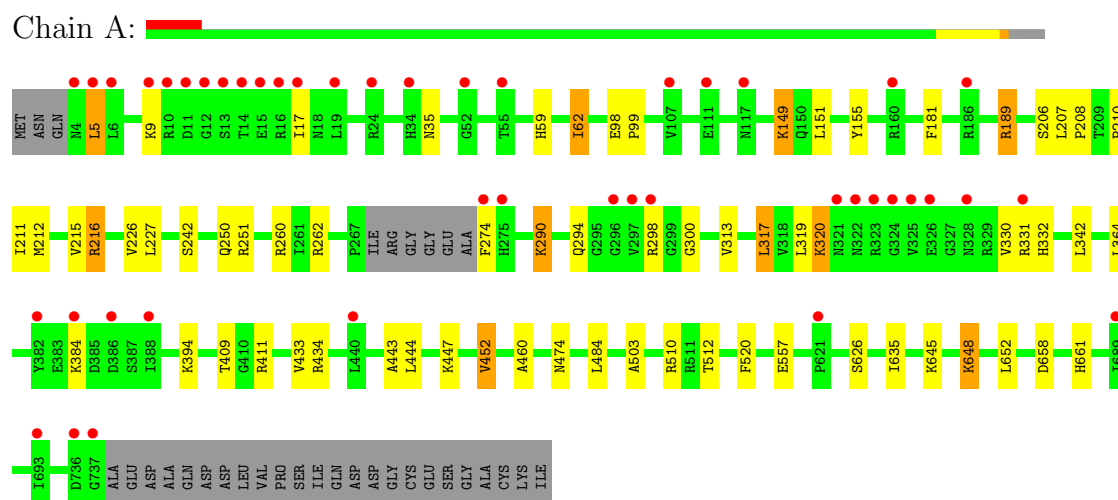
*Continued from previous page...*

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	6	Total	O	0	0
			6	6		
3	F	2	Total	O	0	0
			2	2		

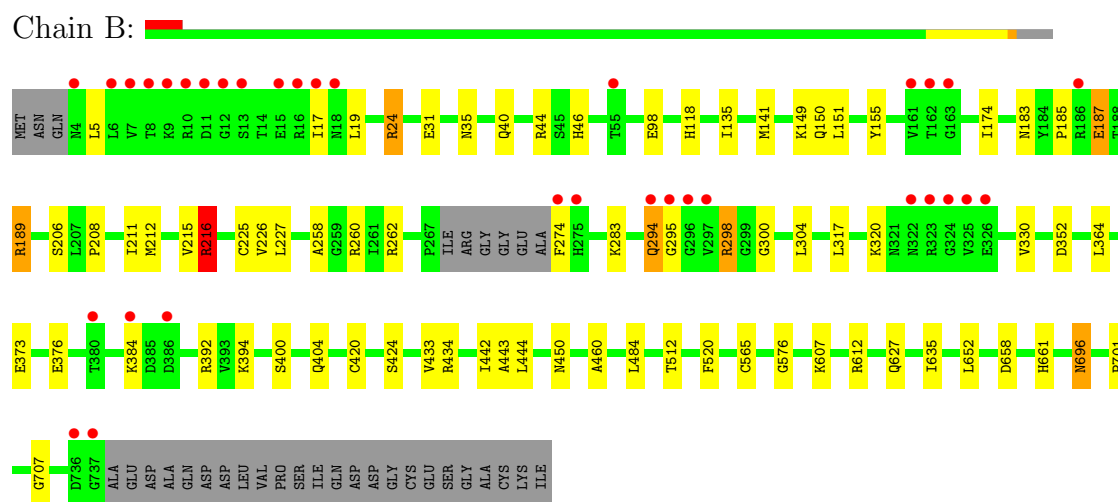
### 3 Residue-property plots

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.

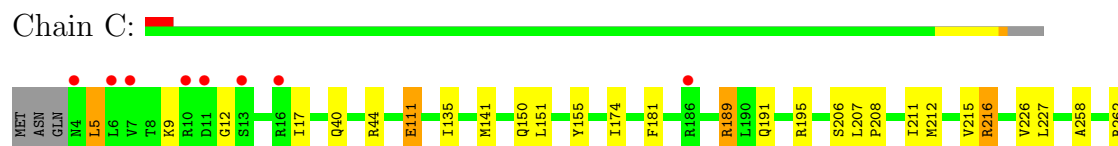
#### • Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATEREDUCTASE 1 SUBUNIT ALPHA

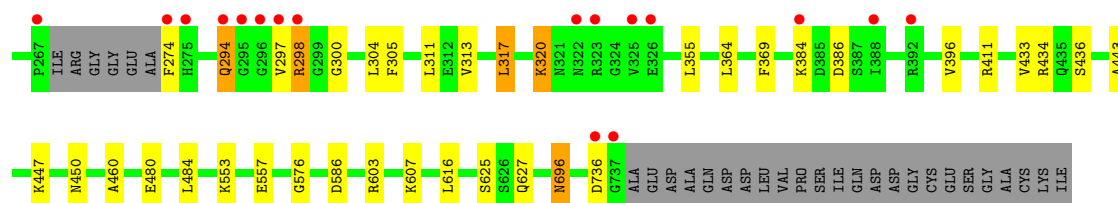


#### • Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATEREDUCTASE 1 SUBUNIT ALPHA



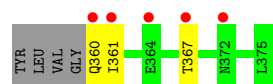
#### • Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATEREDUCTASE 1 SUBUNIT ALPHA





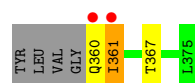
- Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATEREDUCTASE 1 SUBUNIT BETA

Chain D:



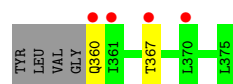
- Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATEREDUCTASE 1 SUBUNIT BETA

Chain E:



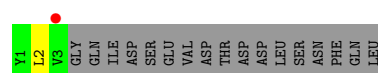
- Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATEREDUCTASE 1 SUBUNIT BETA

Chain F:



- Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATEREDUCTASE 1 SUBUNIT BETA

Chain P:



## 4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	223.98Å 223.98Å 336.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	169.03 – 2.10 55.24 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.8 (169.03-2.10) 91.7 (55.24-2.10)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.31 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, $R_{free}$	0.196 , 0.230 0.198 , 0.232	Depositor DCC
$R_{free}$ test set	8629 reflections (5.29%)	DCC
Wilson B-factor (Å <sup>2</sup> )	31.4	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.37 , 41.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 171841 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	19192	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	35.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.88% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.38	0/5917	0.53	0/8012
1	B	0.37	0/5917	0.53	0/8012
1	C	0.42	0/5917	0.55	0/8012
2	D	0.40	0/129	0.52	0/173
2	E	0.37	0/129	0.53	0/173
2	F	0.38	0/129	0.49	0/173
2	P	0.49	0/27	0.52	0/36
All	All	0.39	0/18165	0.53	0/24591

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

### 5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	5807	0	5725	40	0
1	B	5807	0	5726	41	0
1	C	5807	0	5726	38	0
2	D	129	0	111	0	0
2	E	129	0	111	1	0

*Continued on next page...*



*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	F	129	0	111	0	0
2	P	27	0	31	1	0
3	A	408	0	0	6	0
3	B	394	0	0	5	0
3	C	544	0	0	10	0
3	D	3	0	0	0	0
3	E	6	0	0	0	0
3	F	2	0	0	0	0
All	All	19192	0	17541	120	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 3.

All (120) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:24:ARG:HG3	1:B:24:ARG:HH11	1.13	1.06
1:A:189:ARG:HH11	1:A:189:ARG:HG2	1.20	1.03
1:C:189:ARG:HH11	1:C:189:ARG:HG2	1.29	0.98
1:B:576:GLY:HA3	1:B:607:LYS:HE2	1.57	0.87
1:A:189:ARG:NH1	1:A:189:ARG:HG2	1.87	0.82
1:B:260:ARG:HH21	1:B:434:ARG:HH22	1.32	0.76
1:C:189:ARG:HH11	1:C:189:ARG:CG	1.98	0.75
1:B:24:ARG:HG3	1:B:24:ARG:NH1	1.90	0.74
1:B:40:GLN:HG3	3:B:2008:HOH:O	1.86	0.73
1:B:215:VAL:O	1:B:216:ARG:HB3	1.87	0.73
1:C:576:GLY:HA3	1:C:607:LYS:HE2	1.69	0.73
1:C:189:ARG:NH1	1:C:189:ARG:HG2	2.01	0.72
1:A:189:ARG:HH11	1:A:189:ARG:CG	2.01	0.71
1:A:262:ARG:HD2	1:A:274:PHE:HB3	1.72	0.70
1:C:480:GLU:HB3	3:C:2169:HOH:O	1.92	0.69
1:C:40:GLN:HG3	3:C:2033:HOH:O	1.91	0.69
1:B:208:PRO:HD2	1:B:211:ILE:HD12	1.74	0.69
1:A:260:ARG:HH21	1:A:434:ARG:HH22	1.41	0.68
1:A:181:PHE:O	1:A:189:ARG:HD2	1.93	0.68
1:C:189:ARG:NH1	3:C:2164:HOH:O	2.29	0.66
1:A:215:VAL:O	1:A:216:ARG:HB3	1.96	0.66
1:B:212:MET:O	1:B:216:ARG:NH2	2.23	0.64
1:C:181:PHE:O	1:C:189:ARG:HD2	1.98	0.63
1:B:227:LEU:HB2	1:B:460:ALA:HB3	1.81	0.62
1:B:151:LEU:HA	1:B:155:TYR:HB2	1.81	0.62
1:B:185:PRO:HB2	1:B:187:GLU:HG2	1.80	0.62
1:A:648:LYS:HD2	1:A:648:LYS:H	1.65	0.60

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:242:SER:HB2	1:A:452:VAL:HG13	1.83	0.60
1:B:135:ILE:HD11	1:B:174:ILE:HG21	1.83	0.59
1:A:447:LYS:HD3	3:A:2243:HOH:O	2.03	0.58
1:A:274:PHE:HA	3:A:2151:HOH:O	2.02	0.58
1:C:111:GLU:HG3	2:P:2:LEU:HB2	1.86	0.57
1:A:151:LEU:HA	1:A:155:TYR:HB2	1.85	0.57
1:C:450:ASN:HB2	3:C:2338:HOH:O	2.03	0.57
1:C:274:PHE:HA	3:C:2234:HOH:O	2.05	0.57
1:A:227:LEU:HB2	1:A:460:ALA:HB3	1.88	0.55
1:A:290:LYS:HE2	1:A:332:HIS:HB3	1.88	0.55
1:B:189:ARG:HH11	1:B:189:ARG:CG	2.19	0.55
1:C:44:ARG:HD3	3:C:2040:HOH:O	2.06	0.55
1:C:208:PRO:HG2	1:C:211:ILE:HD12	1.89	0.55
1:C:258:ALA:HB3	1:C:304:LEU:HD21	1.90	0.54
1:A:207:LEU:HD12	1:A:212:MET:CE	2.38	0.54
1:A:212:MET:O	1:A:216:ARG:NH2	2.28	0.54
1:A:444:LEU:HD22	1:A:512:THR:HG21	1.91	0.52
1:B:294:GLN:HB2	1:B:298:ARG:HH11	1.75	0.52
1:C:207:LEU:HD12	1:C:212:MET:HE1	1.91	0.51
1:A:250:GLN:O	1:A:251:ARG:HB2	2.10	0.51
1:C:433:VAL:HG11	1:C:443:ALA:HB1	1.93	0.51
1:B:149:LYS:HG3	1:B:652:LEU:HD21	1.92	0.51
1:B:189:ARG:HH11	1:B:189:ARG:HG2	1.76	0.51
1:A:207:LEU:HD12	1:A:212:MET:HE3	1.93	0.51
1:A:294:GLN:HB3	1:A:298:ARG:HB3	1.93	0.50
1:B:658:ASP:OD1	1:B:661:HIS:HD2	1.94	0.50
1:C:44:ARG:NH1	3:C:2037:HOH:O	2.43	0.50
1:A:648:LYS:HD2	1:A:648:LYS:N	2.26	0.50
1:B:444:LEU:HD22	1:B:512:THR:HG21	1.93	0.50
1:A:320:LYS:HA	1:A:331:ARG:HG2	1.93	0.50
1:C:553:LYS:O	1:C:557:GLU:HG3	2.11	0.49
1:B:400:SER:O	1:B:404:GLN:HB2	2.12	0.49
1:B:373:GLU:HG2	3:B:2205:HOH:O	2.11	0.49
1:B:696:ASN:HD22	1:B:696:ASN:N	2.10	0.49
1:C:155:TYR:CZ	1:C:212:MET:HG3	2.48	0.49
1:B:520:PHE:HB3	1:B:635:ILE:HA	1.94	0.49
1:C:151:LEU:HA	1:C:155:TYR:HB2	1.95	0.49
1:B:258:ALA:HB3	1:B:304:LEU:HD21	1.95	0.49
1:B:44:ARG:NH2	3:B:2023:HOH:O	2.46	0.48
1:C:227:LEU:HB2	1:C:460:ALA:HB3	1.94	0.48
1:B:283:LYS:HG3	1:B:330:VAL:HG22	1.96	0.48
1:C:294:GLN:HB3	1:C:298:ARG:HB2	1.96	0.47

*Continued on next page...*

*Continued from previous page...*

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:396:VAL:HG23	3:C:2272:HOH:O	2.13	0.47
1:C:155:TYR:CE2	1:C:212:MET:SD	3.07	0.47
1:A:503:ALA:HB3	3:A:2141:HOH:O	2.14	0.47
1:B:352:ASP:HB2	1:B:392:ARG:HH11	1.80	0.46
1:C:191:GLN:HE21	1:C:195:ARG:HH21	1.64	0.46
1:B:19:LEU:HD22	1:B:46:HIS:CE1	2.50	0.46
1:B:262:ARG:HD3	1:B:274:PHE:HB3	1.98	0.46
1:C:150:GLN:HE21	1:C:627:GLN:CD	2.20	0.45
1:C:215:VAL:O	1:C:216:ARG:HB3	2.17	0.45
1:B:565:CYS:HB3	1:B:612:ARG:O	2.18	0.44
1:C:447:LYS:HE3	3:C:2344:HOH:O	2.17	0.44
1:B:433:VAL:HG11	1:B:443:ALA:HB1	2.00	0.44
1:B:189:ARG:HH11	1:B:189:ARG:HB3	1.82	0.44
1:C:320:LYS:HE2	1:C:411:ARG:HB2	2.00	0.44
1:B:701:PRO:O	1:B:707:GLY:HA2	2.17	0.44
1:A:433:VAL:HG11	1:A:443:ALA:HB1	1.99	0.44
2:E:361:ILE:HD13	2:E:361:ILE:H	1.83	0.43
1:C:311:LEU:HA	1:C:355:LEU:HB3	2.01	0.43
1:C:603:ARG:HG2	1:C:607:LYS:HE3	2.00	0.43
1:C:313:VAL:HG22	1:C:317:LEU:HD22	2.00	0.43
1:B:450:ASN:HB2	3:B:2240:HOH:O	2.18	0.43
1:A:208:PRO:HD2	1:A:211:ILE:HD12	1.99	0.43
1:A:319:LEU:HD22	1:A:330:VAL:HG23	2.01	0.43
1:B:189:ARG:NH1	1:B:189:ARG:HG2	2.32	0.43
1:A:510:ARG:HB2	1:A:512:THR:HG23	2.01	0.43
1:A:520:PHE:HB3	1:A:635:ILE:HA	2.01	0.43
1:A:242:SER:CB	1:A:452:VAL:HG13	2.48	0.42
1:A:658:ASP:OD1	1:A:661:HIS:HD2	2.02	0.42
1:A:342:LEU:HG	3:A:2179:HOH:O	2.19	0.42
1:A:59:HIS:O	1:A:62:ILE:HD13	2.19	0.42
1:C:262:ARG:HD2	1:C:274:PHE:HB3	2.01	0.42
1:A:98:GLU:HA	1:A:99:PRO:HD3	1.90	0.42
1:A:215:VAL:O	1:A:216:ARG:CB	2.63	0.42
1:C:305:PHE:CZ	1:C:436:SER:HB3	2.55	0.42
1:C:696:ASN:HD22	1:C:696:ASN:N	2.18	0.42
1:A:208:PRO:HB2	1:A:210:PRO:HD2	2.02	0.42
1:C:369:PHE:CD2	1:C:434:ARG:HD2	2.55	0.42
1:B:215:VAL:O	1:B:216:ARG:CB	2.64	0.42
1:B:420:CYS:O	1:B:424:SER:HB2	2.20	0.42
1:B:44:ARG:HD3	3:B:2024:HOH:O	2.19	0.41
1:A:557:GLU:HG3	3:A:2078:HOH:O	2.20	0.41
1:A:320:LYS:HG3	1:A:409:THR:HG21	2.01	0.41

*Continued on next page...*

Continued from previous page...

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:576:GLY:CA	1:B:607:LYS:HE2	2.39	0.41
1:A:313:VAL:HG22	1:A:317:LEU:HD22	2.03	0.41
1:A:274:PHE:N	3:A:2155:HOH:O	2.52	0.41
1:C:111:GLU:HG2	3:C:2097:HOH:O	2.21	0.41
1:A:149:LYS:HG2	1:A:652:LEU:HD11	2.02	0.41
1:B:189:ARG:HH11	1:B:189:ARG:CB	2.34	0.40
1:B:150:GLN:HE21	1:B:627:GLN:CD	2.25	0.40
1:C:135:ILE:HD11	1:C:174:ILE:HG21	2.04	0.40
1:B:225:CYS:SG	1:B:442:ILE:HG13	2.62	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	723/761 (95%)	704 (97%)	16 (2%)	3 (0%)	43	39
1	B	723/761 (95%)	702 (97%)	16 (2%)	5 (1%)	30	23
1	C	723/761 (95%)	706 (98%)	12 (2%)	5 (1%)	30	23
2	D	14/20 (70%)	14 (100%)	0	0	100	100
2	E	14/20 (70%)	14 (100%)	0	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
All	All	2212/2363 (94%)	2155 (97%)	44 (2%)	13 (1%)	33	28

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	ARG
1	A	300	GLY
1	B	216	ARG
1	B	294	GLN
1	C	216	ARG

Continued on next page...

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	5	LEU
1	B	295	GLY
1	B	298	ARG
1	B	300	GLY
1	C	294	GLN
1	C	12	GLY
1	C	5	LEU
1	C	300	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	625/650 (96%)	603 (96%)	22 (4%)	48	48
1	B	625/650 (96%)	603 (96%)	22 (4%)	48	48
1	C	625/650 (96%)	604 (97%)	21 (3%)	49	49
2	D	16/19 (84%)	13 (81%)	3 (19%)	2	1
2	E	16/19 (84%)	13 (81%)	3 (19%)	2	1
2	F	16/19 (84%)	14 (88%)	2 (12%)	7	3
2	P	3/19 (16%)	3 (100%)	0	100	100
All	All	1926/2026 (95%)	1853 (96%)	73 (4%)	44	44

All (73) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	9	LYS
1	A	17	ILE
1	A	35	ASN
1	A	62	ILE
1	A	149	LYS
1	A	189	ARG
1	A	206	SER
1	A	226	VAL
1	A	290	LYS

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	A	317	LEU
1	A	320	LYS
1	A	364	LEU
1	A	384	LYS
1	A	394	LYS
1	A	411	ARG
1	A	452	VAL
1	A	474	ASN
1	A	484	LEU
1	A	626	SER
1	A	645	LYS
1	A	648	LYS
1	B	5	LEU
1	B	17	ILE
1	B	24	ARG
1	B	31	GLU
1	B	35	ASN
1	B	98	GLU
1	B	118	HIS
1	B	141	MET
1	B	183	ASN
1	B	187	GLU
1	B	189	ARG
1	B	206	SER
1	B	216	ARG
1	B	226	VAL
1	B	317	LEU
1	B	320	LYS
1	B	364	LEU
1	B	376	GLU
1	B	384	LYS
1	B	394	LYS
1	B	484	LEU
1	B	696	ASN
1	C	5	LEU
1	C	9	LYS
1	C	17	ILE
1	C	111	GLU
1	C	141	MET
1	C	189	ARG
1	C	206	SER
1	C	226	VAL

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	C	297	VAL
1	C	298	ARG
1	C	317	LEU
1	C	320	LYS
1	C	364	LEU
1	C	384	LYS
1	C	386	ASP
1	C	484	LEU
1	C	586	ASP
1	C	616	LEU
1	C	625	SER
1	C	696	ASN
1	C	736	ASP
2	D	360	GLN
2	D	361	ILE
2	D	367	THR
2	E	360	GLN
2	E	361	ILE
2	E	367	THR
2	F	360	GLN
2	F	367	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	46	HIS
1	A	130	GLN
1	A	183	ASN
1	A	250	GLN
1	A	328	ASN
1	A	609	HIS
1	A	630	ASN
1	A	633	ASN
1	A	661	HIS
1	B	46	HIS
1	B	130	GLN
1	B	183	ASN
1	B	250	GLN
1	B	328	ASN
1	B	630	ASN
1	B	633	ASN

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type
1	B	661	HIS
1	C	46	HIS
1	C	183	ASN
1	C	191	GLN
1	C	250	GLN
1	C	328	ASN
1	C	630	ASN
1	C	661	HIS
2	D	360	GLN
2	F	360	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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	NIY	A	731	1	15,15,16	5.00	2 (13%)	18,20,22	1.00	2 (11%)
1	NIY	B	731	1	15,15,16	4.78	3 (20%)	18,20,22	1.26	1 (5%)
1	NIY	C	731	1	15,15,16	4.72	3 (20%)	18,20,22	1.10	2 (11%)

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	NIY	A	731	1	-	0/8/10/12	0/1/1/1
1	NIY	B	731	1	-	0/8/10/12	0/1/1/1

*Continued on next page...*



*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	NIY	C	731	1	-	0/8/10/12	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	731	NIY	O-C	18.70	1.24	1.11
1	B	731	NIY	O-C	17.80	1.23	1.11
1	C	731	NIY	O-C	17.66	1.23	1.11
1	B	731	NIY	CE1-NN	-4.18	1.40	1.46
1	A	731	NIY	CE1-NN	-4.18	1.40	1.46
1	C	731	NIY	CE1-NN	-3.88	1.40	1.46
1	B	731	NIY	CA-C	2.18	1.52	1.48
1	C	731	NIY	CA-C	2.01	1.52	1.48

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	731	NIY	CD1-CE1-NN	4.50	120.33	115.82
1	C	731	NIY	CB-CG-CD1	-2.56	115.88	120.41
1	A	731	NIY	CB-CG-CD1	-2.12	116.66	120.41
1	C	731	NIY	CZ-CE1-NN	2.03	123.14	118.94
1	A	731	NIY	CD1-CE1-NN	2.03	117.86	115.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

There are no ligands in this entry.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues

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	728/761 (95%)	0.40	45 (6%)	20 22	22, 34, 55, 85	0
1	B	728/761 (95%)	0.32	34 (4%)	30 33	22, 34, 53, 81	0
1	C	728/761 (95%)	0.12	25 (3%)	43 47	15, 26, 45, 72	0
2	D	16/20 (80%)	1.34	5 (31%)	1 1	72, 80, 81, 81	0
2	E	16/20 (80%)	1.19	2 (12%)	5 5	70, 78, 81, 82	0
2	F	16/20 (80%)	1.54	4 (25%)	1 1	62, 72, 75, 76	0
2	P	3/20 (15%)	0.78	1 (33%)	1 1	29, 29, 35, 39	0
All	All	2235/2363 (94%)	0.30	116 (5%)	26 29	15, 32, 56, 85	0

All (116) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	297	VAL	7.8
1	B	297	VAL	7.3
1	C	737	GLY	6.8
1	C	297	VAL	6.5
1	A	737	GLY	6.4
1	B	274	PHE	6.4
1	A	6	LEU	5.6
2	D	361	ILE	5.5
1	B	737	GLY	5.5
2	E	360	GLN	5.5
1	A	17	ILE	5.3
1	A	323	ARG	5.2
1	C	294	GLN	5.1
1	A	322	ASN	5.1
1	B	10	ARG	5.1
1	B	325	VAL	5.0
1	B	296	GLY	4.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	323	ARG	4.8
1	A	13	SER	4.8
1	A	19	LEU	4.7
1	A	12	GLY	4.7
1	A	4	ASN	4.5
1	C	296	GLY	4.4
1	A	325	VAL	4.4
1	B	9	LYS	4.4
2	F	360	GLN	4.4
1	A	274	PHE	4.3
1	A	14	THR	4.3
1	A	296	GLY	4.2
1	B	322	ASN	4.1
1	B	6	LEU	4.1
1	C	274	PHE	4.0
1	C	323	ARG	4.0
1	A	11	ASP	4.0
1	C	13	SER	3.8
1	B	161	VAL	3.8
1	A	9	LYS	3.8
2	E	361	ILE	3.7
2	D	360	GLN	3.7
1	B	11	ASP	3.7
1	C	16	ARG	3.6
1	C	384	LYS	3.6
1	B	384	LYS	3.5
1	C	322	ASN	3.4
1	C	298	ARG	3.4
1	B	17	ILE	3.4
1	B	736	ASP	3.4
1	A	321	ASN	3.2
2	F	361	ILE	3.1
1	A	15	GLU	3.0
1	A	298	ARG	3.0
1	C	186	ARG	3.0
1	C	325	VAL	3.0
1	B	386	ASP	3.0
1	A	16	ARG	3.0
1	C	4	ASN	3.0
1	B	13	SER	3.0
2	F	367	THR	2.9
1	B	4	ASN	2.9

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	B	7	VAL	2.8
1	B	55	THR	2.8
1	C	11	ASP	2.7
1	A	111	GLU	2.7
1	B	324	GLY	2.7
1	A	186	ARG	2.7
1	B	8	THR	2.7
1	A	324	GLY	2.7
1	A	736	ASP	2.6
1	A	55	THR	2.6
1	A	10	ARG	2.6
1	A	328	ASN	2.6
1	A	384	LYS	2.6
1	B	16	ARG	2.6
1	A	275	HIS	2.6
1	A	24	ARG	2.6
1	B	12	GLY	2.6
1	B	294	GLN	2.5
1	B	380	THR	2.5
1	B	18	ASN	2.5
1	B	295	GLY	2.4
1	C	10	ARG	2.4
1	B	275	HIS	2.4
1	B	162	THR	2.4
1	C	326	GLU	2.4
1	A	331	ARG	2.3
1	A	34	HIS	2.3
1	C	388	ILE	2.3
2	P	3	VAL	2.3
2	D	372	ASN	2.3
1	B	15	GLU	2.3
1	C	7	VAL	2.3
1	A	689	ILE	2.3
1	C	392	ARG	2.2
1	C	295	GLY	2.2
1	B	186	ARG	2.2
2	D	364	GLU	2.2
1	A	693	ILE	2.2
1	C	6	LEU	2.2
1	B	163	GLY	2.2
1	A	382	TYR	2.2
1	A	621	PRO	2.2

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	RSRZ
1	A	5	LEU	2.2
1	A	388	ILE	2.2
1	A	326	GLU	2.2
1	A	117	ASN	2.1
1	B	326	GLU	2.1
1	C	275	HIS	2.1
1	A	52	GLY	2.1
2	D	367	THR	2.1
1	A	160	ARG	2.1
1	A	386	ASP	2.1
1	A	107	VAL	2.1
1	C	736	ASP	2.1
1	A	440	LEU	2.0
2	F	370	LEU	2.0
1	C	267	PRO	2.0

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

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, 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	NIY	B	731	15/16	0.14	0.06	27,31,37,38	0
1	NIY	A	731	15/16	0.12	-0.60	28,33,39,39	0
1	NIY	C	731	15/16	0.11	-0.83	20,27,35,35	0

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

There are no ligands in this entry.

## 6.5 Other polymers ⓘ

There are no such residues in this entry.