



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 15, 2017 – 03:37 am 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 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : trunk28620  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : recalc28949

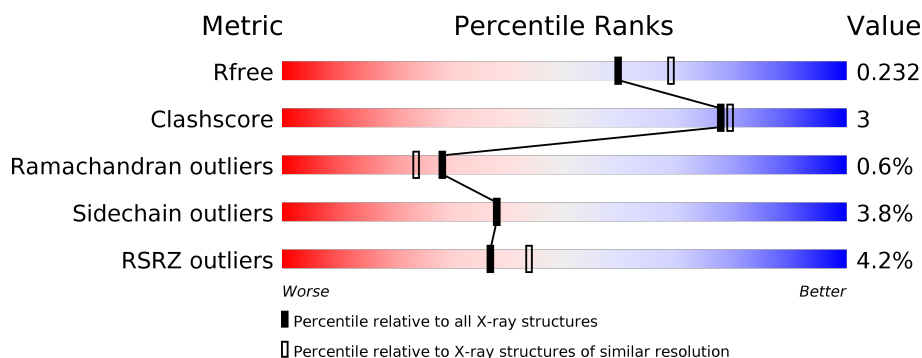
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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))
$R_{free}$	100719	4243 (2.10-2.10)
Clashscore	112137	4788 (2.10-2.10)
Ramachandran outliers	110173	4740 (2.10-2.10)
Sidechain outliers	110143	4741 (2.10-2.10)
RSRZ outliers	101464	4275 (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. 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>5%</div> <div> <div>87%</div> <div>7%</div> <div>• •</div> </div> </div>
1	B	761	<div> <div>3%</div> <div> <div>86%</div> <div>9%</div> <div>• •</div> </div> </div>
1	C	761	<div> <div>2%</div> <div> <div>87%</div> <div>7%</div> <div>• •</div> </div> </div>
2	D	20	<div> <div>20%</div> <div> <div>65%</div> <div>15%</div> <div>20%</div> </div> </div>
2	E	20	<div> <div>15%</div> <div> <div>65%</div> <div>10%</div> <div>5%</div> <div>20%</div> </div> </div>
2	F	20	<div> <div>15%</div> <div> <div>70%</div> <div>10%</div> <div>20%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
2	P	20	<div><div><div></div><div></div><div></div></div><div>5%10%5%85%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 19192 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	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-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	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		

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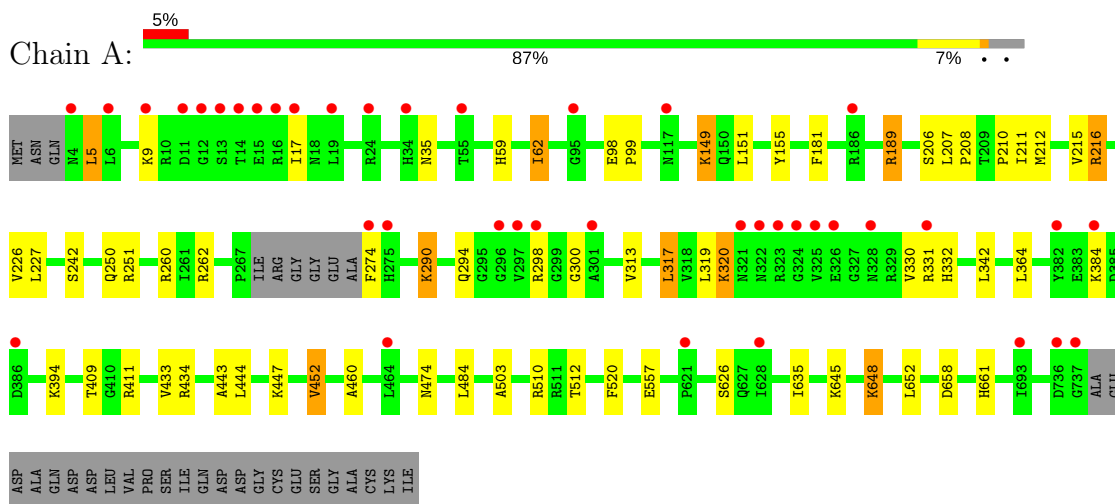
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	6	Total	O	0	0
			6	6		
3	F	2	Total	O	0	0
			2	2		

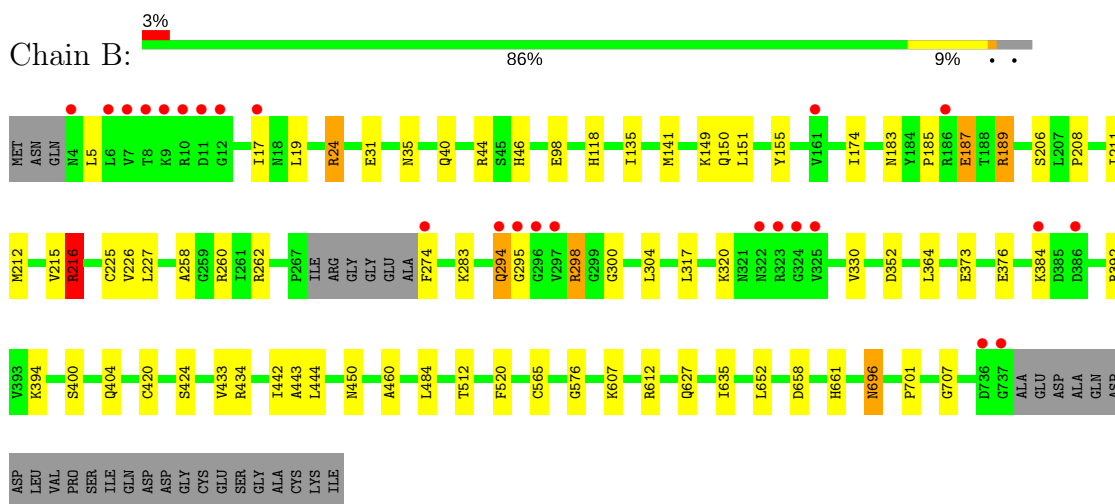
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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.

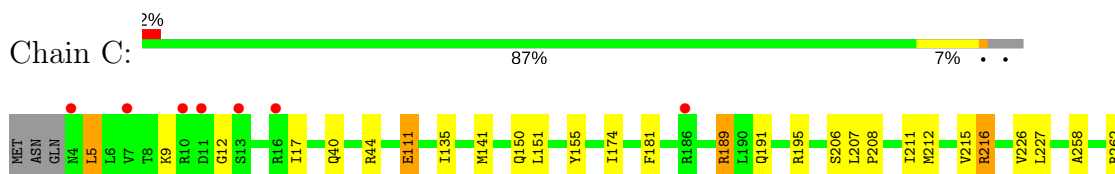
#### • Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT ALPHA

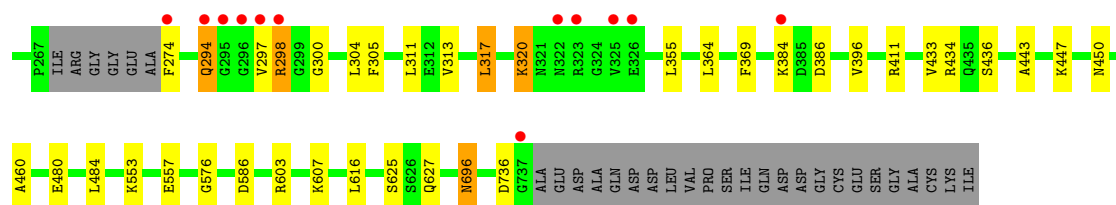


#### • Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT ALPHA

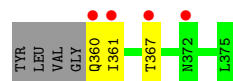


#### • Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT ALPHA

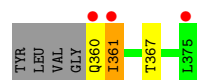




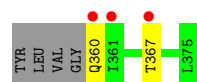
● Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA



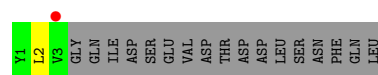
● Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA



● 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, $\alpha$ , $\beta$ , $\gamma$	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 , 52.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	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.

<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 [i](#)

### 5.1 Standard geometry [i](#)

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 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	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
2	F	129	0	111	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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

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 3.

All (120) 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: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:CG	1:A:189:ARG:HH11	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:151:LEU:HA	1:B:155:TYR:HB2	1.81	0.62
1:B:227:LEU:HB2	1:B:460:ALA:HB3	1.81	0.62
1:B:185:PRO:HB2	1:B:187:GLU:HG2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:648:LYS:HD2	1:A:648:LYS:H	1.65	0.60
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:A:151:LEU:HA	1:A:155:TYR:HB2	1.85	0.57
1:C:111:GLU:HG3	2:P:2:LEU:HB2	1.86	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:B:400:SER:O	1:B:404:GLN:HB2	2.12	0.49
1:C:553:LYS:O	1:C:557:GLU:HG3	2.11	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:19:LEU:HD22	1:B:46:HIS:CE1	2.50	0.46
1:C:191:GLN:HE21	1:C:195:ARG:HH21	1.64	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:B:701:PRO:O	1:B:707:GLY:HA2	2.17	0.44
1:C:320:LYS:HE2	1:C:411:ARG:HB2	2.00	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:A:208:PRO:HD2	1:A:211:ILE:HD12	1.99	0.43
1:B:450:ASN:HB2	3:B:2240:HOH:O	2.18	0.43
1:C:313:VAL:HG22	1:C:317:LEU:HD22	2.00	0.43
1:C:603:ARG:HG2	1:C:607:LYS:HE3	2.00	0.43
1:A:319:LEU:HD22	1:A:330:VAL:HG23	2.01	0.43
1:A:510:ARG:HB2	1:A:512:THR:HG23	2.01	0.43
1:B:189:ARG:NH1	1:B:189:ARG:HG2	2.32	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:GLU:HG3	3:A:2078:HOH:O	2.20	0.41
1:B:44:ARG:HD3	3:B:2024:HOH:O	2.19	0.41
1:A:320:LYS:HG3	1:A:409:THR:HG21	2.01	0.41
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%)	38	35
1	B	723/761 (95%)	702 (97%)	16 (2%)	5 (1%)	25	20
1	C	723/761 (95%)	706 (98%)	12 (2%)	5 (1%)	25	20
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%)	28	24

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
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%)	41	42
1	B	625/650 (96%)	603 (96%)	22 (4%)	41	42
1	C	625/650 (96%)	604 (97%)	21 (3%)	42	43
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%)	5	3
2	P	3/19 (16%)	3 (100%)	0	100	100
All	All	1926/2026 (95%)	1853 (96%)	73 (4%)	38	38

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

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Mol	Chain	Res	Type
1	A	149	LYS
1	A	189	ARG
1	A	206	SER
1	A	226	VAL
1	A	290	LYS
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

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Mol	Chain	Res	Type
1	C	111	GLU
1	C	141	MET
1	C	189	ARG
1	C	206	SER
1	C	226	VAL
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

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Mol	Chain	Res	Type
1	B	183	ASN
1	B	250	GLN
1	B	328	ASN
1	B	630	ASN
1	B	633	ASN
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 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	NIY	A	731	1	13,15,16	0.53	0	15,20,22	1.51	2 (13%)
1	NIY	B	731	1	13,15,16	0.61	0	15,20,22	1.55	2 (13%)
1	NIY	C	731	1	13,15,16	0.55	0	15,20,22	1.71	2 (13%)

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	-	0/6/10/12	0/1/1/1
1	NIY	B	731	1	-	0/6/10/12	0/1/1/1
1	NIY	C	731	1	-	0/6/10/12	0/1/1/1

There are no bond length outliers.

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	731	NIY	CB-CA-C	-5.14	101.51	111.41
1	A	731	NIY	CB-CA-C	-4.18	103.35	111.41
1	B	731	NIY	CB-CA-C	-3.38	104.89	111.41
1	C	731	NIY	CB-CG-CD1	-2.50	115.88	120.43
1	A	731	NIY	CB-CG-CD1	-2.07	116.66	120.43
1	B	731	NIY	CD1-CE1-NN	3.89	120.33	115.82

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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

### 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	727/761 (95%)	0.29	40 (5%)	26 32	22, 34, 55, 85	0
1	B	727/761 (95%)	0.15	24 (3%)	47 54	22, 34, 53, 81	0
1	C	727/761 (95%)	0.02	19 (2%)	56 62	15, 26, 45, 72	0
2	D	16/20 (80%)	1.18	4 (25%)	1 1	72, 80, 81, 81	0
2	E	16/20 (80%)	1.03	3 (18%)	1 2	70, 78, 81, 82	0
2	F	16/20 (80%)	1.34	3 (18%)	1 2	62, 72, 75, 76	0
2	P	3/20 (15%)	0.73	1 (33%)	0 0	29, 29, 35, 39	0
All	All	2232/2363 (94%)	0.17	94 (4%)	37 44	15, 32, 56, 85	0

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	297	VAL	8.2
1	C	737	GLY	6.8
1	B	296	GLY	6.5
1	A	737	GLY	6.3
1	B	274	PHE	6.2
1	A	297	VAL	5.9
1	C	297	VAL	5.6
1	C	296	GLY	5.3
1	A	6	LEU	5.2
1	B	737	GLY	4.9
1	B	325	VAL	4.9
1	A	13	SER	4.7
1	A	296	GLY	4.6
1	A	323	ARG	4.6
2	E	360	GLN	4.5
1	A	17	ILE	4.5
2	F	360	GLN	4.4

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Mol	Chain	Res	Type	RSRZ
1	A	12	GLY	4.2
1	B	323	ARG	4.2
1	A	322	ASN	4.0
1	A	4	ASN	4.0
1	C	294	GLN	3.9
1	C	323	ARG	3.9
1	A	14	THR	3.8
1	A	325	VAL	3.8
1	A	274	PHE	3.8
2	D	361	ILE	3.6
1	C	274	PHE	3.6
1	B	6	LEU	3.5
1	C	13	SER	3.4
1	B	10	ARG	3.4
1	B	322	ASN	3.3
1	C	384	LYS	3.2
1	B	384	LYS	3.2
1	C	322	ASN	3.2
1	A	15	GLU	3.2
1	C	16	ARG	3.2
2	D	360	GLN	3.1
1	B	324	GLY	3.0
2	D	372	ASN	2.9
1	A	19	LEU	2.9
1	A	321	ASN	2.9
1	B	295	GLY	2.8
1	C	325	VAL	2.8
1	C	186	ARG	2.8
1	A	275	HIS	2.8
1	B	736	ASP	2.8
1	A	11	ASP	2.8
1	B	9	LYS	2.8
1	C	4	ASN	2.7
1	A	9	LYS	2.7
1	A	298	ARG	2.7
1	A	34	HIS	2.7
1	A	186	ARG	2.7
1	A	16	ARG	2.7
1	C	295	GLY	2.6
2	F	367	THR	2.6
1	C	11	ASP	2.6
2	E	361	ILE	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	326	GLU	2.5
1	A	55	THR	2.5
1	A	384	LYS	2.5
1	B	294	GLN	2.5
1	A	95	GLY	2.5
1	A	324	GLY	2.5
1	B	12	GLY	2.4
2	P	3	VAL	2.4
1	B	386	ASP	2.4
1	B	161	VAL	2.4
1	A	24	ARG	2.4
1	B	186	ARG	2.4
1	C	326	GLU	2.3
1	B	11	ASP	2.3
1	B	4	ASN	2.3
2	D	367	THR	2.2
2	F	361	ILE	2.2
1	A	386	ASP	2.2
1	C	298	ARG	2.2
1	A	117	ASN	2.2
1	A	328	ASN	2.2
1	B	7	VAL	2.2
1	C	10	ARG	2.2
1	A	331	ARG	2.2
1	A	621	PRO	2.1
1	C	7	VAL	2.1
1	A	301	ALA	2.1
1	A	693	ILE	2.1
1	B	8	THR	2.1
1	A	736	ASP	2.1
1	B	17	ILE	2.1
1	A	382	TYR	2.1
2	E	375	LEU	2.0
1	A	464	LEU	2.0
1	A	628	ILE	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	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	NIY	A	731	15/16	0.94	0.11	-	28,33,39,39	0
1	NIY	B	731	15/16	0.88	0.14	-	27,31,37,38	0
1	NIY	C	731	15/16	0.94	0.10	-	20,27,35,35	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.