



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 02:41 PM UTC

PDB ID : 2XAP / pdb_00002xap
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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

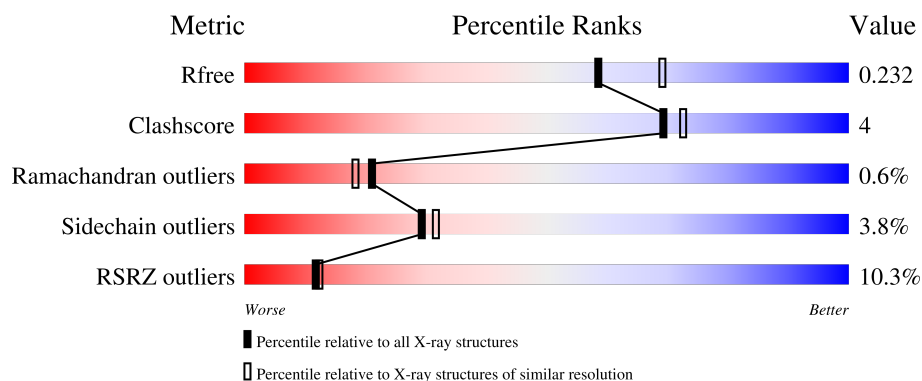
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	761	10% 86% 8% ..
1	B	761	9% 85% 9% ..
1	C	761	7% 86% 8% ..
2	D	20	55% 65% 15% 20%
2	E	20	55% 65% 10% 5% 20%

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Mol	Chain	Length	Quality of chain
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 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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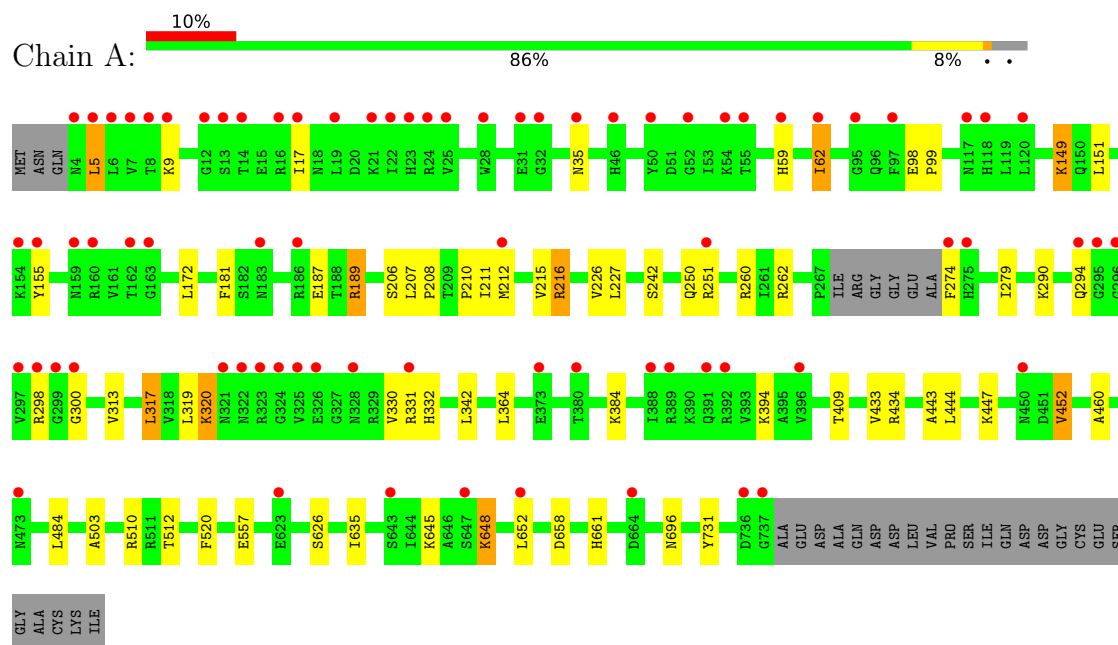
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	E	6	Total	O	0	0
			6	6		
3	F	2	Total	O	0	0
			2	2		

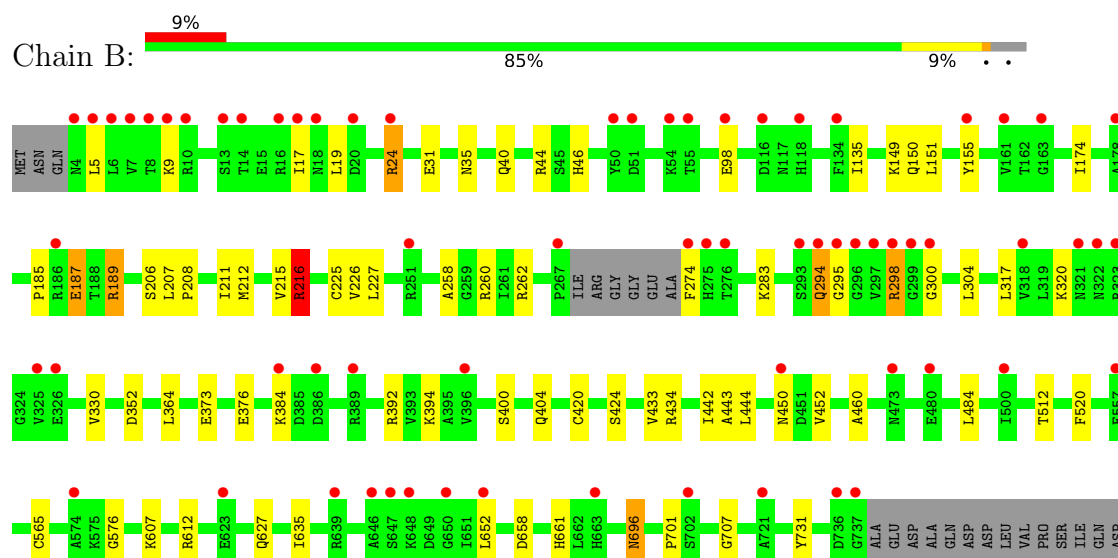
3 Residue-property plots

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

• Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT ALPHA



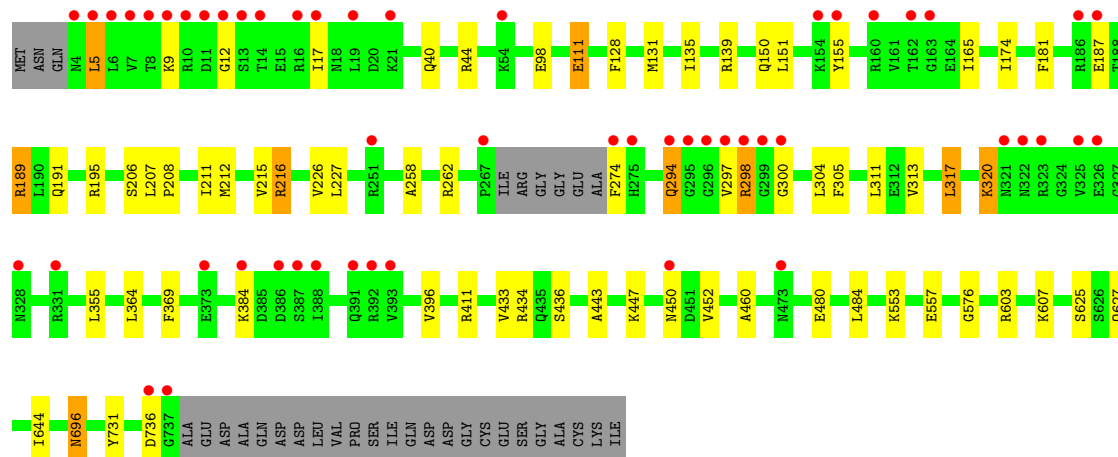
• Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT ALPHA



ASP
GLY
CYS
GLU
SER
GLY
ALA
CYS
LYS
ILE

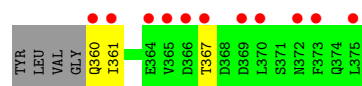
• Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT ALPHA

Chain C: 7% 86% 8% . .



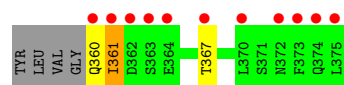
• Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA

Chain D: 55% 65% 15% 20%



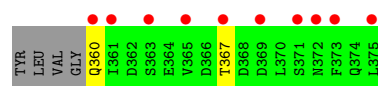
• Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA

Chain E: 55% 65% 10% 5% 20%



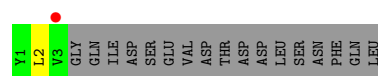
• Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA

Chain F: 50% 70% 10% 20%



• Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA

Chain P: 5% 10% 5% 85%



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	223.98Å 223.98Å 336.03Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	169.03 – 2.10 167.99 – 2.10	Depositor EDS
% Data completeness (in resolution range)	94.8 (169.03-2.10) 91.7 (167.99-2.10)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	31.4	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	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 ²)	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.*

¹Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 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	0.50	1/5917 (0.0%)	0.79	0/8012
1	B	0.49	0/5917	0.79	0/8012
1	C	0.53	0/5917	0.79	0/8012
2	D	0.49	0/129	0.74	0/173
2	E	0.46	0/129	0.77	0/173
2	F	0.44	0/129	0.68	0/173
2	P	0.53	0/27	0.52	0/36
All	All	0.50	1/18165 (0.0%)	0.79	0/24591

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	279	ILE	CA-CB	6.61	1.57	1.54

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	42	0
1	C	5807	0	5726	41	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	129	0	111	0	0
2	E	129	0	111	1	0
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	124	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 4.

All (124) 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:HH11	1:B:24:ARG:HG3	1.13	1.06
1:A:189:ARG:HG2	1:A:189:ARG:HH11	1.20	1.03
1:C:189:ARG:HH11	1:C:189:ARG:HG2	1.29	0.98
1:A:207:LEU:HD12	1:A:212:MET:HE3	1.52	0.89
1:B:576:GLY:HA3	1:B:607:LYS:HE2	1.57	0.87
1:A:189:ARG:HG2	1:A:189:ARG:NH1	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:HG2	1:C:189:ARG:NH1	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	0.64
1:B:212:MET:O	1:B:216:ARG:NH2	2.23	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:B:207:LEU:HB2	1:B:212:MET:HE3	1.88	0.56
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:CG	1:B:189:ARG:HH11	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:207:LEU:HB2	1:C:212:MET:HE3	1.88	0.54
1:C:258:ALA:HB3	1:C:304:LEU:HD21	1.90	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: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: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:150:GLN:HE21	1:C:627:GLN:CD	2.20	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:207:LEU:CD1	1:C:212:MET:HE3	2.42	0.49
1:C:155:TYR:CZ	1:C:212:MET:HG3	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:207:LEU:HD12	1:C:212:MET:HE3	1.97	0.45
1:B:150:GLN:HE21	1:B:627:GLN:CD	2.25	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:172:LEU:HD23	1:A:172:LEU:C	2.43	0.44
1:A:433:VAL:HG11	1:A:443:ALA:HB1	1.99	0.44
2:E:361:ILE:H	2:E:361:ILE:HD13	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:HG2	1:B:189:ARG:NH1	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:59:HIS:O	1:A:62:ILE:HD13	2.19	0.42
1:A:342:LEU:HG	3:A:2179:HOH:O	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:C:128:PHE:HA	1:C:131:MET:HE3	2.03	0.41
1:A:149:LYS:HG2	1:A:652:LEU:HD11	2.02	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:B:189:ARG:HH11	1:B:189:ARG:CB	2.34	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 [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	723/761 (95%)	704 (97%)	16 (2%)	3 (0%)	30	28
1	B	723/761 (95%)	702 (97%)	16 (2%)	5 (1%)	18	15
1	C	723/761 (95%)	706 (98%)	12 (2%)	5 (1%)	18	15
2	D	14/20 (70%)	14 (100%)	0	0	100	100
2	E	14/20 (70%)	14 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
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%)	21	18

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%)	604 (97%)	21 (3%)	32	35
1	B	625/650 (96%)	604 (97%)	21 (3%)	32	35
1	C	625/650 (96%)	602 (96%)	23 (4%)	30	33
2	D	16/19 (84%)	13 (81%)	3 (19%)	1	1
2	E	16/19 (84%)	13 (81%)	3 (19%)	1	1
2	F	16/19 (84%)	14 (88%)	2 (12%)	4	2
2	P	3/19 (16%)	3 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	1926/2026 (95%)	1853 (96%)	73 (4%)	29	32

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	187	GLU
1	A	189	ARG
1	A	206	SER
1	A	226	VAL
1	A	317	LEU
1	A	320	LYS
1	A	364	LEU
1	A	384	LYS
1	A	394	LYS
1	A	452	VAL
1	A	484	LEU
1	A	626	SER
1	A	645	LYS
1	A	648	LYS
1	A	696	ASN
1	B	5	LEU
1	B	9	LYS
1	B	17	ILE
1	B	24	ARG
1	B	31	GLU
1	B	35	ASN
1	B	98	GLU
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

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Mol	Chain	Res	Type
1	B	384	LYS
1	B	394	LYS
1	B	452	VAL
1	B	484	LEU
1	B	696	ASN
1	C	5	LEU
1	C	9	LYS
1	C	17	ILE
1	C	98	GLU
1	C	111	GLU
1	C	139	ARG
1	C	165	ILE
1	C	187	GLU
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	452	VAL
1	C	484	LEU
1	C	625	SER
1	C	644	ILE
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

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (46) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	35	ASN
1	A	46	HIS

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Mol	Chain	Res	Type
1	A	96	GLN
1	A	130	GLN
1	A	183	ASN
1	A	250	GLN
1	A	328	ASN
1	A	332	HIS
1	A	416	ASN
1	A	453	ASN
1	A	609	HIS
1	A	661	HIS
1	A	733	ASN
1	B	18	ASN
1	B	46	HIS
1	B	48	GLN
1	B	130	GLN
1	B	150	GLN
1	B	183	ASN
1	B	250	GLN
1	B	328	ASN
1	B	453	ASN
1	B	456	ASN
1	B	474	ASN
1	B	569	ASN
1	B	630	ASN
1	B	633	ASN
1	B	661	HIS
1	B	696	ASN
1	B	733	ASN
1	C	46	HIS
1	C	130	GLN
1	C	150	GLN
1	C	183	ASN
1	C	191	GLN
1	C	250	GLN
1	C	294	GLN
1	C	328	ASN
1	C	332	HIS
1	C	456	ASN
1	C	613	ASN
1	C	661	HIS
1	C	696	ASN
1	C	733	ASN

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Mol	Chain	Res	Type
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	C	731	1	14,15,16	1.00	1 (7%)	11,20,22	1.21	1 (9%)
1	NIY	B	731	1	14,15,16	1.06	1 (7%)	11,20,22	0.82	0
1	NIY	A	731	1	14,15,16	1.07	1 (7%)	11,20,22	1.03	1 (9%)

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	C	731	1	-	4/7/10/12	0/1/1/1
1	NIY	B	731	1	-	2/7/10/12	0/1/1/1
1	NIY	A	731	1	-	4/7/10/12	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	731	NIY	CE1-NN	-3.14	1.40	1.45
1	A	731	NIY	CE1-NN	-3.13	1.40	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	731	NIY	CE1-NN	-2.88	1.40	1.45

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	731	NIY	CB-CG-CD1	-2.65	115.88	120.43
1	A	731	NIY	CB-CG-CD1	-2.20	116.66	120.43

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	731	NIY	CD1-CE1-NN-O2
1	A	731	NIY	CZ-CE1-NN-O2
1	B	731	NIY	CA-CB-CG-CD2
1	C	731	NIY	CA-CB-CG-CD1
1	C	731	NIY	CA-CB-CG-CD2
1	B	731	NIY	CA-CB-CG-CD1
1	A	731	NIY	CA-CB-CG-CD2
1	A	731	NIY	CA-CB-CG-CD1
1	C	731	NIY	CD1-CE1-NN-O2
1	C	731	NIY	CZ-CE1-NN-O2

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	727/761 (95%)	0.57	76 (10%) 11 12	22, 34, 55, 85	0
1	B	727/761 (95%)	0.65	68 (9%) 14 14	22, 34, 53, 81	0
1	C	727/761 (95%)	0.23	53 (7%) 21 22	15, 26, 45, 72	0
2	D	16/20 (80%)	2.56	11 (68%) 0 0	72, 80, 81, 81	0
2	E	16/20 (80%)	2.46	11 (68%) 0 0	70, 78, 81, 82	0
2	F	16/20 (80%)	2.30	10 (62%) 0 0	62, 72, 75, 76	0
2	P	3/20 (15%)	1.39	1 (33%) 1 1	29, 29, 35, 39	0
All	All	2232/2363 (94%)	0.52	230 (10%) 12 12	15, 32, 56, 85	0

All (230) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	297	VAL	6.9
1	B	297	VAL	6.4
1	B	296	GLY	6.3
1	A	17	ILE	6.2
1	C	294	GLN	6.0
1	C	274	PHE	6.0
1	A	737	GLY	5.8
1	C	297	VAL	5.8
1	A	274	PHE	5.7
1	C	737	GLY	5.6
1	B	274	PHE	5.6
1	C	296	GLY	5.5
1	A	296	GLY	5.3
1	B	736	ASP	5.1
2	E	373	PHE	5.0
2	D	361	ILE	4.9
1	A	5	LEU	4.6

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Mol	Chain	Res	Type	RSRZ
1	A	328	ASN	4.6
1	A	9	LYS	4.4
1	A	295	GLY	4.4
1	A	300	GLY	4.4
1	C	322	ASN	4.4
1	C	16	ARG	4.3
1	B	737	GLY	4.2
1	A	8	THR	4.2
1	A	19	LEU	4.1
2	D	365	VAL	4.1
1	B	251	ARG	4.0
1	A	118	HIS	4.0
2	E	361	ILE	4.0
1	A	321	ASN	4.0
1	A	325	VAL	3.9
1	A	6	LEU	3.9
1	A	14	THR	3.9
2	F	375	LEU	3.9
1	C	275	HIS	3.9
1	A	155	TYR	3.8
1	C	13	SER	3.8
1	B	295	GLY	3.8
1	C	12	GLY	3.8
1	A	299	GLY	3.7
1	A	322	ASN	3.7
1	B	299	GLY	3.7
1	B	325	VAL	3.7
1	A	275	HIS	3.6
2	F	373	PHE	3.6
2	F	361	ILE	3.6
2	D	372	ASN	3.5
2	E	375	LEU	3.5
1	C	325	VAL	3.5
1	B	275	HIS	3.5
1	C	4	ASN	3.5
1	C	5	LEU	3.5
1	A	391	GLN	3.5
1	A	117	ASN	3.5
1	B	7	VAL	3.4
1	A	298	ARG	3.4
1	A	736	ASP	3.4
1	A	4	ASN	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	11	ASP	3.3
1	B	322	ASN	3.3
1	C	298	ARG	3.3
1	C	326	GLU	3.3
1	B	51	ASP	3.3
1	B	8	THR	3.2
1	B	323	ARG	3.2
1	C	295	GLY	3.2
1	A	7	VAL	3.2
1	B	17	ILE	3.1
2	D	367	THR	3.1
1	B	298	ARG	3.1
1	C	9	LYS	3.1
1	B	6	LEU	3.1
2	D	375	LEU	3.1
1	C	384	LYS	3.1
1	C	8	THR	3.1
1	A	450	ASN	3.1
2	F	363	SER	3.1
1	C	299	GLY	3.0
1	B	294	GLN	3.0
1	A	13	SER	3.0
2	P	3	VAL	3.0
1	C	186	ARG	3.0
1	A	35	ASN	3.0
1	A	183	ASN	3.0
1	A	160	ARG	3.0
1	C	251	ARG	2.9
1	A	52	GLY	2.9
1	A	55	THR	2.9
1	A	212	MET	2.9
1	A	643	SER	2.9
1	B	386	ASP	2.8
1	A	251	ARG	2.8
1	B	10	ARG	2.8
1	C	328	ASN	2.8
1	B	646	ALA	2.8
2	D	373	PHE	2.8
1	B	300	GLY	2.8
1	A	22	ILE	2.8
1	C	473	ASN	2.8
1	A	647	SER	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	736	ASP	2.8
1	B	5	LEU	2.8
1	C	54	LYS	2.8
1	C	267	PRO	2.8
1	B	500	ILE	2.8
1	A	16	ARG	2.7
1	C	392	ARG	2.7
1	B	293	SER	2.7
1	C	21	LYS	2.7
1	A	186	ARG	2.7
1	C	7	VAL	2.7
1	B	14	THR	2.7
1	B	50	TYR	2.7
1	A	473	ASN	2.7
1	A	59	HIS	2.7
1	A	294	GLN	2.7
1	B	134	PHE	2.7
1	C	373	GLU	2.6
2	D	364	GLU	2.6
1	B	384	LYS	2.6
1	A	388	ILE	2.6
1	A	331	ARG	2.6
1	A	392	ARG	2.6
1	B	450	ASN	2.6
1	A	162	THR	2.6
1	B	161	VAL	2.6
1	A	46	HIS	2.6
2	E	372	ASN	2.6
1	C	154	LYS	2.6
1	C	160	ARG	2.6
2	E	367	THR	2.6
2	D	370	LEU	2.6
1	B	623	GLU	2.5
2	E	360	GLN	2.5
1	B	55	THR	2.5
1	B	276	THR	2.5
1	C	14	THR	2.5
2	F	365	VAL	2.5
1	B	480	GLU	2.5
1	B	557	GLU	2.5
1	B	574	ALA	2.5
2	E	370	LEU	2.5

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Mol	Chain	Res	Type	RSRZ
1	A	31	GLU	2.4
1	B	647	SER	2.4
1	C	155	TYR	2.4
1	B	267	PRO	2.4
1	A	389	ARG	2.4
1	B	16	ARG	2.4
1	B	163	GLY	2.4
1	B	20	ASP	2.4
1	C	386	ASP	2.4
1	C	388	ILE	2.4
1	C	331	ARG	2.4
1	B	389	ARG	2.3
1	B	13	SER	2.3
1	B	396	VAL	2.3
2	D	360	GLN	2.3
1	C	321	ASN	2.3
1	B	652	LEU	2.3
1	B	321	ASN	2.3
1	A	652	LEU	2.3
1	C	10	ARG	2.3
1	C	300	GLY	2.3
2	D	369	ASP	2.3
1	B	326	GLU	2.3
1	C	17	ILE	2.3
2	F	360	GLN	2.3
1	A	54	LYS	2.3
2	E	362	ASP	2.3
1	A	120	LEU	2.3
1	A	25	VAL	2.2
1	B	318	VAL	2.2
1	A	159	ASN	2.2
1	B	721	ALA	2.2
1	B	155	TYR	2.2
1	C	387	SER	2.2
2	F	371	SER	2.2
1	A	154	LYS	2.2
1	B	18	ASN	2.2
2	F	367	THR	2.2
1	A	12	GLY	2.2
1	B	178	ALA	2.2
2	E	374	GLN	2.2
1	B	24	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	450	ASN	2.2
2	F	372	ASN	2.2
2	F	369	ASP	2.2
1	C	187	GLU	2.2
1	B	118	HIS	2.2
1	C	391	GLN	2.2
1	A	373	GLU	2.1
1	B	98	GLU	2.1
1	A	32	GLY	2.1
1	A	163	GLY	2.1
1	B	650	GLY	2.1
1	B	186	ARG	2.1
1	B	648	LYS	2.1
1	B	4	ASN	2.1
1	B	116	ASP	2.1
2	D	366	ASP	2.1
1	C	162	THR	2.1
1	A	95	GLY	2.1
1	A	396	VAL	2.1
1	A	323	ARG	2.1
2	E	363	SER	2.1
1	B	473	ASN	2.1
1	A	24	ARG	2.1
1	C	323	ARG	2.1
1	A	28	TRP	2.1
1	C	393	VAL	2.1
1	A	21	LYS	2.1
1	B	9	LYS	2.1
1	C	6	LEU	2.1
1	C	19	LEU	2.1
1	A	326	GLU	2.1
1	A	623	GLU	2.1
2	E	364	GLU	2.1
1	A	50	TYR	2.1
1	B	639	ARG	2.1
1	A	62	ILE	2.1
1	B	54	LYS	2.1
1	B	702	SER	2.1
1	A	664	ASP	2.0
1	A	23	HIS	2.0
1	A	97	PHE	2.0
1	B	663	HIS	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	380	THR	2.0
1	A	324	GLY	2.0
1	C	163	GLY	2.0

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

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	NIY	B	731	15/16	0.83	0.14	27,31,37,38	0
1	NIY	A	731	15/16	0.90	0.13	28,33,39,39	0
1	NIY	C	731	15/16	0.91	0.11	20,27,35,35	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.