



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 03:30 PM GMT

PDB ID : 2XAY
Title : RIBONUCLEOTIDE REDUCTASE Y730NO2Y AND C439A MODIFIED R1
SUBUNIT OF E. COLI
Authors : Yokoyama, K.; Uhlin, U.; Stubbe, J.
Deposited on : 2010-04-01
Resolution : 2.65 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

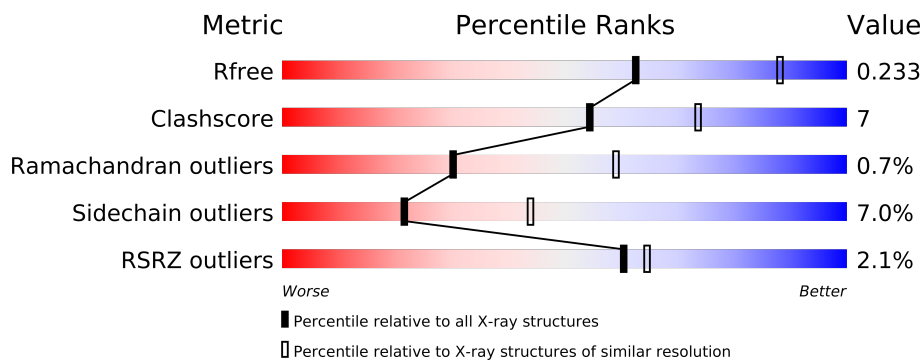
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.65 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	2232 (2.70-2.62)
Clashscore	79885	2700 (2.70-2.62)
Ramachandran outliers	78287	2657 (2.70-2.62)
Sidechain outliers	78261	2657 (2.70-2.62)
RSRZ outliers	66119	2234 (2.70-2.62)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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 18579 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
			5806	3688	996	1099	23			
1	B	728	Total	C	N	O	S	0	0	0
			5806	3688	996	1099	23			
1	C	728	Total	C	N	O	S	0	0	0
			5806	3688	996	1099	23			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	439	ALA	CYS	ENGINEERED MUTATION	UNP P00452
B	439	ALA	CYS	ENGINEERED MUTATION	UNP P00452
C	439	ALA	CYS	ENGINEERED MUTATION	UNP P00452

- 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	11	Total	C	N	O	0	0	0
			89	54	13	22			
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	229	Total	O	0	0
			229	229		

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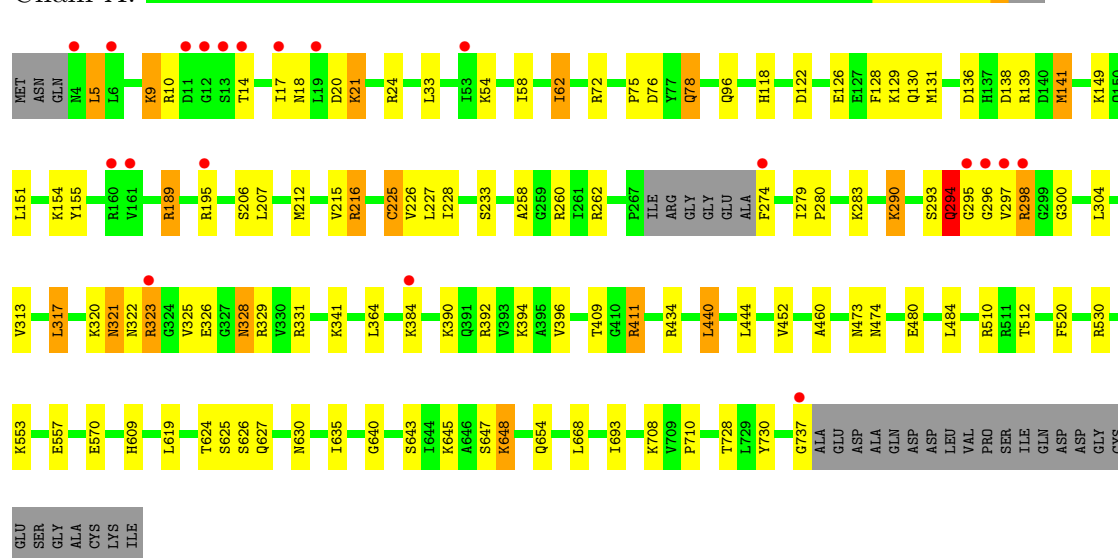
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	245	Total 245	O 245	0	0
3	C	299	Total 299	O 299	0	0
3	D	5	Total 5	O 5	0	0
3	F	5	Total 5	O 5	0	0
3	P	4	Total 4	O 4	0	0

3 Residue-property plots

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

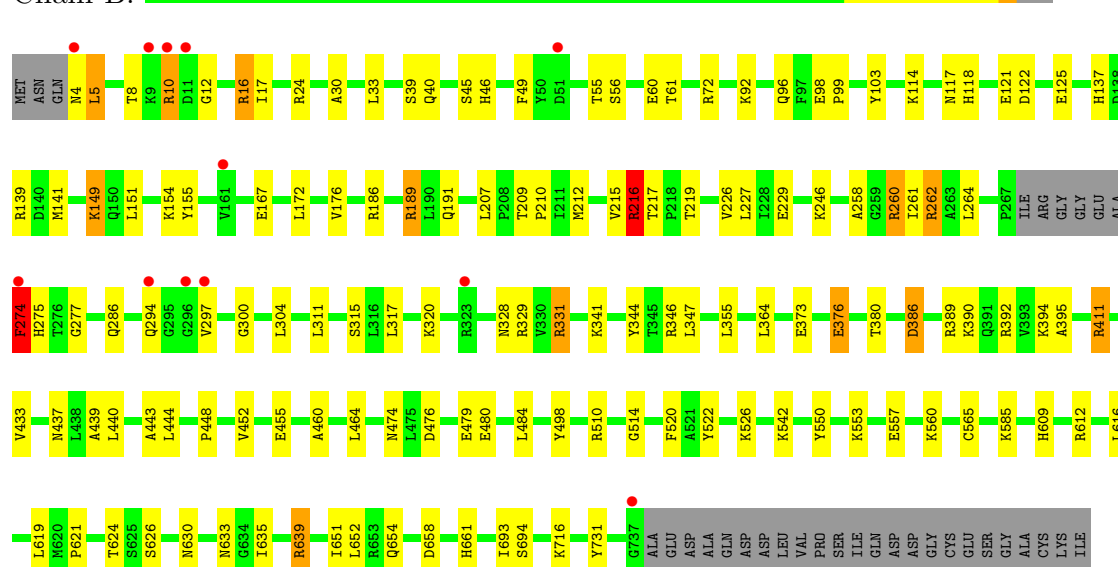
• Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATEREDUCTASE 1 SUBUNIT ALPHA

Chain A:



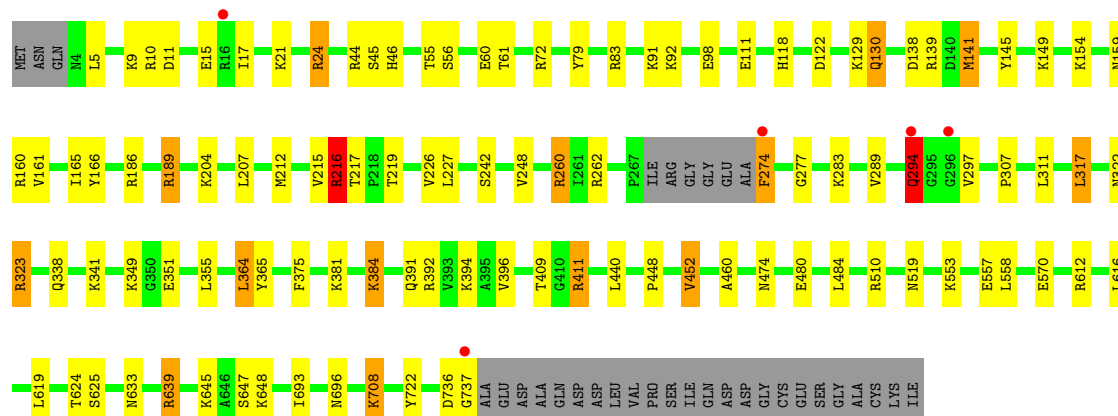
• Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATEREDUCTASE 1 SUBUNIT ALPHA

Chain B:



- Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATEREDUCTASE 1 SUBUNIT ALPHA

Chain C:



4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	224.50Å 224.50Å 337.84Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	169.03 – 2.65 79.50 – 2.65	Depositor EDS
% Data completeness (in resolution range)	98.5 (169.03-2.65) 98.5 (79.50-2.65)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.96 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.182 , 0.235 0.182 , 0.233	Depositor DCC
R_{free} test set	4667 reflections (5.27%)	DCC
Wilson B-factor (Å ²)	41.3	Xtriage
Anisotropy	0.070	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 23.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	4 of 93249 reflections (0.004%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18579	wwPDB-VP
Average B, all atoms (Å ²)	40.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities 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	0.45	0/5916	0.58	0/8011
1	B	0.46	0/5916	0.58	0/8011
1	C	0.51	0/5916	0.62	1/8011 (0.0%)
2	D	0.47	0/129	0.58	0/173
2	E	0.38	0/89	0.59	0/119
2	F	0.45	0/129	0.62	0/173
2	P	0.66	0/27	0.72	0/36
All	All	0.47	0/18122	0.60	1/24534 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	317	LEU	CA-CB-CG	5.10	127.03	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	274	PHE	Peptide

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	5806	0	5725	82	0
1	B	5806	0	5725	87	0
1	C	5806	0	5725	67	0
2	D	129	0	111	3	0
2	E	89	0	77	0	0
2	F	129	0	111	1	0
2	P	27	0	31	1	0
3	A	229	0	0	25	0
3	B	245	0	0	30	0
3	C	299	0	0	28	0
3	D	5	0	0	1	0
3	F	5	0	0	1	0
3	P	4	0	0	2	0
All	All	18579	0	17505	239	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 7.

All (239) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:216:ARG:HD2	3:B:2052:HOH:O	1.34	1.22
1:B:526:LYS:HD2	3:B:2173:HOH:O	1.47	1.13
1:B:155:TYR:HE1	3:B:2067:HOH:O	1.31	1.11
1:B:346:ARG:HB3	3:B:2118:HOH:O	1.52	1.09
1:A:274:PHE:HA	3:A:2091:HOH:O	1.54	1.06
1:B:260:ARG:HH11	1:B:260:ARG:HG2	1.24	0.98
1:C:274:PHE:HA	3:C:2115:HOH:O	1.62	0.98
1:A:294:GLN:HG3	1:A:295:GLY:N	1.84	0.91
1:C:24:ARG:HD3	3:C:2009:HOH:O	1.70	0.89
1:C:262:ARG:HG2	1:C:274:PHE:HB2	1.58	0.85
1:A:233:SER:HA	1:A:274:PHE:HZ	1.42	0.84
1:A:510:ARG:NH2	1:A:570:GLU:OE1	2.10	0.83
1:C:262:ARG:CG	1:C:274:PHE:HB2	2.09	0.83
1:B:260:ARG:HG2	1:B:260:ARG:NH1	1.98	0.79

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:476:ASP:HB2	3:B:2160:HOH:O	1.83	0.77
1:B:480:GLU:HB3	3:B:2164:HOH:O	1.83	0.77
1:C:633:ASN:HB3	3:C:2247:HOH:O	1.86	0.76
1:A:283:LYS:HG2	3:A:2095:HOH:O	1.85	0.76
1:B:619:LEU:HD12	1:B:693:ILE:HG12	1.68	0.76
1:A:233:SER:HA	1:A:274:PHE:CZ	2.21	0.75
1:A:207:LEU:HD12	1:A:212:MET:HE3	1.68	0.75
1:A:207:LEU:HD12	1:A:212:MET:CE	2.17	0.74
1:C:294:GLN:HB3	3:C:2121:HOH:O	1.88	0.74
1:C:212:MET:O	1:C:216:ARG:NH2	2.21	0.74
1:C:392:ARG:HD2	3:C:2146:HOH:O	1.88	0.73
1:A:328:ASN:HB2	1:A:329:ARG:NH1	2.04	0.73
1:C:215:VAL:O	1:C:216:ARG:HB3	1.87	0.73
1:C:260:ARG:HH11	1:C:260:ARG:HG2	1.53	0.72
1:C:639:ARG:NH1	3:C:2259:HOH:O	2.21	0.72
1:A:215:VAL:O	1:A:216:ARG:HB3	1.87	0.72
1:B:167:GLU:OE1	3:B:2052:HOH:O	2.08	0.71
1:B:411:ARG:NH1	1:B:731:TYR:HE1	1.87	0.71
1:A:294:GLN:HG3	1:A:295:GLY:H	1.56	0.71
1:C:262:ARG:HG2	1:C:274:PHE:CB	2.21	0.70
1:A:331:ARG:HD3	3:A:2114:HOH:O	1.92	0.70
1:C:480:GLU:HB3	3:C:2082:HOH:O	1.90	0.70
1:B:215:VAL:O	1:B:216:ARG:HB3	1.90	0.69
1:B:40:GLN:HG3	3:B:2018:HOH:O	1.92	0.69
1:B:212:MET:O	1:B:216:ARG:NH2	2.25	0.69
1:C:639:ARG:HH11	1:C:639:ARG:HG3	1.56	0.69
1:C:260:ARG:HD2	1:C:365:TYR:CE2	2.26	0.69
1:B:262:ARG:HG3	1:B:274:PHE:HB2	1.75	0.69
1:A:480:GLU:HB3	3:A:2059:HOH:O	1.92	0.69
1:A:473:ASN:HB2	3:A:2152:HOH:O	1.94	0.68
1:A:75:PRO:O	1:A:78:GLN:HB2	1.95	0.67
1:A:9:LYS:HE3	1:A:10:ARG:H	1.59	0.66
1:C:130:GLN:HG2	3:C:2057:HOH:O	1.95	0.66
1:A:619:LEU:HD12	1:A:693:ILE:HG12	1.77	0.66
1:B:479:GLU:HB2	1:B:550:TYR:CE1	2.31	0.66
1:A:212:MET:O	1:A:216:ARG:NH2	2.29	0.65
1:A:24:ARG:HH11	1:A:24:ARG:HG2	1.61	0.65
1:A:648:LYS:N	1:A:648:LYS:HD2	2.13	0.64
1:C:44:ARG:HD3	3:C:2020:HOH:O	1.96	0.64
1:B:411:ARG:NH1	1:B:731:TYR:CE1	2.65	0.64
1:A:129:LYS:HG3	3:A:2039:HOH:O	1.97	0.64
1:A:58:ILE:O	1:A:62:ILE:HG23	1.97	0.64

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:10:ARG:HG2	3:C:2004:HOH:O	1.97	0.63
1:A:130:GLN:HG3	3:A:2040:HOH:O	1.98	0.63
1:B:258:ALA:HB3	1:B:304:LEU:HD21	1.81	0.62
1:A:326:GLU:HA	3:A:2109:HOH:O	1.99	0.61
1:B:149:LYS:HG2	1:B:652:LEU:HD11	1.81	0.61
1:A:227:LEU:HB2	1:A:460:ALA:HB3	1.82	0.61
1:B:118:HIS:HB3	3:B:2042:HOH:O	1.99	0.61
1:A:233:SER:CA	1:A:274:PHE:HZ	2.12	0.61
1:C:737:GLY:HA2	3:C:2299:HOH:O	2.01	0.60
1:A:322:ASN:HB2	3:A:2108:HOH:O	2.02	0.59
1:A:126:GLU:HG3	3:A:2016:HOH:O	2.02	0.59
1:A:737:GLY:HA3	3:A:2226:HOH:O	2.02	0.59
1:B:217:THR:OG1	1:B:219:THR:HG22	2.03	0.59
1:C:384:LYS:HA	1:C:384:LYS:HE3	1.85	0.58
1:B:56:SER:O	1:B:60:GLU:HG2	2.02	0.58
1:C:297:VAL:HG12	3:C:2123:HOH:O	2.03	0.58
1:A:130:GLN:CG	3:A:2040:HOH:O	2.52	0.57
1:B:189:ARG:NE	3:B:2059:HOH:O	2.37	0.57
1:B:264:LEU:O	1:B:389:ARG:NH2	2.37	0.56
1:A:293:SER:HB2	1:A:298:ARG:O	2.05	0.56
1:C:647:SER:HB2	3:C:2268:HOH:O	2.06	0.56
1:A:151:LEU:HA	1:A:155:TYR:HB2	1.87	0.56
1:A:647:SER:HB3	3:A:2203:HOH:O	2.04	0.56
1:B:151:LEU:HA	1:B:155:TYR:HB2	1.88	0.56
1:A:122:ASP:O	1:A:189:ARG:NH2	2.39	0.55
1:C:311:LEU:HA	1:C:355:LEU:HB3	1.88	0.55
2:D:368:ASP:HB3	3:D:2004:HOH:O	2.06	0.55
1:A:262:ARG:HD2	1:A:274:PHE:HB3	1.90	0.54
1:A:328:ASN:HB2	1:A:329:ARG:HH11	1.71	0.54
1:B:117:ASN:HB2	3:B:2039:HOH:O	2.07	0.54
1:C:558:LEU:HD23	1:C:612:ARG:HG2	1.90	0.53
1:B:274:PHE:HA	1:B:277:GLY:H	1.74	0.53
1:A:24:ARG:HH11	1:A:24:ARG:CG	2.21	0.53
1:B:386:ASP:HA	1:B:390:LYS:NZ	2.23	0.53
1:C:91:LYS:HG2	3:C:2041:HOH:O	2.08	0.53
1:C:260:ARG:NH1	1:C:260:ARG:HG2	2.13	0.53
1:A:648:LYS:HD2	1:A:648:LYS:H	1.73	0.53
1:C:217:THR:OG1	1:C:219:THR:HG22	2.10	0.52
1:B:373:GLU:HA	1:B:376:GLU:HB2	1.92	0.52
1:B:386:ASP:N	1:B:386:ASP:OD2	2.38	0.52
1:B:433:VAL:HG11	1:B:443:ALA:HB1	1.90	0.52
1:B:227:LEU:HB2	1:B:460:ALA:HB3	1.92	0.52

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:122:ASP:O	1:C:189:ARG:NH2	2.42	0.51
1:B:262:ARG:HG3	1:B:274:PHE:CB	2.41	0.51
1:B:331:ARG:H	1:B:331:ARG:HH11	1.56	0.51
1:B:24:ARG:HD2	3:B:2009:HOH:O	2.11	0.51
1:B:716:LYS:HE3	3:B:2236:HOH:O	2.11	0.51
1:A:138:ASP:O	1:A:141:MET:HB2	2.12	0.50
1:B:10:ARG:HD3	3:B:2004:HOH:O	2.11	0.50
1:B:10:ARG:HD2	1:B:55:THR:HG21	1.94	0.50
1:C:260:ARG:HH21	1:C:448:PRO:HG2	1.75	0.50
1:A:300:GLY:HA2	3:A:2083:HOH:O	2.11	0.50
1:B:331:ARG:HD3	1:B:331:ARG:N	2.27	0.49
1:B:311:LEU:HA	1:B:355:LEU:HB3	1.93	0.49
1:A:390:LYS:HD2	1:A:392:ARG:NH2	2.26	0.49
1:B:386:ASP:HA	1:B:390:LYS:HZ3	1.78	0.49
1:A:321:ASN:HB2	3:A:2132:HOH:O	2.12	0.49
1:C:138:ASP:O	1:C:141:MET:HB2	2.12	0.49
1:C:242:SER:HB3	1:C:452:VAL:HG13	1.93	0.49
1:C:92:LYS:HE3	3:C:2028:HOH:O	2.13	0.49
1:B:630:ASN:ND2	1:B:654:GLN:HG2	2.28	0.48
1:A:609:HIS:HD2	3:P:2001:HOH:O	1.96	0.48
1:C:409:THR:O	1:C:411:ARG:HG2	2.13	0.48
1:C:207:LEU:HD12	1:C:212:MET:HE3	1.95	0.48
1:B:520:PHE:HB3	1:B:635:ILE:HA	1.95	0.48
1:A:313:VAL:HG22	1:A:317:LEU:HD22	1.95	0.48
1:C:56:SER:HB2	3:C:2029:HOH:O	2.13	0.48
1:A:710:PRO:HA	2:D:362:ASP:HB3	1.95	0.48
1:A:474:ASN:ND2	3:A:2152:HOH:O	2.33	0.48
1:A:195:ARG:NH1	3:A:2058:HOH:O	2.44	0.48
1:B:92:LYS:HG2	3:B:2032:HOH:O	2.13	0.48
1:A:280:PRO:HA	1:A:283:LYS:HD2	1.95	0.47
1:A:708:LYS:HD3	2:D:362:ASP:HB2	1.96	0.47
1:B:639:ARG:HB2	1:B:639:ARG:HH11	1.79	0.47
1:C:558:LEU:CD2	1:C:612:ARG:HG2	2.44	0.47
2:F:372:ASN:HA	3:F:2005:HOH:O	2.14	0.47
1:A:341:LYS:HB3	3:A:2122:HOH:O	2.15	0.47
1:B:331:ARG:H	1:B:331:ARG:HD3	1.80	0.47
1:B:585:LYS:HB2	3:B:2198:HOH:O	2.15	0.47
1:B:99:PRO:HG2	1:B:137:HIS:CG	2.50	0.47
1:B:246:LYS:HE3	3:B:2166:HOH:O	2.14	0.47
1:A:645:LYS:HG3	3:A:2201:HOH:O	2.15	0.47
1:B:4:ASN:HD22	1:B:16:ARG:CZ	2.28	0.46
1:A:444:LEU:HD22	1:A:512:THR:HG21	1.97	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:307:PRO:HA	1:C:338:GLN:HB2	1.97	0.46
1:A:294:GLN:HB2	3:A:2101:HOH:O	2.15	0.46
1:A:258:ALA:HB3	1:A:304:LEU:HD21	1.96	0.46
1:A:136:ASP:HB3	1:A:139:ARG:HG3	1.96	0.46
1:B:621:PRO:HD3	1:B:694:SER:OG	2.15	0.46
1:C:619:LEU:HD12	1:C:693:ILE:HG12	1.97	0.46
1:B:498:TYR:HB3	3:B:2167:HOH:O	2.16	0.46
1:A:215:VAL:O	1:A:216:ARG:CB	2.61	0.46
1:C:9:LYS:HD3	3:C:2004:HOH:O	2.16	0.45
1:A:640:GLY:HA2	1:A:668:LEU:HD13	1.97	0.45
1:C:260:ARG:HH11	1:C:260:ARG:CG	2.23	0.45
1:C:79:TYR:O	1:C:83:ARG:HG3	2.16	0.45
1:B:297:VAL:HG13	3:B:2092:HOH:O	2.16	0.45
1:C:349:LYS:HD3	1:C:351:GLU:OE2	2.17	0.45
1:B:522:TYR:CZ	3:B:2173:HOH:O	2.56	0.45
1:C:159:ASN:HB2	1:C:166:TYR:OH	2.16	0.45
1:A:274:PHE:CA	3:A:2091:HOH:O	2.32	0.45
1:C:394:LYS:HD3	3:C:2145:HOH:O	2.16	0.45
1:B:411:ARG:HH12	1:B:731:TYR:HE1	1.60	0.45
1:C:46:HIS:HB3	3:C:2022:HOH:O	2.17	0.45
1:C:708:LYS:HB3	1:C:708:LYS:NZ	2.32	0.45
1:A:225:CYS:HB2	3:A:2141:HOH:O	2.17	0.45
1:B:565:CYS:HB3	1:B:612:ARG:O	2.17	0.45
1:C:510:ARG:NH2	1:C:570:GLU:OE1	2.50	0.45
1:B:4:ASN:N	3:B:2001:HOH:O	2.50	0.44
1:A:322:ASN:HB3	1:A:331:ARG:HD2	1.98	0.44
1:A:18:ASN:CG	1:A:21:LYS:HB2	2.37	0.44
1:C:10:ARG:NH1	1:C:56:SER:HB3	2.32	0.44
1:C:45:SER:HB2	1:C:61:THR:HG22	2.00	0.44
1:B:553:LYS:O	1:B:557:GLU:HG2	2.18	0.44
1:C:341:LYS:HB2	1:C:722:TYR:OH	2.18	0.44
1:A:33:LEU:HB3	1:A:76:ASP:HB3	1.98	0.44
1:B:331:ARG:H	1:B:331:ARG:NH1	2.16	0.44
1:A:279:ILE:HG22	1:A:283:LYS:HE2	2.00	0.44
1:A:290:LYS:HG2	1:A:296:GLY:O	2.18	0.44
1:B:464:LEU:HA	1:B:514:GLY:O	2.18	0.44
1:C:384:LYS:HA	1:C:384:LYS:CE	2.47	0.43
2:P:3:VAL:N	3:P:2004:HOH:O	2.51	0.43
1:B:286:GLN:HE22	1:B:331:ARG:HH12	1.65	0.43
1:C:154:LYS:HD2	1:C:624:THR:HG21	2.00	0.43
1:B:45:SER:HB2	1:B:61:THR:HG22	2.00	0.43
1:A:294:GLN:CG	1:A:295:GLY:N	2.67	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:24:ARG:CG	1:A:24:ARG:NH1	2.81	0.43
1:C:260:ARG:HB2	3:C:2095:HOH:O	2.18	0.43
1:B:658:ASP:OD1	1:B:661:HIS:HD2	2.01	0.43
1:B:630:ASN:HD21	1:B:654:GLN:HG2	1.83	0.43
1:B:439:ALA:O	1:B:440:LEU:HB2	2.17	0.43
1:C:145:TYR:CZ	1:C:149:LYS:HD3	2.54	0.43
1:B:639:ARG:NH1	3:B:2213:HOH:O	2.51	0.43
1:B:344:TYR:O	1:B:347:LEU:HB3	2.18	0.43
1:B:260:ARG:NE	3:B:2081:HOH:O	2.52	0.43
1:A:283:LYS:HD3	3:B:2036:HOH:O	2.17	0.43
1:C:277:GLY:N	3:C:2115:HOH:O	2.47	0.42
1:B:261:ILE:HG23	1:B:274:PHE:HD1	1.84	0.42
1:C:381:LYS:HE3	3:C:2161:HOH:O	2.19	0.42
1:A:260:ARG:HH21	1:A:434:ARG:NH2	2.18	0.42
1:A:24:ARG:HD2	3:A:2009:HOH:O	2.19	0.42
1:B:154:LYS:HD2	1:B:624:THR:HG21	2.00	0.42
1:A:609:HIS:HE1	3:A:2193:HOH:O	2.01	0.42
1:A:553:LYS:O	1:A:557:GLU:HG2	2.19	0.42
1:B:122:ASP:O	1:B:189:ARG:NH2	2.52	0.42
1:B:633:ASN:HB3	3:B:2206:HOH:O	2.19	0.42
1:B:395:ALA:HB2	3:B:2118:HOH:O	2.20	0.42
1:B:103:TYR:CG	1:B:125:GLU:HG3	2.54	0.42
1:A:619:LEU:HB2	1:A:693:ILE:HG23	2.02	0.42
1:C:118:HIS:CE1	3:C:2048:HOH:O	2.72	0.42
1:C:215:VAL:O	1:C:216:ARG:CB	2.63	0.42
1:B:172:LEU:O	1:B:176:VAL:HG23	2.20	0.42
1:B:30:ALA:HA	1:B:33:LEU:HD12	2.01	0.42
1:C:364:LEU:HD22	1:C:375:PHE:CE1	2.55	0.42
1:B:392:ARG:HD3	3:B:2134:HOH:O	2.20	0.42
1:C:553:LYS:O	1:C:557:GLU:HG3	2.20	0.42
1:B:215:VAL:O	1:B:216:ARG:CB	2.62	0.42
1:A:128:PHE:HA	1:A:131:MET:HE3	2.02	0.42
1:B:560:LYS:HG2	1:B:609:HIS:CG	2.55	0.42
1:B:155:TYR:CE1	3:B:2067:HOH:O	2.23	0.42
1:B:328:ASN:HB3	1:B:329:ARG:NH1	2.35	0.42
1:A:440:LEU:HD12	1:A:728:THR:HB	2.00	0.42
1:B:46:HIS:HA	1:B:49:PHE:CD2	2.55	0.41
1:A:730:NIY:O1	1:A:730:NIY:OH	2.37	0.41
1:C:129:LYS:HG3	3:C:2054:HOH:O	2.20	0.41
1:C:384:LYS:HD2	3:C:2159:HOH:O	2.20	0.41
1:A:154:LYS:C	1:A:155:TYR:HD1	2.23	0.41
1:A:630:ASN:ND2	1:A:654:GLN:HG2	2.35	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:624:THR:O	1:A:627:GLN:HB2	2.19	0.41
1:C:283:LYS:HG2	3:C:2116:HOH:O	2.19	0.41
1:A:396:VAL:HG23	3:A:2117:HOH:O	2.20	0.41
1:A:409:THR:O	1:A:411:ARG:HG2	2.21	0.41
1:B:229:GLU:HG2	1:B:448:PRO:HG3	2.03	0.41
1:C:160:ARG:HB2	3:C:2066:HOH:O	2.21	0.41
1:B:209:THR:HB	1:B:210:PRO:HD3	2.02	0.41
1:C:248:VAL:HG11	1:C:289:VAL:HA	2.03	0.41
1:C:118:HIS:HB3	3:C:2047:HOH:O	2.20	0.41
1:B:207:LEU:HD12	1:B:212:MET:HE3	2.03	0.40
1:C:227:LEU:HB2	1:C:460:ALA:HB3	2.03	0.40
1:A:520:PHE:HB3	1:A:635:ILE:HA	2.03	0.40
1:B:437:ASN:HB2	3:B:2145:HOH:O	2.21	0.40
1:A:207:LEU:HD12	1:A:212:MET:HE2	1.99	0.40
1:B:444:LEU:O	3:B:2147:HOH:O	2.22	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%)	696 (96%)	23 (3%)	4 (1%)	33	63
1	B	723/761 (95%)	682 (94%)	36 (5%)	5 (1%)	30	59
1	C	723/761 (95%)	698 (96%)	19 (3%)	6 (1%)	27	55
2	D	14/20 (70%)	13 (93%)	1 (7%)	0	100	100
2	E	9/20 (45%)	7 (78%)	2 (22%)	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	2207/2363 (93%)	2111 (96%)	81 (4%)	15 (1%)	30	59

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	294	GLN
1	A	323	ARG
1	B	216	ARG
1	C	216	ARG
1	C	294	GLN
1	A	5	LEU
1	A	216	ARG
1	B	5	LEU
1	B	12	GLY
1	B	294	GLN
1	B	300	GLY
1	C	323	ARG
1	C	5	LEU
1	C	322	ASN
1	C	161	VAL

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	624/649 (96%)	583 (93%)	41 (7%)	24	47
1	B	624/649 (96%)	580 (93%)	44 (7%)	21	43
1	C	624/649 (96%)	582 (93%)	42 (7%)	23	46
2	D	16/19 (84%)	13 (81%)	3 (19%)	2	5
2	E	11/19 (58%)	10 (91%)	1 (9%)	14	28
2	F	16/19 (84%)	12 (75%)	4 (25%)	1	2
2	P	3/19 (16%)	3 (100%)	0	100	100
All	All	1918/2023 (95%)	1783 (93%)	135 (7%)	21	44

All (135) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	9	LYS
1	A	14	THR
1	A	17	ILE

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Mol	Chain	Res	Type
1	A	20	ASP
1	A	21	LYS
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	141	MET
1	A	149	LYS
1	A	189	ARG
1	A	206	SER
1	A	225	CYS
1	A	226	VAL
1	A	228	ILE
1	A	290	LYS
1	A	294	GLN
1	A	297	VAL
1	A	298	ARG
1	A	317	LEU
1	A	320	LYS
1	A	321	ASN
1	A	323	ARG
1	A	325	VAL
1	A	328	ASN
1	A	364	LEU
1	A	384	LYS
1	A	394	LYS
1	A	411	ARG
1	A	440	LEU
1	A	452	VAL
1	A	484	LEU
1	A	530	ARG
1	A	625	SER
1	A	626	SER
1	A	643	SER
1	A	648	LYS
1	B	5	LEU
1	B	8	THR
1	B	10	ARG
1	B	16	ARG
1	B	17	ILE

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Mol	Chain	Res	Type
1	B	39	SER
1	B	72	ARG
1	B	96	GLN
1	B	98	GLU
1	B	114	LYS
1	B	121	GLU
1	B	139	ARG
1	B	141	MET
1	B	149	LYS
1	B	186	ARG
1	B	189	ARG
1	B	191	GLN
1	B	216	ARG
1	B	226	VAL
1	B	260	ARG
1	B	262	ARG
1	B	274	PHE
1	B	275	HIS
1	B	315	SER
1	B	317	LEU
1	B	320	LYS
1	B	331	ARG
1	B	341	LYS
1	B	364	LEU
1	B	376	GLU
1	B	380	THR
1	B	386	ASP
1	B	394	LYS
1	B	411	ARG
1	B	452	VAL
1	B	455	GLU
1	B	474	ASN
1	B	484	LEU
1	B	510	ARG
1	B	542	LYS
1	B	616	LEU
1	B	626	SER
1	B	639	ARG
1	B	651	ILE
1	C	11	ASP
1	C	15	GLU
1	C	17	ILE

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Mol	Chain	Res	Type
1	C	21	LYS
1	C	24	ARG
1	C	55	THR
1	C	60	GLU
1	C	72	ARG
1	C	98	GLU
1	C	111	GLU
1	C	130	GLN
1	C	139	ARG
1	C	141	MET
1	C	165	ILE
1	C	186	ARG
1	C	189	ARG
1	C	204	LYS
1	C	216	ARG
1	C	226	VAL
1	C	260	ARG
1	C	274	PHE
1	C	294	GLN
1	C	317	LEU
1	C	323	ARG
1	C	364	LEU
1	C	384	LYS
1	C	391	GLN
1	C	396	VAL
1	C	411	ARG
1	C	440	LEU
1	C	452	VAL
1	C	474	ASN
1	C	484	LEU
1	C	519	ASN
1	C	616	LEU
1	C	625	SER
1	C	639	ARG
1	C	645	LYS
1	C	648	LYS
1	C	696	ASN
1	C	708	LYS
1	C	736	ASP
2	D	360	GLN
2	D	361	ILE
2	D	368	ASP

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Mol	Chain	Res	Type
2	E	372	ASN
2	F	360	GLN
2	F	361	ILE
2	F	367	THR
2	F	374	GLN

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

Mol	Chain	Res	Type
1	A	4	ASN
1	A	40	GLN
1	A	46	HIS
1	A	117	ASN
1	A	183	ASN
1	A	322	ASN
1	A	332	HIS
1	A	527	HIS
1	A	609	HIS
1	A	630	ASN
1	A	696	ASN
1	A	713	GLN
1	B	4	ASN
1	B	35	ASN
1	B	130	GLN
1	B	183	ASN
1	B	191	GLN
1	B	250	GLN
1	B	328	ASN
1	B	456	ASN
1	B	630	ASN
1	B	633	ASN
1	B	661	HIS
1	B	663	HIS
1	B	696	ASN
1	C	46	HIS
1	C	59	HIS
1	C	96	GLN
1	C	183	ASN
1	C	328	ASN
1	C	527	HIS
1	C	630	ASN
1	C	661	HIS

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Mol	Chain	Res	Type
2	E	372	ASN

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	730	1	15,15,16	4.74	3 (20%)	18,20,22	1.71	4 (22%)
1	NIY	B	730	1	15,15,16	4.88	3 (20%)	18,20,22	1.48	2 (11%)
1	NIY	C	730	1	15,15,16	4.63	3 (20%)	18,20,22	1.65	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	730	1	-	0/8/10/12	0/1/1/1
1	NIY	B	730	1	-	0/8/10/12	0/1/1/1
1	NIY	C	730	1	-	0/8/10/12	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	NIY	O-C	18.28	1.24	1.11
1	A	730	NIY	O-C	17.61	1.23	1.11
1	C	730	NIY	O-C	16.81	1.23	1.11
1	C	730	NIY	CE1-NN	-5.04	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	730	NIY	CE1-NN	-3.78	1.40	1.46
1	B	730	NIY	CE1-NN	-3.66	1.40	1.46
1	B	730	NIY	CA-C	2.57	1.53	1.48
1	A	730	NIY	CA-C	2.49	1.52	1.48
1	C	730	NIY	CA-C	2.23	1.52	1.48

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	730	NIY	C-CA-N	-4.67	109.16	113.83
1	B	730	NIY	C-CA-N	-4.07	109.76	113.83
1	A	730	NIY	C-CA-N	-3.95	109.88	113.83
1	A	730	NIY	CD1-CE1-NN	3.16	118.99	115.82
1	B	730	NIY	CD1-CE1-NN	3.07	118.90	115.82
1	C	730	NIY	CB-CG-CD1	-3.01	115.08	120.41
1	A	730	NIY	CB-CG-CD1	-2.74	115.55	120.41
1	A	730	NIY	CD2-CG-CD1	2.08	121.68	118.53

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, 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	728/761 (95%)	0.03	20 (2%) 52 55	23, 40, 62, 91	0
1	B	728/761 (95%)	0.02	12 (1%) 68 72	27, 41, 60, 92	0
1	C	728/761 (95%)	-0.15	5 (0%) 84 88	19, 30, 51, 78	0
2	D	16/20 (80%)	1.58	5 (31%) 1 1	82, 91, 97, 97	0
2	E	11/20 (55%)	1.23	3 (27%) 1 1	75, 82, 93, 94	0
2	F	16/20 (80%)	0.93	2 (12%) 5 4	67, 81, 86, 86	0
2	P	3/20 (15%)	0.36	0 100 100	33, 33, 37, 42	0
All	All	2230/2363 (94%)	-0.01	47 (2%) 60 64	19, 38, 64, 97	0

All (47) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	6	LEU	5.7
1	B	296	GLY	5.4
1	A	14	THR	4.3
1	A	296	GLY	4.2
1	B	737	GLY	4.1
1	A	4	ASN	3.7
1	A	297	VAL	3.6
1	B	297	VAL	3.6
1	A	737	GLY	3.3
1	A	13	SER	3.2
1	A	274	PHE	3.2
1	B	294	GLN	3.2
1	A	17	ILE	3.2
2	D	361	ILE	3.1
1	A	12	GLY	3.1
1	A	11	ASP	2.8
1	C	737	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
2	D	372	ASN	2.7
2	F	361	ILE	2.6
2	D	364	GLU	2.6
1	B	10	ARG	2.6
1	A	160	ARG	2.5
1	C	16	ARG	2.5
1	A	161	VAL	2.5
1	B	323	ARG	2.5
1	B	11	ASP	2.5
1	A	19	LEU	2.5
2	E	372	ASN	2.5
2	E	368	ASP	2.4
1	B	4	ASN	2.4
2	E	367	THR	2.4
1	C	294	GLN	2.3
1	A	53	ILE	2.3
1	A	323	ARG	2.3
1	B	274	PHE	2.2
1	C	274	PHE	2.2
1	B	51	ASP	2.2
2	D	375	LEU	2.2
1	B	161	VAL	2.1
1	A	298	ARG	2.1
1	C	296	GLY	2.1
2	D	373	PHE	2.1
1	A	295	GLY	2.1
1	A	384	LYS	2.1
1	B	9	LYS	2.1
1	A	195	ARG	2.0
2	F	360	GLN	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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
1	NIY	A	730	15/16	0.18	0.92	30,31,39,39	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	NIY	C	730	15/16	0.16	0.31	24,25,35,36	0
1	NIY	B	730	15/16	0.15	-0.60	31,33,41,42	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.