



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:58 AM UTC

PDB ID : 2XAZ / pdb_00002xaz
Title : Ribonucleotide reductase Y730NO2Y and C439S modified R1 subunit of E. coli
Authors : Yokoyama, K.; Uhlin, U.; Stubbe, J.
Deposited on : 2010-04-01
Resolution : 2.60 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

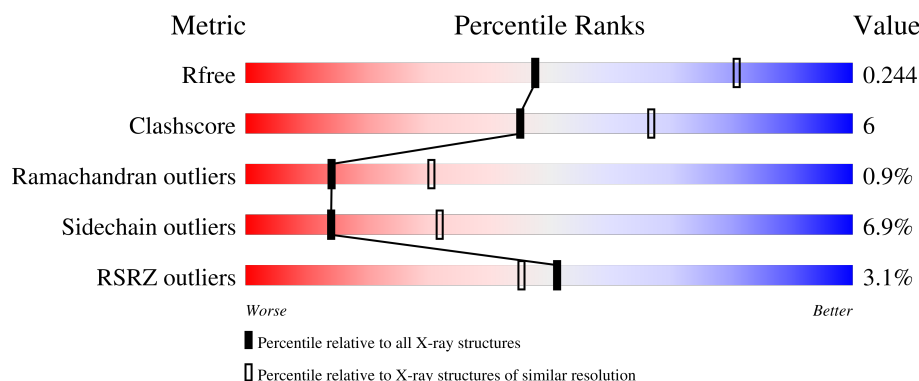
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	3% 80% 14% • •
1	B	761	2% 79% 15% • •
1	C	761	2% 80% 13% • •
2	D	20	10% 35% 20% 45%
2	E	20	35% 45% 25% 10% 20%

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Mol	Chain	Length	Quality of chain
2	F	20	15% 60% 15% 5% 20%
2	P	20	5% 10% 5% 85%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 18144 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	1100	23			
1	B	728	Total	C	N	O	S	0	0	0
			5807	3688	996	1100	23			
1	C	728	Total	C	N	O	S	0	0	0
			5807	3688	996	1100	23			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	439	SER	CYS	engineered mutation	UNP P00452
B	439	SER	CYS	engineered mutation	UNP P00452
C	439	SER	CYS	engineered mutation	UNP P00452

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	D	11	Total	C	N	O	0	0	0
			89	54	13	22			
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.

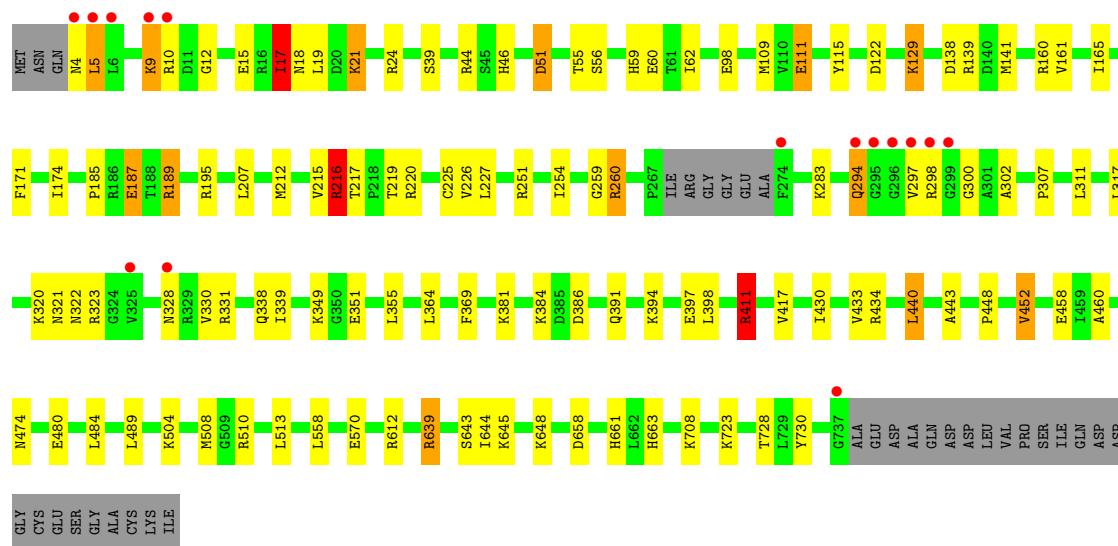
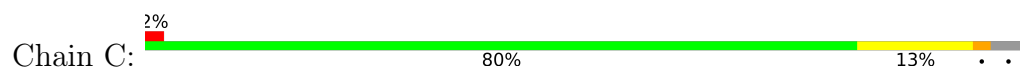
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	85	Total	O	0	0
			85	85		

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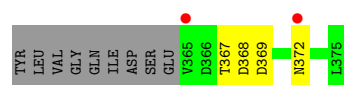
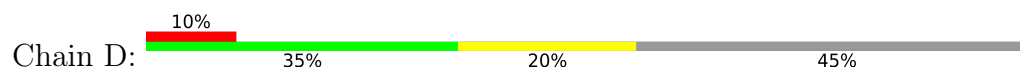
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	97	Total 97	O 97	0	0
3	C	163	Total 163	O 163	0	0
3	F	1	Total 1	O 1	0	0
3	P	3	Total 3	O 3	0	0

● Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT ALPHA



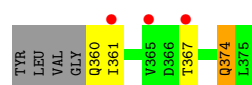
• Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA



• Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA



● Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA



• Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA



Y1	L2	V3	GLY	GLN	ILE	ASP	SER	GLU	VAL	ASP	THR	ASP	ASP	LEU	SER	ASN	PHE	GLN	LEU
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4 Data and refinement statistics

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α , β , γ	224.81Å 224.81Å 337.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	169.03 – 2.60 168.59 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.4 (169.03-2.60) 94.8 (168.59-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.21 (at 2.62Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.196 , 0.246 0.195 , 0.244	Depositor DCC
R_{free} test set	4755 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	44.6	Xtriage
Anisotropy	0.058	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 35.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	18144	wwPDB-VP
Average B, all atoms (Å ²)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.76% 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	0.58	0/5917	0.86	1/8012 (0.0%)
1	B	0.59	0/5917	0.85	1/8012 (0.0%)
1	C	0.67	1/5917 (0.0%)	0.88	2/8012 (0.0%)
2	D	0.51	0/89	0.77	0/119
2	E	0.60	0/129	0.95	0/173
2	F	0.52	0/129	0.85	0/173
2	P	0.88	0/27	1.24	0/36
All	All	0.61	1/18125 (0.0%)	0.86	4/24537 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	17	ILE	CA-CB	5.20	1.60	1.54

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	411	ARG	N-CA-C	5.58	118.02	110.88
1	C	452	VAL	CB-CA-C	-5.50	104.02	112.05
1	A	452	VAL	CB-CA-C	-5.28	105.12	112.04
1	B	622	SER	N-CA-C	-5.14	101.78	109.95

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	66	0
1	B	5807	0	5725	71	0
1	C	5807	0	5726	69	0
2	D	89	0	77	1	0
2	E	129	0	111	4	0
2	F	129	0	111	1	0
2	P	27	0	31	1	0
3	A	85	0	0	8	0
3	B	97	0	0	11	0
3	C	163	0	0	12	0
3	F	1	0	0	0	0
3	P	3	0	0	1	0
All	All	18144	0	17506	209	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (209) 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:299:GLY:HA3	3:B:2039:HOH:O	1.59	1.02
1:A:294:GLN:HG3	1:A:295:GLY:H	0.90	1.02
1:C:207:LEU:HB2	1:C:212:MET:HE3	1.43	1.00
1:A:294:GLN:HG3	1:A:295:GLY:N	1.74	0.98
1:C:9:LYS:HD3	1:C:10:ARG:H	1.35	0.91
1:C:480:GLU:HB3	3:C:2039:HOH:O	1.70	0.90
1:A:294:GLN:CG	1:A:295:GLY:H	1.75	0.90
1:C:260:ARG:HH11	1:C:260:ARG:HG2	1.42	0.84
1:B:323:ARG:NH1	1:B:323:ARG:HB3	1.98	0.79
1:A:215:VAL:O	1:A:216:ARG:HB3	1.82	0.78
1:B:323:ARG:HB3	1:B:323:ARG:HH11	1.44	0.78
1:B:274:PHE:HA	3:B:2034:HOH:O	1.82	0.78
1:B:10:ARG:H	1:B:10:ARG:HD2	1.50	0.77
1:A:212:MET:O	1:A:216:ARG:NH2	2.19	0.75
1:B:122:ASP:O	1:B:189:ARG:NH2	2.21	0.73
1:A:195:ARG:NH1	3:A:2022:HOH:O	2.20	0.73
1:C:212:MET:O	1:C:216:ARG:NH2	2.22	0.72
1:C:320:LYS:HE2	1:C:411:ARG:HG3	1.71	0.72
1:C:9:LYS:HZ3	1:C:10:ARG:HG2	1.53	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:9:LYS:NZ	1:C:10:ARG:HG2	2.06	0.70
1:A:233:SER:HA	1:A:274:PHE:HZ	1.55	0.69
1:A:9:LYS:HE3	1:A:10:ARG:H	1.58	0.69
1:A:207:LEU:HB2	1:A:212:MET:HE3	1.75	0.69
1:C:260:ARG:HG2	1:C:260:ARG:NH1	2.04	0.69
1:A:242:SER:HB2	1:A:452:VAL:HG13	1.76	0.68
1:B:480:GLU:HB3	3:B:2026:HOH:O	1.93	0.68
1:C:24:ARG:HD2	3:C:2003:HOH:O	1.93	0.67
1:C:639:ARG:HD2	3:C:2139:HOH:O	1.93	0.67
1:C:227:LEU:HB2	1:C:460:ALA:HB3	1.77	0.67
1:B:217:THR:OG1	1:B:219:THR:HG22	1.96	0.66
1:A:75:PRO:O	1:A:78:GLN:HB2	1.96	0.66
1:C:122:ASP:O	1:C:189:ARG:NH2	2.28	0.65
1:B:56:SER:O	1:B:60:GLU:HG2	1.96	0.65
1:A:648:LYS:HD2	1:A:648:LYS:H	1.62	0.65
1:B:730:NIY:HD1	3:B:2094:HOH:O	1.96	0.64
1:A:510:ARG:NH2	1:A:570:GLU:OE1	2.32	0.63
1:B:621:PRO:HD3	1:B:694:SER:OG	1.99	0.62
1:B:215:VAL:O	1:B:216:ARG:HB3	1.99	0.62
1:B:10:ARG:H	1:B:10:ARG:CD	2.12	0.61
1:A:88:HIS:ND1	3:A:2010:HOH:O	2.31	0.61
1:C:260:ARG:HH11	1:C:260:ARG:CG	2.11	0.61
1:C:298:ARG:HB3	1:C:298:ARG:HH11	1.66	0.61
1:B:472:ILE:O	1:B:472:ILE:HG13	2.01	0.61
1:B:623:GLU:HG3	3:B:2080:HOH:O	2.00	0.61
1:A:4:ASN:HB2	3:A:2001:HOH:O	2.01	0.60
1:C:195:ARG:HD3	3:C:2040:HOH:O	2.00	0.60
1:B:619:LEU:HD12	1:B:693:ILE:HG12	1.83	0.59
1:B:212:MET:O	1:B:216:ARG:NH2	2.36	0.59
1:A:262:ARG:HG3	1:A:274:PHE:HA	1.84	0.59
1:C:4:ASN:O	1:C:5:LEU:HB2	2.03	0.59
1:B:207:LEU:HD12	1:B:212:MET:HE3	1.84	0.59
1:C:215:VAL:O	1:C:216:ARG:HB3	2.02	0.59
1:C:283:LYS:HG3	1:C:330:VAL:HG22	1.85	0.58
1:B:696:ASN:ND2	1:B:731:TYR:HB2	2.18	0.58
1:B:55:THR:HG23	3:B:2011:HOH:O	2.02	0.58
1:C:10:ARG:NH1	1:C:56:SER:HB3	2.19	0.58
1:A:207:LEU:HD12	1:A:212:MET:HE3	1.86	0.57
1:A:619:LEU:HD12	1:A:693:ILE:HG12	1.85	0.57
1:A:233:SER:CA	1:A:274:PHE:HZ	2.17	0.57
1:C:510:ARG:NH2	1:C:570:GLU:OE1	2.38	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:609:HIS:HD2	3:P:2001:HOH:O	1.87	0.56
1:A:58:ILE:O	1:A:62:ILE:HG23	2.06	0.56
1:B:4:ASN:HD22	1:B:16:ARG:CZ	2.19	0.56
1:C:260:ARG:HH21	1:C:448:PRO:HG2	1.70	0.56
1:C:369:PHE:CD2	1:C:434:ARG:HD2	2.41	0.55
1:C:207:LEU:CB	1:C:212:MET:HE3	2.28	0.55
1:B:311:LEU:HA	1:B:355:LEU:HB3	1.88	0.55
1:A:633:ASN:HB3	3:A:2074:HOH:O	2.07	0.54
1:A:138:ASP:HA	1:A:141:MET:HE2	1.89	0.54
1:A:227:LEU:HB2	1:A:460:ALA:HB3	1.89	0.54
1:B:439:SER:O	1:B:440:LEU:HB2	2.07	0.54
1:C:440:LEU:HD12	1:C:728:THR:HB	1.89	0.54
1:A:233:SER:HA	1:A:274:PHE:CZ	2.39	0.53
1:A:62:ILE:HD11	1:A:84:LEU:HD22	1.91	0.53
1:C:294:GLN:HB3	3:C:2069:HOH:O	2.09	0.53
1:C:311:LEU:HA	1:C:355:LEU:HB3	1.91	0.53
1:B:386:ASP:OD2	1:B:386:ASP:N	2.41	0.52
1:A:207:LEU:HD12	1:A:212:MET:CE	2.39	0.52
1:C:207:LEU:HD12	1:C:212:MET:CE	2.39	0.52
1:B:8:THR:O	1:B:55:THR:HG22	2.10	0.52
1:B:227:LEU:HB2	1:B:460:ALA:HB3	1.92	0.52
1:B:320:LYS:HE2	1:B:411:ARG:HB2	1.91	0.51
1:C:322:ASN:O	1:C:331:ARG:NH1	2.42	0.51
1:B:558:LEU:HD23	1:B:612:ARG:HG2	1.92	0.51
1:C:217:THR:OG1	1:C:219:THR:HG22	2.09	0.51
1:A:258:ALA:HB3	1:A:304:LEU:HD21	1.91	0.51
1:B:159:ASN:HB2	1:B:166:TYR:OH	2.11	0.51
1:B:409:THR:O	1:B:411:ARG:HG2	2.11	0.51
1:B:258:ALA:HB3	1:B:304:LEU:HD21	1.92	0.51
1:C:430:ILE:HG21	1:C:570:GLU:HG2	1.93	0.51
1:C:639:ARG:H	1:C:639:ARG:CD	2.24	0.51
1:A:126:GLU:HG3	3:A:2016:HOH:O	2.10	0.50
1:A:294:GLN:CG	1:A:295:GLY:N	2.49	0.50
1:B:321:ASN:C	1:B:323:ARG:H	2.19	0.50
1:B:262:ARG:HD2	1:B:274:PHE:HB3	1.94	0.50
1:A:480:GLU:O	1:A:484:LEU:HD22	2.12	0.49
1:C:225:CYS:HB2	3:C:2058:HOH:O	2.12	0.49
1:A:259:GLY:HA3	1:A:307:PRO:HD3	1.94	0.49
1:C:658:ASP:OD1	1:C:661:HIS:HD2	1.96	0.49
1:C:558:LEU:HD23	1:C:612:ARG:HG2	1.94	0.49
1:A:214:GLY:HA3	1:A:222:PHE:HE1	1.76	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:135:ILE:HD11	1:B:174:ILE:HG21	1.95	0.48
1:C:138:ASP:O	1:C:141:MET:HB2	2.13	0.48
1:C:297:VAL:HG23	1:C:298:ARG:HG3	1.96	0.48
1:C:508:MET:HA	1:C:508:MET:HE2	1.96	0.48
1:B:297:VAL:HG13	3:B:2038:HOH:O	2.13	0.48
1:C:349:LYS:HD3	1:C:351:GLU:OE2	2.14	0.48
1:B:45:SER:HB2	1:B:61:THR:HG22	1.96	0.48
1:A:630:ASN:HD22	1:A:654:GLN:NE2	2.12	0.48
1:A:648:LYS:HD2	1:A:648:LYS:N	2.28	0.48
1:B:433:VAL:HG11	1:B:443:ALA:HB1	1.96	0.47
1:B:373:GLU:O	1:B:376:GLU:HB2	2.13	0.47
1:C:9:LYS:HD3	1:C:10:ARG:N	2.17	0.47
2:E:367:THR:HA	2:E:370:LEU:HD12	1.96	0.47
1:A:37:SER:HB3	1:A:40:GLN:HG3	1.96	0.47
1:A:294:GLN:HG2	1:A:297:VAL:HG23	1.97	0.47
1:A:126:GLU:O	1:A:129:LYS:HB2	2.14	0.47
1:C:489:LEU:HB3	1:C:513:LEU:HD22	1.97	0.47
1:C:663:HIS:HD2	3:C:2150:HOH:O	1.97	0.47
1:A:105:HIS:CD2	1:A:171:PHE:CD2	3.03	0.46
1:B:225:CYS:HB2	3:B:2050:HOH:O	2.14	0.46
1:B:565:CYS:HB3	1:B:612:ARG:O	2.16	0.46
1:C:138:ASP:HA	1:C:141:MET:HE2	1.97	0.46
1:B:437:ASN:HB2	3:B:2050:HOH:O	2.15	0.46
1:A:30:ALA:O	1:A:31:GLU:C	2.59	0.46
1:B:330:VAL:HB	1:B:335:TYR:OH	2.16	0.46
1:A:225:CYS:HB2	3:A:2034:HOH:O	2.16	0.46
1:B:215:VAL:O	1:B:216:ARG:CB	2.64	0.45
1:B:511:ARG:O	1:B:613:ASN:HB3	2.16	0.45
1:A:510:ARG:HB2	1:A:512:THR:HG23	1.98	0.45
1:A:622:SER:O	1:A:626:SER:OG	2.34	0.45
1:A:215:VAL:O	1:A:216:ARG:CB	2.56	0.45
1:A:221:GLN:CD	1:A:250:GLN:HG2	2.41	0.45
1:A:226:VAL:C	1:A:227:LEU:HD12	2.42	0.45
1:B:138:ASP:O	1:B:141:MET:HB2	2.16	0.45
1:C:558:LEU:CD2	1:C:612:ARG:HG2	2.47	0.45
1:B:639:ARG:NH1	3:B:2085:HOH:O	2.49	0.45
1:A:244:ILE:O	1:A:248:VAL:HG22	2.17	0.45
1:C:111:GLU:HG3	2:P:2:LEU:HB2	1.99	0.45
2:D:369:ASP:HA	2:D:372:ASN:ND2	2.32	0.44
1:A:400:SER:O	1:A:404:GLN:HB2	2.17	0.44
1:B:157:VAL:HG23	1:B:216:ARG:NH1	2.33	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:394:LYS:HB2	1:C:397:GLU:OE1	2.18	0.44
1:A:283:LYS:HG3	1:A:330:VAL:HG22	1.99	0.44
1:C:328:ASN:HD22	1:C:328:ASN:HA	1.68	0.44
1:A:331:ARG:HD3	3:A:2043:HOH:O	2.17	0.44
1:A:735:ARG:HG2	1:A:736:ASP:N	2.32	0.44
1:B:172:LEU:C	1:B:172:LEU:HD23	2.43	0.44
1:C:46:HIS:HB3	3:C:2009:HOH:O	2.17	0.44
2:E:361:ILE:H	2:E:361:ILE:HD13	1.83	0.44
1:B:517:VAL:HG22	1:B:619:LEU:HD22	1.99	0.44
1:B:109:MET:HB2	1:B:115:TYR:CD2	2.53	0.43
1:B:464:LEU:HB3	1:B:620:MET:HE2	2.00	0.43
1:B:226:VAL:HG11	1:B:247:TYR:CG	2.53	0.43
1:C:219:THR:O	1:C:220:ARG:HD3	2.19	0.43
1:A:463:THR:HG21	1:A:492:LEU:HD23	1.99	0.43
1:A:621:PRO:HD3	1:A:694:SER:OG	2.18	0.43
1:B:145:TYR:CZ	1:B:149:LYS:HD3	2.54	0.43
1:B:298:ARG:HH11	1:B:298:ARG:HB3	1.83	0.43
1:C:18:ASN:ND2	1:C:21:LYS:HB2	2.34	0.43
1:C:639:ARG:H	1:C:639:ARG:HD3	1.84	0.43
1:A:221:GLN:OE1	1:A:250:GLN:HG2	2.19	0.43
1:B:376:GLU:HG2	3:B:2046:HOH:O	2.19	0.42
1:C:17:ILE:HG22	3:C:2001:HOH:O	2.18	0.42
1:B:149:LYS:HE2	1:B:152:GLU:OE1	2.19	0.42
1:B:328:ASN:HD22	1:B:328:ASN:HA	1.73	0.42
1:C:109:MET:HB2	1:C:115:TYR:CD2	2.54	0.42
1:C:381:LYS:HE3	3:C:2090:HOH:O	2.18	0.42
1:A:385:ASP:O	1:A:390:LYS:NZ	2.51	0.42
1:C:5:LEU:HA	1:C:51:ASP:OD1	2.18	0.42
2:E:362:ASP:OD1	2:E:364:GLU:HB2	2.18	0.42
1:C:723:LYS:NZ	2:F:374:GLN:O	2.45	0.42
1:C:433:VAL:HG11	1:C:443:ALA:HB1	2.01	0.42
1:A:109:MET:HB2	1:A:115:TYR:CD2	2.55	0.42
1:B:116:ASP:CG	1:B:220:ARG:HH22	2.27	0.42
1:B:298:ARG:HB3	1:B:298:ARG:NH1	2.34	0.42
1:B:520:PHE:HB3	1:B:635:ILE:HA	2.02	0.42
1:C:259:GLY:HA3	1:C:307:PRO:HD3	2.02	0.42
1:C:338:GLN:HB3	1:C:417:VAL:CG1	2.50	0.42
1:A:479:GLU:HB2	1:A:550:TYR:CE1	2.55	0.42
1:B:319:LEU:HD22	1:B:330:VAL:HG23	2.01	0.42
1:B:715:LEU:O	1:B:719:LEU:HG	2.20	0.42
1:C:17:ILE:HD12	1:C:19:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:SER:CB	1:A:452:VAL:HG13	2.48	0.41
1:A:260:ARG:HH21	1:A:434:ARG:NH2	2.18	0.41
1:C:59:HIS:O	1:C:62:ILE:HG12	2.19	0.41
1:C:185:PRO:HB2	1:C:187:GLU:HG2	2.01	0.41
1:C:298:ARG:HB3	1:C:298:ARG:NH1	2.35	0.41
1:A:284:HIS:CE1	1:B:284:HIS:CE1	3.09	0.41
1:B:447:LYS:HD3	1:B:448:PRO:HD2	2.01	0.41
1:B:294:GLN:HE22	1:B:297:VAL:HG23	1.85	0.41
1:C:458:GLU:OE2	1:C:510:ARG:HD2	2.21	0.41
1:A:444:LEU:HD22	1:A:512:THR:HG21	2.02	0.41
1:B:321:ASN:OD1	1:B:323:ARG:HB2	2.21	0.41
1:C:21:LYS:HD3	3:C:2002:HOH:O	2.19	0.41
1:C:398:LEU:HD12	1:C:398:LEU:HA	1.94	0.41
1:A:98:GLU:HA	1:A:99:PRO:HD3	1.90	0.41
1:A:262:ARG:HD3	1:A:266:SER:HB2	2.02	0.41
1:B:259:GLY:HA3	1:B:307:PRO:HD3	2.02	0.41
1:C:171:PHE:HA	1:C:174:ILE:HG22	2.03	0.41
1:A:21:LYS:NZ	3:A:2003:HOH:O	2.53	0.41
1:B:711:MET:HG2	2:E:365:VAL:HG22	2.02	0.40
1:C:254:ILE:O	1:C:302:ALA:HA	2.21	0.40
1:A:465:SER:HB2	1:A:489:LEU:HD11	2.02	0.40
1:B:420:CYS:O	1:B:424:SER:HB2	2.22	0.40
1:B:480:GLU:H	1:B:480:GLU:CD	2.28	0.40
1:C:129:LYS:HG2	3:C:2027:HOH:O	2.21	0.40
1:A:138:ASP:O	1:A:141:MET:HB2	2.21	0.40
1:B:264:LEU:O	1:B:389:ARG:NH2	2.54	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%)	695 (96%)	24 (3%)	4 (1%)	21	42
1	B	723/761 (95%)	683 (94%)	31 (4%)	9 (1%)	10	23
1	C	723/761 (95%)	692 (96%)	25 (4%)	6 (1%)	16	34
2	D	9/20 (45%)	9 (100%)	0	0	100	100
2	E	14/20 (70%)	11 (79%)	3 (21%)	0	100	100
2	F	14/20 (70%)	14 (100%)	0	0	100	100
2	P	1/20 (5%)	1 (100%)	0	0	100	100
All	All	2207/2363 (93%)	2105 (95%)	83 (4%)	19 (1%)	14	30

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	ARG
1	C	294	GLN
1	B	5	LEU
1	B	216	ARG
1	B	300	GLY
1	B	322	ASN
1	C	216	ARG
1	A	300	GLY
1	B	12	GLY
1	C	5	LEU
1	A	31	GLU
1	B	294	GLN
1	C	161	VAL
1	A	323	ARG
1	B	297	VAL
1	B	630	ASN
1	C	12	GLY
1	B	186	ARG
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%)	585 (94%)	40 (6%)	16	35
1	B	625/650 (96%)	583 (93%)	42 (7%)	15	33
1	C	625/650 (96%)	584 (93%)	41 (7%)	15	34
2	D	11/19 (58%)	9 (82%)	2 (18%)	2	3
2	E	16/19 (84%)	13 (81%)	3 (19%)	1	2
2	F	16/19 (84%)	12 (75%)	4 (25%)	0	1
2	P	3/19 (16%)	3 (100%)	0	100	100
All	All	1921/2026 (95%)	1789 (93%)	132 (7%)	14	32

All (132) 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
1	A	21	LYS
1	A	27	ASP
1	A	62	ILE
1	A	78	GLN
1	A	98	GLU
1	A	118	HIS
1	A	130	GLN
1	A	149	LYS
1	A	187	GLU
1	A	189	ARG
1	A	216	ARG
1	A	226	VAL
1	A	228	ILE
1	A	249	SER
1	A	290	LYS
1	A	297	VAL
1	A	298	ARG
1	A	314	GLU
1	A	315	SER
1	A	317	LEU
1	A	322	ASN
1	A	364	LEU
1	A	384	LYS
1	A	391	GLN
1	A	396	VAL

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Mol	Chain	Res	Type
1	A	404	GLN
1	A	440	LEU
1	A	452	VAL
1	A	484	LEU
1	A	625	SER
1	A	626	SER
1	A	629	SER
1	A	643	SER
1	A	647	SER
1	A	648	LYS
1	A	708	LYS
1	B	5	LEU
1	B	10	ARG
1	B	16	ARG
1	B	17	ILE
1	B	35	ASN
1	B	55	THR
1	B	72	ARG
1	B	98	GLU
1	B	139	ARG
1	B	149	LYS
1	B	189	ARG
1	B	191	GLN
1	B	216	ARG
1	B	226	VAL
1	B	256	ILE
1	B	264	LEU
1	B	294	GLN
1	B	297	VAL
1	B	317	LEU
1	B	318	VAL
1	B	320	LYS
1	B	330	VAL
1	B	331	ARG
1	B	341	LYS
1	B	364	LEU
1	B	380	THR
1	B	394	LYS
1	B	400	SER
1	B	414	ILE
1	B	439	SER
1	B	440	LEU

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Mol	Chain	Res	Type
1	B	447	LYS
1	B	452	VAL
1	B	484	LEU
1	B	542	LYS
1	B	607	LYS
1	B	616	LEU
1	B	626	SER
1	B	639	ARG
1	B	645	LYS
1	B	651	ILE
1	B	706	SER
1	C	9	LYS
1	C	15	GLU
1	C	17	ILE
1	C	21	LYS
1	C	39	SER
1	C	44	ARG
1	C	51	ASP
1	C	55	THR
1	C	60	GLU
1	C	98	GLU
1	C	111	GLU
1	C	129	LYS
1	C	139	ARG
1	C	160	ARG
1	C	165	ILE
1	C	187	GLU
1	C	189	ARG
1	C	216	ARG
1	C	226	VAL
1	C	251	ARG
1	C	260	ARG
1	C	317	LEU
1	C	321	ASN
1	C	323	ARG
1	C	339	ILE
1	C	364	LEU
1	C	384	LYS
1	C	386	ASP
1	C	391	GLN
1	C	411	ARG
1	C	440	LEU

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Mol	Chain	Res	Type
1	C	452	VAL
1	C	474	ASN
1	C	484	LEU
1	C	504	LYS
1	C	639	ARG
1	C	643	SER
1	C	644	ILE
1	C	645	LYS
1	C	648	LYS
1	C	708	LYS
2	D	367	THR
2	D	368	ASP
2	E	360	GLN
2	E	361	ILE
2	E	367	THR
2	F	360	GLN
2	F	361	ILE
2	F	367	THR
2	F	374	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (37) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	40	GLN
1	A	46	HIS
1	A	96	GLN
1	A	137	HIS
1	A	150	GLN
1	A	183	ASN
1	A	328	ASN
1	A	609	HIS
1	A	630	ASN
1	A	661	HIS
1	B	4	ASN
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	696	ASN
1	B	733	ASN

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Mol	Chain	Res	Type
1	C	18	ASN
1	C	40	GLN
1	C	250	GLN
1	C	275	HIS
1	C	322	ASN
1	C	328	ASN
1	C	332	HIS
1	C	416	ASN
1	C	453	ASN
1	C	609	HIS
1	C	630	ASN
1	C	633	ASN
1	C	661	HIS
1	C	663	HIS
1	C	733	ASN
2	E	360	GLN
2	F	360	GLN
2	F	374	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	730	1	14,15,16	0.96	1 (7%)	11,20,22	1.16	1 (9%)
1	NIY	B	730	1	14,15,16	0.99	1 (7%)	11,20,22	1.11	1 (9%)
1	NIY	C	730	1	14,15,16	1.26	1 (7%)	11,20,22	1.58	2 (18%)

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	-	3/7/10/12	0/1/1/1
1	NIY	B	730	1	-	3/7/10/12	0/1/1/1
1	NIY	C	730	1	-	3/7/10/12	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	730	NIY	CE1-NN	-3.36	1.39	1.45
1	B	730	NIY	CE1-NN	-2.57	1.41	1.45
1	A	730	NIY	CE1-NN	-2.40	1.41	1.45

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	730	NIY	CB-CG-CD1	-3.43	114.54	120.43
1	A	730	NIY	CB-CG-CD1	-2.34	116.42	120.43
1	B	730	NIY	CB-CG-CD1	-2.14	116.75	120.43
1	C	730	NIY	CB-CG-CD2	2.08	124.77	120.90

There are no chirality outliers.

All (9) torsion outliers are listed below:

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

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	730	NIY	1	0

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 [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, 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%)	-0.05	24 (3%)	49 43	29, 45, 68, 98	0
1	B	727/761 (95%)	0.03	18 (2%)	58 52	31, 45, 66, 93	0
1	C	727/761 (95%)	-0.37	15 (2%)	63 58	21, 33, 56, 80	0
2	D	11/20 (55%)	1.37	2 (18%)	3 3	77, 84, 90, 90	0
2	E	16/20 (80%)	1.83	7 (43%)	0 0	77, 91, 98, 98	0
2	F	16/20 (80%)	1.19	3 (18%)	3 2	69, 88, 97, 97	0
2	P	3/20 (15%)	0.99	1 (33%)	1 1	37, 37, 40, 44	0
All	All	2227/2363 (94%)	-0.10	70 (3%)	51 45	21, 42, 70, 98	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	296	GLY	5.8
1	A	296	GLY	5.6
1	B	297	VAL	5.3
1	B	296	GLY	5.2
2	F	361	ILE	4.3
1	C	297	VAL	4.3
1	A	737	GLY	4.2
1	A	274	PHE	4.1
2	E	361	ILE	4.0
1	A	295	GLY	4.0
1	A	297	VAL	3.8
1	B	274	PHE	3.8
1	B	5	LEU	3.6
2	D	365	VAL	3.5
1	B	10	ARG	3.3
1	A	299	GLY	3.3
1	B	737	GLY	3.3

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Mol	Chain	Res	Type	RSRZ
1	B	4	ASN	3.0
1	B	325	VAL	3.0
1	A	118	HIS	3.0
2	P	3	VAL	3.0
1	C	4	ASN	3.0
1	C	295	GLY	2.9
1	C	294	GLN	2.8
1	A	9	LYS	2.8
1	A	5	LEU	2.8
1	C	6	LEU	2.8
1	A	14	THR	2.8
1	A	622	SER	2.7
2	F	367	THR	2.7
1	A	6	LEU	2.7
1	C	737	GLY	2.7
1	A	322	ASN	2.7
1	C	274	PHE	2.6
1	B	118	HIS	2.6
1	A	298	ARG	2.6
1	A	325	VAL	2.6
2	E	365	VAL	2.6
2	E	364	GLU	2.5
1	A	17	ILE	2.5
2	E	372	ASN	2.5
1	A	161	VAL	2.5
1	B	6	LEU	2.4
1	C	5	LEU	2.4
1	B	7	VAL	2.4
2	E	360	GLN	2.4
1	A	323	ARG	2.4
1	B	187	GLU	2.4
1	C	9	LYS	2.4
2	E	367	THR	2.4
1	C	299	GLY	2.3
1	B	622	SER	2.3
1	C	325	VAL	2.3
1	B	736	ASP	2.2
2	E	363	SER	2.2
1	A	46	HIS	2.2
1	B	275	HIS	2.2
1	C	10	ARG	2.2
1	A	19	LEU	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	323	ARG	2.2
1	C	328	ASN	2.2
1	A	13	SER	2.2
1	A	331	ARG	2.1
1	B	450	ASN	2.1
2	D	372	ASN	2.1
1	A	7	VAL	2.1
2	F	365	VAL	2.1
1	B	294	GLN	2.1
1	A	95	GLY	2.0
1	C	298	ARG	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	A	730	15/16	0.92	0.13	43,45,51,51	0
1	NIY	B	730	15/16	0.94	0.12	40,43,48,49	0
1	NIY	C	730	15/16	0.95	0.09	30,34,42,42	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.