Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:30 AM GMT

PDB ID	:	2XAZ
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
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

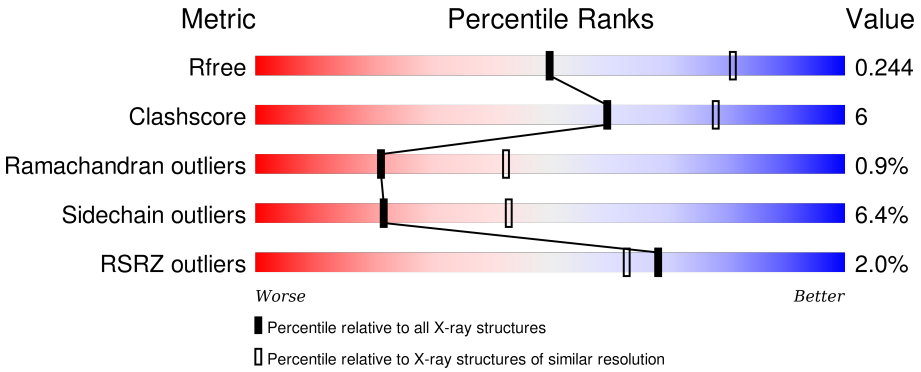
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

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}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (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 on the lower bar indicate the fraction of residues that contain outliers for >=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 <=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% 81% 13%
1	B	761	2% 80% 13%
1	C	761	% 81% 13%
2	D	20	10% 35% 20% 45%
2	E	20	20% 45% 25% 10% 20%

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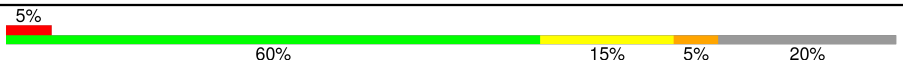
Mol	Chain	Length	Quality of chain
2	F	20	
2	P	20	

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 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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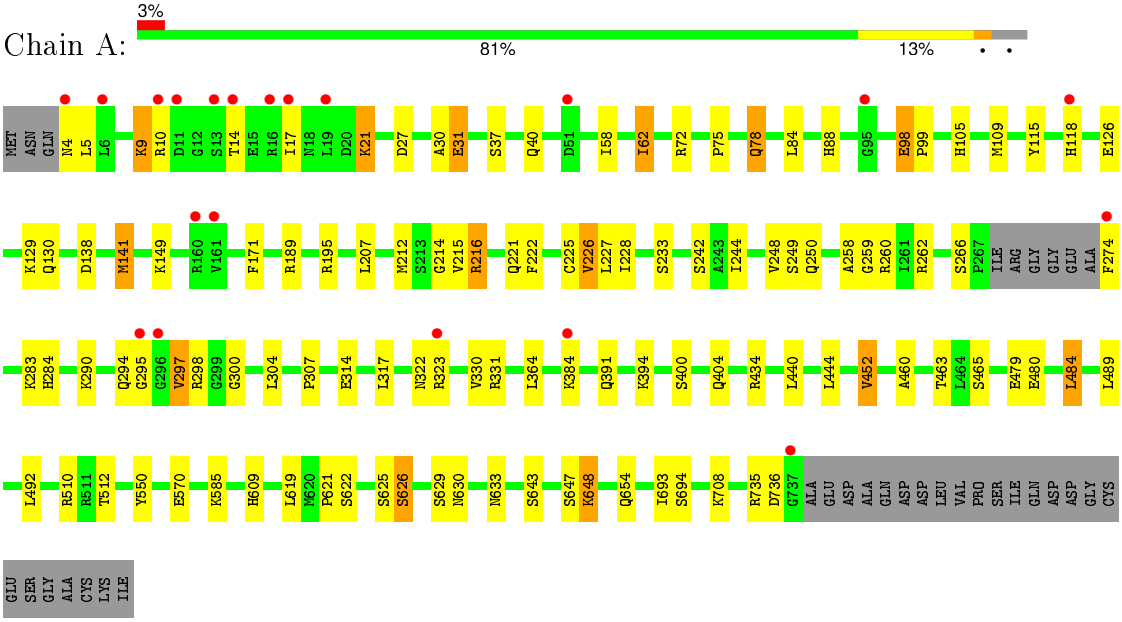
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	97	Total O 97 97	0	0
3	C	163	Total O 163 163	0	0
3	F	1	Total O 1 1	0	0
3	P	3	Total O 3 3	0	0

3 Residue-property plots (i)

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.

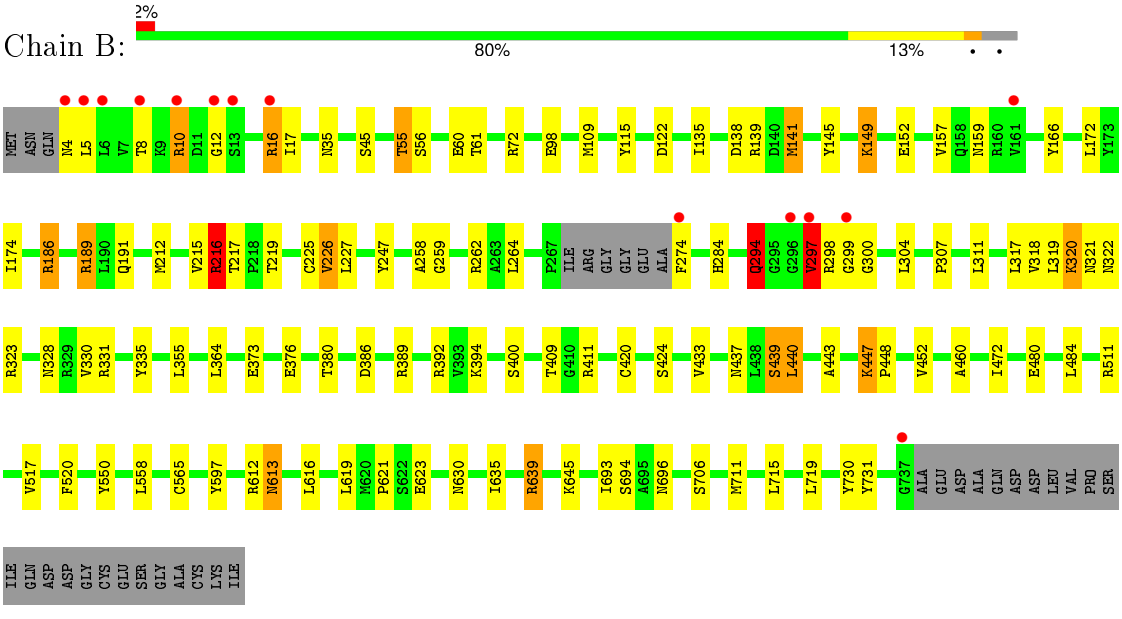
- Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT ALPHA

Chain A:



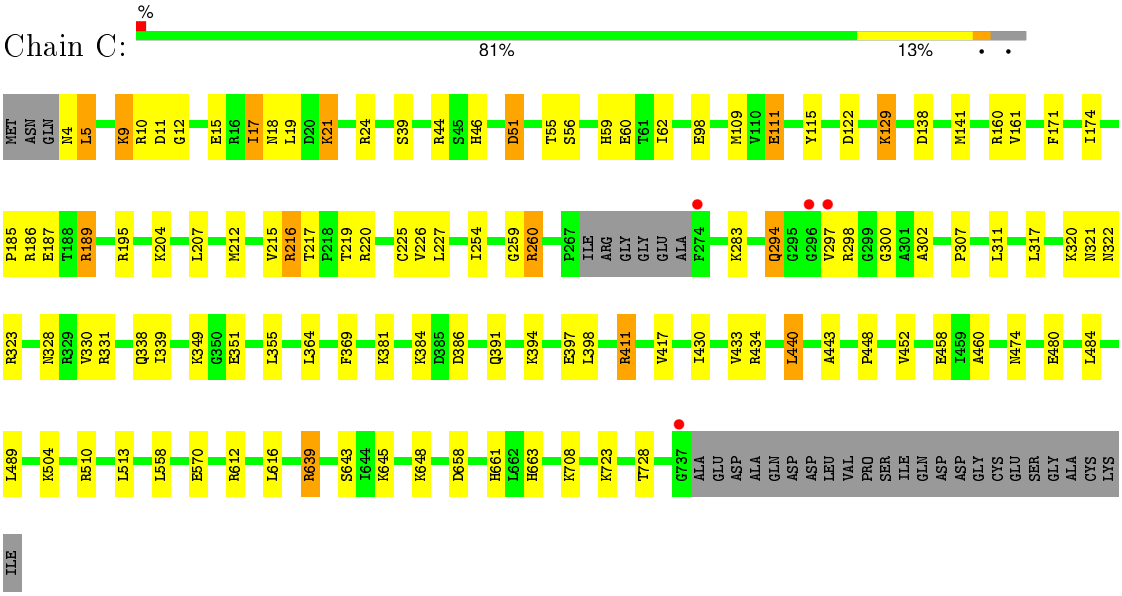
- Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT ALPHA

Chain B:



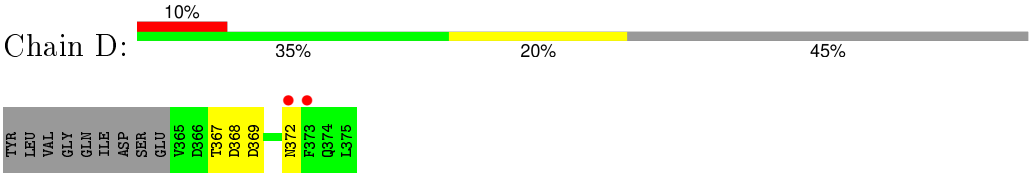
• Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT ALPHA

Chain C:



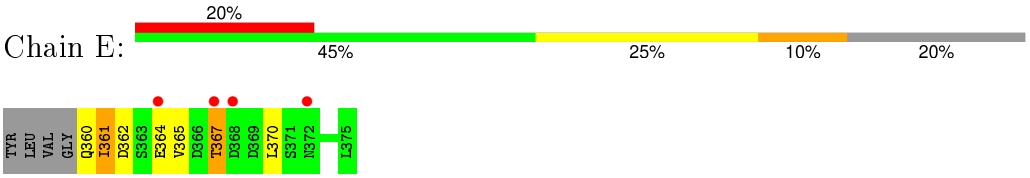
• Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA

Chain D:



• Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA

Chain E:



• Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA

Chain F:

• Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA

Chain P:

4 Data and refinement statistics (i)

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 79.47 – 2.60	Depositor EDS
% Data completeness (in resolution range)	96.4 (169.03-2.60) 94.8 (79.47-2.60)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [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 (5.27%)	DCC
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 , 39.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Outliers	2 of 95052 reflections (0.002%)	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

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	0.47	0/5917	0.59	0/8012
1	B	0.48	0/5917	0.59	0/8012
1	C	0.54	0/5917	0.64	0/8012
2	D	0.44	0/89	0.59	0/119
2	E	0.46	0/129	0.61	0/173
2	F	0.44	0/129	0.58	0/173
2	P	0.81	0/27	0.86	0/36
All	All	0.50	0/18125	0.61	0/24537

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

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	63	0
1	B	5807	0	5725	68	0
1	C	5807	0	5726	67	0
2	D	89	0	77	1	0
2	E	129	0	111	4	0
2	F	129	0	111	1	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	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	201	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 (201) 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: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:HB3	1:B:323:ARG:NH1	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:C:9:LYS:HZ3	1:C:10:ARG:HG2	1.51	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: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: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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:C:260:ARG:HH11	1:C:260:ARG:CG	2.11	0.61
1:A:88:HIS:ND1	3:A:2010:HOH:O	2.31	0.61
1:C:298:ARG:HB3	1:C:298:ARG:HH11	1.66	0.61
1:B:472:ILE:HG13	1:B:472:ILE:O	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: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: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
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: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: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:C:207:LEU:HB2	1:C:212:MET:CE	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:ILE:HD11	1:A:84:LEU:HD22	1.91	0.53
1:C:311:LEU:HA	1:C:355:LEU:HB3	1.91	0.53
1:C:294:GLN:HB3	3:C:2069:HOH:O	2.09	0.53
1:B:386:ASP:N	1:B:386:ASP:OD2	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:C:217:THR:OG1	1:C:219:THR:HG22	2.09	0.51
1:B:558:LEU:HD23	1:B:612:ARG:HG2	1.92	0.51
1:A:258:ALA:HB3	1:A:304:LEU:HD21	1.91	0.51
1:A:207:LEU:HD12	1:A:212:MET:HE3	1.93	0.51
1:B:409:THR:O	1:B:411:ARG:HG2	2.11	0.51
1:B:159:ASN:HB2	1:B:166:TYR:OH	2.11	0.51
1:C:639:ARG:CD	1:C:639:ARG:H	2.24	0.51
1:C:430:ILE:HG21	1:C:570:GLU:HG2	1.93	0.51
1:B:258:ALA:HB3	1:B:304:LEU:HD21	1.92	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: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:C:658:ASP:OD1	1:C:661:HIS:HD2	1.96	0.49
1:A:259:GLY:HA3	1:A:307:PRO:HD3	1.94	0.49
1:C:558:LEU:HD23	1:C:612:ARG:HG2	1.94	0.49
1:C:207:LEU:HB2	1:C:212:MET:HE3	1.94	0.49
1:C:138:ASP:O	1:C:141:MET:HB2	2.13	0.48
1:A:214:GLY:HA3	1:A:222:PHE:HE1	1.76	0.48
1:B:135:ILE:HD11	1:B:174:ILE:HG21	1.95	0.48
1:C:297:VAL:HG23	1:C:298:ARG:HG3	1.96	0.48
1:C:349:LYS:HD3	1:C:351:GLU:OE2	2.14	0.48
1:B:297:VAL:HG13	3:B:2038:HOH:O	2.13	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:N	1:A:648:LYS:HD2	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:294:GLN:HG2	1:A:297:VAL:HG23	1.97	0.47
1:A:37:SER:HB3	1:A:40:GLN:HG3	1.96	0.47
1:A:126:GLU:O	1:A:129:LYS:HB2	2.14	0.47
1:C:663:HIS:HD2	3:C:2150:HOH:O	1.97	0.47
1:C:489:LEU:HB3	1:C:513:LEU:HD22	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:B:437:ASN:HB2	3:B:2050:HOH:O	2.15	0.46
1:B:321:ASN:C	1:B:323:ARG:H	2.19	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:C:558:LEU:CD2	1:C:612:ARG:HG2	2.47	0.45
1:B:138:ASP:O	1:B:141:MET:HB2	2.16	0.45
1:B:639:ARG:NH1	3:B:2085:HOH:O	2.49	0.45
1:B:172:LEU:HD21	1:B:212:MET:HE2	1.98	0.45
1:C:111:GLU:HG3	2:P:2:LEU:HB2	1.99	0.45
1:A:244:ILE:O	1:A:248:VAL:HG22	2.17	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
1:C:394:LYS:HB2	1:C:397:GLU:OE1	2.18	0.44
1:C:328:ASN:HA	1:C:328:ASN:HD22	1.68	0.44
1:A:283:LYS:HG3	1:A:330:VAL:HG22	1.99	0.44
1:A:331:ARG:HD3	3:A:2043:HOH:O	2.17	0.44
1:C:46:HIS:HB3	3:C:2009:HOH:O	2.17	0.44
1:A:735:ARG:HG2	1:A:736:ASP:N	2.32	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:C:219:THR:O	1:C:220:ARG:HD3	2.19	0.43
1:B:226:VAL:HG11	1:B:247:TYR:CG	2.53	0.43
1:A:463:THR:HG21	1:A:492:LEU:HD23	1.99	0.43
1:C:639:ARG:HD3	1:C:639:ARG:H	1.84	0.43
1:C:18:ASN:ND2	1:C:21:LYS:HB2	2.34	0.43
1:B:298:ARG:HH11	1:B:298:ARG:HB3	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:HA	1:B:328:ASN:HD22	1.73	0.42
1:C:381:LYS:HE3	3:C:2090:HOH:O	2.18	0.42
1:C:109:MET:HB2	1:C:115:TYR:CD2	2.54	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:B:298:ARG:NH1	1:B:298:ARG:HB3	2.34	0.42
1:A:109:MET:HB2	1:A:115:TYR:CD2	2.55	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:B:319:LEU:HD22	1:B:330:VAL:HG23	2.01	0.42
1:C:17:ILE:HD12	1:C:19:LEU:HD23	2.01	0.42
1:B:715:LEU:O	1:B:719:LEU:HG	2.20	0.42
1:A:479:GLU:HB2	1:A:550:TYR:CE1	2.55	0.42
1:A:242:SER:CB	1:A:452:VAL:HG13	2.48	0.41
1:C:298:ARG:HB3	1:C:298:ARG:NH1	2.35	0.41
1:C:185:PRO:HB2	1:C:187:GLU:HG2	2.01	0.41
1:C:59:HIS:O	1:C:62:ILE:HG12	2.19	0.41
1:A:260:ARG:HH21	1:A:434:ARG:NH2	2.18	0.41
1:A:284:HIS:CE1	1:B:284:HIS:CE1	3.09	0.41
1:B:550:TYR:HH	1:B:597:TYR:HE1	1.68	0.41
1:B:447:LYS:HD3	1:B:448:PRO:HD2	2.01	0.41
1:C:458:GLU:OE2	1:C:510:ARG:HD2	2.21	0.41
1:B:294:GLN:HE22	1:B:297:VAL:HG23	1.85	0.41
1:B:321:ASN:OD1	1:B:323:ARG:HB2	2.21	0.41
1:A:444:LEU:HD22	1:A:512:THR:HG21	2.02	0.41
1:A:30:ALA:O	1:A:31:GLU:C	2.59	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: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:A:98:GLU:HA	1:A:99:PRO:HD3	1.90	0.41
1:C:171:PHE:HA	1:C:174:ILE:HG22	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:LYS:NZ	3:A:2003:HOH:O	2.53	0.41
1:A:226:VAL:C	1:A:227:LEU:HD12	2.42	0.40
1:A:221:GLN:CD	1:A:250:GLN:HG2	2.41	0.40
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: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%)	30	56
1	B	723/761 (95%)	683 (94%)	31 (4%)	9 (1%)	16	33
1	C	723/761 (95%)	692 (96%)	25 (4%)	6 (1%)	24	46
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%)	21	42

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	ARG

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Mol	Chain	Res	Type
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%)	586 (94%)	39 (6%)	23 45
1	B	625/650 (96%)	589 (94%)	36 (6%)	25 49
1	C	625/650 (96%)	586 (94%)	39 (6%)	23 45
2	D	11/19 (58%)	9 (82%)	2 (18%)	2 3
2	E	16/19 (84%)	13 (81%)	3 (19%)	2 3
2	F	16/19 (84%)	12 (75%)	4 (25%)	1 1
2	P	3/19 (16%)	3 (100%)	0	100 100
All	All	1921/2026 (95%)	1798 (94%)	123 (6%)	22 43

All (123) 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	72	ARG
1	A	78	GLN
1	A	98	GLU
1	A	118	HIS
1	A	130	GLN
1	A	141	MET
1	A	149	LYS
1	A	189	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	317	LEU
1	A	322	ASN
1	A	364	LEU
1	A	384	LYS
1	A	391	GLN
1	A	394	LYS
1	A	440	LEU
1	A	452	VAL
1	A	484	LEU
1	A	585	LYS
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	10	ARG
1	B	16	ARG
1	B	17	ILE
1	B	35	ASN

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Mol	Chain	Res	Type
1	B	55	THR
1	B	72	ARG
1	B	98	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	294	GLN
1	B	297	VAL
1	B	317	LEU
1	B	318	VAL
1	B	320	LYS
1	B	331	ARG
1	B	364	LEU
1	B	380	THR
1	B	392	ARG
1	B	394	LYS
1	B	400	SER
1	B	439	SER
1	B	440	LEU
1	B	447	LYS
1	B	452	VAL
1	B	484	LEU
1	B	613	ASN
1	B	616	LEU
1	B	639	ARG
1	B	645	LYS
1	B	706	SER
1	C	9	LYS
1	C	11	ASP
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

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Mol	Chain	Res	Type
1	C	98	GLU
1	C	111	GLU
1	C	129	LYS
1	C	160	ARG
1	C	186	ARG
1	C	189	ARG
1	C	204	LYS
1	C	226	VAL
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
1	C	452	VAL
1	C	474	ASN
1	C	484	LEU
1	C	504	LYS
1	C	616	LEU
1	C	639	ARG
1	C	643	SER
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

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	40	GLN
1	A	46	HIS
1	A	150	GLN
1	A	183	ASN
1	A	294	GLN
1	A	609	HIS
1	A	630	ASN
1	A	661	HIS
1	A	696	ASN
1	A	713	GLN
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	713	GLN
1	C	40	GLN
1	C	250	GLN
1	C	328	ASN
1	C	630	ASN
1	C	633	ASN
1	C	661	HIS
1	C	663	HIS
2	E	360	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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	11,15,16	0.55	0	10,20,22	1.34	2 (20%)
1	NIY	B	730	1	11,15,16	0.55	0	10,20,22	1.24	1 (10%)
1	NIY	C	730	1	11,15,16	0.75	0	10,20,22	1.62	2 (20%)

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

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	730	NIY	CB-CG-CD1	-3.02	114.54	120.36
1	C	730	NIY	O-C-CA	-2.58	118.76	125.49
1	A	730	NIY	O-C-CA	-2.49	119.02	125.49
1	B	730	NIY	O-C-CA	-2.08	120.08	125.49
1	A	730	NIY	CB-CG-CD1	-2.04	116.42	120.36

There are no chirality outliers.

There are no torsion outliers.

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 carbohydrates in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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%)	0.09	20 (2%) 56 49	29, 45, 68, 98	0
1	B	727/761 (95%)	0.07	14 (1%) 70 64	31, 45, 67, 93	0
1	C	727/761 (95%)	-0.08	4 (0%) 90 88	21, 33, 56, 80	0
2	D	11/20 (55%)	1.02	2 (18%) 2 1	77, 84, 90, 90	0
2	E	16/20 (80%)	1.39	4 (25%) 1 0	77, 91, 98, 98	0
2	F	16/20 (80%)	1.21	1 (6%) 23 17	69, 88, 97, 97	0
2	P	3/20 (15%)	0.67	0 100 100	37, 37, 40, 44	0
All	All	2227/2363 (94%)	0.05	45 (2%) 68 63	21, 42, 70, 98	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	296	GLY	5.7
1	B	296	GLY	5.4
1	A	6	LEU	5.3
1	A	14	THR	5.2
1	A	274	PHE	5.1
2	E	372	ASN	4.4
1	B	4	ASN	3.9
1	C	737	GLY	3.9
2	F	361	ILE	3.8
1	A	13	SER	3.8
1	A	17	ILE	3.7
1	B	737	GLY	3.5
1	B	274	PHE	3.5
1	A	4	ASN	3.4
1	B	297	VAL	3.4
1	A	161	VAL	3.4
1	A	19	LEU	3.1

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Mol	Chain	Res	Type	RSRZ
2	E	364	GLU	2.9
1	C	296	GLY	2.9
1	A	323	ARG	2.9
1	B	13	SER	2.8
1	A	737	GLY	2.8
1	A	118	HIS	2.7
1	C	297	VAL	2.6
2	E	368	ASP	2.5
2	D	372	ASN	2.5
1	A	295	GLY	2.4
1	B	12	GLY	2.4
1	B	6	LEU	2.4
1	C	274	PHE	2.4
1	B	161	VAL	2.4
1	A	160	ARG	2.3
1	B	299	GLY	2.3
1	B	5	LEU	2.3
1	A	51	ASP	2.3
1	A	11	ASP	2.3
1	B	10	ARG	2.3
1	B	8	THR	2.2
1	A	10	ARG	2.2
2	D	373	PHE	2.2
1	A	384	LYS	2.1
2	E	367	THR	2.1
1	B	16	ARG	2.1
1	A	95	GLY	2.1
1	A	16	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. 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^{th} 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(Å^2)	Q<0.9
1	NIY	B	730	15/16	0.92	0.16	-	40,43,48,49	0
1	NIY	A	730	15/16	0.92	0.19	-	43,45,51,51	0
1	NIY	C	730	15/16	0.96	0.15	-	30,34,42,42	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.