Full wwPDB X-ray Structure Validation Report ⓘ

May 15, 2020 – 07:27 am BST

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

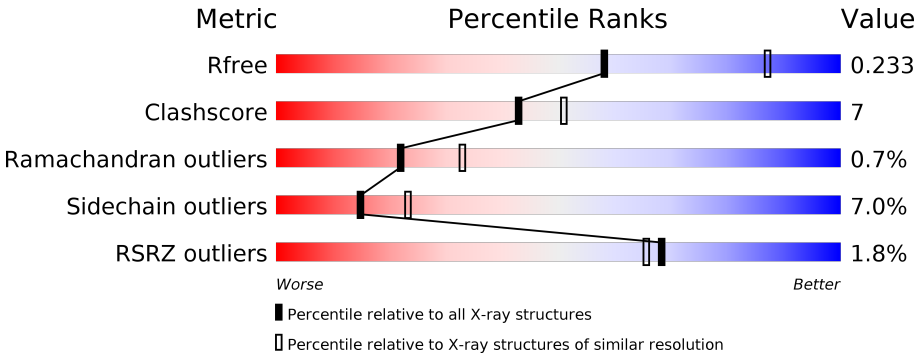
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

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 2.65 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}	130704	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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 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 <=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	2% 80% 13%
1	B	761	% 77% 17%
1	C	761	% 81% 12%
2	D	20	20% 60% 15% 5% 20%
2	E	20	15% 50% 5% 45%
2	F	20	5% 55% 25% 20%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
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 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
			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-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	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		

Continued on next page...

Continued from previous page...

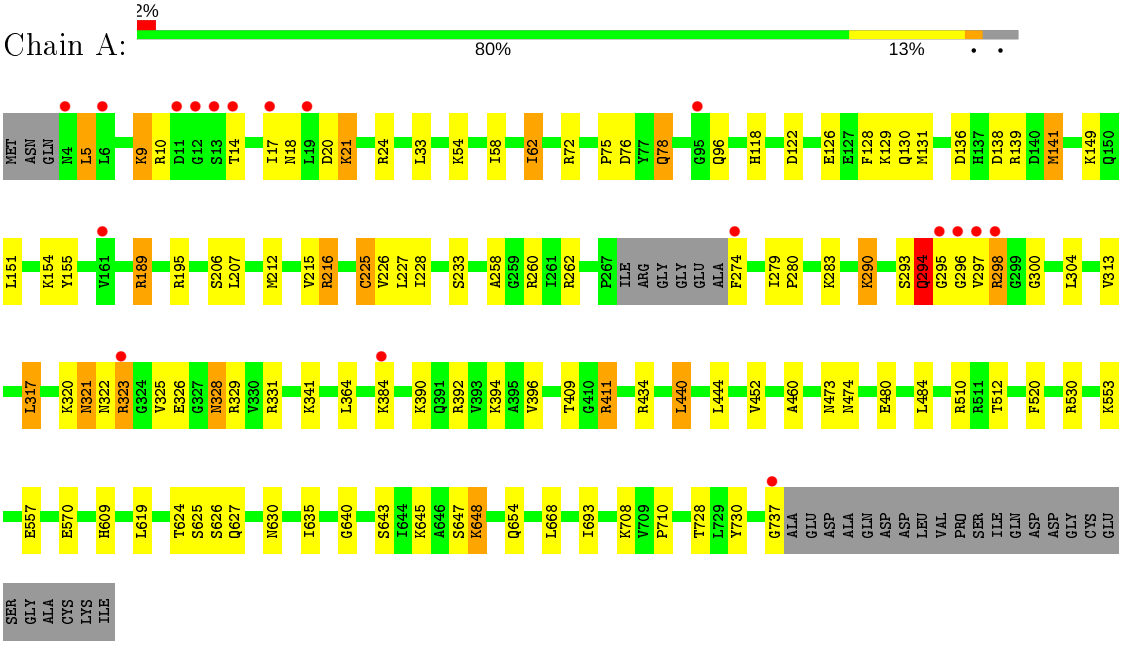
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	245	Total O 245 245	0	0
3	C	299	Total O 299 299	0	0
3	D	5	Total O 5 5	0	0
3	F	5	Total O 5 5	0	0
3	P	4	Total O 4 4	0	0

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 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.

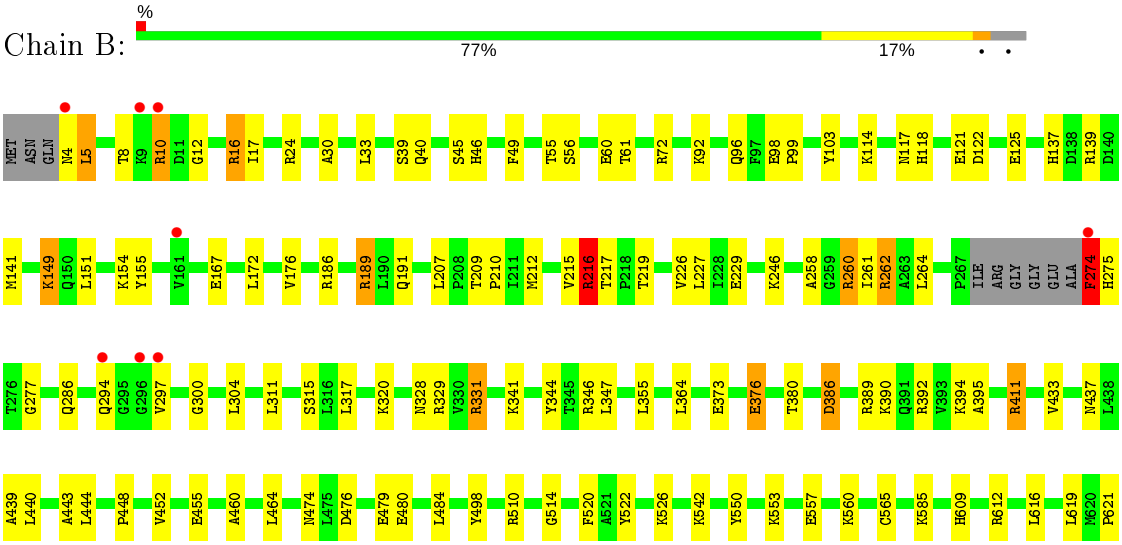
• Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT ALPHA

Chain A:

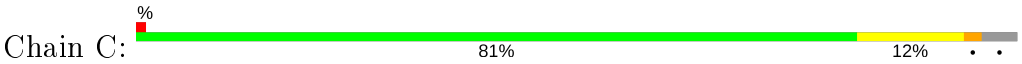


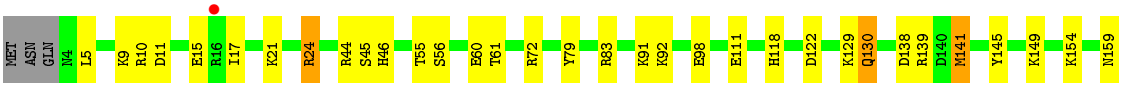
• Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT ALPHA

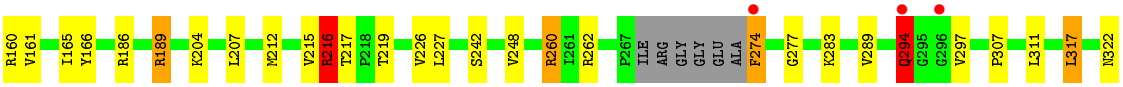
Chain B:

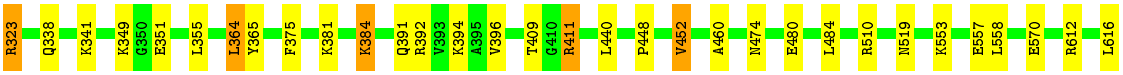


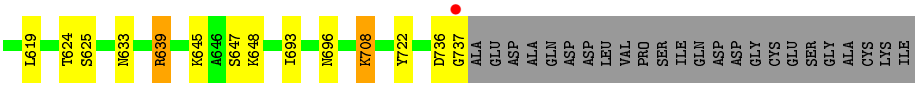
• Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT ALPHA



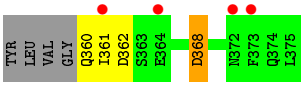




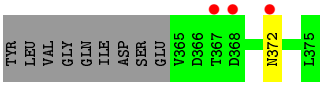




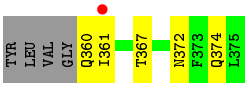
• Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA



• Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA



• Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA



• Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA

4 Data and refinement statistics (i)

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
$< I/\sigma(I) >$ [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 (5.00%)	wwPDB-VP
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 , 44.6	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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	0.45	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(^{o})	Ideal(^{o})
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 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	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

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 7.

All (239) 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: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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (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:212:MET:O	1:C:216:ARG:NH2	2.21	0.74
1:C:294:GLN:HB3	3:C:2121:HOH:O	1.88	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:A:331:ARG:HD3	3:A:2114:HOH:O	1.92	0.70
1:C:262:ARG:HG2	1:C:274:PHE:CB	2.21	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:A:480:GLU:HB3	3:A:2059:HOH:O	1.92	0.69
1:B:262:ARG:HG3	1:B:274:PHE:HB2	1.75	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:58:ILE:O	1:A:62:ILE:HG23	1.97	0.64
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:A:293:SER:HB2	1:A:298:ARG:O	2.05	0.56
1:B:264:LEU:O	1:B:389:ARG:NH2	2.37	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:A:24:ARG:HH11	1:A:24:ARG:CG	2.21	0.53
1:B:274:PHE:HA	1:B:277:GLY:H	1.74	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:A:648:LYS:HD2	1:A:648:LYS:H	1.73	0.53
1:C:260:ARG:NH1	1:C:260:ARG:HG2	2.13	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:311:LEU:HA	1:B:355:LEU:HB3	1.93	0.49
1:B:331:ARG:HD3	1:B:331:ARG:N	2.27	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:A:313:VAL:HG22	1:A:317:LEU:HD22	1.95	0.48
1:B:520:PHE:HB3	1:B:635:ILE:HA	1.95	0.48
1:C:207:LEU:HD12	1:C:212:MET:HE3	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:195:ARG:NH1	3:A:2058:HOH:O	2.44	0.48
1:A:474:ASN:ND2	3:A:2152:HOH:O	2.33	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:B:639:ARG:HB2	1:B:639:ARG:HH11	1.79	0.47
1:A:708:LYS:HD3	2:D:362:ASP:HB2	1.96	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:645:LYS:HG3	3:A:2201:HOH:O	2.15	0.47
1:A:444:LEU:HD22	1:A:512:THR:HG21	1.97	0.46
1:B:4:ASN:HD22	1:B:16:ARG:CZ	2.28	0.46
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:A:640:GLY:HA2	1:A:668:LEU:HD13	1.97	0.45
1:C:9:LYS:HD3	3:C:2004:HOH:O	2.16	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: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:C:708:LYS:HB3	1:C:708:LYS:NZ	2.32	0.45
1:B:4:ASN:N	3:B:2001:HOH:O	2.50	0.44
1:A:18:ASN:CG	1:A:21:LYS:HB2	2.37	0.44
1:A:322:ASN:HB3	1:A:331:ARG:HD2	1.98	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:GLN:HE22	1:B:331:ARG:HH12	1.65	0.43
1:B:45:SER:HB2	1:B:61:THR:HG22	2.00	0.43
1:C:154:LYS:HD2	1:C:624:THR:HG21	2.00	0.43
1:A:24:ARG:CG	1:A:24:ARG:NH1	2.81	0.43
1:A:294:GLN:CG	1:A:295:GLY:N	2.67	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:439:ALA:O	1:B:440:LEU:HB2	2.17	0.43
1:B:630:ASN:HD21	1:B:654:GLN:HG2	1.83	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:A:283:LYS:HD3	3:B:2036:HOH:O	2.17	0.43
1:B:260:ARG:NE	3:B:2081:HOH:O	2.52	0.43
1:A:260:ARG:HH21	1:A:434:ARG:NH2	2.18	0.42
1:B:261:ILE:HG23	1:B:274:PHE:HD1	1.84	0.42
1:C:277:GLY:N	3:C:2115:HOH:O	2.47	0.42
1:C:381:LYS:HE3	3:C:2161:HOH:O	2.19	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:553:LYS:O	1:A:557:GLU:HG2	2.19	0.42
1:A:609:HIS:HE1	3:A:2193:HOH:O	2.01	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:103:TYR:CG	1:B:125:GLU:HG3	2.54	0.42
1:B:395:ALA:HB2	3:B:2118:HOH:O	2.20	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: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:B:392:ARG:HD3	3:B:2134:HOH:O	2.20	0.42
1:C:215:VAL:O	1:C:216:ARG:CB	2.63	0.42
1:C:364:LEU:HD22	1:C:375:PHE:CE1	2.55	0.42
1:C:553:LYS:O	1:C:557:GLU:HG3	2.20	0.42
1:A:128:PHE:HA	1:A:131:MET:HE3	2.02	0.42
1:B:215:VAL:O	1:B:216:ARG:CB	2.62	0.42
1:B:560:LYS:HG2	1:B:609:HIS:CG	2.55	0.42
1:A:440:LEU:HD12	1:A:728:THR:HB	2.00	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:730:NIY:O1	1:A:730:NIY:OH	2.37	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:46:HIS:HA	1:B:49:PHE:CD2	2.55	0.41
1:C:129:LYS:HG3	3:C:2054:HOH:O	2.20	0.41
1:A:154:LYS:C	1:A:155:TYR:HD1	2.23	0.41
1:A:624:THR:O	1:A:627:GLN:HB2	2.19	0.41
1:A:630:ASN:ND2	1:A:654:GLN:HG2	2.35	0.41
1:C:384:LYS:HD2	3:C:2159:HOH:O	2.20	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 (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%)	696 (96%)	23 (3%)	4 (1%)	25	37
1	B	723/761 (95%)	682 (94%)	36 (5%)	5 (1%)	22	33
1	C	723/761 (95%)	698 (96%)	19 (3%)	6 (1%)	19	29
2	D	14/20 (70%)	13 (93%)	1 (7%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
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%)	22 33

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 (i)

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%)	16 25
1	B	624/649 (96%)	580 (93%)	44 (7%)	14 22
1	C	624/649 (96%)	582 (93%)	42 (7%)	16 25
2	D	16/19 (84%)	13 (81%)	3 (19%)	1 1
2	E	11/19 (58%)	10 (91%)	1 (9%)	9 13

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	F	16/19 (84%)	12 (75%)	4 (25%)	0 0
2	P	3/19 (16%)	3 (100%)	0	100 100
All	All	1918/2023 (95%)	1783 (93%)	135 (7%)	15 23

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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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
2	E	372	ASN

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	B	730	1	13,15,16	0.94	1 (7%)	13,20,22	1.06	1 (7%)
1	NIY	C	730	1	13,15,16	1.32	1 (7%)	13,20,22	1.57	3 (23%)
1	NIY	A	730	1	13,15,16	1.01	1 (7%)	13,20,22	1.57	3 (23%)

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	B	730	1	-	3/7/10/12	0/1/1/1
1	NIY	C	730	1	-	3/7/10/12	0/1/1/1
1	NIY	A	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	-3.86	1.38	1.45
1	A	730	NIY	CE1-NN	-2.80	1.40	1.45
1	B	730	NIY	CE1-NN	-2.70	1.40	1.45

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	730	NIY	CB-CA-C	3.15	117.37	111.47
1	C	730	NIY	CB-CG-CD1	-3.12	115.08	120.44
1	A	730	NIY	CB-CG-CD1	-2.85	115.55	120.44
1	A	730	NIY	CB-CA-C	2.68	116.49	111.47
1	A	730	NIY	CD2-CG-CD1	2.24	121.68	118.54
1	B	730	NIY	CB-CA-C	2.15	115.49	111.47
1	C	730	NIY	CD2-CE2-CZ	-2.03	118.42	120.50

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	B	730	NIY	O-C-CA-CB
1	C	730	NIY	O-C-CA-CB
1	A	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	A	730	NIY	1	0

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, 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%)	0.02	18 (2%) 57 53	23, 40, 62, 91	0
1	B	727/761 (95%)	0.01	9 (1%) 79 77	27, 41, 60, 92	0
1	C	727/761 (95%)	-0.14	5 (0%) 87 87	19, 30, 51, 78	0
2	D	16/20 (80%)	1.50	4 (25%) 0 0	82, 91, 97, 97	0
2	E	11/20 (55%)	1.29	3 (27%) 0 0	75, 82, 93, 94	0
2	F	16/20 (80%)	0.81	1 (6%) 20 17	67, 81, 86, 86	0
2	P	3/20 (15%)	0.47	0 100 100	33, 33, 37, 42	0
All	All	2227/2363 (94%)	-0.01	40 (1%) 68 65	19, 38, 64, 97	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	296	GLY	5.4
1	A	6	LEU	4.7
1	A	14	THR	3.9
1	A	296	GLY	3.8
1	A	12	GLY	3.7
1	A	13	SER	3.7
1	B	737	GLY	3.6
1	B	294	GLN	3.5
1	C	737	GLY	3.4
1	A	737	GLY	3.4
1	A	274	PHE	3.3
2	D	372	ASN	3.1
1	B	297	VAL	3.0
1	A	11	ASP	2.9
1	A	19	LEU	2.9
1	A	4	ASN	2.9
2	D	361	ILE	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	E	367	THR	2.7
1	B	161	VAL	2.6
2	E	372	ASN	2.6
1	A	17	ILE	2.6
1	C	274	PHE	2.5
1	A	298	ARG	2.5
1	A	323	ARG	2.5
1	A	295	GLY	2.5
2	D	364	GLU	2.5
2	F	361	ILE	2.4
2	D	373	PHE	2.4
2	E	368	ASP	2.4
1	A	161	VAL	2.3
1	C	296	GLY	2.3
1	C	16	ARG	2.3
1	B	9	LYS	2.3
1	A	384	LYS	2.2
1	B	10	ARG	2.1
1	A	95	GLY	2.1
1	B	4	ASN	2.1
1	B	274	PHE	2.0
1	C	294	GLN	2.0
1	A	297	VAL	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, 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	B-factors(Å^2)	Q<0.9
1	NIY	A	730	15/16	0.93	0.19	30,31,39,39	0
1	NIY	B	730	15/16	0.94	0.17	31,33,41,42	0
1	NIY	C	730	15/16	0.96	0.17	24,25,35,36	0

6.3 Carbohydrates (i)

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.