Full wwPDB X-ray Structure Validation Report (i)

Dec 17, 2023 – 06:46 am GMT

PDB ID	:	2XAW
Title	:	Ribonucleotide reductase Y730NO2Y and Y731F modified R1 subunit of E. coli
Authors	:	Yokoyama, K.; Uhlin, U.; Stubbe, J.
Deposited on	:	2010-03-31
Resolution	:	3.10 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) 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 (i)) were used in the production of this report:

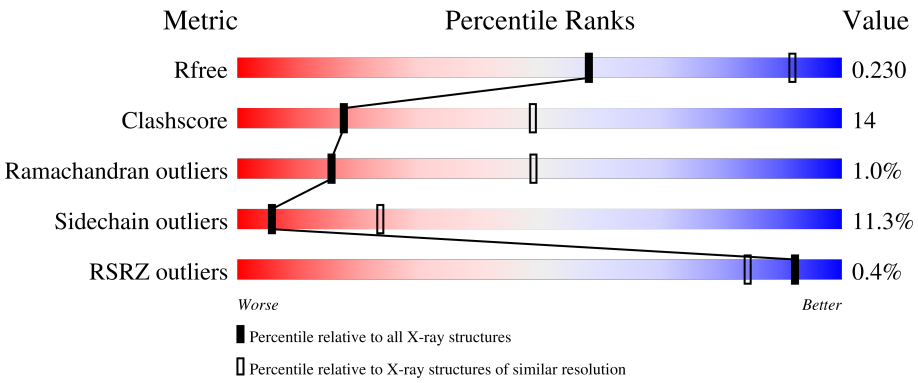
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 3.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1094 (3.10-3.10)
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)
RSRZ outliers	127900	1067 (3.10-3.10)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=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	.% 64% 27% • •
1	B	761	65% 25% 5% •
1	C	761	70% 23% • •
2	D	20	10% 30% 25% 45%
2	E	20	35% 15% 5% 45%

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Mol	Chain	Length	Quality of chain
2	F	20	35% 25% 40%
2	P	20	5% 10% 85%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 18220 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
			Total	C	N	O	S			
1	A	727	5795	3679	995	1097	24	0	0	0
1	B	727	5795	3679	995	1097	24	0	0	0
1	C	727	5795	3679	995	1097	24	0	0	0

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	731	PHE	TYR	engineered mutation	UNP P00452
B	731	PHE	TYR	engineered mutation	UNP P00452
C	731	PHE	TYR	engineered mutation	UNP P00452

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

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
			Total	C	N	O			
2	D	11	89	54	13	22	0	0	0
2	E	11	89	54	13	22	0	0	0
2	F	12	98	59	14	25	0	0	0
2	P	3	27	20	3	4	0	0	0

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	A	152	152	152	0	0

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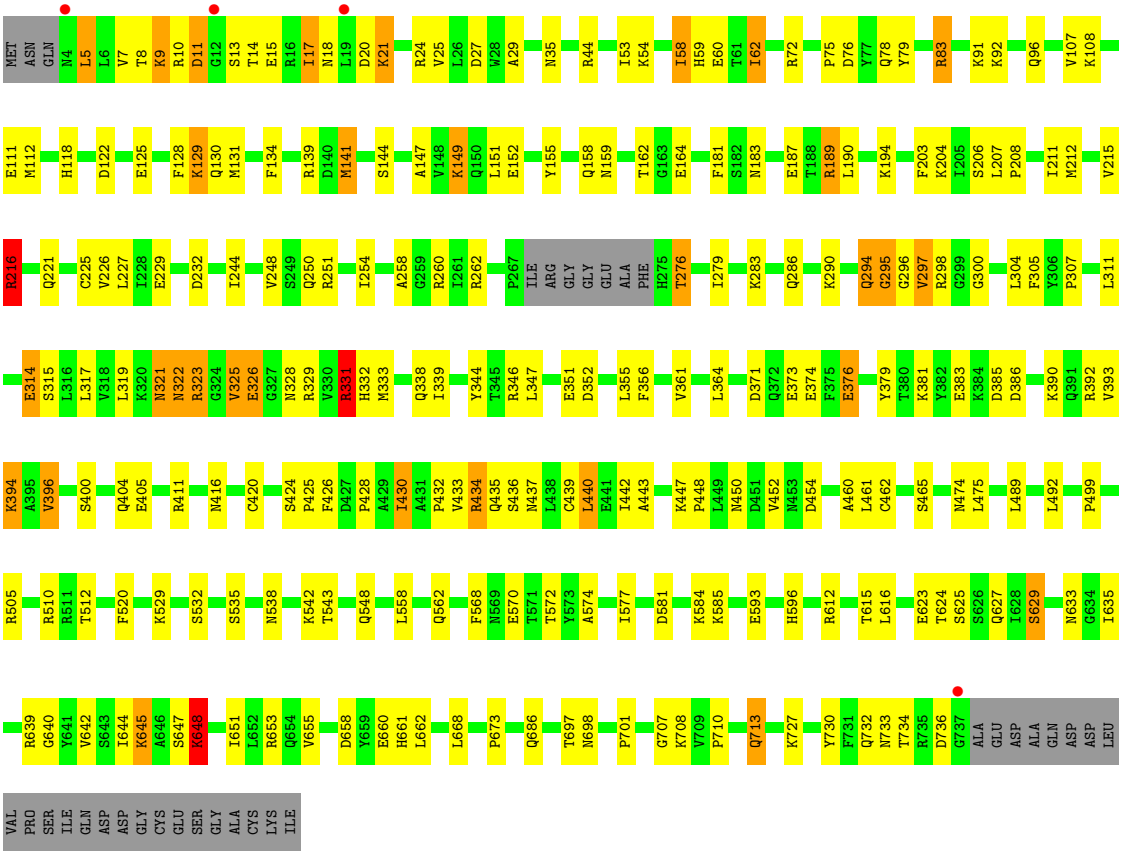
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	B	179	179	179	0	0
			Total	O		
3	C	195	195	195	0	0
			Total	O		
3	D	2	2	2	0	0
			Total	O		
3	E	1	1	1	0	0
			Total	O		
3	F	2	2	2	0	0
			Total	O		
3	P	1	1	1	0	0

3 Residue-property plots (i)

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

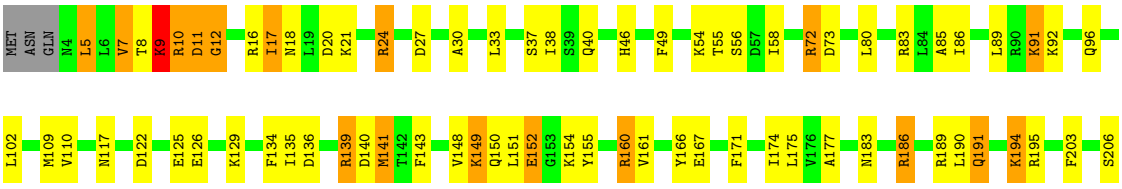
• Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT ALPHA

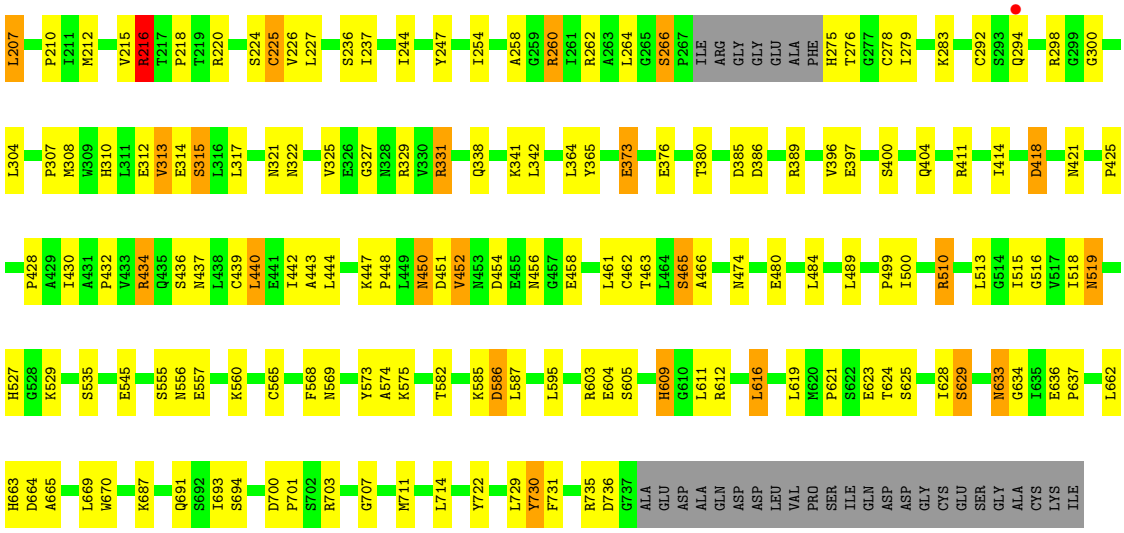
Chain A:



• Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT ALPHA

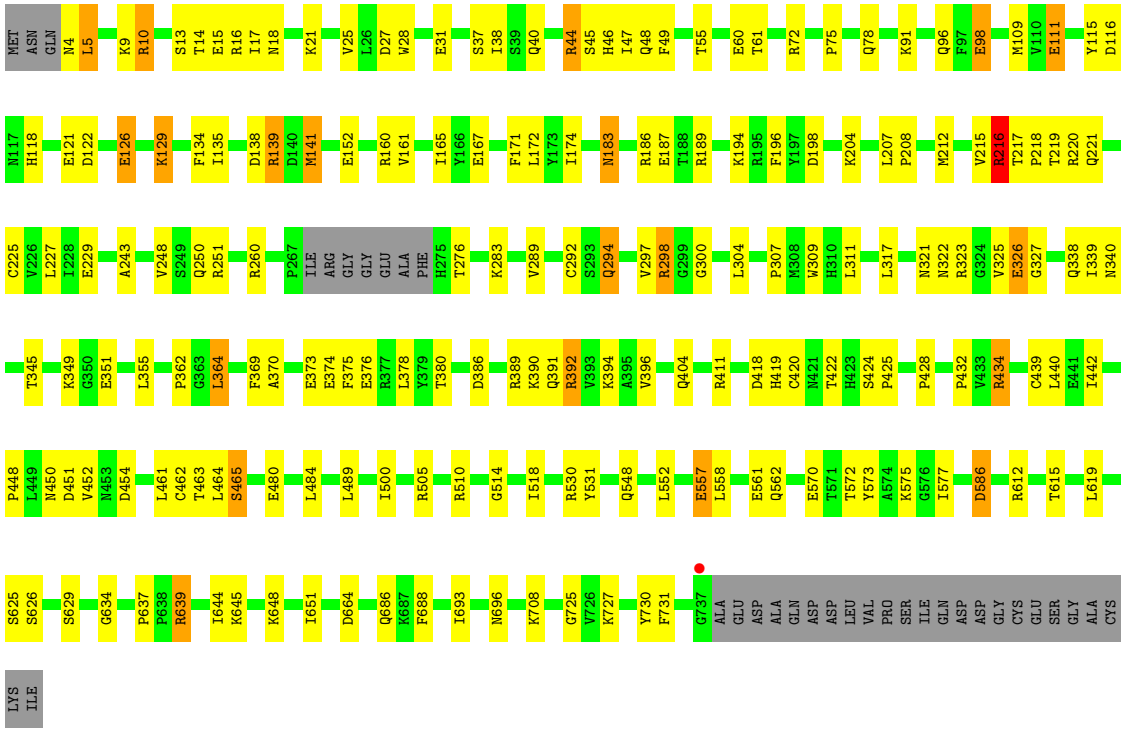
Chain B:





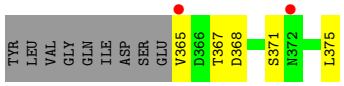
• Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT ALPHA

Chain C:



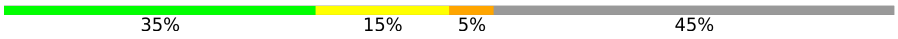
• Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA

Chain D:



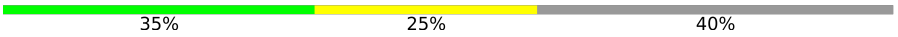
• Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA

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	223.89Å 223.89Å 336.73Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	169.03 – 3.10 84.02 – 3.10	Depositor EDS
% Data completeness (in resolution range)	98.6 (169.03-3.10) 97.2 (84.02-3.10)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.41 (at 3.13Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.165 , 0.234 0.165 , 0.230	Depositor DCC
R_{free} test set	2894 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å^2)	51.5	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 51.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	18220	wwPDB-VP
Average B, all atoms (Å^2)	43.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.06% 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 (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	0.55	0/5904	0.70	2/7994 (0.0%)
1	B	0.55	0/5904	0.69	1/7994 (0.0%)
1	C	0.61	0/5904	0.73	0/7994
2	D	0.53	0/89	0.69	0/119
2	E	0.52	0/89	0.83	0/119
2	F	0.50	0/98	0.69	0/131
2	P	0.88	0/27	1.13	0/36
All	All	0.57	0/18015	0.71	3/24387 (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 (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	331	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	B	616	LEU	CA-CB-CG	-5.53	102.59	115.30
1	A	295	GLY	N-CA-C	-5.33	99.79	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	450	ASN	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	5795	0	5714	162	0
1	B	5795	0	5714	174	0
1	C	5795	0	5715	143	0
2	D	89	0	77	1	0
2	E	89	0	77	4	0
2	F	98	0	83	1	0
2	P	27	0	31	1	0
3	A	152	0	0	29	0
3	B	179	0	0	27	0
3	C	195	0	0	37	0
3	D	2	0	0	0	0
3	E	1	0	0	0	0
3	F	2	0	0	0	0
3	P	1	0	0	0	0
All	All	18220	0	17411	482	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 14.

All (482) 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:117:ASN:HB2	3:B:2034:HOH:O	1.41	1.20
1:A:294:GLN:HE21	1:A:294:GLN:HA	0.97	1.12
1:C:126:GLU:HA	1:C:129:LYS:HB2	1.30	1.10
1:B:160:ARG:HE	1:B:160:ARG:HA	0.98	1.08
1:A:83:ARG:HG3	1:A:83:ARG:HH11	1.12	1.08
1:C:160:ARG:HG3	3:C:2048:HOH:O	1.56	1.03
1:C:404:GLN:HB2	3:C:2119:HOH:O	1.57	1.02
1:B:10:ARG:H	1:B:10:ARG:HD2	1.24	0.99
1:A:79:TYR:O	1:A:83:ARG:HG2	1.63	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:160:ARG:HA	1:B:160:ARG:NE	1.80	0.97
1:A:294:GLN:HA	1:A:294:GLN:NE2	1.78	0.95
1:A:9:LYS:CE	3:A:2002:HOH:O	2.14	0.95
1:C:283:LYS:HG3	3:C:2083:HOH:O	1.64	0.95
1:A:346:ARG:HD2	1:A:352:ASP:O	1.68	0.93
1:C:480:GLU:HB2	3:C:2139:HOH:O	1.70	0.92
1:C:44:ARG:HG2	1:C:44:ARG:HH11	1.35	0.91
1:B:160:ARG:HE	1:B:160:ARG:CA	1.84	0.91
1:C:294:GLN:HG3	1:C:298:ARG:HB2	1.53	0.90
1:A:351:GLU:HB3	3:A:2081:HOH:O	1.73	0.88
1:B:314:GLU:HG2	3:B:2073:HOH:O	1.74	0.86
1:C:373:GLU:HG2	3:C:2112:HOH:O	1.75	0.86
1:B:91:LYS:HD3	3:B:2025:HOH:O	1.76	0.85
1:A:215:VAL:O	1:A:216:ARG:HB3	1.75	0.85
1:B:11:ASP:CG	1:B:12:GLY:H	1.80	0.85
1:A:294:GLN:HE21	1:A:294:GLN:CA	1.82	0.85
1:C:251:ARG:HD3	3:C:2073:HOH:O	1.76	0.85
1:C:212:MET:O	1:C:216:ARG:NH2	2.10	0.84
1:A:9:LYS:HE2	3:A:2002:HOH:O	1.70	0.83
1:A:125:GLU:HG2	1:A:129:LYS:HE3	1.58	0.83
1:C:75:PRO:O	1:C:78:GLN:HG2	1.80	0.82
1:B:10:ARG:HD2	1:B:10:ARG:N	1.93	0.81
1:A:221:GLN:OE1	1:A:250:GLN:HG2	1.81	0.81
1:A:376:GLU:HB2	3:A:2085:HOH:O	1.81	0.81
2:E:372:ASN:H	2:E:372:ASN:ND2	1.78	0.81
1:B:225:CYS:HB3	3:B:2113:HOH:O	1.81	0.80
1:C:480:GLU:HB3	3:C:2056:HOH:O	1.80	0.80
1:A:294:GLN:HG3	1:A:295:GLY:H	1.45	0.80
1:B:603:ARG:HG3	1:B:603:ARG:HH11	1.47	0.79
1:C:111:GLU:HG2	3:C:2038:HOH:O	1.82	0.78
1:C:362:PRO:HA	3:C:2106:HOH:O	1.81	0.78
1:C:373:GLU:CG	3:C:2112:HOH:O	2.30	0.78
1:B:10:ARG:H	1:B:10:ARG:CD	1.96	0.78
1:C:46:HIS:HD2	1:C:49:PHE:CE2	2.02	0.77
1:A:425:PRO:HG3	1:A:615:THR:HG22	1.67	0.77
1:B:18:ASN:ND2	1:B:21:LYS:HB2	1.99	0.77
1:C:46:HIS:CD2	1:C:49:PHE:HE2	2.02	0.76
1:A:9:LYS:HE3	1:A:10:ARG:H	1.51	0.76
1:C:111:GLU:HG3	2:P:2:LEU:HB2	1.68	0.75
1:A:686:GLN:NE2	1:A:727:LYS:HE3	2.01	0.75
1:B:619:LEU:HD12	1:B:693:ILE:HG12	1.66	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:ARG:HG2	3:C:2010:HOH:O	1.85	0.75
1:B:215:VAL:O	1:B:216:ARG:HB3	1.86	0.75
1:A:322:ASN:O	1:A:323:ARG:HB2	1.86	0.75
1:B:450:ASN:HB2	1:B:454:ASP:HB2	1.69	0.73
1:A:532:SER:HB2	1:A:673:PRO:HD2	1.70	0.73
1:B:203:PHE:HB3	1:B:629:SER:HB3	1.70	0.73
1:C:215:VAL:O	1:C:216:ARG:HB3	1.89	0.73
1:C:28:TRP:HZ2	1:C:141:MET:CE	2.02	0.73
1:A:59:HIS:HA	1:A:62:ILE:HD13	1.71	0.73
1:C:326:GLU:OE1	1:C:326:GLU:HA	1.89	0.72
1:C:46:HIS:HD2	1:C:49:PHE:HE2	1.36	0.72
1:A:300:GLY:HA2	3:A:2057:HOH:O	1.88	0.72
1:B:404:GLN:HG2	3:B:2106:HOH:O	1.90	0.72
1:C:349:LYS:HE2	3:C:2101:HOH:O	1.89	0.72
1:C:129:LYS:HE2	3:C:2040:HOH:O	1.89	0.71
1:B:480:GLU:HA	3:B:2049:HOH:O	1.89	0.71
1:A:279:ILE:HG12	1:A:319:LEU:HD21	1.72	0.71
1:B:207:LEU:HB2	1:B:212:MET:CE	2.21	0.70
1:B:633:ASN:HB3	3:B:2146:HOH:O	1.91	0.70
1:B:191:GLN:O	1:B:195:ARG:HG3	1.92	0.70
1:C:122:ASP:O	1:C:189:ARG:NH2	2.26	0.69
1:A:393:VAL:HB	3:A:2093:HOH:O	1.91	0.69
2:E:372:ASN:H	2:E:372:ASN:HD22	1.38	0.69
1:B:474:ASN:HB2	3:B:2119:HOH:O	1.93	0.69
1:A:83:ARG:HH11	1:A:83:ARG:CG	1.99	0.68
1:C:619:LEU:HD12	1:C:693:ILE:HG12	1.75	0.68
1:C:557:GLU:HB3	3:C:2155:HOH:O	1.94	0.68
1:C:44:ARG:HG2	1:C:44:ARG:NH1	2.07	0.68
1:C:664:ASP:HB2	3:C:2185:HOH:O	1.94	0.68
1:A:331:ARG:HG3	1:A:331:ARG:HH11	1.57	0.67
1:B:186:ARG:HB3	3:B:2046:HOH:O	1.92	0.67
1:B:122:ASP:O	1:B:189:ARG:NH2	2.26	0.67
1:C:167:GLU:OE2	1:C:216:ARG:NH1	2.28	0.66
1:B:582:THR:HA	3:B:2139:HOH:O	1.96	0.66
1:C:696:ASN:OD1	1:C:731:PHE:HB2	1.95	0.66
1:C:28:TRP:HZ2	1:C:141:MET:HE1	1.59	0.66
1:C:126:GLU:CA	1:C:129:LYS:HB2	2.18	0.66
1:A:450:ASN:HB2	1:A:454:ASP:OD2	1.96	0.66
1:C:505:ARG:HD2	3:C:2142:HOH:O	1.95	0.66
1:A:639:ARG:HD3	3:A:2150:HOH:O	1.95	0.65
1:C:46:HIS:CD2	1:C:49:PHE:CE2	2.80	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:LYS:HE3	3:A:2102:HOH:O	1.96	0.65
1:B:568:PHE:CE2	1:B:574:ALA:HA	2.31	0.65
1:B:621:PRO:HD3	1:B:694:SER:OG	1.97	0.64
1:A:226:VAL:HG12	1:A:461:LEU:HD23	1.79	0.64
1:A:321:ASN:HB3	1:A:405:GLU:OE1	1.97	0.64
1:B:560:LYS:HG3	1:B:609:HIS:CD2	2.31	0.64
1:A:296:GLY:HA3	3:A:2072:HOH:O	1.96	0.64
1:B:603:ARG:HG3	1:B:603:ARG:NH1	2.12	0.64
1:B:565:CYS:HB3	1:B:612:ARG:O	1.98	0.64
1:C:480:GLU:CB	3:C:2056:HOH:O	2.42	0.64
1:A:221:GLN:HG2	3:A:2056:HOH:O	1.98	0.63
1:B:633:ASN:N	1:B:633:ASN:HD22	1.94	0.63
1:B:110:VAL:CG1	1:B:117:ASN:HB3	2.29	0.63
1:A:83:ARG:HG3	1:A:83:ARG:NH1	1.91	0.62
1:B:24:ARG:HD2	3:B:2014:HOH:O	1.99	0.62
1:B:260:ARG:HH21	1:B:448:PRO:HG3	1.63	0.62
1:B:136:ASP:HB3	1:B:139:ARG:NH1	2.14	0.62
1:B:298:ARG:HG2	3:B:2071:HOH:O	1.97	0.62
1:B:11:ASP:CG	1:B:12:GLY:N	2.52	0.62
1:B:260:ARG:HD2	1:B:365:TYR:CE2	2.35	0.62
1:C:376:GLU:HG2	3:C:2113:HOH:O	1.98	0.62
1:B:207:LEU:HB2	1:B:212:MET:HE3	1.79	0.62
1:B:298:ARG:HB3	1:B:298:ARG:NH1	2.16	0.61
1:B:55:THR:HG23	1:B:56:SER:H	1.64	0.61
1:C:183:ASN:HB3	3:C:2053:HOH:O	2.01	0.60
1:C:196:PHE:HZ	1:C:207:LEU:HD11	1.66	0.60
1:B:331:ARG:HD2	3:B:2082:HOH:O	2.01	0.60
1:B:86:ILE:HG21	1:B:140:ASP:HB3	1.82	0.60
1:B:466:ALA:HA	1:B:516:GLY:O	2.00	0.60
1:B:46:HIS:HD2	1:B:49:PHE:CE2	2.20	0.60
1:B:215:VAL:O	1:B:216:ARG:CB	2.50	0.60
1:C:225:CYS:HB2	3:C:2128:HOH:O	2.02	0.60
1:C:392:ARG:NH1	1:C:392:ARG:HB3	2.17	0.60
1:C:307:PRO:HA	1:C:338:GLN:HB2	1.85	0.59
1:B:294:GLN:HG2	3:B:2066:HOH:O	2.03	0.59
1:A:260:ARG:HH21	1:A:434:ARG:NH2	2.01	0.59
1:B:266:SER:O	1:B:275:HIS:CD2	2.56	0.59
1:A:108:LYS:O	1:A:112:MET:HG2	2.02	0.58
1:B:376:GLU:HG3	3:B:2093:HOH:O	2.03	0.58
1:A:141:MET:HG2	3:A:2010:HOH:O	2.02	0.58
1:A:208:PRO:HG2	1:A:211:ILE:HD12	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:75:PRO:HD2	3:A:2012:HOH:O	2.04	0.58
1:A:584:LYS:HD2	3:A:2119:HOH:O	2.03	0.58
1:B:298:ARG:HD3	3:B:2068:HOH:O	2.02	0.58
1:B:397:GLU:HA	1:B:400:SER:HB2	1.84	0.58
1:B:283:LYS:NZ	1:B:327:GLY:HA2	2.19	0.58
1:A:558:LEU:HD23	1:A:612:ARG:HG2	1.85	0.57
1:B:298:ARG:HB2	3:B:2070:HOH:O	2.04	0.57
1:A:633:ASN:HB3	3:A:2128:HOH:O	2.04	0.57
1:B:443:ALA:O	1:B:444:LEU:HD23	2.04	0.57
1:A:75:PRO:O	1:A:78:GLN:HB2	2.04	0.57
1:A:439:CYS:O	1:A:440:LEU:HB2	2.03	0.57
1:C:462:CYS:HB2	1:C:464:LEU:HD21	1.85	0.57
1:C:28:TRP:CZ2	1:C:141:MET:CE	2.88	0.56
1:B:109:MET:CE	1:B:166:TYR:HB3	2.35	0.56
1:B:568:PHE:HE2	1:B:574:ALA:HA	1.69	0.56
1:C:21:LYS:O	1:C:25:VAL:HG23	2.05	0.56
1:B:700:ASP:OD2	1:B:735:ARG:HD3	2.05	0.56
1:A:532:SER:CB	1:A:673:PRO:HD2	2.36	0.56
1:B:110:VAL:HG13	1:B:117:ASN:HB3	1.88	0.56
1:A:144:SER:O	1:A:147:ALA:HB3	2.05	0.56
1:B:10:ARG:HH21	1:B:91:LYS:HE2	1.71	0.55
1:B:149:LYS:HE3	1:B:152:GLU:OE1	2.05	0.55
1:B:258:ALA:HB3	1:B:304:LEU:HD21	1.88	0.55
1:C:644:ILE:HG23	1:C:651:ILE:HG23	1.89	0.55
1:A:258:ALA:HB3	1:A:304:LEU:HD21	1.88	0.55
1:B:46:HIS:CD2	1:B:49:PHE:CE2	2.94	0.55
1:A:648:LYS:HG3	3:A:2137:HOH:O	2.07	0.55
1:B:5:LEU:O	1:B:17:ILE:HB	2.06	0.55
1:B:447:LYS:HD2	1:B:456:ASN:O	2.07	0.55
1:C:28:TRP:CZ2	1:C:141:MET:HE3	2.42	0.55
1:C:207:LEU:HD13	1:C:212:MET:HE1	1.88	0.55
1:A:11:ASP:OD1	1:A:13:SER:OG	2.25	0.55
1:B:49:PHE:CZ	1:B:58:ILE:HG23	2.42	0.55
1:B:83:ARG:HG2	1:B:141:MET:HG3	1.88	0.55
1:B:439:CYS:O	1:B:694:SER:HB3	2.06	0.55
1:C:518:ILE:HA	1:C:634:GLY:HA2	1.88	0.55
1:A:331:ARG:HH11	1:A:331:ARG:H	1.54	0.54
1:A:442:ILE:HG13	1:A:462:CYS:HB3	1.89	0.54
1:B:212:MET:O	1:B:216:ARG:NH2	2.38	0.54
1:A:212:MET:O	1:A:216:ARG:NH2	2.40	0.54
1:A:297:VAL:CG2	3:A:2074:HOH:O	2.55	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:510:ARG:HB2	1:A:512:THR:HG23	1.90	0.54
1:C:45:SER:HB2	1:C:61:THR:HG22	1.90	0.54
1:C:98:GLU:OE2	1:C:98:GLU:HA	2.07	0.54
1:B:418:ASP:HB2	3:B:2109:HOH:O	2.07	0.54
1:A:18:ASN:CG	1:A:21:LYS:HB2	2.28	0.54
1:A:425:PRO:HG2	1:A:426:PHE:CD2	2.43	0.54
1:C:419:HIS:CD2	1:C:725:GLY:HA2	2.42	0.54
1:C:118:HIS:HA	1:C:121:GLU:HB2	1.90	0.54
1:A:558:LEU:CD2	1:A:612:ARG:HG2	2.37	0.54
1:B:18:ASN:HD22	1:B:21:LYS:HE2	1.70	0.54
1:B:46:HIS:CD2	1:B:49:PHE:HE2	2.25	0.54
1:C:44:ARG:HH11	1:C:44:ARG:CG	2.15	0.54
1:C:135:ILE:HD11	1:C:174:ILE:HG21	1.90	0.54
1:C:686:GLN:CD	1:C:727:LYS:HD2	2.28	0.54
1:B:195:ARG:HD3	3:B:2047:HOH:O	2.07	0.54
1:C:171:PHE:HA	1:C:174:ILE:HG22	1.90	0.54
1:B:10:ARG:HH21	1:B:91:LYS:CE	2.21	0.54
1:C:139:ARG:NH2	1:C:198:ASP:OD1	2.41	0.54
1:A:294:GLN:CG	1:A:295:GLY:H	2.14	0.53
1:B:136:ASP:HB3	1:B:139:ARG:HH11	1.73	0.53
1:B:432:PRO:CG	1:B:434:ARG:HD3	2.37	0.53
1:A:227:LEU:HD11	1:A:437:ASN:HB3	1.90	0.53
1:A:181:PHE:O	1:A:189:ARG:HD2	2.08	0.53
1:A:203:PHE:HB3	1:A:629:SER:HB3	1.89	0.53
1:A:520:PHE:HB3	1:A:635:ILE:HA	1.89	0.53
1:C:134:PHE:CE2	1:C:194:LYS:HB2	2.44	0.53
1:C:9:LYS:NZ	3:C:2005:HOH:O	2.42	0.53
1:C:548:GLN:HB2	1:C:688:PHE:HB3	1.91	0.53
1:A:710:PRO:HG2	1:A:713:GLN:HB2	1.91	0.53
1:C:321:ASN:HA	3:C:2120:HOH:O	2.08	0.53
1:B:207:LEU:HB2	1:B:212:MET:HE2	1.91	0.52
1:A:29:ALA:O	1:A:83:ARG:NH1	2.41	0.52
1:B:396:VAL:HG23	3:B:2103:HOH:O	2.08	0.52
1:C:425:PRO:HG2	1:C:615:THR:HG22	1.92	0.52
1:C:18:ASN:ND2	1:C:21:LYS:HB2	2.25	0.52
1:A:627:GLN:OE1	1:A:645:LYS:HE3	2.10	0.52
1:C:298:ARG:HB3	1:C:298:ARG:CZ	2.40	0.52
1:A:305:PHE:CZ	1:A:436:SER:HB3	2.45	0.52
1:B:27:ASP:HA	1:B:38:ILE:HD11	1.92	0.52
1:C:464:LEU:HA	1:C:514:GLY:O	2.10	0.51
1:A:648:LYS:HD2	1:A:648:LYS:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:CYS:HA	1:A:727:LYS:HD3	1.92	0.51
1:A:432:PRO:HG2	1:A:434:ARG:HD3	1.92	0.51
1:B:499:PRO:O	1:B:500:ILE:HG13	2.10	0.51
1:B:439:CYS:O	1:B:440:LEU:HB2	2.11	0.51
1:C:420:CYS:O	1:C:424:SER:HB2	2.11	0.51
1:B:134:PHE:CE2	1:B:194:LYS:HB2	2.46	0.51
1:A:344:TYR:O	1:A:347:LEU:HB3	2.11	0.51
1:B:700:ASP:OD2	1:B:735:ARG:CD	2.59	0.51
1:A:433:VAL:HG11	1:A:443:ALA:HB1	1.93	0.51
1:A:648:LYS:HD2	1:A:648:LYS:H	1.75	0.51
1:A:640:GLY:HA2	1:A:668:LEU:HD13	1.92	0.51
1:B:210:PRO:HG3	1:B:224:SER:HB3	1.93	0.51
1:A:648:LYS:HD3	3:A:2136:HOH:O	2.10	0.50
1:B:527:HIS:O	1:B:529:LYS:HE2	2.12	0.50
1:B:55:THR:HG23	1:B:56:SER:N	2.26	0.50
1:A:54:LYS:HE3	3:A:2001:HOH:O	2.11	0.50
1:A:568:PHE:CE2	1:A:574:ALA:HA	2.46	0.50
1:B:283:LYS:HZ1	1:B:327:GLY:HA2	1.77	0.50
1:C:28:TRP:HZ2	1:C:141:MET:HE3	1.75	0.50
1:B:308:MET:O	1:B:313:VAL:HG21	2.11	0.50
1:C:44:ARG:NH1	1:C:44:ARG:CG	2.73	0.50
1:C:373:GLU:HG3	3:C:2112:HOH:O	2.04	0.50
1:A:8:THR:HB	1:A:54:LYS:HA	1.93	0.50
1:A:328:ASN:O	1:A:329:ARG:HD3	2.12	0.50
1:A:660:GLU:HG3	1:A:661:HIS:N	2.26	0.50
1:B:310:HIS:O	1:B:313:VAL:HB	2.11	0.50
1:B:312:GLU:HG2	3:B:2075:HOH:O	2.11	0.50
1:C:138:ASP:O	1:C:141:MET:HB2	2.12	0.50
1:A:5:LEU:HB3	1:A:17:ILE:HG21	1.94	0.50
1:B:373:GLU:HA	1:B:376:GLU:HB2	1.94	0.49
1:B:46:HIS:HA	1:B:49:PHE:CD2	2.46	0.49
1:C:221:GLN:OE1	1:C:250:GLN:HG2	2.12	0.49
1:C:373:GLU:HB2	3:C:2111:HOH:O	2.12	0.49
1:A:356:PHE:CD1	1:A:361:VAL:HG11	2.47	0.49
1:A:21:LYS:O	1:A:25:VAL:HG23	2.13	0.49
1:B:298:ARG:HB3	1:B:298:ARG:HH11	1.76	0.49
1:A:58:ILE:O	1:A:62:ILE:HG23	2.13	0.49
1:B:329:ARG:HB3	1:B:331:ARG:HD3	1.94	0.49
1:B:568:PHE:CE2	1:B:574:ALA:CA	2.95	0.49
1:C:21:LYS:HD3	3:C:2011:HOH:O	2.13	0.49
1:C:91:LYS:HB3	3:C:2007:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:30:ALA:HA	1:B:33:LEU:HD12	1.94	0.48
1:A:128:PHE:CD1	1:A:131:MET:CE	2.96	0.48
1:A:331:ARG:HH11	1:A:331:ARG:CG	2.26	0.48
1:B:637:PRO:HG2	1:B:669:LEU:HD12	1.95	0.48
1:C:298:ARG:HB3	1:C:298:ARG:NH1	2.29	0.48
1:A:311:LEU:HA	1:A:355:LEU:HB3	1.94	0.48
1:C:243:ALA:HA	1:C:500:ILE:HD11	1.95	0.48
1:C:369:PHE:CD1	1:C:434:ARG:HB3	2.49	0.48
1:C:463:THR:HG22	1:C:489:LEU:HD22	1.95	0.48
1:A:260:ARG:HH21	1:A:434:ARG:HH22	1.60	0.48
1:B:529:LYS:HD2	1:B:535:SER:O	2.13	0.48
1:A:396:VAL:CG1	2:D:365:VAL:HG11	2.43	0.48
1:B:342:LEU:HD12	1:B:376:GLU:HG2	1.96	0.48
1:A:426:PHE:O	1:A:428:PRO:HD3	2.13	0.48
1:A:229:GLU:O	1:A:448:PRO:HA	2.13	0.48
1:A:314:GLU:HB2	3:A:2078:HOH:O	2.13	0.48
1:B:266:SER:O	1:B:275:HIS:HD2	1.95	0.48
1:A:430:ILE:HD12	1:A:570:GLU:HA	1.95	0.47
1:B:633:ASN:N	1:B:633:ASN:ND2	2.62	0.47
1:B:489:LEU:HB3	1:B:513:LEU:HD22	1.97	0.47
1:A:18:ASN:ND2	1:A:21:LYS:HB2	2.29	0.47
1:B:264:LEU:O	1:B:389:ARG:NH2	2.47	0.47
1:A:373:GLU:HA	1:A:376:GLU:HB3	1.95	0.47
1:B:465:SER:O	1:B:515:ILE:HA	2.14	0.47
1:B:150:GLN:HB2	1:B:628:ILE:HD13	1.97	0.47
1:B:160:ARG:NE	1:B:160:ARG:CA	2.57	0.47
1:B:236:SER:O	1:B:237:ILE:C	2.52	0.47
1:B:442:ILE:HG13	1:B:462:CYS:SG	2.54	0.47
1:A:644:ILE:HG23	1:A:651:ILE:HG23	1.97	0.47
1:C:172:LEU:HD23	1:C:172:LEU:C	2.35	0.47
1:C:219:THR:O	1:C:220:ARG:NH1	2.44	0.47
1:C:227:LEU:N	1:C:227:LEU:HD12	2.30	0.47
1:C:418:ASP:O	1:C:422:THR:HG23	2.15	0.47
1:A:244:ILE:O	1:A:248:VAL:HG22	2.14	0.47
1:A:339:ILE:O	1:A:416:ASN:HA	2.15	0.47
1:A:435:GLN:HG2	3:A:2060:HOH:O	2.15	0.47
1:B:7:VAL:HG22	1:B:17:ILE:HG12	1.96	0.47
1:C:572:THR:HB	1:C:577:ILE:HB	1.96	0.47
1:A:83:ARG:HD2	1:A:141:MET:HG3	1.96	0.47
1:A:542:LYS:HG3	1:A:596:HIS:CD2	2.50	0.47
1:B:8:THR:HB	1:B:54:LYS:HA	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:151:LEU:HA	1:B:155:TYR:HB2	1.97	0.47
1:B:425:PRO:HB3	1:B:573:TYR:CE2	2.50	0.47
1:B:711:MET:HE3	3:B:2105:HOH:O	2.15	0.47
1:B:9:LYS:NZ	1:B:10:ARG:HD3	2.30	0.47
1:C:207:LEU:HD23	1:C:465:SER:OG	2.15	0.47
1:C:248:VAL:HG11	1:C:289:VAL:HA	1.97	0.47
1:C:294:GLN:HB2	1:C:298:ARG:O	2.15	0.47
1:C:531:TYR:CE2	1:C:637:PRO:HD3	2.50	0.47
1:A:437:ASN:ND2	1:A:439:CYS:H	2.13	0.46
1:B:307:PRO:HA	1:B:338:GLN:HB2	1.95	0.46
1:C:225:CYS:CB	3:C:2128:HOH:O	2.62	0.46
1:A:134:PHE:CD1	1:A:194:LYS:HD2	2.51	0.46
1:A:623:GLU:O	1:A:627:GLN:HB2	2.15	0.46
1:B:458:GLU:OE1	1:B:510:ARG:NH1	2.48	0.46
1:B:226:VAL:HG12	1:B:461:LEU:HD23	1.97	0.46
1:B:711:MET:HA	1:B:714:LEU:HD12	1.96	0.46
1:C:311:LEU:HA	1:C:355:LEU:HB3	1.96	0.46
1:C:558:LEU:HD23	1:C:612:ARG:HG2	1.97	0.46
1:C:109:MET:HG3	1:C:115:TYR:CE2	2.51	0.46
1:C:552:LEU:HD21	1:C:573:TYR:CZ	2.50	0.46
1:A:424:SER:HB2	1:A:425:PRO:HD2	1.96	0.46
1:B:134:PHE:CD2	1:B:194:LYS:HB2	2.50	0.46
1:C:389:ARG:HA	3:C:2116:HOH:O	2.16	0.46
1:A:379:TYR:O	1:A:383:GLU:HG2	2.15	0.46
1:C:283:LYS:HZ1	1:C:327:GLY:HA2	1.81	0.46
1:A:548:GLN:OE1	1:A:548:GLN:HA	2.15	0.46
1:A:325:VAL:HG13	1:A:328:ASN:HD21	1.79	0.46
1:B:226:VAL:HG11	1:B:247:TYR:CD2	2.51	0.46
1:A:307:PRO:HA	1:A:338:GLN:HB2	1.97	0.46
1:C:364:LEU:CD2	1:C:375:PHE:CE1	2.99	0.46
1:B:418:ASP:N	1:B:418:ASP:OD1	2.46	0.45
1:A:122:ASP:O	1:A:189:ARG:NH2	2.50	0.45
1:A:159:ASN:OD1	1:A:162:THR:N	2.47	0.45
1:B:102:LEU:HD11	1:B:175:LEU:HD21	1.99	0.45
1:C:44:ARG:NH1	3:C:2022:HOH:O	2.50	0.45
1:C:134:PHE:CD2	1:C:194:LYS:HB2	2.51	0.45
1:A:91:LYS:HE2	3:A:2028:HOH:O	2.17	0.45
1:A:190:LEU:HD23	1:A:190:LEU:HA	1.72	0.45
1:A:697:THR:OG1	1:A:732:GLN:HG3	2.17	0.45
1:B:670:TRP:CE2	1:B:735:ARG:HG3	2.51	0.45
1:C:47:ILE:HG13	1:C:47:ILE:O	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:PRO:HD3	3:C:2098:HOH:O	2.16	0.45
1:C:386:ASP:HA	1:C:390:LYS:NZ	2.30	0.45
1:B:171:PHE:HA	1:B:174:ILE:HG22	1.98	0.45
1:B:279:ILE:HD11	1:B:315:SER:HB3	1.99	0.45
1:B:10:ARG:NH1	1:B:55:THR:HG21	2.32	0.45
1:C:297:VAL:HG22	3:C:2086:HOH:O	2.17	0.45
1:A:149:LYS:HE2	1:A:152:GLU:OE1	2.17	0.45
1:A:294:GLN:CG	1:A:295:GLY:N	2.80	0.45
1:A:5:LEU:HB3	1:A:17:ILE:CG2	2.47	0.44
1:B:85:ALA:O	1:B:89:LEU:HG	2.18	0.44
1:C:229:GLU:O	1:C:448:PRO:HA	2.18	0.44
1:A:76:ASP:C	1:A:78:GLN:N	2.71	0.44
1:A:658:ASP:HB3	1:A:662:LEU:HD12	1.99	0.44
1:B:568:PHE:CE2	1:B:574:ALA:HB2	2.51	0.44
1:B:662:LEU:O	1:B:665:ALA:HB3	2.17	0.44
1:A:227:LEU:HB2	1:A:460:ALA:HB3	2.00	0.44
1:A:338:GLN:NE2	1:A:434:ARG:O	2.50	0.44
1:B:154:LYS:HD2	1:B:624:THR:HG21	1.99	0.44
1:A:736:ASP:OD2	1:A:736:ASP:N	2.43	0.44
1:B:568:PHE:CD2	1:B:574:ALA:HB2	2.53	0.44
1:C:212:MET:HA	1:C:212:MET:HE2	1.99	0.44
1:C:304:LEU:HD23	1:C:304:LEU:C	2.37	0.44
1:C:420:CYS:HA	1:C:727:LYS:HE2	1.99	0.44
1:A:232:ASP:HB2	1:A:260:ARG:O	2.18	0.44
1:A:276:THR:HG21	1:B:292:CYS:O	2.18	0.44
1:A:286:GLN:HG3	1:A:333:MET:HG3	2.00	0.44
1:C:392:ARG:HB3	1:C:392:ARG:HH11	1.83	0.44
1:B:109:MET:HE1	1:B:166:TYR:HB3	2.00	0.44
1:A:332:HIS:CD2	3:A:2075:HOH:O	2.71	0.44
1:A:510:ARG:NH2	1:A:570:GLU:OE1	2.51	0.44
2:F:369:ASP:O	2:F:370:LEU:C	2.56	0.44
1:B:619:LEU:HB2	1:B:693:ILE:HG23	2.00	0.43
1:C:27:ASP:HA	1:C:38:ILE:HD11	2.00	0.43
1:C:442:ILE:HD11	1:C:464:LEU:HD21	1.98	0.43
1:B:91:LYS:HE3	3:B:2007:HOH:O	2.18	0.43
1:B:191:GLN:HE21	1:B:191:GLN:HB2	1.51	0.43
1:B:341:LYS:HG2	1:B:722:TYR:OH	2.18	0.43
1:B:421:ASN:HB3	1:B:428:PRO:HB3	2.00	0.43
1:C:37:SER:CB	1:C:40:GLN:HB2	2.48	0.43
1:C:586:ASP:OD1	1:C:586:ASP:N	2.49	0.43
1:B:167:GLU:OE2	1:B:216:ARG:NH1	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:221:GLN:HG2	3:C:2072:HOH:O	2.18	0.43
1:B:37:SER:HB3	1:B:40:GLN:HB2	2.01	0.43
1:B:331:ARG:HH11	1:B:331:ARG:H	1.65	0.43
1:B:587:LEU:CD1	1:B:687:LYS:HB2	2.48	0.43
1:C:46:HIS:HA	1:C:49:PHE:CD2	2.54	0.43
1:C:215:VAL:O	1:C:216:ARG:CB	2.65	0.43
1:C:283:LYS:NZ	1:C:327:GLY:HA2	2.34	0.43
1:B:729:LEU:HA	1:B:729:LEU:HD23	1.71	0.43
1:A:296:GLY:CA	3:A:2072:HOH:O	2.61	0.43
1:A:383:GLU:HA	1:A:390:LYS:HE2	1.99	0.43
1:A:642:VAL:HG22	1:A:655:VAL:HG22	2.00	0.43
1:C:37:SER:HB3	1:C:40:GLN:HB2	2.00	0.43
1:A:701:PRO:HB3	1:A:707:GLY:O	2.19	0.43
1:B:110:VAL:HG11	1:B:117:ASN:HB3	2.00	0.43
1:B:227:LEU:HD11	1:B:437:ASN:HB3	2.00	0.43
1:A:24:ARG:HD2	3:A:2009:HOH:O	2.18	0.43
1:C:561:GLU:HB3	1:C:562:GLN:HG3	2.01	0.43
1:C:432:PRO:HG2	1:C:434:ARG:HD3	2.00	0.42
1:A:294:GLN:HG3	1:A:295:GLY:N	2.25	0.42
1:A:436:SER:OG	1:A:440:LEU:HA	2.19	0.42
1:A:529:LYS:HD2	1:A:535:SER:O	2.19	0.42
1:C:37:SER:OG	1:C:40:GLN:HB2	2.19	0.42
1:C:558:LEU:CD2	1:C:612:ARG:HG2	2.49	0.42
1:C:639:ARG:HH11	1:C:639:ARG:H	1.66	0.42
1:A:475:LEU:HD21	1:A:543:THR:HG23	2.01	0.42
1:A:639:ARG:NH1	3:A:2134:HOH:O	2.48	0.42
1:B:663:HIS:CD2	3:B:2155:HOH:O	2.72	0.42
1:B:701:PRO:C	1:B:703:ARG:H	2.22	0.42
1:A:10:ARG:HB3	3:A:2003:HOH:O	2.19	0.42
1:A:322:ASN:O	1:A:323:ARG:CB	2.63	0.42
1:B:9:LYS:NZ	3:B:2006:HOH:O	2.51	0.42
1:C:116:ASP:OD2	1:C:220:ARG:NH2	2.44	0.42
1:B:72:ARG:H	1:B:72:ARG:HG2	1.34	0.42
1:B:207:LEU:CD2	1:B:465:SER:OG	2.67	0.42
1:B:322:ASN:HA	3:B:2082:HOH:O	2.19	0.42
1:A:352:ASP:OD2	1:A:394:LYS:HD3	2.18	0.42
1:A:572:THR:HB	1:A:577:ILE:HB	2.01	0.42
1:B:135:ILE:HD11	1:B:174:ILE:HG21	2.01	0.42
1:B:218:PRO:O	1:B:220:ARG:NH1	2.52	0.42
1:B:325:VAL:HG12	3:B:2079:HOH:O	2.19	0.42
1:B:518:ILE:O	1:B:518:ILE:HG13	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:633:ASN:O	1:B:634:GLY:C	2.58	0.42
1:A:83:ARG:CG	1:A:83:ARG:NH1	2.68	0.42
1:C:309:TRP:O	1:C:355:LEU:HA	2.20	0.42
1:C:322:ASN:HD22	1:C:322:ASN:HA	1.64	0.42
1:C:557:GLU:H	1:C:557:GLU:HG2	1.72	0.42
1:A:131:MET:HA	1:A:134:PHE:CD2	2.55	0.42
1:A:385:ASP:OD1	1:A:386:ASP:N	2.52	0.42
1:B:385:ASP:OD1	1:B:386:ASP:N	2.53	0.42
1:C:450:ASN:HB2	1:C:454:ASP:OD2	2.19	0.42
1:C:96:GLN:HE21	1:C:98:GLU:HB3	1.85	0.41
1:C:208:PRO:HB2	3:C:2062:HOH:O	2.19	0.41
1:C:349:LYS:O	1:C:351:GLU:HG3	2.20	0.41
1:A:244:ILE:HG12	1:A:254:ILE:HG21	2.01	0.41
1:A:297:VAL:HG23	3:A:2074:HOH:O	2.19	0.41
1:A:538:ASN:HB3	1:A:593:GLU:OE1	2.20	0.41
1:B:463:THR:HG22	1:B:489:LEU:HD22	2.03	0.41
1:B:545:GLU:HG3	1:B:595:LEU:HD23	2.02	0.41
1:B:701:PRO:O	1:B:707:GLY:HA2	2.20	0.41
1:B:86:ILE:HD11	1:B:148:VAL:HG22	2.02	0.41
1:B:190:LEU:HD23	1:B:190:LEU:HA	1.82	0.41
1:B:568:PHE:HE1	1:B:611:LEU:HB2	1.85	0.41
1:C:31:GLU:OE1	1:C:31:GLU:HA	2.21	0.41
1:A:151:LEU:HA	1:A:155:TYR:HB2	2.02	0.41
1:A:331:ARG:HD3	3:A:2079:HOH:O	2.20	0.41
1:B:149:LYS:HA	1:B:149:LYS:HD2	1.41	0.41
1:B:262:ARG:HD3	1:B:266:SER:HB2	2.01	0.41
1:C:374:GLU:HG3	1:C:378:LEU:HD12	2.03	0.41
1:A:290:LYS:NZ	1:A:297:VAL:O	2.42	0.41
1:C:639:ARG:H	1:C:639:ARG:NH1	2.17	0.41
1:A:294:GLN:NE2	1:A:294:GLN:CA	2.56	0.41
1:A:390:LYS:HD2	1:A:392:ARG:NH2	2.35	0.41
1:B:730:NIY:CG	1:B:731:PHE:H	2.33	0.41
1:C:10:ARG:HB2	3:C:2009:HOH:O	2.19	0.41
1:A:7:VAL:HG23	1:A:17:ILE:HB	2.03	0.41
1:A:385:ASP:OD1	1:A:385:ASP:C	2.59	0.41
1:C:339:ILE:HG22	1:C:340:ASN:N	2.35	0.41
2:E:372:ASN:ND2	2:E:372:ASN:N	2.56	0.41
1:A:262:ARG:HE	1:A:262:ARG:HB3	1.62	0.41
1:B:244:ILE:HG12	1:B:254:ILE:HG21	2.01	0.41
1:B:586:ASP:OD1	1:B:586:ASP:N	2.53	0.41
1:C:394:LYS:HD3	3:C:2103:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:107:VAL:O	1:A:111:GLU:HB2	2.21	0.41
1:B:174:ILE:O	1:B:177:ALA:HB3	2.21	0.41
1:C:45:SER:HA	1:C:48:GLN:HE21	1.86	0.41
1:C:292:CYS:HB3	3:C:2084:HOH:O	2.20	0.41
1:C:323:ARG:HG3	1:C:323:ARG:O	2.20	0.41
1:C:548:GLN:CB	1:C:688:PHE:HB3	2.50	0.41
1:B:711:MET:HB3	2:E:365:VAL:HG22	2.03	0.41
1:A:371:ASP:CG	1:A:374:GLU:HB3	2.42	0.40
1:B:143:PHE:CE1	1:B:203:PHE:HE1	2.38	0.40
1:B:568:PHE:CE1	1:B:611:LEU:HB2	2.56	0.40
1:A:701:PRO:O	1:A:707:GLY:HA2	2.21	0.40
1:B:489:LEU:HD23	1:B:489:LEU:HA	1.92	0.40
1:C:370:ALA:HA	1:C:428:PRO:HB2	2.02	0.40
1:A:207:LEU:HD13	1:A:212:MET:HE1	2.04	0.40
1:A:400:SER:O	1:A:404:GLN:HB2	2.21	0.40
1:A:639:ARG:NH2	3:A:2134:HOH:O	2.48	0.40
1:C:297:VAL:CG2	3:C:2086:HOH:O	2.69	0.40
1:A:159:ASN:HB3	1:A:164:GLU:H	1.87	0.40
1:A:294:GLN:HB3	1:A:297:VAL:H	1.87	0.40
1:A:489:LEU:O	1:A:492:LEU:HB3	2.22	0.40
1:B:518:ILE:O	1:B:519:ASN:CB	2.69	0.40
1:C:217:THR:HB	1:C:218:PRO:CD	2.51	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	722/761 (95%)	670 (93%)	47 (6%)	5 (1%)	22 57
1	B	722/761 (95%)	656 (91%)	56 (8%)	10 (1%)	11 40
1	C	722/761 (95%)	665 (92%)	52 (7%)	5 (1%)	22 57

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	9/20 (45%)	5 (56%)	3 (33%)	1 (11%)	0	2
2	E	9/20 (45%)	7 (78%)	1 (11%)	1 (11%)	0	2
2	F	10/20 (50%)	9 (90%)	1 (10%)	0	100	100
2	P	1/20 (5%)	1 (100%)	0	0	100	100
All	All	2195/2363 (93%)	2013 (92%)	160 (7%)	22 (1%)	15	49

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	216	ARG
1	A	323	ARG
1	B	216	ARG
1	A	648	LYS
1	B	11	ASP
1	B	125	GLU
1	B	300	GLY
1	C	161	VAL
1	C	216	ARG
1	A	326	GLU
1	A	499	PRO
1	B	9	LYS
1	B	321	ASN
1	C	10	ARG
1	C	300	GLY
2	D	371	SER
2	E	371	SER
1	B	519	ASN
1	B	691	GLN
1	C	5	LEU
1	B	12	GLY
1	B	452	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	624/650 (96%)	548 (88%)	76 (12%)	5 19
1	B	624/650 (96%)	553 (89%)	71 (11%)	5 23
1	C	624/650 (96%)	565 (90%)	59 (10%)	8 31
2	D	11/19 (58%)	8 (73%)	3 (27%)	0 1
2	E	11/19 (58%)	9 (82%)	2 (18%)	1 7
2	F	12/19 (63%)	9 (75%)	3 (25%)	0 2
2	P	3/19 (16%)	2 (67%)	1 (33%)	0 0
All	All	1909/2026 (94%)	1694 (89%)	215 (11%)	6 23

All (215) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	9	LYS
1	A	11	ASP
1	A	14	THR
1	A	15	GLU
1	A	17	ILE
1	A	20	ASP
1	A	21	LYS
1	A	27	ASP
1	A	35	ASN
1	A	44	ARG
1	A	53	ILE
1	A	58	ILE
1	A	60	GLU
1	A	62	ILE
1	A	72	ARG
1	A	83	ARG
1	A	92	LYS
1	A	96	GLN
1	A	118	HIS
1	A	129	LYS
1	A	130	GLN
1	A	139	ARG
1	A	141	MET
1	A	149	LYS
1	A	158	GLN
1	A	183	ASN
1	A	187	GLU
1	A	189	ARG

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Mol	Chain	Res	Type
1	A	204	LYS
1	A	206	SER
1	A	216	ARG
1	A	225	CYS
1	A	251	ARG
1	A	276	THR
1	A	283	LYS
1	A	294	GLN
1	A	297	VAL
1	A	298	ARG
1	A	314	GLU
1	A	315	SER
1	A	317	LEU
1	A	321	ASN
1	A	322	ASN
1	A	325	VAL
1	A	326	GLU
1	A	331	ARG
1	A	364	LEU
1	A	376	GLU
1	A	381	LYS
1	A	394	LYS
1	A	396	VAL
1	A	411	ARG
1	A	430	ILE
1	A	434	ARG
1	A	440	LEU
1	A	452	VAL
1	A	465	SER
1	A	474	ASN
1	A	505	ARG
1	A	562	GLN
1	A	581	ASP
1	A	585	LYS
1	A	616	LEU
1	A	624	THR
1	A	625	SER
1	A	629	SER
1	A	645	LYS
1	A	647	SER
1	A	648	LYS
1	A	653	ARG

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Mol	Chain	Res	Type
1	A	698	ASN
1	A	708	LYS
1	A	713	GLN
1	A	733	ASN
1	A	734	THR
1	B	5	LEU
1	B	7	VAL
1	B	9	LYS
1	B	10	ARG
1	B	16	ARG
1	B	17	ILE
1	B	20	ASP
1	B	24	ARG
1	B	72	ARG
1	B	73	ASP
1	B	80	LEU
1	B	91	LYS
1	B	92	LYS
1	B	96	GLN
1	B	126	GLU
1	B	129	LYS
1	B	139	ARG
1	B	141	MET
1	B	149	LYS
1	B	152	GLU
1	B	160	ARG
1	B	161	VAL
1	B	183	ASN
1	B	186	ARG
1	B	191	GLN
1	B	194	LYS
1	B	206	SER
1	B	207	LEU
1	B	216	ARG
1	B	225	CYS
1	B	260	ARG
1	B	266	SER
1	B	276	THR
1	B	278	CYS
1	B	313	VAL
1	B	315	SER
1	B	317	LEU

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Mol	Chain	Res	Type
1	B	331	ARG
1	B	364	LEU
1	B	373	GLU
1	B	380	THR
1	B	411	ARG
1	B	414	ILE
1	B	418	ASP
1	B	430	ILE
1	B	434	ARG
1	B	436	SER
1	B	440	LEU
1	B	451	ASP
1	B	452	VAL
1	B	465	SER
1	B	484	LEU
1	B	510	ARG
1	B	555	SER
1	B	556	ASN
1	B	557	GLU
1	B	569	ASN
1	B	575	LYS
1	B	585	LYS
1	B	586	ASP
1	B	604	GLU
1	B	605	SER
1	B	609	HIS
1	B	616	LEU
1	B	623	GLU
1	B	625	SER
1	B	629	SER
1	B	633	ASN
1	B	636	GLU
1	B	664	ASP
1	B	736	ASP
1	C	4	ASN
1	C	5	LEU
1	C	13	SER
1	C	14	THR
1	C	15	GLU
1	C	16	ARG
1	C	17	ILE
1	C	44	ARG

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Mol	Chain	Res	Type
1	C	55	THR
1	C	60	GLU
1	C	72	ARG
1	C	98	GLU
1	C	111	GLU
1	C	126	GLU
1	C	129	LYS
1	C	139	ARG
1	C	141	MET
1	C	152	GLU
1	C	165	ILE
1	C	183	ASN
1	C	186	ARG
1	C	187	GLU
1	C	204	LYS
1	C	216	ARG
1	C	260	ARG
1	C	276	THR
1	C	294	GLN
1	C	298	ARG
1	C	317	LEU
1	C	325	VAL
1	C	326	GLU
1	C	345	THR
1	C	364	LEU
1	C	380	THR
1	C	391	GLN
1	C	392	ARG
1	C	396	VAL
1	C	411	ARG
1	C	434	ARG
1	C	439	CYS
1	C	440	LEU
1	C	451	ASP
1	C	452	VAL
1	C	461	LEU
1	C	465	SER
1	C	484	LEU
1	C	510	ARG
1	C	530	ARG
1	C	557	GLU
1	C	570	GLU

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Mol	Chain	Res	Type
1	C	575	LYS
1	C	586	ASP
1	C	625	SER
1	C	626	SER
1	C	629	SER
1	C	639	ARG
1	C	645	LYS
1	C	648	LYS
1	C	708	LYS
2	D	367	THR
2	D	368	ASP
2	D	375	LEU
2	E	367	THR
2	E	372	ASN
2	F	364	GLU
2	F	368	ASP
2	F	374	GLN
2	P	3	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (32) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	ASN
1	A	294	GLN
1	A	609	HIS
1	A	696	ASN
1	A	698	ASN
1	A	733	ASN
1	B	4	ASN
1	B	18	ASN
1	B	46	HIS
1	B	59	HIS
1	B	130	GLN
1	B	191	GLN
1	B	250	GLN
1	B	275	HIS
1	B	435	GLN
1	B	556	ASN
1	B	633	ASN
1	B	661	HIS
1	B	663	HIS
1	B	696	ASN

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Mol	Chain	Res	Type
1	C	46	HIS
1	C	48	GLN
1	C	88	HIS
1	C	322	ASN
1	C	328	ASN
1	C	456	ASN
1	C	596	HIS
1	C	609	HIS
1	C	630	ASN
1	C	661	HIS
1	C	663	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	0.91	1 (7%)	13,20,22	1.07	0
1	NIY	A	730	1	13,15,16	0.86	1 (7%)	13,20,22	1.59	3 (23%)
1	NIY	C	730	1	13,15,16	0.89	1 (7%)	13,20,22	1.32	2 (15%)

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	A	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	B	730	NIY	CE1-NN	-2.74	1.40	1.45
1	C	730	NIY	CE1-NN	-2.64	1.40	1.45
1	A	730	NIY	CE1-NN	-2.63	1.40	1.45

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	730	NIY	CB-CA-C	3.53	118.09	111.47
1	A	730	NIY	CB-CG-CD1	-2.65	115.88	120.44
1	C	730	NIY	CB-CA-C	2.47	116.11	111.47
1	A	730	NIY	CD2-CG-CD1	2.25	121.69	118.54
1	C	730	NIY	CB-CG-CD1	-2.10	116.83	120.44

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	C	730	NIY	CA-CB-CG-CD1
1	A	730	NIY	CA-CB-CG-CD2
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 monosaccharides 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 (i)

6.1 Protein, DNA and RNA chains (i)

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	726/761 (95%)	-0.11	4 (0%)	89	78	26, 44, 66, 93	0
1	B	726/761 (95%)	-0.23	1 (0%)	95	92	32, 46, 64, 89	0
1	C	726/761 (95%)	-0.35	1 (0%)	95	92	20, 34, 54, 82	0
2	D	11/20 (55%)	0.96	2 (18%)	1	0	74, 84, 90, 91	0
2	E	11/20 (55%)	0.31	0	100	100	77, 82, 88, 89	0
2	F	12/20 (60%)	0.29	0	100	100	71, 80, 88, 88	0
2	P	3/20 (15%)	0.43	0	100	100	43, 43, 46, 47	0
All	All	2215/2363 (93%)	-0.22	8 (0%)	92	84	20, 41, 67, 93	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	737	GLY	3.2
1	A	4	ASN	2.8
1	A	737	GLY	2.6
1	A	19	LEU	2.6
2	D	365	VAL	2.6
1	A	12	GLY	2.4
2	D	372	ASN	2.3
1	B	294	GLN	2.1

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	0.96	0.20	40,42,47,49	0
1	NIY	B	730	15/16	0.97	0.18	37,40,43,45	0
1	NIY	C	730	15/16	0.98	0.18	30,34,39,40	0

6.3 Carbohydrates (i)

There are no monosaccharides 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.