Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:31 AM GMT

PDB ID	:	2XAK
Title	:	RIBONUCLEOTIDE REDUCTASE Y730NO2Y MODIFIED R1 SUBUNIT OF E. COLI
Authors	:	Yokoyama, K.; Uhlin, U.; Stubbe, J.
Deposited on	:	2010-03-31
Resolution	:	2.80 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:

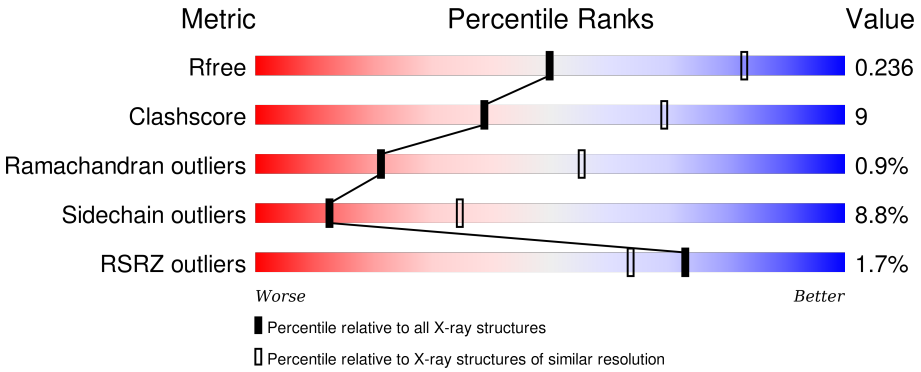
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 2.80 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	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	2% 74% 19%
1	B	761	2% 75% 18%
1	C	761	77% 16%
2	D	20	5% 55% 20% 5% 20%
2	E	20	20% 50% 20% 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 18274 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	1099	24			
1	B	728	Total	C	N	O	S	0	0	0
			5807	3688	996	1099	24			
1	C	728	Total	C	N	O	S	0	0	0
			5807	3688	996	1099	24			

- 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	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	138	Total	O	0	0
			138	138		
3	B	118	Total	O	0	0
			118	118		
3	C	178	Total	O	0	0
			178	178		
3	D	1	Total	O	0	0
			1	1		

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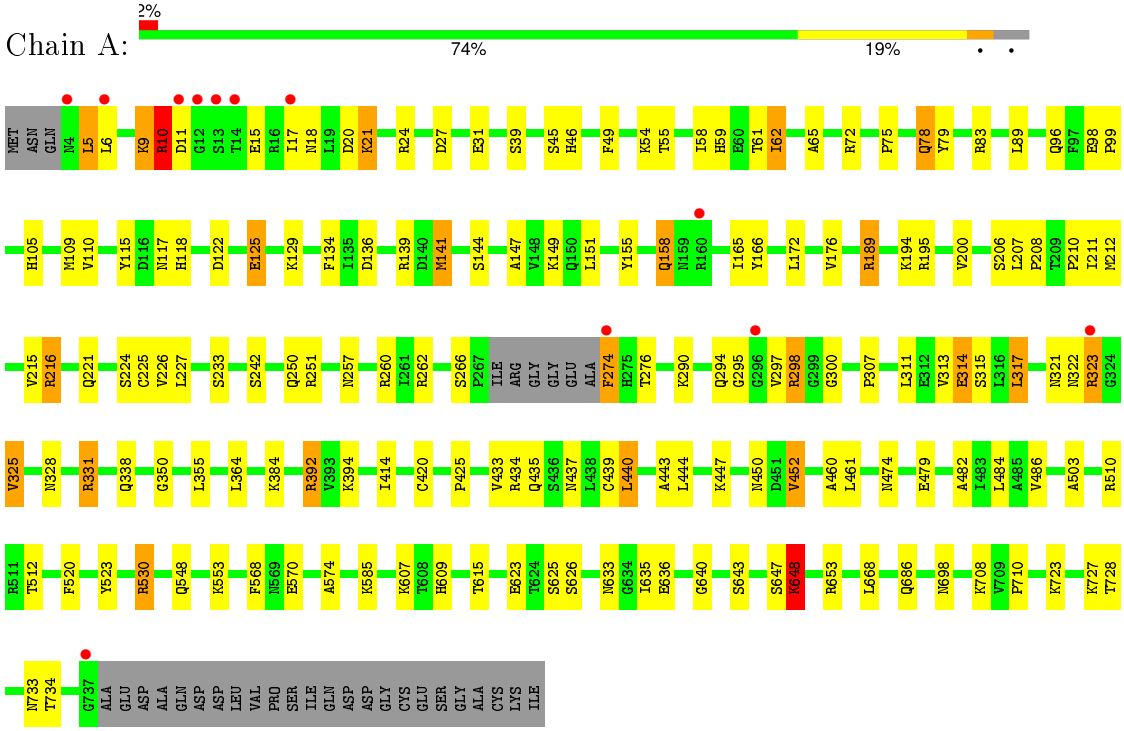
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	E	1	Total O 1 1	0	0
3	F	1	Total O 1 1	0	0
3	P	2	Total O 2 2	0	0

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.

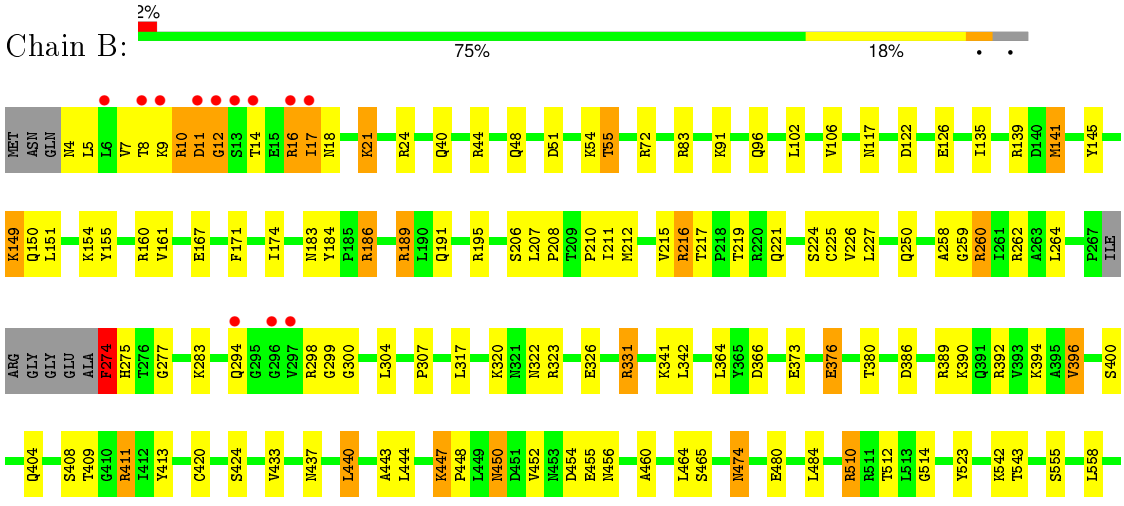
- Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT ALPHA

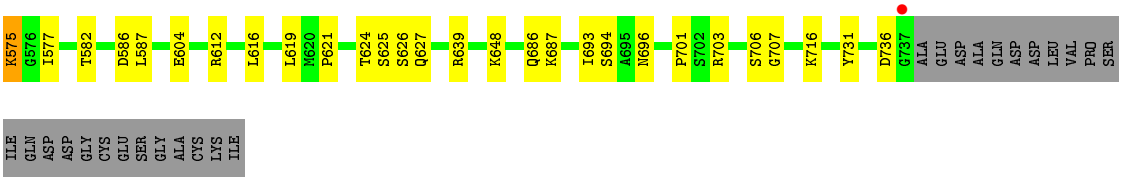
Chain A:



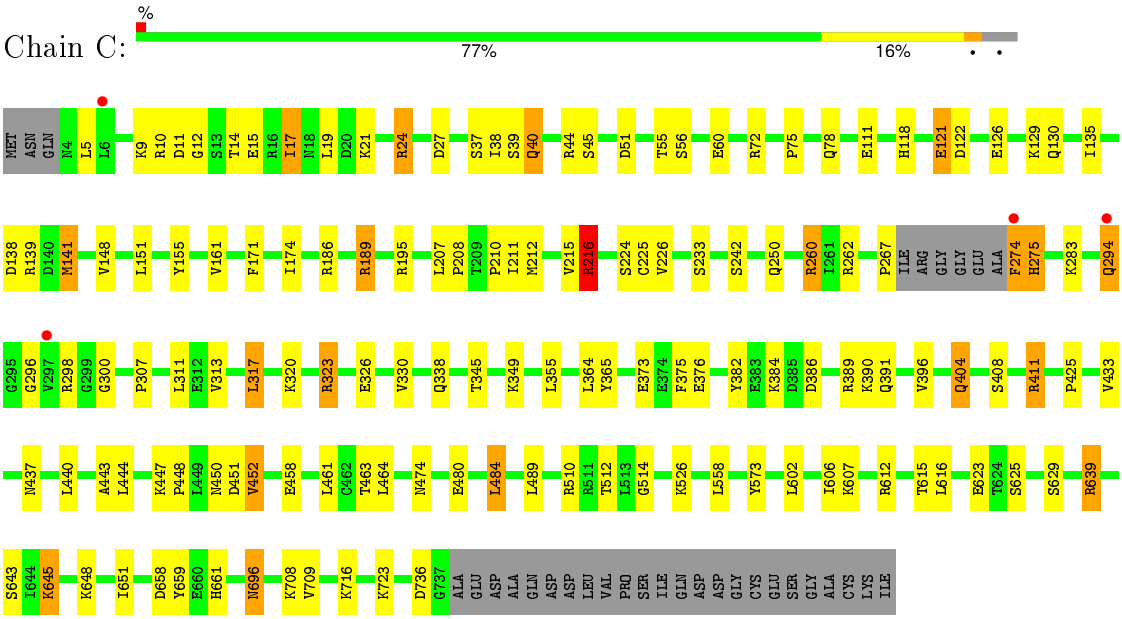
- Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT ALPHA

Chain B:



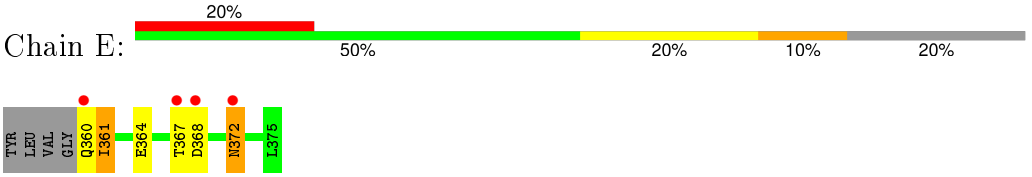


• Molecule 1: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT ALPHA

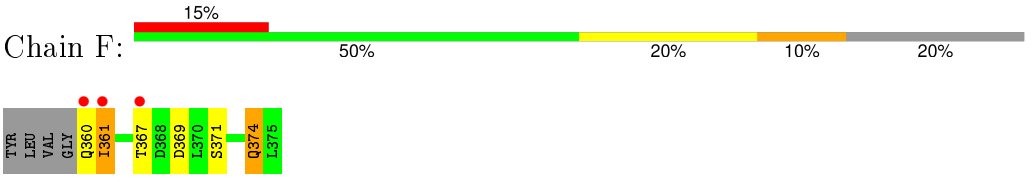


• Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA

• Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA



• Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA



• Molecule 2: RIBONUCLEOSIDE-DIPHOSPHATE REDUCTASE 1 SUBUNIT BETA


Y1
L2
V3
GLY
GLN
ILE
ASP
SER
GLU
VAL
ASP
THR
ASP
ASP
LEU
SER
ASN
PHE
GLN
LEU

4 Data and refinement statistics (i)

Property	Value	Source
Space group	H 3 2	Depositor
Cell constants a, b, c, α, β, γ	224.09Å 224.09Å 337.16Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	169.03 – 2.80 67.26 – 2.80	Depositor EDS
% Data completeness (in resolution range)	100.0 (169.03-2.80) 99.9 (67.26-2.80)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.53 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.178 , 0.241 0.177 , 0.236	Depositor DCC
R_{free} test set	4006 reflections (5.28%)	DCC
Wilson B-factor (Å^2)	39.8	Xtriage
Anisotropy	0.040	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 47.4	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 79849 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	18274	wwPDB-VP
Average B, all atoms (Å^2)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.97% 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	0.50	0/5917	0.64	0/8012
1	B	0.50	0/5917	0.63	0/8012
1	C	0.56	0/5917	0.67	0/8012
2	D	0.56	0/129	0.72	0/173
2	E	0.52	0/129	0.68	0/173
2	F	0.48	0/129	0.70	0/173
2	P	0.88	0/27	0.82	0/36
All	All	0.52	0/18165	0.65	0/24591

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	2

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	274	PHE	Peptide
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	5807	0	5725	114	0
1	B	5807	0	5725	97	0
1	C	5807	0	5726	99	0
2	D	129	0	111	3	0
2	E	129	0	111	4	0
2	F	129	0	111	3	0
2	P	27	0	31	1	0
3	A	138	0	0	16	0
3	B	118	0	0	20	1
3	C	178	0	0	27	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	P	2	0	0	2	0
All	All	18274	0	17540	317	1

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 9.

All (317) 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:C:274:PHE:HA	3:C:2073:HOH:O	1.51	1.10
1:C:260:ARG:HH11	1:C:260:ARG:HG2	1.14	1.06
1:A:294:GLN:HG3	1:A:295:GLY:H	1.18	1.03
1:B:480:GLU:HB3	3:B:2031:HOH:O	1.62	1.00
1:C:450:ASN:HB2	3:C:2112:HOH:O	1.61	0.98
1:B:260:ARG:HG2	1:B:260:ARG:HH11	1.28	0.98
1:B:392:ARG:HH11	1:B:392:ARG:HG3	1.30	0.96
1:C:480:GLU:HB3	3:C:2048:HOH:O	1.71	0.91
1:A:10:ARG:HG3	1:A:10:ARG:HH11	1.35	0.90
1:C:639:ARG:NH1	3:C:2151:HOH:O	2.04	0.89
1:B:91:LYS:HE2	3:B:2017:HOH:O	1.69	0.89
1:A:207:LEU:HD13	1:A:212:MET:CE	2.03	0.87
1:C:75:PRO:O	1:C:78:GLN:HG3	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:404:GLN:HG3	3:C:2102:HOH:O	1.74	0.86
1:C:122:ASP:O	1:C:189:ARG:NH2	2.10	0.84
1:C:260:ARG:HG2	1:C:260:ARG:NH1	1.88	0.83
1:C:24:ARG:HD3	3:C:2005:HOH:O	1.80	0.81
1:A:215:VAL:O	1:A:216:ARG:HB3	1.79	0.81
1:B:703:ARG:NH1	3:B:2114:HOH:O	2.12	0.81
1:A:9:LYS:HE3	1:A:10:ARG:H	1.44	0.81
1:A:294:GLN:HG3	1:A:295:GLY:N	1.95	0.80
1:C:607:LYS:HE3	3:C:2140:HOH:O	1.81	0.80
1:B:299:GLY:HA3	3:B:2045:HOH:O	1.81	0.80
1:C:195:ARG:HD3	3:C:2047:HOH:O	1.82	0.79
1:A:151:LEU:HA	1:A:155:TYR:HB2	1.65	0.79
1:B:5:LEU:O	1:B:17:ILE:HB	1.84	0.77
1:C:225:CYS:CB	3:C:2108:HOH:O	2.31	0.77
1:B:215:VAL:O	1:B:216:ARG:HB3	1.83	0.77
1:C:9:LYS:HD3	1:C:10:ARG:H	1.50	0.76
1:A:207:LEU:HD13	1:A:212:MET:HE1	1.65	0.76
1:A:212:MET:O	1:A:216:ARG:NH2	2.19	0.75
1:C:226:VAL:HG12	1:C:461:LEU:HD23	1.68	0.75
1:A:294:GLN:HB2	1:A:298:ARG:HD3	1.68	0.74
1:C:275:HIS:CD2	3:C:2072:HOH:O	2.39	0.73
1:C:225:CYS:HB3	3:C:2108:HOH:O	1.86	0.73
1:C:27:ASP:HA	1:C:38:ILE:HD11	1.71	0.73
1:C:215:VAL:O	1:C:216:ARG:HB3	1.89	0.73
1:B:262:ARG:HG3	1:B:274:PHE:HB2	1.71	0.72
1:C:207:LEU:HD13	1:C:212:MET:HE1	1.72	0.72
1:C:639:ARG:HG3	1:C:639:ARG:HH11	1.55	0.71
1:C:558:LEU:HD23	1:C:612:ARG:HG2	1.72	0.71
1:A:58:ILE:O	1:A:62:ILE:HG23	1.92	0.70
1:C:364:LEU:HD21	1:C:375:PHE:CE1	2.27	0.70
1:A:262:ARG:HG3	1:A:274:PHE:HB3	1.74	0.69
1:B:260:ARG:HH21	1:B:448:PRO:HG3	1.57	0.69
1:B:225:CYS:CB	3:B:2066:HOH:O	2.40	0.68
1:A:392:ARG:HG2	1:A:392:ARG:HH11	1.57	0.68
1:A:226:VAL:HG12	1:A:461:LEU:HD23	1.74	0.68
1:C:260:ARG:HD2	1:C:365:TYR:CE2	2.29	0.68
1:B:474:ASN:HB3	3:B:2074:HOH:O	1.94	0.67
1:A:10:ARG:CG	1:A:10:ARG:HH11	2.08	0.67
1:A:233:SER:HA	1:A:274:PHE:HZ	1.60	0.67
1:C:558:LEU:CD2	1:C:612:ARG:HG2	2.25	0.67
1:A:75:PRO:O	1:A:78:GLN:HB2	1.94	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:79:TYR:O	1:A:83:ARG:HG2	1.96	0.66
1:B:225:CYS:HB3	3:B:2066:HOH:O	1.93	0.66
1:A:225:CYS:HB2	3:A:2070:HOH:O	1.93	0.66
1:A:331:ARG:HG3	3:A:2056:HOH:O	1.95	0.66
1:C:207:LEU:HD13	1:C:212:MET:CE	2.25	0.65
1:B:117:ASN:HB2	3:B:2018:HOH:O	1.95	0.65
1:B:274:PHE:N	1:B:274:PHE:CD2	2.61	0.65
1:A:609:HIS:HD2	3:P:2001:HOH:O	1.80	0.65
1:B:122:ASP:O	1:B:189:ARG:NH2	2.30	0.65
1:B:575:LYS:HB3	1:B:577:ILE:HD12	1.77	0.65
1:B:716:LYS:HE3	3:B:2115:HOH:O	1.96	0.65
1:A:227:LEU:HB2	1:A:460:ALA:HB3	1.80	0.64
1:A:207:LEU:HD13	1:A:212:MET:HE3	1.79	0.64
1:A:65:ALA:HA	3:A:2009:HOH:O	1.98	0.64
1:A:262:ARG:HG3	1:A:274:PHE:CB	2.27	0.64
1:B:212:MET:O	1:B:216:ARG:NH2	2.31	0.64
1:B:392:ARG:NH1	1:B:392:ARG:HG3	2.07	0.63
1:B:11:ASP:CG	1:B:12:GLY:H	2.02	0.63
1:A:392:ARG:HH11	1:A:392:ARG:CG	2.11	0.63
1:B:210:PRO:HG2	1:B:224:SER:HB3	1.81	0.63
1:A:710:PRO:HA	2:D:362:ASP:HB3	1.81	0.63
1:C:260:ARG:NH2	1:C:448:PRO:HG2	2.14	0.62
1:B:186:ARG:HB2	3:B:2027:HOH:O	1.99	0.62
1:C:450:ASN:CB	3:C:2112:HOH:O	2.33	0.62
1:B:260:ARG:HG2	1:B:260:ARG:NH1	2.01	0.62
1:A:260:ARG:HH21	1:A:434:ARG:NH2	1.97	0.62
1:C:226:VAL:HG12	1:C:461:LEU:CD2	2.29	0.62
1:A:633:ASN:HB3	3:A:2107:HOH:O	1.98	0.62
1:A:233:SER:HA	1:A:274:PHE:CZ	2.35	0.61
1:B:619:LEU:HD12	1:B:693:ILE:HG12	1.80	0.61
1:B:10:ARG:HD2	1:B:55:THR:HG21	1.83	0.61
1:A:294:GLN:CG	1:A:295:GLY:H	1.94	0.61
1:A:59:HIS:HA	1:A:62:ILE:HD13	1.82	0.61
1:B:208:PRO:HD2	1:B:211:ILE:HD12	1.82	0.61
1:A:510:ARG:NH2	1:A:570:GLU:OE1	2.34	0.61
1:B:154:LYS:HD2	1:B:624:THR:HG21	1.82	0.60
1:C:233:SER:HA	1:C:274:PHE:HZ	1.67	0.60
1:C:364:LEU:HD23	1:C:364:LEU:O	2.02	0.60
1:C:389:ARG:HA	3:C:2100:HOH:O	2.01	0.60
1:A:262:ARG:CG	1:A:274:PHE:CB	2.80	0.60
1:B:18:ASN:ND2	1:B:21:LYS:HB2	2.16	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:260:ARG:HH11	1:C:260:ARG:CG	2.03	0.59
1:A:24:ARG:HH11	1:A:24:ARG:CG	2.16	0.59
1:C:283:LYS:HG3	1:C:330:VAL:HG22	1.85	0.59
1:B:24:ARG:HD2	3:B:2003:HOH:O	2.03	0.58
1:B:411:ARG:NH1	1:B:731:TYR:HE1	2.02	0.58
1:A:10:ARG:NH1	1:A:10:ARG:HG3	2.14	0.58
1:B:558:LEU:HD23	1:B:612:ARG:HG2	1.84	0.58
1:C:37:SER:HB3	1:C:40:GLN:HB2	1.86	0.58
1:C:212:MET:O	1:C:216:ARG:NH2	2.33	0.58
1:A:636:GLU:OE2	3:A:2112:HOH:O	2.17	0.58
1:B:274:PHE:HA	1:B:277:GLY:H	1.67	0.58
1:B:621:PRO:HD3	1:B:694:SER:OG	2.02	0.58
1:A:262:ARG:CG	1:A:274:PHE:HB3	2.33	0.57
1:B:11:ASP:CG	1:B:12:GLY:N	2.57	0.57
1:A:647:SER:HB2	1:A:648:LYS:HD2	1.86	0.57
1:C:274:PHE:CA	3:C:2073:HOH:O	2.28	0.57
1:C:658:ASP:OD1	1:C:661:HIS:HD2	1.88	0.57
1:A:24:ARG:HH11	1:A:24:ARG:HG2	1.70	0.57
1:B:217:THR:OG1	1:B:219:THR:HG22	2.05	0.56
1:A:294:GLN:HB2	1:A:298:ARG:HH11	1.71	0.56
1:A:9:LYS:HE3	1:A:10:ARG:N	2.19	0.56
1:A:262:ARG:HD2	1:A:274:PHE:HB2	1.88	0.55
1:C:262:ARG:HG2	1:C:274:PHE:CB	2.35	0.55
1:B:151:LEU:HA	1:B:155:TYR:HB2	1.89	0.55
1:B:225:CYS:HB2	3:B:2066:HOH:O	2.04	0.55
1:B:392:ARG:HH11	1:B:392:ARG:CG	2.12	0.55
1:B:21:LYS:HD3	3:B:2002:HOH:O	2.07	0.54
1:B:83:ARG:HG2	1:B:141:MET:HG3	1.88	0.54
1:A:548:GLN:HA	1:A:548:GLN:OE1	2.08	0.54
2:E:372:ASN:H	2:E:372:ASN:HD22	1.54	0.54
1:C:425:PRO:HG2	1:C:615:THR:HG22	1.90	0.54
1:A:45:SER:HB2	1:A:61:THR:HG22	1.90	0.53
1:B:331:ARG:NH1	1:B:331:ARG:H	2.06	0.53
1:A:450:ASN:HB3	3:A:2076:HOH:O	2.08	0.53
1:C:242:SER:HB2	1:C:452:VAL:HG13	1.90	0.53
2:E:361:ILE:H	2:E:361:ILE:HD13	1.74	0.53
1:C:386:ASP:HA	1:C:390:LYS:HZ1	1.74	0.53
1:A:89:LEU:CD2	1:A:165:ILE:HD13	2.39	0.53
1:A:314:GLU:HB2	3:A:2053:HOH:O	2.09	0.53
1:C:376:GLU:HG2	3:C:2097:HOH:O	2.09	0.53
1:C:208:PRO:HD2	1:C:211:ILE:HD12	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:461:LEU:HD11	1:A:503:ALA:HB1	1.92	0.52
1:B:331:ARG:H	1:B:331:ARG:HH11	1.56	0.52
1:C:311:LEU:HA	1:C:355:LEU:HB3	1.92	0.52
1:B:411:ARG:HH11	1:B:731:TYR:HE1	1.58	0.52
1:A:435:GLN:HG2	3:A:2045:HOH:O	2.10	0.52
1:C:320:LYS:HE2	1:C:411:ARG:HG3	1.92	0.52
1:B:411:ARG:NH1	1:B:731:TYR:CE1	2.77	0.52
1:B:150:GLN:HE21	1:B:627:GLN:CD	2.12	0.52
1:A:136:ASP:HB3	1:A:139:ARG:HG3	1.92	0.52
2:P:3:VAL:C	3:P:2002:HOH:O	2.49	0.52
1:A:530:ARG:HG3	3:A:2091:HOH:O	2.10	0.52
1:B:396:VAL:HG22	3:B:2054:HOH:O	2.10	0.51
1:B:227:LEU:HB2	1:B:460:ALA:HB3	1.91	0.51
1:A:643:SER:O	1:A:653:ARG:HA	2.11	0.51
1:B:587:LEU:CD1	1:B:687:LYS:HB2	2.41	0.51
1:A:313:VAL:HG22	1:A:317:LEU:HD22	1.92	0.51
1:A:568:PHE:CE2	1:A:574:ALA:HA	2.46	0.51
1:C:262:ARG:HG2	1:C:274:PHE:HB3	1.91	0.51
1:B:258:ALA:HB3	1:B:304:LEU:HD21	1.92	0.51
1:A:225:CYS:CB	3:A:2070:HOH:O	2.55	0.51
1:C:275:HIS:HD2	3:C:2072:HOH:O	1.87	0.51
1:B:207:LEU:HD13	1:B:212:MET:HE1	1.93	0.50
2:E:372:ASN:H	2:E:372:ASN:ND2	2.09	0.50
1:B:135:ILE:HD11	1:B:174:ILE:HG21	1.93	0.50
3:A:2052:HOH:O	1:B:283:LYS:HD2	2.10	0.50
1:A:200:VAL:HG11	1:A:207:LEU:HD11	1.93	0.50
1:A:392:ARG:NH1	1:A:392:ARG:CG	2.74	0.50
1:A:83:ARG:CD	1:A:141:MET:HG3	2.42	0.49
1:B:523:TYR:HH	1:B:543:THR:HG1	1.59	0.49
1:B:342:LEU:HD12	1:B:376:GLU:HG2	1.95	0.49
1:B:298:ARG:NH1	1:B:298:ARG:HB3	2.28	0.49
1:A:110:VAL:HG11	1:A:117:ASN:HD22	1.77	0.49
1:C:433:VAL:HG11	1:C:443:ALA:HB1	1.95	0.49
1:C:464:LEU:HA	1:C:514:GLY:O	2.12	0.49
1:A:262:ARG:HD3	1:A:266:SER:HB2	1.95	0.49
1:C:17:ILE:HD12	1:C:19:LEU:HD23	1.95	0.49
1:C:40:GLN:HE21	1:C:44:ARG:HD2	1.76	0.49
1:C:225:CYS:HB2	3:C:2108:HOH:O	2.04	0.48
1:B:215:VAL:O	1:B:216:ARG:CB	2.57	0.48
1:C:723:LYS:NZ	2:F:374:GLN:O	2.45	0.48
1:C:262:ARG:CG	1:C:274:PHE:CB	2.92	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:364:LEU:CD2	1:C:375:PHE:CE1	2.95	0.48
1:A:262:ARG:CG	1:A:274:PHE:HB2	2.43	0.48
1:A:215:VAL:O	1:A:216:ARG:CB	2.58	0.48
1:A:723:LYS:NZ	2:D:374:GLN:O	2.40	0.48
1:C:250:GLN:HG2	3:C:2057:HOH:O	2.15	0.47
1:A:325:VAL:HG12	1:A:328:ASN:OD1	2.13	0.47
1:C:210:PRO:HG2	1:C:224:SER:HB3	1.96	0.47
1:C:215:VAL:O	1:C:216:ARG:CB	2.62	0.47
1:A:479:GLU:OE2	1:A:553:LYS:NZ	2.47	0.47
1:A:257:ASN:HB2	1:A:435:GLN:HB3	1.96	0.47
1:C:151:LEU:HA	1:C:155:TYR:HB2	1.95	0.47
1:C:526:LYS:HE2	3:C:2115:HOH:O	2.14	0.47
1:B:621:PRO:HD3	1:B:694:SER:CB	2.45	0.47
1:C:135:ILE:HD11	1:C:174:ILE:HG21	1.97	0.47
1:B:44:ARG:O	1:B:48:GLN:NE2	2.48	0.47
1:C:709:VAL:HB	2:F:361:ILE:HG22	1.97	0.47
1:C:148:VAL:HA	1:C:151:LEU:HD12	1.97	0.47
1:A:482:ALA:O	1:A:486:VAL:HG23	2.15	0.47
1:A:221:GLN:HG2	3:A:2043:HOH:O	2.14	0.47
1:C:56:SER:O	1:C:60:GLU:HG2	2.14	0.47
1:C:364:LEU:HD23	1:C:364:LEU:C	2.35	0.46
1:A:331:ARG:CG	3:A:2056:HOH:O	2.60	0.46
1:A:452:VAL:HG22	3:A:2077:HOH:O	2.15	0.46
1:A:122:ASP:O	1:A:189:ARG:NH2	2.48	0.46
1:A:322:ASN:O	1:A:323:ARG:HB2	2.15	0.46
1:B:400:SER:O	1:B:404:GLN:HB2	2.15	0.46
1:A:444:LEU:HD22	1:A:512:THR:HG21	1.97	0.46
1:C:643:SER:OG	1:C:645:LYS:HE3	2.16	0.46
1:A:439:CYS:O	1:A:440:LEU:HB2	2.16	0.46
1:A:294:GLN:CG	1:A:295:GLY:N	2.60	0.46
1:B:184:TYR:O	1:B:189:ARG:HD3	2.16	0.46
1:B:40:GLN:HG3	3:B:2007:HOH:O	2.15	0.46
1:B:221:GLN:OE1	1:B:250:GLN:HG2	2.16	0.46
1:A:24:ARG:CG	1:A:24:ARG:NH1	2.76	0.46
1:C:72:ARG:HB2	1:C:659:TYR:CE2	2.51	0.46
1:A:226:VAL:HG12	1:A:461:LEU:CD2	2.42	0.46
1:A:46:HIS:HA	1:A:49:PHE:CD2	2.51	0.45
1:B:433:VAL:HG11	1:B:443:ALA:HB1	1.97	0.45
1:B:264:LEU:O	1:B:389:ARG:NH2	2.49	0.45
1:C:262:ARG:HD2	1:C:274:PHE:HB2	1.98	0.45
1:B:207:LEU:HD23	1:B:465:SER:OG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:37:SER:CB	1:C:40:GLN:HB2	2.46	0.45
1:B:386:ASP:HA	1:B:390:LYS:NZ	2.31	0.45
1:A:520:PHE:HB3	1:A:635:ILE:HA	1.99	0.45
1:C:313:VAL:HG22	1:C:317:LEU:HD22	1.97	0.45
1:A:46:HIS:CD2	1:A:49:PHE:CE2	3.03	0.45
1:C:171:PHE:HA	1:C:174:ILE:HG22	1.98	0.45
1:B:4:ASN:HB3	1:B:16:ARG:NH2	2.32	0.45
1:B:227:LEU:HD11	1:B:437:ASN:HB3	1.99	0.45
1:A:520:PHE:O	1:A:523:TYR:HB3	2.17	0.45
1:A:144:SER:O	1:A:147:ALA:HB3	2.16	0.45
1:C:138:ASP:O	1:C:141:MET:HB2	2.16	0.45
1:B:510:ARG:HB2	1:B:512:THR:HG23	1.98	0.45
1:A:311:LEU:HA	1:A:355:LEU:HB3	1.98	0.45
1:B:8:THR:HB	1:B:54:LYS:HD2	1.99	0.44
1:B:373:GLU:HA	1:B:376:GLU:HB2	1.99	0.44
1:C:17:ILE:HD12	1:C:19:LEU:CD2	2.47	0.44
1:B:326:GLU:HA	1:B:326:GLU:OE2	2.17	0.44
1:C:463:THR:HG22	1:C:489:LEU:HD22	1.99	0.44
1:B:437:ASN:HB2	3:B:2067:HOH:O	2.16	0.44
1:A:433:VAL:HG11	1:A:443:ALA:HB1	1.99	0.44
1:C:307:PRO:HA	1:C:338:GLN:HB2	1.98	0.44
2:D:368:ASP:O	2:D:371:SER:OG	2.32	0.44
1:A:10:ARG:CG	1:A:10:ARG:NH1	2.70	0.44
1:B:9:LYS:NZ	1:B:10:ARG:HD3	2.33	0.44
1:B:409:THR:O	1:B:411:ARG:HG2	2.18	0.44
1:C:716:LYS:HE3	3:C:2174:HOH:O	2.18	0.44
1:C:696:ASN:N	1:C:696:ASN:HD22	2.15	0.44
1:B:701:PRO:O	1:B:707:GLY:HA2	2.18	0.44
1:C:262:ARG:CG	1:C:274:PHE:HB2	2.48	0.44
1:B:195:ARG:HD3	3:B:2028:HOH:O	2.17	0.44
1:A:221:GLN:OE1	1:A:250:GLN:HG2	2.18	0.44
1:C:296:GLY:HA3	3:C:2078:HOH:O	2.18	0.43
1:A:686:GLN:NE2	1:A:727:LYS:HE3	2.33	0.43
1:B:696:ASN:ND2	1:B:731:TYR:HB2	2.34	0.43
1:B:686:GLN:HB3	3:B:2111:HOH:O	2.19	0.43
3:C:2102:HOH:O	2:F:361:ILE:HD11	2.18	0.43
1:C:658:ASP:OD1	1:C:661:HIS:CD2	2.71	0.43
1:C:526:LYS:CE	3:C:2115:HOH:O	2.65	0.43
1:A:125:GLU:O	1:A:129:LYS:HG2	2.19	0.43
1:C:373:GLU:OE2	1:C:373:GLU:HA	2.18	0.43
1:A:425:PRO:HG3	1:A:615:THR:HG22	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:46:HIS:CD2	1:A:49:PHE:HE2	2.37	0.43
1:A:447:LYS:HE3	3:A:2074:HOH:O	2.17	0.43
1:B:195:ARG:NH1	3:B:2031:HOH:O	2.52	0.43
1:B:7:VAL:O	1:B:14:THR:HA	2.19	0.43
1:B:450:ASN:HB2	1:B:454:ASP:OD2	2.19	0.43
1:C:425:PRO:HB3	1:C:573:TYR:CE2	2.54	0.43
1:B:259:GLY:HA3	1:B:307:PRO:HD3	1.99	0.43
1:A:109:MET:HB2	1:A:115:TYR:CD2	2.54	0.43
1:C:437:ASN:HB2	3:C:2109:HOH:O	2.17	0.43
1:A:98:GLU:HA	1:A:99:PRO:HD3	1.93	0.43
1:A:242:SER:HB2	1:A:452:VAL:HG13	2.01	0.43
1:B:413:TYR:CD2	1:B:440:LEU:HD21	2.54	0.43
1:C:326:GLU:OE1	1:C:326:GLU:HA	2.18	0.43
1:C:651:ILE:HA	3:C:2156:HOH:O	2.18	0.43
1:A:18:ASN:CG	1:A:21:LYS:HB2	2.39	0.43
1:B:171:PHE:HA	1:B:174:ILE:HG22	2.00	0.42
1:A:105:HIS:HE1	1:A:166:TYR:O	2.02	0.42
1:A:698:ASN:OD1	1:A:733:ASN:ND2	2.40	0.42
1:B:102:LEU:O	1:B:106:VAL:HG23	2.19	0.42
1:C:364:LEU:HD12	1:C:382:TYR:HD2	1.84	0.42
1:C:294:GLN:HB3	3:C:2077:HOH:O	2.18	0.42
1:A:210:PRO:HG2	1:A:224:SER:HB3	2.01	0.42
1:A:9:LYS:O	1:A:11:ASP:N	2.45	0.42
1:C:444:LEU:HD22	1:C:512:THR:HG21	2.01	0.42
1:A:195:ARG:HD3	3:A:2026:HOH:O	2.19	0.42
1:A:158:GLN:HB3	1:A:158:GLN:HE21	1.61	0.42
1:B:155:TYR:CE2	1:B:212:MET:HB3	2.54	0.42
1:A:83:ARG:HD2	1:A:141:MET:HG3	2.02	0.42
1:A:260:ARG:NH2	1:A:434:ARG:NH2	2.65	0.42
2:E:368:ASP:O	2:E:372:ASN:ND2	2.53	0.42
1:C:602:LEU:HG	1:C:606:ILE:HD12	1.99	0.42
1:C:364:LEU:HD21	1:C:375:PHE:HE1	1.78	0.42
1:A:208:PRO:HG2	1:A:211:ILE:HD12	2.02	0.42
1:B:420:CYS:O	1:B:424:SER:HB2	2.20	0.42
1:B:145:TYR:CZ	1:B:149:LYS:HD3	2.55	0.42
1:A:134:PHE:CD1	1:A:194:LYS:HD2	2.55	0.41
1:B:443:ALA:O	1:B:444:LEU:HD23	2.20	0.41
1:C:345:THR:HG22	1:C:349:LYS:HD2	2.02	0.41
1:A:221:GLN:CD	1:A:250:GLN:HG2	2.40	0.41
1:A:262:ARG:HG3	1:A:274:PHE:HB2	2.00	0.41
1:B:260:ARG:CG	1:B:260:ARG:HH11	2.12	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:451:ASP:O	1:C:452:VAL:C	2.58	0.41
1:B:447:LYS:HD2	1:B:456:ASN:O	2.21	0.41
1:B:366:ASP:HB2	3:B:2056:HOH:O	2.20	0.41
1:C:484:LEU:HD12	1:C:484:LEU:HA	1.91	0.41
1:C:118:HIS:HA	1:C:121:GLU:HB2	2.03	0.41
1:A:227:LEU:HD11	1:A:437:ASN:HB3	2.02	0.41
1:C:267:PRO:HD2	3:C:2091:HOH:O	2.20	0.41
1:C:458:GLU:OE2	1:C:510:ARG:HD2	2.21	0.40
1:C:38:ILE:HD13	1:C:38:ILE:HG21	1.87	0.40
1:A:307:PRO:HA	1:A:338:GLN:HB2	2.03	0.40
1:A:172:LEU:O	1:A:176:VAL:HG23	2.21	0.40
1:B:207:LEU:HB2	1:B:212:MET:HE3	2.03	0.40
1:A:414:ILE:O	1:A:728:THR:HA	2.20	0.40
1:B:392:ARG:NH1	1:B:392:ARG:CG	2.74	0.40
1:A:420:CYS:HA	1:A:727:LYS:HD3	2.03	0.40
1:B:464:LEU:HA	1:B:514:GLY:O	2.21	0.40
1:A:640:GLY:HA2	1:A:668:LEU:HD13	2.04	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2010:HOH:O	3:B:2114:HOH:O[2_665]	2.03	0.17

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%)	679 (94%)	37 (5%)	7 (1%)	19	52
1	B	723/761 (95%)	685 (95%)	33 (5%)	5 (1%)	26	62
1	C	723/761 (95%)	688 (95%)	27 (4%)	8 (1%)	17	50

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	14/20 (70%)	11 (79%)	3 (21%)	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	2212/2363 (94%)	2089 (94%)	103 (5%)	20 (1%)	21	55

All (20) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	323	ARG
1	A	10	ARG
1	A	216	ARG
1	B	216	ARG
1	B	294	GLN
1	C	161	VAL
1	C	216	ARG
1	C	294	GLN
1	B	12	GLY
1	C	12	GLY
1	A	5	LEU
1	A	648	LYS
1	B	300	GLY
1	C	323	ARG
1	C	5	LEU
1	C	623	GLU
1	B	51	ASP
1	A	350	GLY
1	C	300	GLY
1	A	300	GLY

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	625/650 (96%)	572 (92%)	53 (8%)	13 36
1	B	625/650 (96%)	568 (91%)	57 (9%)	12 33
1	C	625/650 (96%)	578 (92%)	47 (8%)	17 43
2	D	16/19 (84%)	14 (88%)	2 (12%)	6 17
2	E	16/19 (84%)	11 (69%)	5 (31%)	0 1
2	F	16/19 (84%)	10 (62%)	6 (38%)	0 0
2	P	3/19 (16%)	3 (100%)	0	100 100
All	All	1926/2026 (95%)	1756 (91%)	170 (9%)	12 35

All (170) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	LEU
1	A	6	LEU
1	A	9	LYS
1	A	10	ARG
1	A	15	GLU
1	A	17	ILE
1	A	20	ASP
1	A	21	LYS
1	A	27	ASP
1	A	31	GLU
1	A	39	SER
1	A	54	LYS
1	A	55	THR
1	A	62	ILE
1	A	72	ARG
1	A	78	GLN
1	A	96	GLN
1	A	118	HIS
1	A	125	GLU
1	A	141	MET
1	A	149	LYS
1	A	158	GLN
1	A	189	ARG
1	A	206	SER
1	A	251	ARG
1	A	274	PHE
1	A	276	THR
1	A	290	LYS
1	A	297	VAL

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Mol	Chain	Res	Type
1	A	298	ARG
1	A	314	GLU
1	A	315	SER
1	A	317	LEU
1	A	321	ASN
1	A	325	VAL
1	A	331	ARG
1	A	364	LEU
1	A	384	LYS
1	A	392	ARG
1	A	394	LYS
1	A	440	LEU
1	A	452	VAL
1	A	474	ASN
1	A	484	LEU
1	A	530	ARG
1	A	585	LYS
1	A	607	LYS
1	A	623	GLU
1	A	625	SER
1	A	626	SER
1	A	648	LYS
1	A	708	LYS
1	A	734	THR
1	B	10	ARG
1	B	11	ASP
1	B	16	ARG
1	B	17	ILE
1	B	21	LYS
1	B	55	THR
1	B	72	ARG
1	B	96	GLN
1	B	126	GLU
1	B	139	ARG
1	B	141	MET
1	B	149	LYS
1	B	160	ARG
1	B	161	VAL
1	B	167	GLU
1	B	183	ASN
1	B	186	ARG
1	B	189	ARG

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Mol	Chain	Res	Type
1	B	191	GLN
1	B	206	SER
1	B	226	VAL
1	B	260	ARG
1	B	274	PHE
1	B	275	HIS
1	B	317	LEU
1	B	320	LYS
1	B	322	ASN
1	B	323	ARG
1	B	331	ARG
1	B	341	LYS
1	B	364	LEU
1	B	376	GLU
1	B	380	THR
1	B	394	LYS
1	B	396	VAL
1	B	408	SER
1	B	411	ARG
1	B	440	LEU
1	B	447	LYS
1	B	452	VAL
1	B	455	GLU
1	B	474	ASN
1	B	484	LEU
1	B	510	ARG
1	B	542	LYS
1	B	555	SER
1	B	575	LYS
1	B	582	THR
1	B	586	ASP
1	B	604	GLU
1	B	616	LEU
1	B	625	SER
1	B	626	SER
1	B	639	ARG
1	B	648	LYS
1	B	706	SER
1	B	736	ASP
1	C	11	ASP
1	C	14	THR
1	C	15	GLU

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Mol	Chain	Res	Type
1	C	17	ILE
1	C	21	LYS
1	C	24	ARG
1	C	39	SER
1	C	40	GLN
1	C	45	SER
1	C	51	ASP
1	C	55	THR
1	C	111	GLU
1	C	121	GLU
1	C	126	GLU
1	C	129	LYS
1	C	130	GLN
1	C	139	ARG
1	C	141	MET
1	C	186	ARG
1	C	189	ARG
1	C	216	ARG
1	C	260	ARG
1	C	274	PHE
1	C	275	HIS
1	C	298	ARG
1	C	317	LEU
1	C	323	ARG
1	C	384	LYS
1	C	391	GLN
1	C	396	VAL
1	C	404	GLN
1	C	408	SER
1	C	411	ARG
1	C	440	LEU
1	C	447	LYS
1	C	452	VAL
1	C	474	ASN
1	C	484	LEU
1	C	616	LEU
1	C	625	SER
1	C	629	SER
1	C	639	ARG
1	C	645	LYS
1	C	648	LYS
1	C	696	ASN

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Mol	Chain	Res	Type
1	C	708	LYS
1	C	736	ASP
2	D	361	ILE
2	D	374	GLN
2	E	360	GLN
2	E	361	ILE
2	E	364	GLU
2	E	367	THR
2	E	372	ASN
2	F	360	GLN
2	F	361	ILE
2	F	367	THR
2	F	369	ASP
2	F	371	SER
2	F	374	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	46	HIS
1	A	117	ASN
1	A	158	GLN
1	A	183	ASN
1	A	250	GLN
1	A	294	GLN
1	A	609	HIS
1	A	630	ASN
1	A	696	ASN
1	A	713	GLN
1	B	4	ASN
1	B	150	GLN
1	B	183	ASN
1	B	191	GLN
1	B	328	ASN
1	B	456	ASN
1	B	609	HIS
1	B	630	ASN
1	B	661	HIS
1	B	663	HIS
1	B	696	ASN
1	B	713	GLN
1	B	732	GLN

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Mol	Chain	Res	Type
1	C	40	GLN
1	C	46	HIS
1	C	59	HIS
1	C	183	ASN
1	C	221	GLN
1	C	275	HIS
1	C	456	ASN
1	C	609	HIS
1	C	630	ASN
1	C	661	HIS
1	C	663	HIS
2	E	372	ASN
2	F	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	A	730	1	11,15,16	0.71	0	10,20,22	1.75	4 (40%)
1	NIY	B	730	1	11,15,16	0.60	0	10,20,22	1.38	1 (10%)
1	NIY	C	730	1	11,15,16	0.91	0	10,20,22	1.59	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 (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	730	NIY	CB-CG-CD1	-3.01	114.55	120.36
1	A	730	NIY	CB-CG-CD1	-2.70	115.15	120.36
1	C	730	NIY	O-C-CA	-2.51	118.94	125.49
1	A	730	NIY	O-C-CA	-2.47	119.05	125.49
1	A	730	NIY	CD1-CE1-CZ	-2.38	118.82	121.34
1	B	730	NIY	O-C-CA	-2.21	119.73	125.49
1	A	730	NIY	CE2-CD2-CG	-2.13	118.12	121.04

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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%)	-0.06	12 (1%) 73 63	20, 36, 59, 93	0
1	B	727/761 (95%)	-0.03	13 (1%) 71 61	25, 38, 56, 91	0
1	C	727/761 (95%)	-0.18	4 (0%) 90 86	14, 27, 47, 82	0
2	D	16/20 (80%)	0.79	1 (6%) 23 14	68, 86, 96, 97	0
2	E	16/20 (80%)	1.64	4 (25%) 1 0	71, 85, 95, 96	0
2	F	16/20 (80%)	1.39	3 (18%) 2 1	65, 80, 89, 90	0
2	P	3/20 (15%)	0.24	0 100 100	27, 27, 30, 35	0
All	All	2232/2363 (94%)	-0.06	37 (1%) 73 63	14, 34, 63, 97	0

All (37) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	737	GLY	5.0
1	B	296	GLY	4.7
1	A	6	LEU	4.0
1	A	296	GLY	3.8
2	F	367	THR	3.7
2	F	360	GLN	3.4
2	E	368	ASP	3.3
1	B	6	LEU	3.3
1	A	14	THR	3.3
1	B	13	SER	3.2
1	B	14	THR	3.1
2	E	367	THR	3.1
2	F	361	ILE	2.9
1	B	297	VAL	2.8
1	A	323	ARG	2.8
1	B	17	ILE	2.7
1	A	160	ARG	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	11	ASP	2.7
1	C	297	VAL	2.6
1	B	12	GLY	2.6
2	E	372	ASN	2.6
1	A	737	GLY	2.5
1	A	4	ASN	2.5
1	A	11	ASP	2.4
1	C	294	GLN	2.4
1	B	9	LYS	2.4
1	B	8	THR	2.3
1	A	17	ILE	2.3
1	C	274	PHE	2.2
1	A	13	SER	2.2
1	B	294	GLN	2.2
2	E	360	GLN	2.1
1	C	6	LEU	2.1
2	D	360	GLN	2.1
1	B	16	ARG	2.1
1	A	274	PHE	2.1
1	A	12	GLY	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	A	730	15/16	0.94	0.21	-	28,29,35,37	0
1	NIY	B	730	15/16	0.94	0.17	-	29,33,40,40	0
1	NIY	C	730	15/16	0.96	0.17	-	21,25,34,36	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.