Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:51 PM GMT

PDB ID	:	3V8V
Title	:	Crystal structure of bifunctional methyltransferase YcbY (RlmLK) from Escherichia coli, SAM binding
Authors	:	Su, X.D.; Wang, K.T.
Deposited on	:	2011-12-23
Resolution	:	2.60 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

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

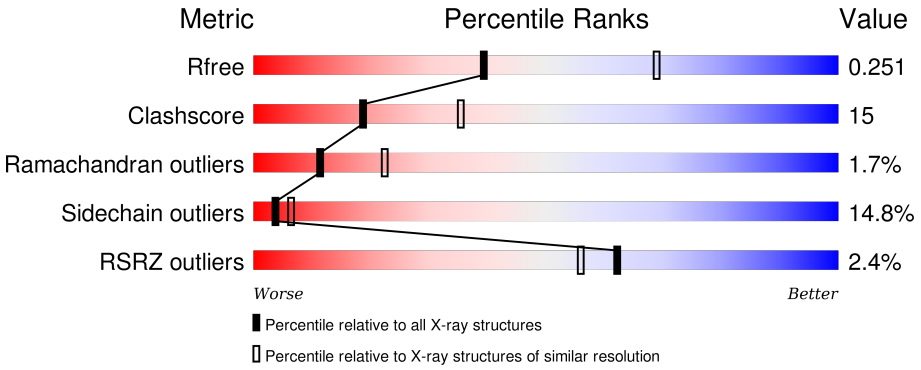
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2328 (2.60-2.60)
Clashscore	102246	2679 (2.60-2.60)
Ramachandran outliers	100387	2635 (2.60-2.60)
Sidechain outliers	100360	2635 (2.60-2.60)
RSRZ outliers	91569	2334 (2.60-2.60)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	702	% 68% 22% 5% 5%
1	B	702	4% 63% 20% 6% • 9%

2 Entry composition

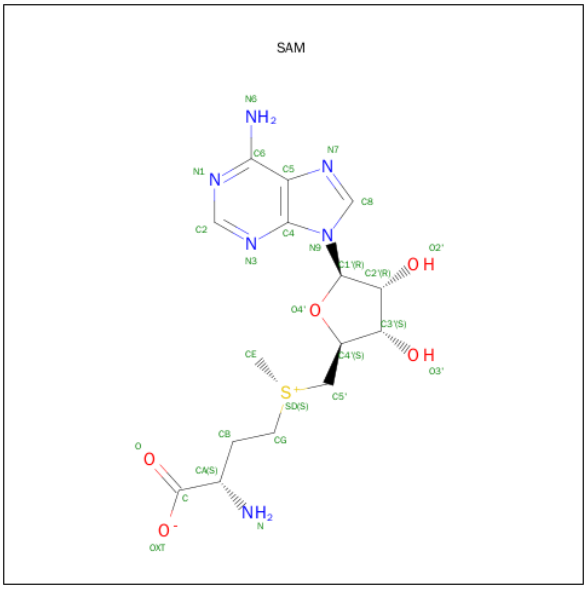
There are 4 unique types of molecules in this entry. The entry contains 10456 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Ribosomal RNA large subunit methyltransferase L.

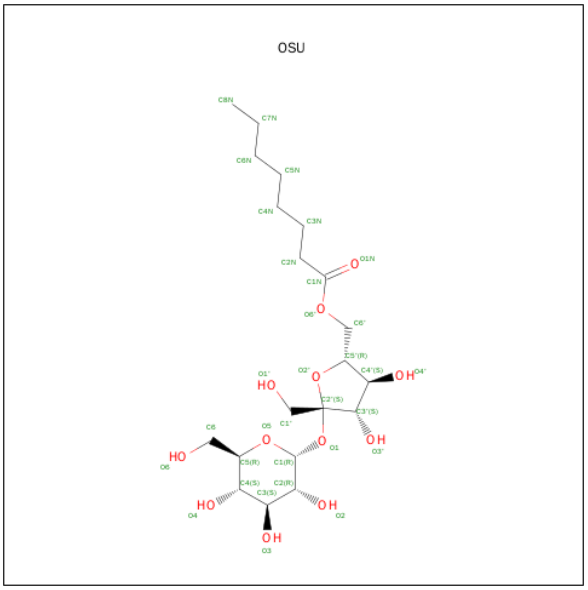
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	664	Total	C	N	O	S	0	1	0
			5139	3269	901	946	23			
1	B	636	Total	C	N	O	S	0	1	0
			4788	3035	836	895	22			

- Molecule 2 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	A	1	Total	C	N	O	S	0	0
			19	10	5	3	1		
2	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			25	14	6	4	1		

- Molecule 3 is N-OCTANOYLSUCROSE (three-letter code: OSU) (formula: $C_{20}H_{36}O_{12}$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 31 19 12	0	0
3	B	1	Total C O 30 18 12	0	0

- Molecule 4 is water.

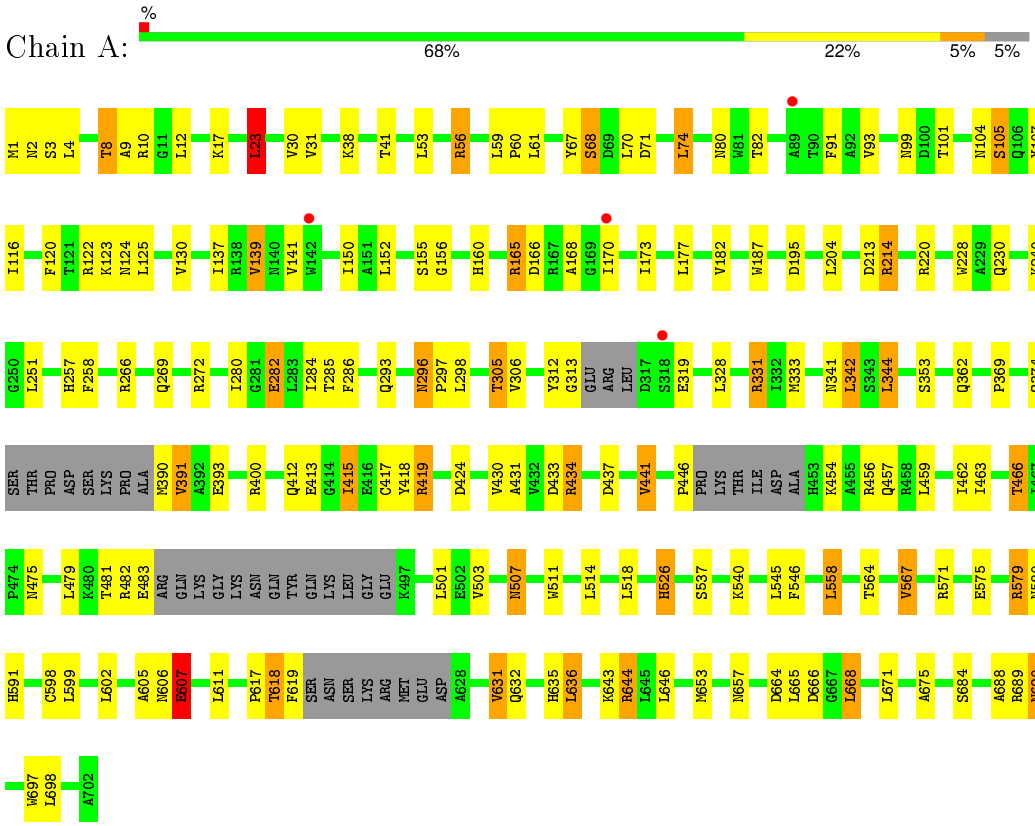
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	211	Total O 211 211	0	0
4	B	161	Total O 161 161	0	0

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.

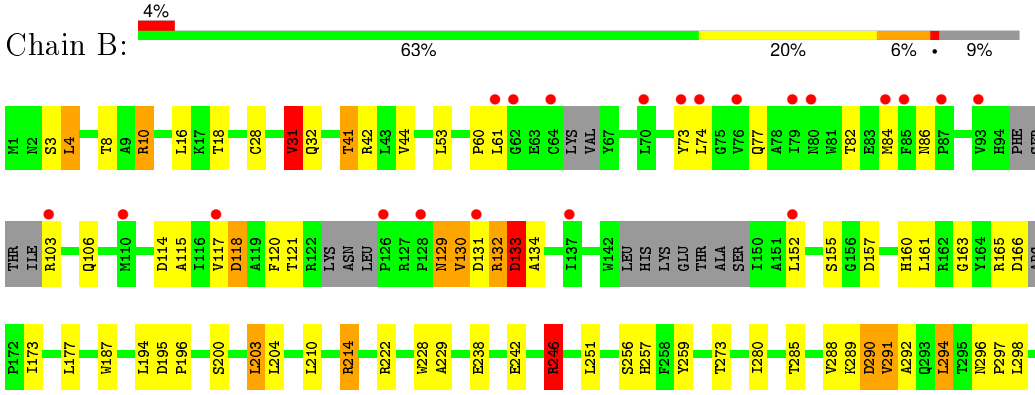
- Molecule 1: Ribosomal RNA large subunit methyltransferase L

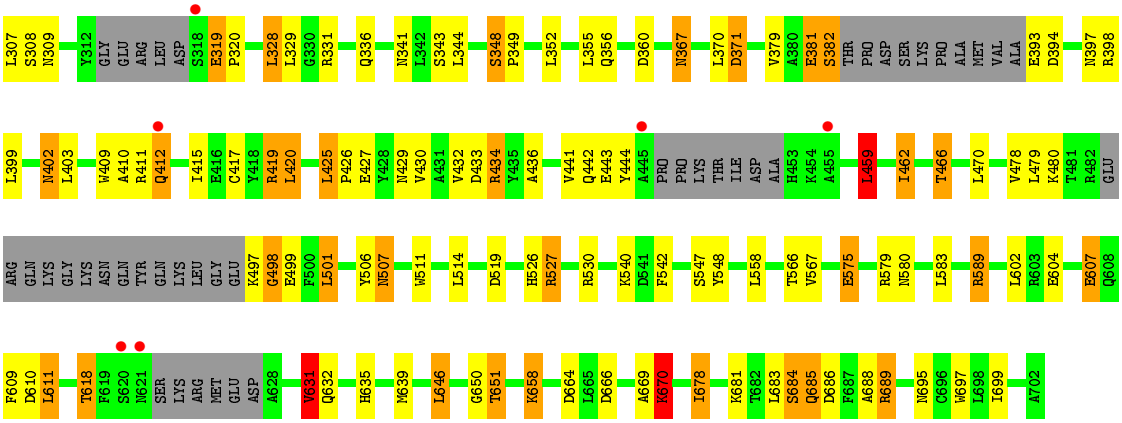
Chain A:



- Molecule 1: Ribosomal RNA large subunit methyltransferase L

Chain B:




L307 S308 N309 Y312 GLY GLU ARG LEU ASP S318 E319 P320 L328 L329 G330 R331 Q336 N341 L342 S343 L344 S348 P349 L352 L355 Q356 D360 N367 L370 D371 V379 A380 E381 S382 THR PRO ASP SER LYS PRO ALA MET VAL ALA E393 D394 N397 R398
L399 N402 L403 W409 A410 R411 Q412 I415 E416 C417 Y418 R419 L420 L425 P426 E427 Y428 N429 V430 A431 V432 D433 R434 Y435 A436 V441 Q442 E443 Y444 A445 PRO PRO LYS THR ILE ASP ALA H453 K454 A455 L459 I462 T466 L470 V478 L479 K480 T481 R482 GLU
ARG GLN LYS GLY LYS ASN GLN TYR GLN LYS LEU GLY GLU K497 G498 E499 F500 L501 Y506 N507 W511 L514 D519 H526 R527 R530 K540 D541 F542 S547 Y548 L558 T566 V567 E575 R579 N580 L583 R589 L602 R603 E604 E607 Q608
F609 D610 L611 T618 F619 S620 N621 SER LYS ARG MET GLU ASP A628 V631 Q632 H635 M639 L646 G650 T651 K658 D664 L665 D666 A669 K670 I678 K681 T682 L683 S684 Q685 D686 F687 A688 R689 N695 C696 W697 L698 I699 A702

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	73.72Å 140.59Å 102.10Å 90.00° 101.88° 90.00°	Depositor
Resolution (Å)	42.57 – 2.60 42.57 – 2.60	Depositor EDS
% Data completeness (in resolution range)	94.6 (42.57-2.60) 94.6 (42.57-2.60)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	3.89 (at 2.61Å)	Xtriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.182 , 0.247 0.191 , 0.251	Depositor DCC
R_{free} test set	3163 reflections (5.66%)	DCC
Wilson B-factor (Å^2)	55.8	Xtriage
Anisotropy	0.199	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 61.3	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 58905 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	10456	wwPDB-VP
Average B, all atoms (Å^2)	63.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.72% 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: OSU, SAM

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	0.91	1/5248 (0.0%)	0.95	15/7115 (0.2%)
1	B	0.82	1/4882 (0.0%)	0.92	12/6625 (0.2%)
All	All	0.86	2/10130 (0.0%)	0.94	27/13740 (0.2%)

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

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	282	GLU	CG-CD	5.53	1.60	1.51
1	B	499	GLU	CG-CD	5.52	1.60	1.51

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	214	ARG	NE-CZ-NH2	-7.87	116.37	120.30
1	B	459	LEU	CA-CB-CG	7.58	132.72	115.30
1	B	246	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	A	579	ARG	NE-CZ-NH2	7.02	123.81	120.30
1	A	56	ARG	NE-CZ-NH2	-6.36	117.12	120.30
1	B	246	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	A	214	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	B	631	VAL	CB-CA-C	-6.10	99.81	111.40
1	A	4	LEU	CA-CB-CG	-6.09	101.28	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	686	ASP	CB-CG-OD1	5.98	123.69	118.30
1	A	437	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	195	ASP	CB-CG-OD1	5.92	123.63	118.30
1	A	579	ARG	NE-CZ-NH1	-5.82	117.39	120.30
1	B	402	ASN	CB-CA-C	5.58	121.56	110.40
1	A	220	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	B	498	GLY	N-CA-C	5.54	126.95	113.10
1	A	558	LEU	CB-CG-CD1	5.41	120.20	111.00
1	A	23	LEU	CA-CB-CG	5.36	127.63	115.30
1	B	501	LEU	CA-CB-CG	5.32	127.54	115.30
1	B	4	LEU	CA-CB-CG	5.27	127.42	115.30
1	A	56	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	B	589	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	A	220	ARG	NE-CZ-NH1	5.15	122.88	120.30
1	B	434	ARG	NE-CZ-NH2	-5.10	117.75	120.30
1	A	342	LEU	CA-CB-CG	5.09	127.02	115.30
1	A	582	ARG	CB-CG-CD	-5.08	98.39	111.60
1	B	214	ARG	NE-CZ-NH2	-5.02	117.79	120.30

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	131	ASP	Peptide
1	B	498	GLY	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	5139	0	5025	143	1
1	B	4788	0	4539	155	0
2	A	45	0	31	0	0
2	B	51	0	38	5	0
3	A	31	0	27	4	0
3	B	30	0	25	3	0
4	A	211	0	0	35	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	B	161	0	0	29	0
All	All	10456	0	9685	305	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 15.

All (305) 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)
3:B:803:OSU:O5	3:B:803:OSU:C1	1.65	1.43
3:A:803:OSU:C1	3:A:803:OSU:O5	1.65	1.41
2:B:801:SAM:H8	4:B:1047:HOH:O	1.09	1.26
1:B:165:ARG:HG3	1:B:166:ASP:H	1.05	1.19
1:A:165:ARG:HG3	1:A:166:ASP:H	0.99	1.15
1:B:651:THR:HG22	4:B:983:HOH:O	1.46	1.15
1:B:669:ALA:O	1:B:670:LYS:CB	2.02	1.02
1:B:669:ALA:O	1:B:670:LYS:HB3	1.20	1.02
1:A:165:ARG:HG3	1:A:166:ASP:N	1.76	0.99
1:A:165:ARG:CG	1:A:166:ASP:H	1.78	0.97
3:B:803:OSU:O5	3:B:803:OSU:C2	2.18	0.92
1:A:507:ASN:HD22	1:A:507:ASN:H	1.11	0.91
1:B:73:TYR:CE1	1:B:115:ALA:HB2	2.04	0.91
1:A:246:ARG:HG2	1:A:246:ARG:HH11	1.38	0.89
1:A:446:PRO:HD2	4:A:1099:HOH:O	1.72	0.89
1:B:165:ARG:HG3	1:B:166:ASP:N	1.86	0.89
1:B:511:TRP:H	1:B:580:ASN:HD21	1.18	0.88
1:A:419:ARG:HD2	1:A:433:ASP:OD1	1.78	0.84
1:B:133:ASP:HA	4:B:1039:HOH:O	1.78	0.83
1:A:137:ILE:HD12	1:A:228[B]:TRP:HE3	1.43	0.82
1:B:635:HIS:HE1	1:B:664:ASP:H	1.27	0.81
1:B:685:GLN:N	4:B:1027:HOH:O	1.65	0.81
1:B:84[A]:MET:HA	1:B:84[A]:MET:CE	2.09	0.80
1:B:618:THR:HA	1:B:631:VAL:CG2	2.11	0.80
1:B:319:GLU:HG2	4:B:955:HOH:O	1.82	0.80
1:A:511:TRP:H	1:A:580:ASN:HD21	1.26	0.80
1:A:618:THR:HA	1:A:631:VAL:HG22	1.62	0.79
1:B:478:VAL:CB	4:B:1052:HOH:O	2.30	0.79
1:A:415:ILE:HD11	1:A:418:TYR:HB3	1.66	0.78
1:B:196:PRO:HB3	4:B:1030:HOH:O	1.84	0.77
1:B:462:ILE:O	1:B:466:THR:HG22	1.85	0.76
1:A:434:ARG:HD2	4:A:926:HOH:O	1.86	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:105:SER:HB3	4:A:1096:HOH:O	1.87	0.75
1:B:173:ILE:HG23	1:B:177:LEU:HD23	1.67	0.74
1:A:296:ASN:HD22	1:A:296:ASN:C	1.89	0.74
1:B:530:ARG:HD3	4:B:1034:HOH:O	1.88	0.73
1:B:511:TRP:H	1:B:580:ASN:ND2	1.85	0.73
1:A:67:TYR:O	1:A:68:SER:O	2.06	0.73
1:B:157:ASP:OD1	1:B:222:ARG:NH1	2.21	0.73
1:B:84[A]:MET:HA	1:B:84[A]:MET:HE3	1.69	0.73
1:A:296:ASN:ND2	1:A:298:LEU:H	1.87	0.72
1:A:381:GLU:HB2	4:A:1018:HOH:O	1.87	0.72
1:A:690:ASN:HD22	1:A:690:ASN:C	1.93	0.72
1:B:165:ARG:CG	1:B:166:ASP:H	1.88	0.72
1:B:441:VAL:O	1:B:479:LEU:O	2.08	0.72
1:B:684:SER:O	4:B:1033:HOH:O	2.07	0.72
1:A:617:PRO:HG2	4:A:1076:HOH:O	1.89	0.71
1:B:507:ASN:HD22	1:B:507:ASN:H	1.37	0.71
1:B:246:ARG:HG2	1:B:246:ARG:HH11	1.55	0.71
1:A:257:HIS:HE1	1:A:285:THR:OG1	1.73	0.70
1:B:8:THR:HG23	1:B:16:LEU:HD22	1.73	0.70
1:B:684:SER:O	1:B:685:GLN:CB	2.39	0.70
1:A:511:TRP:H	1:A:580:ASN:ND2	1.90	0.69
1:A:319:GLU:HB2	4:A:1016:HOH:O	1.93	0.69
1:A:618:THR:HA	1:A:631:VAL:CG2	2.23	0.69
1:A:462:ILE:O	1:A:466:THR:HG22	1.93	0.68
1:A:104:ASN:HD22	1:A:107:TYR:H	1.40	0.68
1:A:56:ARG:NH2	1:A:156:GLY:O	2.27	0.68
1:B:73:TYR:CD1	1:B:115:ALA:HB2	2.29	0.68
1:A:567:VAL:HG22	1:A:598:CYS:SG	2.34	0.68
1:B:8:THR:HG22	1:B:53:LEU:O	1.94	0.68
1:B:73:TYR:CE1	1:B:115:ALA:CB	2.77	0.68
1:A:419:ARG:CD	1:A:433:ASP:OD1	2.42	0.67
1:B:294:LEU:HD21	4:B:1030:HOH:O	1.94	0.66
1:A:605:ALA:O	1:A:644:ARG:NH2	2.25	0.66
1:A:17:LYS:HE3	4:A:963:HOH:O	1.96	0.66
1:A:526:HIS:ND1	1:A:694:HIS:HD2	1.94	0.66
1:B:548:TYR:HB2	2:B:802:SAM:HG2	1.76	0.66
1:B:575:GLU:HG3	1:B:579:ARG:HH12	1.61	0.66
1:A:472:ILE:HG23	1:A:473:ALA:H	1.61	0.66
1:B:639:MET:HE1	1:B:699:ILE:HG21	1.77	0.66
1:A:582:ARG:NH2	1:B:163:GLY:O	2.30	0.65
1:A:305:THR:HB	1:A:341:ASN:HB3	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:187:TRP:HD1	1:A:305:THR:HG23	1.61	0.65
1:A:99:ASN:HB2	4:A:981:HOH:O	1.96	0.64
1:A:462:ILE:O	1:A:466:THR:CG2	2.45	0.64
1:B:132:ARG:C	1:B:134:ALA:H	2.00	0.64
1:A:507:ASN:H	1:A:507:ASN:ND2	1.91	0.64
1:A:8:THR:HG22	1:A:53:LEU:O	1.97	0.64
1:A:507:ASN:N	1:A:507:ASN:HD22	1.89	0.64
1:B:28:CYS:HB2	4:B:1012:HOH:O	1.98	0.64
1:B:257:HIS:HE1	1:B:285:THR:OG1	1.80	0.64
1:A:1:MET:N	4:A:1038:HOH:O	2.30	0.63
1:A:228[A]:TRP:NE1	1:A:230:GLN:HB2	2.13	0.63
1:A:213:ASP:OD1	1:A:246:ARG:HG2	1.99	0.63
1:B:305:THR:HB	1:B:341:ASN:HB3	1.81	0.63
1:B:3:SER:O	1:B:60:PRO:HD2	1.97	0.63
1:B:84[A]:MET:CA	1:B:84[A]:MET:HE3	2.26	0.63
1:A:70:LEU:HG	1:A:74:LEU:HD22	1.80	0.63
1:A:690:ASN:ND2	1:A:692:GLN:H	1.97	0.62
1:A:306:VAL:HG13	1:A:333:MET:HE1	1.82	0.62
1:B:604:GLU:CB	4:B:1007:HOH:O	2.46	0.62
1:A:296:ASN:HD22	1:A:298:LEU:H	1.47	0.62
1:A:165:ARG:HA	4:A:1069:HOH:O	2.01	0.61
1:A:380:ALA:O	1:A:381:GLU:CB	2.48	0.61
1:B:646:LEU:HD22	1:B:650:GLY:HA3	1.82	0.61
1:B:381:GLU:CB	4:B:1060:HOH:O	2.47	0.61
1:B:31:VAL:HG13	1:B:31:VAL:O	2.01	0.61
1:B:635:HIS:CE1	1:B:664:ASP:H	2.14	0.60
1:B:194:LEU:HD21	4:B:1030:HOH:O	2.01	0.60
1:B:688:ALA:O	1:B:689:ARG:CB	2.48	0.60
1:A:187:TRP:HA	1:A:305:THR:HG21	1.84	0.60
1:A:3:SER:O	1:A:60:PRO:HD2	2.02	0.60
1:A:257:HIS:HD2	4:A:1080:HOH:O	1.85	0.59
1:B:328:LEU:HD23	1:B:331:ARG:NH2	2.16	0.59
1:B:695:ASN:HD22	1:B:697:TRP:HE1	1.49	0.59
1:B:507:ASN:H	1:B:507:ASN:ND2	2.00	0.59
1:A:137:ILE:HD12	1:A:228[B]:TRP:CE3	2.32	0.59
1:B:8:THR:CG2	1:B:16:LEU:HD22	2.33	0.59
1:B:430:VAL:HG21	1:B:462:ILE:CD1	2.34	0.58
1:B:187:TRP:HD1	1:B:305:THR:HG23	1.68	0.58
1:B:497:LYS:N	4:B:998:HOH:O	2.36	0.58
1:A:635:HIS:HE1	1:A:664:ASP:H	1.52	0.57
1:A:463:ILE:CD1	1:A:479:LEU:HD22	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:390:MET:CB	4:A:1058:HOH:O	2.52	0.57
1:B:479:LEU:O	1:B:480:LYS:HB2	2.05	0.56
1:A:10:ARG:HG2	4:A:986:HOH:O	2.05	0.56
1:B:309:ASN:HD21	2:B:801:SAM:HB2	1.69	0.56
1:A:463:ILE:HD11	1:A:479:LEU:HD22	1.86	0.56
1:B:397:ASN:HA	4:B:978:HOH:O	2.04	0.56
1:B:393:GLU:HB2	4:B:949:HOH:O	2.04	0.56
1:B:397:ASN:ND2	4:B:978:HOH:O	2.38	0.56
1:B:575:GLU:HG3	1:B:579:ARG:NH1	2.21	0.56
1:A:9:ALA:HB3	1:A:12:LEU:HD12	1.87	0.56
1:A:545:LEU:HD23	1:A:567:VAL:HG13	1.87	0.56
1:B:412:GLN:HA	1:B:412:GLN:HE21	1.69	0.56
1:B:443:GLU:OE2	1:B:459:LEU:HD22	2.06	0.55
1:B:589:ARG:HG2	1:B:589:ARG:O	2.05	0.55
1:B:427:GLU:N	1:B:427:GLU:OE2	2.33	0.55
1:A:91:PHE:HA	1:A:137:ILE:O	2.06	0.55
1:A:296:ASN:HD22	1:A:297:PRO:N	2.03	0.55
1:A:8:THR:HG22	4:A:921:HOH:O	2.05	0.55
1:A:482:ARG:CB	4:A:1040:HOH:O	2.54	0.55
1:B:684:SER:O	1:B:685:GLN:HB3	2.07	0.55
1:B:639:MET:CE	1:B:699:ILE:HG21	2.36	0.54
1:B:84[A]:MET:HE1	1:B:229:ALA:HB3	1.88	0.54
1:A:400:ARG:HD3	4:A:1020:HOH:O	2.07	0.54
1:B:246:ARG:HG2	1:B:246:ARG:NH1	2.17	0.54
3:A:803:OSU:C1	3:A:803:OSU:C5	2.71	0.54
1:A:165:ARG:CG	1:A:166:ASP:N	2.47	0.54
1:A:246:ARG:NH1	1:A:246:ARG:HG2	2.12	0.54
1:A:8:THR:CG2	1:A:53:LEU:O	2.54	0.54
1:A:579:ARG:NH2	4:A:983:HOH:O	2.41	0.54
1:B:666:ASP:O	1:B:669:ALA:O	2.25	0.54
1:A:137:ILE:CD1	1:A:228[B]:TRP:HE3	2.20	0.53
1:A:694:HIS:HB3	4:A:1060:HOH:O	2.08	0.53
1:A:353:SER:OG	1:A:457:GLN:HG2	2.09	0.53
1:B:292:ALA:HA	1:B:328:LEU:HD11	1.90	0.53
1:B:73:TYR:HE1	1:B:115:ALA:HB2	1.68	0.53
1:B:479:LEU:O	1:B:480:LYS:CB	2.56	0.52
1:A:319:GLU:OE2	1:A:456:ARG:NH2	2.42	0.52
1:B:187:TRP:CD1	1:B:305:THR:HG23	2.45	0.52
1:B:309:ASN:ND2	2:B:801:SAM:HB2	2.23	0.52
1:A:168:ALA:HB1	4:A:1072:HOH:O	2.09	0.52
1:A:390:MET:O	1:A:391:VAL:HG12	2.09	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:618:THR:HA	1:B:631:VAL:HG22	1.88	0.52
1:A:93:VAL:HG22	1:A:139:VAL:HG22	1.92	0.52
1:B:540:LYS:HB3	1:B:610:ASP:HB2	1.92	0.52
1:B:430:VAL:HA	4:B:1059:HOH:O	2.09	0.52
1:B:419:ARG:HD2	1:B:433:ASP:OD1	2.09	0.52
1:B:429:ASN:HD21	1:B:444:TYR:HB2	1.75	0.52
1:B:290:ASP:OD2	2:B:801:SAM:N6	2.42	0.51
1:A:481:THR:OG1	1:A:482:ARG:N	2.39	0.51
1:B:210:LEU:O	1:B:210:LEU:HD23	2.11	0.51
1:B:618:THR:HG21	4:B:939:HOH:O	2.10	0.51
1:B:214:ARG:HD3	1:B:280:ILE:HD13	1.93	0.51
1:A:431:ALA:O	1:A:441:VAL:HA	2.11	0.51
1:B:430:VAL:HG21	1:B:462:ILE:HD12	1.91	0.51
1:A:526:HIS:CE1	1:A:694:HIS:HD2	2.28	0.51
1:B:419:ARG:CD	1:B:433:ASP:OD1	2.59	0.51
1:B:542:PHE:CD1	1:B:611:LEU:HD13	2.45	0.51
1:A:107:TYR:HA	4:A:1084:HOH:O	2.10	0.50
1:B:381:GLU:O	1:B:382:SER:HB2	2.11	0.50
1:A:635:HIS:CE1	1:A:664:ASP:H	2.27	0.50
1:A:472:ILE:HG12	1:A:473:ALA:N	2.27	0.50
3:B:803:OSU:C5	3:B:803:OSU:C1	2.74	0.50
1:B:117:VAL:O	1:B:118:ASP:HB3	2.11	0.50
1:A:82:THR:HA	1:A:120:PHE:CE2	2.47	0.49
1:A:30:VAL:HG13	4:A:1106:HOH:O	2.11	0.49
1:A:296:ASN:ND2	1:A:296:ASN:C	2.62	0.49
1:B:203:LEU:HB2	4:B:993:HOH:O	2.12	0.49
1:A:391:VAL:O	1:A:391:VAL:HG13	2.13	0.49
1:A:258:PHE:HB2	1:A:284:ILE:HG12	1.95	0.49
1:B:519:ASP:HB3	4:B:947:HOH:O	2.13	0.49
1:A:472:ILE:HG23	1:A:473:ALA:N	2.26	0.49
1:A:305:THR:CG2	4:A:1062:HOH:O	2.60	0.49
1:A:643:LYS:HE2	1:A:671:LEU:O	2.13	0.48
1:B:352:LEU:O	1:B:355:LEU:HD23	2.13	0.48
1:A:619:PHE:C	4:A:1097:HOH:O	2.51	0.48
1:B:10:ARG:CB	4:B:1022:HOH:O	2.61	0.48
1:B:635:HIS:O	1:B:639:MET:HG2	2.13	0.48
1:B:631:VAL:O	1:B:635:HIS:HB3	2.13	0.48
1:B:187:TRP:HA	1:B:305:THR:HG21	1.96	0.48
1:B:152:LEU:HD22	1:B:228:TRP:CD2	2.49	0.48
1:B:417:CYS:HA	1:B:434:ARG:O	2.13	0.48
1:A:631:VAL:HG23	4:A:1091:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:ARG:C	1:B:134:ALA:N	2.67	0.48
1:A:571:ARG:O	1:A:575:GLU:HG2	2.13	0.48
1:B:348:SER:N	1:B:349:PRO:HD3	2.29	0.48
3:A:803:OSU:H3N2	3:A:803:OSU:H6N1	1.67	0.47
1:A:579:ARG:NH1	4:A:941:HOH:O	2.47	0.47
1:B:542:PHE:HD1	1:B:611:LEU:HD13	1.80	0.47
1:A:413:GLU:HB3	1:A:415:ILE:HG23	1.96	0.47
1:A:305:THR:HG21	1:A:341:ASN:HD22	1.79	0.47
1:A:23:LEU:HD23	1:A:23:LEU:O	2.15	0.47
1:A:306:VAL:HG13	1:A:333:MET:CE	2.46	0.46
1:B:349:PRO:HD2	4:B:953:HOH:O	2.15	0.46
1:A:369:PRO:HG2	4:A:1085:HOH:O	2.14	0.46
1:B:292:ALA:HA	1:B:328:LEU:CD1	2.45	0.46
1:B:420:LEU:HA	1:B:420:LEU:HD12	1.62	0.46
1:B:371:ASP:OD1	1:B:371:ASP:N	2.49	0.46
1:A:173:ILE:HG23	1:A:177:LEU:HD23	1.96	0.46
1:A:312:TYR:O	1:A:313:GLY:C	2.54	0.46
1:A:228[A]:TRP:CE2	1:A:230:GLN:HB2	2.50	0.46
1:B:684:SER:O	1:B:685:GLN:HB2	2.14	0.46
1:B:84[B]:MET:HG2	1:B:228:TRP:CZ2	2.51	0.46
1:B:442:GLN:HB3	4:B:943:HOH:O	2.16	0.46
1:A:41:THR:HG23	4:A:974:HOH:O	2.16	0.46
1:A:344:LEU:O	1:A:374:GLN:HA	2.16	0.46
1:B:257:HIS:CE1	1:B:285:THR:OG1	2.65	0.45
1:A:564:THR:OG1	1:A:591:HIS:HD2	1.98	0.45
1:B:166:ASP:HB2	4:B:1026:HOH:O	2.17	0.45
1:B:319:GLU:HA	1:B:320:PRO:HD3	1.74	0.45
1:A:152:LEU:HD22	1:A:228[B]:TRP:CD2	2.52	0.45
1:B:443:GLU:HA	4:B:1059:HOH:O	2.16	0.45
1:A:591:HIS:HE1	4:A:1013:HOH:O	1.98	0.45
1:A:240:LYS:HE2	4:A:950:HOH:O	2.16	0.45
1:A:417:CYS:HA	1:A:434:ARG:O	2.16	0.45
1:A:632:GLN:O	1:A:635:HIS:HD2	2.00	0.45
1:B:103:ARG:O	1:B:106:GLN:HB2	2.17	0.45
1:A:400:ARG:CD	4:A:1020:HOH:O	2.62	0.45
1:A:446:PRO:HA	4:A:1035:HOH:O	2.16	0.44
1:B:305:THR:HG22	4:B:929:HOH:O	2.17	0.44
1:A:472:ILE:HG12	1:A:473:ALA:H	1.81	0.44
1:B:132:ARG:O	1:B:134:ALA:N	2.36	0.44
1:A:690:ASN:C	1:A:690:ASN:ND2	2.66	0.44
1:B:607:GLU:HG2	1:B:607:GLU:H	1.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:194:LEU:HD23	1:B:195:ASP:N	2.33	0.44
1:B:214:ARG:CD	1:B:280:ILE:HD13	2.48	0.44
1:A:82:THR:HG21	1:A:123:LYS:HD2	1.98	0.44
1:B:352:LEU:O	1:B:355:LEU:CD2	2.66	0.44
1:A:668:LEU:HD23	1:A:675:ALA:HB2	2.00	0.44
1:A:56:ARG:HA	1:A:155:SER:OG	2.17	0.44
1:A:475:ASN:HB2	4:A:1073:HOH:O	2.17	0.43
1:A:160:HIS:CD2	1:A:160:HIS:H	2.35	0.43
1:B:632:GLN:HB2	1:B:658:LYS:HE3	1.99	0.43
1:B:399:LEU:O	1:B:403:LEU:HB2	2.18	0.43
1:A:380:ALA:O	1:A:381:GLU:HB2	2.18	0.43
1:A:380:ALA:O	1:A:381:GLU:HB3	2.17	0.43
1:A:546:PHE:CD1	1:A:617:PRO:HD3	2.53	0.43
1:A:657:ASN:HB3	1:A:694:HIS:ND1	2.33	0.43
3:A:803:OSU:C2	3:A:803:OSU:O5	2.30	0.43
1:A:214:ARG:HD2	1:A:280:ILE:HD13	2.00	0.43
1:A:82:THR:HA	1:A:120:PHE:CZ	2.53	0.43
1:B:296:ASN:HA	1:B:297:PRO:HD3	1.88	0.43
1:B:432:VAL:HG22	1:B:441:VAL:HG22	2.01	0.43
1:A:214:ARG:CD	1:A:280:ILE:HD13	2.49	0.43
1:A:112:VAL:O	1:A:116:ILE:HG13	2.19	0.43
1:B:160:HIS:CD2	1:B:160:HIS:H	2.37	0.43
1:B:403:LEU:O	1:B:403:LEU:HD23	2.19	0.42
1:A:2:ASN:O	1:A:38:LYS:HA	2.19	0.42
1:A:272:ARG:NH1	1:A:286:PHE:O	2.52	0.42
1:B:296:ASN:HB2	1:B:336:GLN:HG2	2.01	0.42
1:B:398:ARG:HE	1:B:402:ASN:HD22	1.68	0.42
1:B:367:ASN:OD1	1:B:367:ASN:C	2.57	0.42
1:B:129:ASN:O	1:B:130:VAL:CB	2.67	0.42
1:B:410:ALA:O	1:B:411:ARG:CB	2.66	0.42
1:A:653:MET:HA	1:A:697:TRP:O	2.20	0.42
1:B:196:PRO:HD2	1:B:308:SER:HB2	2.00	0.42
1:A:602:LEU:HD23	1:A:602:LEU:HA	1.78	0.42
1:B:695:ASN:ND2	1:B:697:TRP:HE1	2.16	0.42
1:B:355:LEU:O	1:B:356:GLN:HB2	2.19	0.42
1:B:506:TYR:CE2	1:B:527:ARG:HG3	2.55	0.42
1:B:429:ASN:ND2	1:B:444:TYR:HB2	2.35	0.42
1:B:618:THR:HA	1:B:631:VAL:HG23	1.97	0.42
1:B:242:GLU:O	1:B:246:ARG:HB2	2.19	0.42
1:A:526:HIS:ND1	1:A:694:HIS:CD2	2.82	0.42
1:A:606:ASN:O	1:A:607:GLU:O	2.38	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:425:LEU:HA	1:B:426:PRO:HD3	1.80	0.42
1:A:305:THR:HG22	4:A:1062:HOH:O	2.21	0.41
1:A:636:LEU:HD22	1:A:671:LEU:HD11	2.01	0.41
1:A:187:TRP:CD1	1:A:305:THR:HG23	2.50	0.41
1:A:305:THR:CB	1:A:341:ASN:HB3	2.50	0.41
1:B:165:ARG:CG	1:B:166:ASP:N	2.62	0.41
1:A:152:LEU:HD22	1:A:228[B]:TRP:CE2	2.55	0.41
1:A:462:ILE:O	1:A:466:THR:HG23	2.18	0.41
1:B:678:ILE:HG13	1:B:678:ILE:H	1.73	0.41
1:B:114:ASP:HA	1:B:115:ALA:HA	1.94	0.41
1:A:369:PRO:HD2	4:A:1085:HOH:O	2.20	0.41
1:B:607:GLU:HG3	1:B:609:PHE:CZ	2.56	0.41
1:B:632:GLN:O	1:B:635:HIS:HD2	2.04	0.41
1:B:194:LEU:C	1:B:194:LEU:HD23	2.41	0.41
1:B:259:TYR:N	1:B:259:TYR:CD2	2.89	0.41
1:A:688:ALA:C	1:A:690:ASN:H	2.23	0.41
1:B:187:TRP:HA	1:B:305:THR:CG2	2.51	0.41
1:B:602:LEU:HA	1:B:602:LEU:HD23	1.91	0.41
1:A:618:THR:HG22	4:A:937:HOH:O	2.20	0.40
1:B:86:ASN:HA	1:B:86:ASN:HD22	1.74	0.40
1:B:547:SER:CB	1:B:566:THR:HG23	2.51	0.40
1:B:291:VAL:O	1:B:294:LEU:HB2	2.21	0.40
1:B:497:LYS:N	4:B:997:HOH:O	2.53	0.40
1:B:409:TRP:C	1:B:410:ALA:O	2.57	0.40
1:A:580:ASN:HA	1:A:580:ASN:HD22	1.69	0.40
1:B:41:THR:O	1:B:44:VAL:HB	2.21	0.40
1:B:307:LEU:HA	1:B:343:SER:O	2.21	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)
1:A:71:ASP:OD1	1:A:331:ARG:NH1[1_455]	2.10	0.10

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	653/702 (93%)	616 (94%)	31 (5%)	6 (1%)	21 42
1	B	615/702 (88%)	560 (91%)	39 (6%)	16 (3%)	7 11
All	All	1268/1404 (90%)	1176 (93%)	70 (6%)	22 (2%)	11 22

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	68	SER
1	A	472	ILE
1	B	130	VAL
1	A	607	GLU
1	B	31	VAL
1	B	32	GLN
1	B	118	ASP
1	B	132	ARG
1	B	133	ASP
1	B	367	ASN
1	B	381	GLU
1	B	670	LYS
1	B	685	GLN
1	B	10	ARG
1	B	120	PHE
1	A	689	ARG
1	B	689	ARG
1	A	170	ILE
1	B	129	ASN
1	B	436	ALA
1	A	391	VAL
1	B	301	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	519/581 (89%)	444 (86%)	75 (14%)	4 6
1	B	466/581 (80%)	396 (85%)	70 (15%)	3 6
All	All	985/1162 (85%)	840 (85%)	145 (15%)	4 6

All (145) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	8	THR
1	A	23	LEU
1	A	31	VAL
1	A	59	LEU
1	A	61	LEU
1	A	74	LEU
1	A	80	ASN
1	A	101	THR
1	A	105	SER
1	A	111	LYS
1	A	122	ARG
1	A	124	ASN
1	A	125	LEU
1	A	130	VAL
1	A	139	VAL
1	A	141	VAL
1	A	150	ILE
1	A	165	ARG
1	A	182	VAL
1	A	204	LEU
1	A	246	ARG
1	A	249	LYS
1	A	251	LEU
1	A	266	ARG
1	A	269	GLN
1	A	282	GLU
1	A	293	GLN
1	A	296	ASN
1	A	305	THR
1	A	328	LEU
1	A	331	ARG
1	A	342	LEU
1	A	344	LEU
1	A	362	GLN
1	A	379	VAL

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Mol	Chain	Res	Type
1	A	393	GLU
1	A	412	GLN
1	A	415	ILE
1	A	419	ARG
1	A	424	ASP
1	A	430	VAL
1	A	434	ARG
1	A	441	VAL
1	A	454	LYS
1	A	459	LEU
1	A	466	THR
1	A	468	SER
1	A	483	GLU
1	A	501	LEU
1	A	503	VAL
1	A	507	ASN
1	A	514	LEU
1	A	518	LEU
1	A	526	HIS
1	A	537	SER
1	A	540	LYS
1	A	558	LEU
1	A	567	VAL
1	A	582	ARG
1	A	583	LEU
1	A	599	LEU
1	A	607	GLU
1	A	611	LEU
1	A	618	THR
1	A	631	VAL
1	A	636	LEU
1	A	644	ARG
1	A	646	LEU
1	A	665	LEU
1	A	666	ASP
1	A	668	LEU
1	A	684	SER
1	A	690	ASN
1	A	694	HIS
1	A	698	LEU
1	B	4	LEU
1	B	18	THR

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Mol	Chain	Res	Type
1	B	31	VAL
1	B	41	THR
1	B	42	ARG
1	B	61	LEU
1	B	74	LEU
1	B	77	GLN
1	B	82	THR
1	B	121	THR
1	B	133	ASP
1	B	155	SER
1	B	161	LEU
1	B	200	SER
1	B	203	LEU
1	B	204	LEU
1	B	238	GLU
1	B	246	ARG
1	B	251	LEU
1	B	256	SER
1	B	273	THR
1	B	288	VAL
1	B	289	LYS
1	B	290	ASP
1	B	291	VAL
1	B	294	LEU
1	B	298	LEU
1	B	305	THR
1	B	306	VAL
1	B	319	GLU
1	B	328	LEU
1	B	329	LEU
1	B	344	LEU
1	B	348	SER
1	B	360	ASP
1	B	370	LEU
1	B	371	ASP
1	B	379	VAL
1	B	382	SER
1	B	394	ASP
1	B	412	GLN
1	B	415	ILE
1	B	419	ARG
1	B	420	LEU

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Mol	Chain	Res	Type
1	B	425	LEU
1	B	459	LEU
1	B	462	ILE
1	B	466	THR
1	B	470	LEU
1	B	501	LEU
1	B	507	ASN
1	B	514	LEU
1	B	526	HIS
1	B	527	ARG
1	B	558	LEU
1	B	567	VAL
1	B	575	GLU
1	B	583	LEU
1	B	607	GLU
1	B	611	LEU
1	B	618	THR
1	B	631	VAL
1	B	646	LEU
1	B	651	THR
1	B	658	LYS
1	B	670	LYS
1	B	678	ILE
1	B	681	LYS
1	B	683	LEU
1	B	684	SER

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

Mol	Chain	Res	Type
1	A	22	ASN
1	A	80	ASN
1	A	104	ASN
1	A	160	HIS
1	A	257	HIS
1	A	269	GLN
1	A	293	GLN
1	A	296	ASN
1	A	309	ASN
1	A	341	ASN
1	A	402	ASN
1	A	507	ASN

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Mol	Chain	Res	Type
1	A	509	HIS
1	A	580	ASN
1	A	591	HIS
1	A	635	HIS
1	A	685	GLN
1	A	690	ASN
1	A	694	HIS
1	B	77	GLN
1	B	86	ASN
1	B	140	ASN
1	B	160	HIS
1	B	257	HIS
1	B	309	ASN
1	B	336	GLN
1	B	397	ASN
1	B	402	ASN
1	B	412	GLN
1	B	429	ASN
1	B	507	ASN
1	B	580	ASN
1	B	591	HIS
1	B	608	GLN
1	B	635	HIS
1	B	676	GLN
1	B	695	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

6 ligands 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	$\#\|Z\| > 2$
2	SAM	A	801	-	20,28,29	1.21	1 (5%)	19,40,42	3.14	2 (10%)
2	SAM	A	802	-	15,21,29	1.35	2 (13%)	14,31,42	3.10	3 (21%)
3	OSU	A	803	-	32,32,33	5.30	8 (25%)	45,45,46	2.15	14 (31%)
2	SAM	B	801	-	20,28,29	1.42	2 (10%)	19,40,42	2.18	2 (10%)
2	SAM	B	802	-	21,27,29	1.15	2 (9%)	20,38,42	2.14	3 (15%)
3	OSU	B	803	-	31,31,33	5.66	10 (32%)	44,44,46	1.96	9 (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
2	SAM	A	801	-	-	0/7/31/33	0/3/3/3
2	SAM	A	802	-	-	0/2/22/33	0/3/3/3
3	OSU	A	803	-	-	0/21/60/61	0/2/2/2
2	SAM	B	801	-	-	0/7/31/33	0/3/3/3
2	SAM	B	802	-	-	0/7/29/33	0/3/3/3
3	OSU	B	803	-	-	0/20/59/61	0/2/2/2

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	803	OSU	C4-C5	-22.03	1.06	1.53
3	A	803	OSU	C4-C5	-21.42	1.07	1.53
3	B	803	OSU	C1-C2	-15.26	1.06	1.52
3	A	803	OSU	C1-C2	-14.89	1.08	1.52
2	B	802	SAM	O4'-C4'	-2.32	1.39	1.45
3	B	803	OSU	O2'-C2'	-2.03	1.37	1.42
3	A	803	OSU	O6'-C1N	2.43	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	803	OSU	C2N-C1N	2.46	1.58	1.50
2	A	802	SAM	C2-N1	2.66	1.39	1.33
2	B	802	SAM	C2-N3	2.93	1.37	1.32
2	B	801	SAM	C2-N1	3.10	1.39	1.33
2	A	802	SAM	C2-N3	3.31	1.38	1.32
3	B	803	OSU	O6'-C1N	3.42	1.43	1.33
2	A	801	SAM	C2-N3	3.47	1.38	1.32
3	A	803	OSU	O1N-C1N	4.31	1.35	1.22
3	A	803	OSU	C3-C2	4.45	1.64	1.52
3	A	803	OSU	O5-C5	4.88	1.56	1.44
2	B	801	SAM	C2-N3	4.94	1.40	1.32
3	B	803	OSU	C3-C2	5.05	1.65	1.52
3	B	803	OSU	O5-C5	5.62	1.58	1.44
3	A	803	OSU	C4-C3	6.40	1.69	1.52
3	B	803	OSU	O1N-C1N	6.74	1.42	1.22
3	B	803	OSU	C4-C3	6.92	1.70	1.52
3	A	803	OSU	O5-C1	9.37	1.65	1.41
3	B	803	OSU	O5-C1	9.39	1.65	1.41

All (33) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	801	SAM	N3-C2-N1	-12.93	118.99	128.89
2	A	802	SAM	N3-C2-N1	-10.41	120.92	128.89
2	B	801	SAM	N3-C2-N1	-8.64	122.28	128.89
2	B	802	SAM	N3-C2-N1	-8.06	122.72	128.89
3	B	803	OSU	O6'-C1N-O1N	-4.99	110.62	123.49
3	A	803	OSU	O4-C4-C3	-4.94	99.22	110.34
3	A	803	OSU	O1N-C1N-C2N	-4.60	105.32	123.72
3	A	803	OSU	O2-C2-C3	-3.40	102.67	110.34
2	A	802	SAM	C1'-N9-C4	-3.29	121.97	126.94
3	A	803	OSU	O6'-C1N-O1N	-3.28	115.03	123.49
3	B	803	OSU	O5-C5-C4	-3.15	103.78	109.68
3	B	803	OSU	O5-C1-C2	-2.97	104.19	110.28
3	A	803	OSU	O5-C5-C6	-2.53	99.95	106.36
2	A	801	SAM	C4-C5-N7	-2.52	107.16	109.48
2	B	801	SAM	C4-C5-N7	-2.23	107.43	109.48
2	B	802	SAM	C4'-O4'-C1'	-2.10	107.41	109.72
2	B	802	SAM	CB-CG-SD	2.08	117.58	113.57
3	A	803	OSU	C2'-O1-C1	2.19	123.30	117.53
2	A	802	SAM	O2'-C2'-C3'	2.19	118.95	111.83
3	B	803	OSU	O6'-C6'-C5'	2.34	113.59	108.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	803	OSU	O3-C3-C2	2.45	115.86	110.34
3	A	803	OSU	O6'-C1N-C2N	2.48	119.45	111.90
3	B	803	OSU	O6'-C1N-C2N	2.64	119.95	111.90
3	B	803	OSU	O3-C3-C2	2.68	116.36	110.34
3	A	803	OSU	C4N-C3N-C2N	2.69	123.14	113.29
3	B	803	OSU	O1-C1-C2	2.99	118.35	108.36
3	A	803	OSU	O1'-C1'-C2'	3.03	121.59	111.91
3	A	803	OSU	O1-C1-C2	3.10	118.70	108.36
3	A	803	OSU	O4'-C4'-C3'	3.25	122.33	112.01
3	A	803	OSU	O4-C4-C5	4.69	121.66	109.24
3	B	803	OSU	O2-C2-C1	5.18	121.38	110.02
3	B	803	OSU	O4-C4-C5	5.72	124.41	109.24
3	A	803	OSU	O2-C2-C1	6.19	123.59	110.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	803	OSU	4	0
2	B	801	SAM	4	0
2	B	802	SAM	1	0
3	B	803	OSU	3	0

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	664/702 (94%)	-0.36	4 (0%) 90 88	33, 55, 85, 101	0
1	B	636/702 (90%)	-0.15	27 (4%) 40 32	33, 69, 112, 139	0
All	All	1300/1404 (92%)	-0.26	31 (2%) 62 56	33, 62, 100, 139	0

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	61	LEU	4.3
1	B	131	ASP	3.8
1	B	85	PHE	3.7
1	B	318	SER	3.6
1	B	62	GLY	3.6
1	B	64	CYS	3.4
1	B	117	VAL	3.1
1	B	455	ALA	3.1
1	B	84[A]	MET	3.0
1	A	142	TRP	2.9
1	B	74	LEU	2.9
1	B	70	LEU	2.9
1	B	110	MET	2.9
1	B	103	ARG	2.8
1	B	137	ILE	2.8
1	B	152	LEU	2.6
1	A	318	SER	2.6
1	B	128	PRO	2.5
1	B	620	SER	2.5
1	B	87	PRO	2.5
1	B	73	TYR	2.4
1	B	93	VAL	2.3
1	B	76	VAL	2.2
1	B	126	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	621	ASN	2.2
1	B	445	ALA	2.2
1	B	80	ASN	2.1
1	B	412	GLN	2.1
1	B	79	ILE	2.1
1	A	170	ILE	2.0
1	A	89	ALA	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (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
2	SAM	B	801	26/27	0.94	0.17	0.54	54,76,98,99	0
3	OSU	B	803	30/32	0.97	0.16	0.11	48,56,67,72	0
2	SAM	B	802	25/27	0.96	0.15	-0.17	52,58,84,85	0
3	OSU	A	803	31/32	0.97	0.16	-0.22	31,42,50,50	0
2	SAM	A	801	26/27	0.97	0.13	-0.46	35,49,81,81	0
2	SAM	A	802	19/27	0.97	0.13	-0.47	65,69,71,74	0

6.5 Other polymers (i)

There are no such residues in this entry.