Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 06:34 AM GMT

PDB ID	:	2XJA
Title	:	STRUCTURE OF MURE FROM M.TUBERCULOSIS WITH DIPEPTIDE AND ADP
Authors	:	Basavannacharya, C.; Moody, P.R.; Bhakta, S.; Keep, N.
Deposited on	:	2010-07-03
Resolution	:	3.00 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:

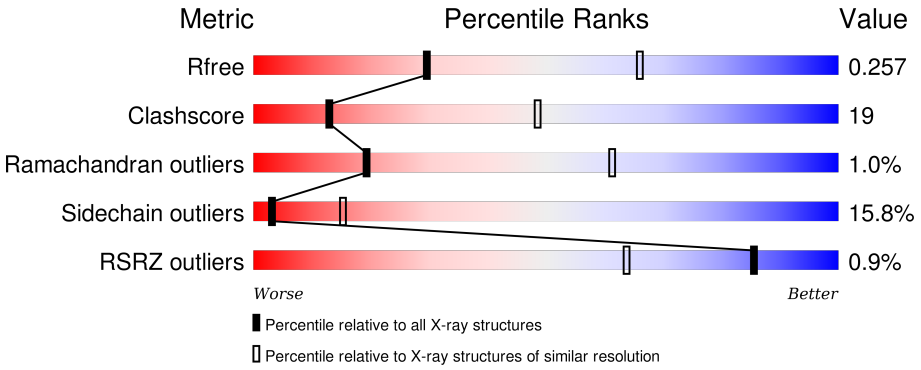
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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	535	60% 29% 5% 6%
1	B	535	59% 29% 5% 7%
1	C	535	% 58% 30% • 7%
1	D	535	% 57% 29% 5% 9%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	MG	D	1537	-	-	-	X

2 Entry composition

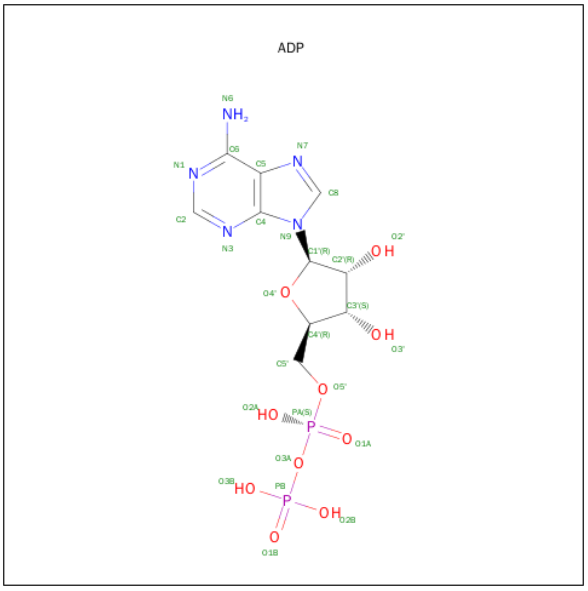
There are 5 unique types of molecules in this entry. The entry contains 14477 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 UDP-N-ACETYLMURAMOYL-L-ALANYL-D-GLUTAMATE--2,6-DIAMINOPIMELATE LIGASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	502	Total	C	N	O	S	0	0	0
			3567	2220	659	680	8			
1	B	500	Total	C	N	O	S	0	0	0
			3556	2211	660	677	8			
1	C	498	Total	C	N	O	S	0	0	0
			3538	2203	655	672	8			
1	D	488	Total	C	N	O	S	0	0	0
			3462	2159	633	662	8			

- Molecule 2 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

Continued on next page...

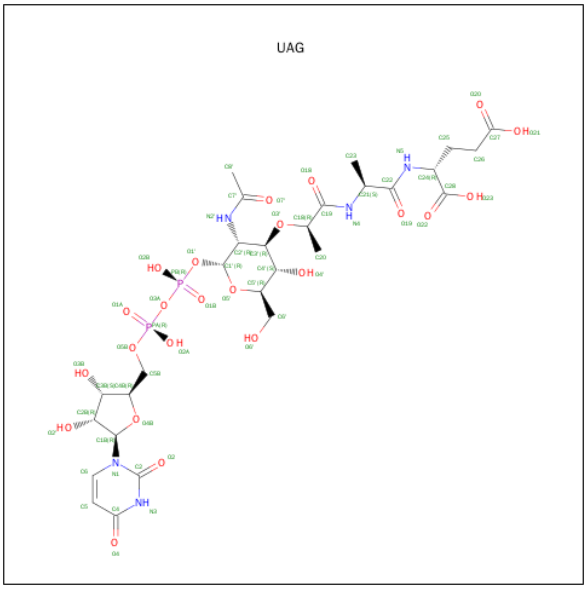
Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
2	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	3	Total	Mg	0	0
			3	3		
3	A	2	Total	Mg	0	0
			2	2		
3	D	3	Total	Mg	0	0
			3	3		
3	C	2	Total	Mg	0	0
			2	2		

- Molecule 4 is URIDINE-5'-DIPHOSPHATE-N-ACETYLMURAMOYL-L-ALANINE-D-GLUTAMATE (three-letter code: UAG) (formula: $C_{28}H_{43}N_5O_{23}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			58	28	5	23	2		
4	B	1	Total	C	N	O	P	0	0
			58	28	5	23	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	C	1	Total	C	N	O	P	0	0
			58	28	5	23	2		
4	D	1	Total	C	N	O	P	0	0
			58	28	5	23	2		

- Molecule 5 is water.

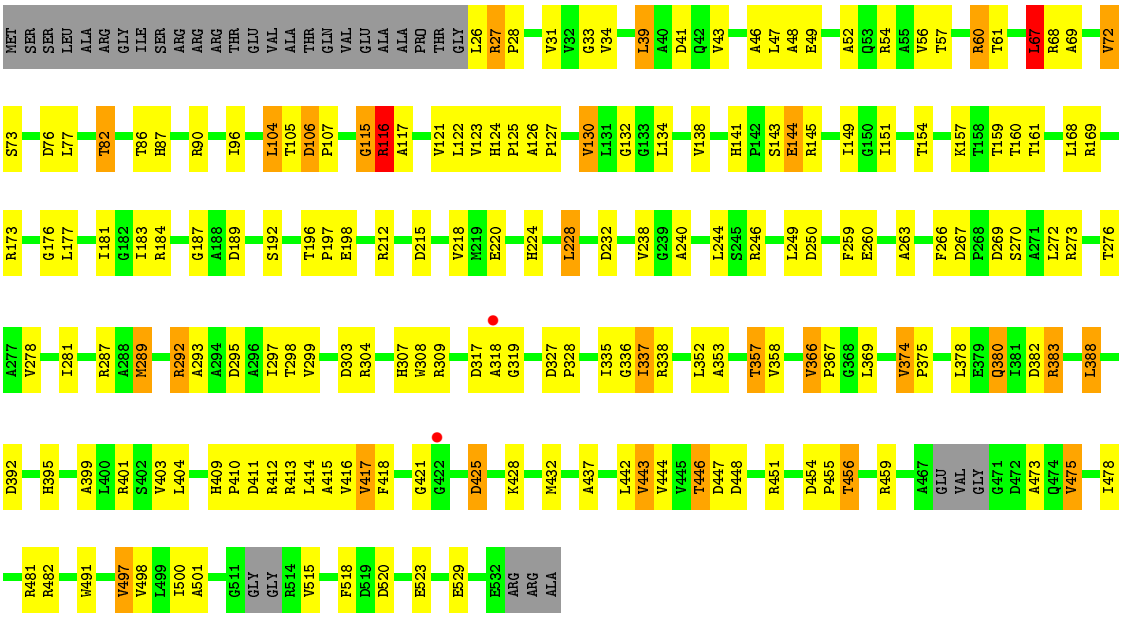
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	O	0	0
			1	1		
5	B	1	Total	O	0	0
			1	1		
5	C	1	Total	O	0	0
			1	1		
5	D	1	Total	O	0	0
			1	1		

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.

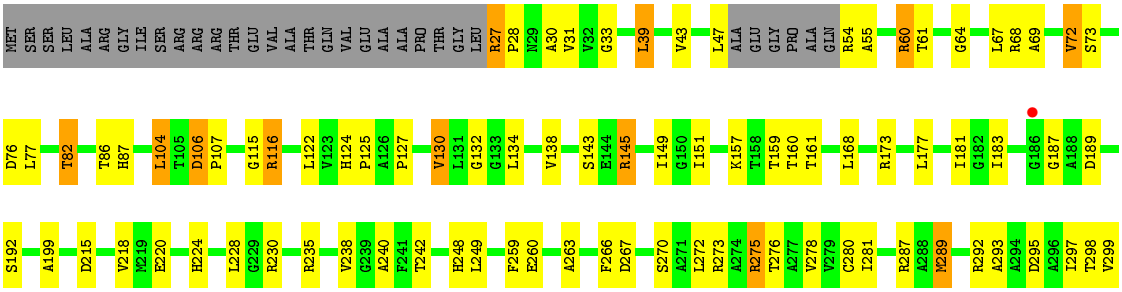
• Molecule 1: UDP-N-ACETYLMURAMOYL-L-ALANYL-D-GLUTAMATE--2,6-DIAMINOPIMELATE LIGASE

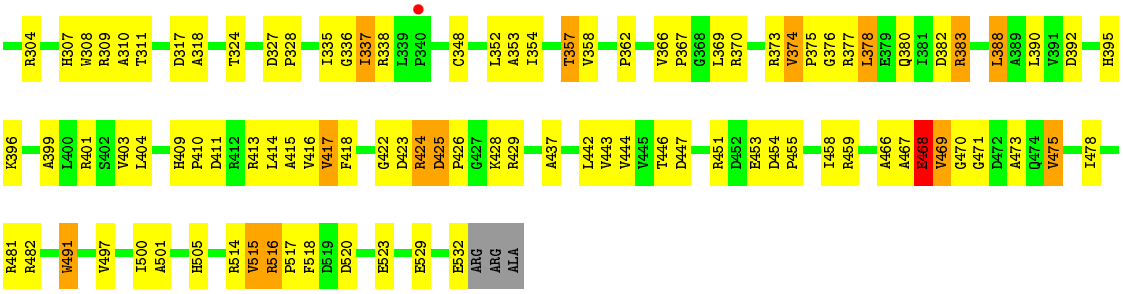
Chain A:



• Molecule 1: UDP-N-ACETYLMURAMOYL-L-ALANYL-D-GLUTAMATE--2,6-DIAMINOPIMELATE LIGASE

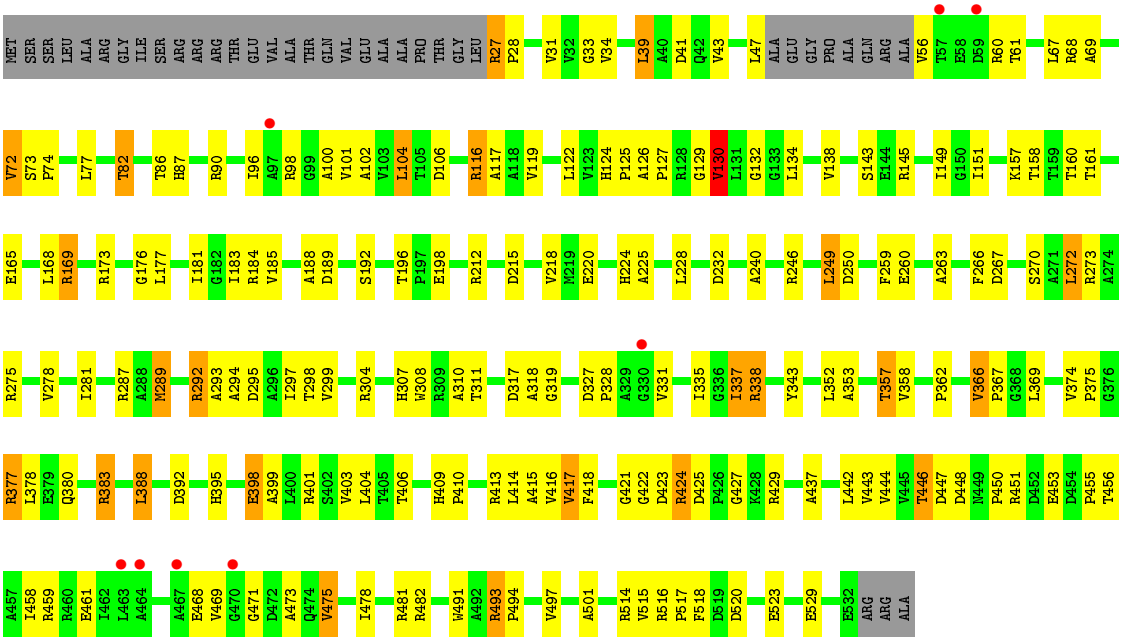
Chain B:





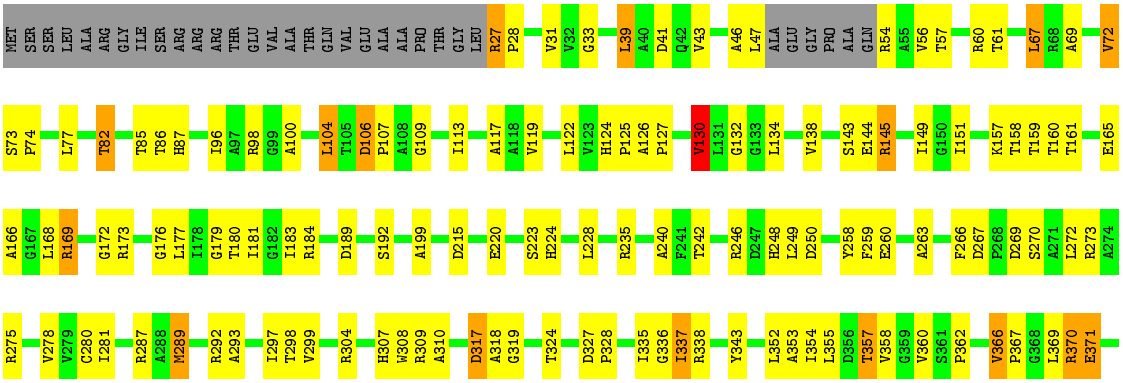
• Molecule 1: UDP-N-ACETYLMURAMOYL-L-ALANYL-D-GLUTAMATE--2,6-DIAMINOPIMELATE LIGASE

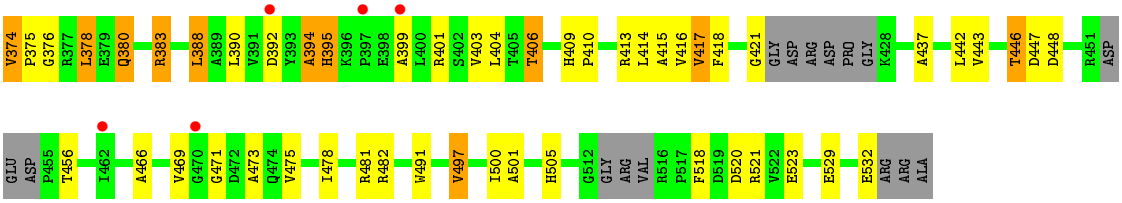
Chain C:



• Molecule 1: UDP-N-ACETYLMURAMOYL-L-ALANYL-D-GLUTAMATE--2,6-DIAMINOPIMELATE LIGASE

Chain D:




V374 P375 G376 R377 L378 E379 Q380 R383 L388 A389 L390 V391 D392 Y393 A394 H395 K396 P397 E398 A399 L400 R401 S402 V403 L404 T405 T406 H409 P410 R413 L414 A415 V416 V417 F418 G421 GLY ASP ARG ASP PRO GLY K428 A437 L442 V443 T446 D447 D448 R451 ASP
GLU ASP P455 T456 I462 A466 V469 G470 G471 D472 A473 Q474 V475 I478 R481 R482 W491 V497 I500 A501 H505 G512 GLY ARG VAL R516 P517 F518 D519 D520 R521 V522 E523 E529 E532 ARG ARG ALA

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	75.04Å 76.32Å 81.99Å 111.32° 91.42° 92.90°	Depositor
Resolution (Å)	76.30 – 3.00 74.86 – 3.00	Depositor EDS
% Data completeness (in resolution range)	95.9 (76.30-3.00) 83.5 (74.86-3.00)	Depositor EDS
R_{merge}	0.12	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.39 (at 3.01Å)	Xtriage
Refinement program	REFMAC 5.6.0077	Depositor
R, R_{free}	0.189 , 0.258 0.189 , 0.257	Depositor DCC
R_{free} test set	1598 reflections (5.18%)	DCC
Wilson B-factor (Å^2)	62.6	Xtriage
Anisotropy	0.065	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 65.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.45$, $< L^2 > = 0.27$	Xtriage
Outliers	0 of 32473 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	14477	wwPDB-VP
Average B, all atoms (Å^2)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.17% 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: MG, ADP, UAG, KCX

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	0.69	0/3612	0.79	1/4939 (0.0%)
1	B	0.73	1/3601 (0.0%)	0.82	1/4921 (0.0%)
1	C	0.68	0/3583	0.78	2/4898 (0.0%)
1	D	0.69	0/3503	0.78	1/4787 (0.0%)
All	All	0.70	1/14299 (0.0%)	0.79	5/19545 (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	A	0	2
1	C	0	1
All	All	0	3

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	348	CYS	CB-SG	-7.75	1.69	1.82

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	67	LEU	CA-CB-CG	5.96	129.00	115.30
1	C	377	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	B	348	CYS	CA-CB-SG	-5.30	104.46	114.00
1	C	427	GLY	N-CA-C	5.20	126.10	113.10
1	D	67	LEU	CA-CB-CG	5.05	126.92	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	115	GLY	Peptide
1	A	116	ARG	Peptide
1	C	116	ARG	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	3567	0	3524	144	1
1	B	3556	0	3520	144	0
1	C	3538	0	3504	144	0
1	D	3462	0	3424	141	1
2	A	27	0	12	1	0
2	B	27	0	12	2	0
2	C	27	0	12	5	0
2	D	27	0	12	5	0
3	A	2	0	0	0	0
3	B	3	0	0	0	0
3	C	2	0	0	0	0
3	D	3	0	0	0	0
4	A	58	0	39	5	0
4	B	58	0	39	4	0
4	C	58	0	39	2	0
4	D	58	0	39	7	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
All	All	14477	0	14176	547	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 19.

All (547) 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:A:383:ARG:HG3	1:A:383:ARG:HH11	1.14	1.07
1:C:424:ARG:HH11	1:C:424:ARG:HG3	1.16	1.07
1:A:116:ARG:HG2	1:A:116:ARG:NH1	1.60	1.04
1:D:383:ARG:HH11	1:D:383:ARG:HG3	1.24	1.02
1:B:383:ARG:HH11	1:B:383:ARG:HG3	1.23	1.02
1:D:165:GLU:OE2	1:D:169:ARG:HD3	1.60	1.01
1:A:116:ARG:HH11	1:A:116:ARG:CG	1.74	0.99
1:D:86:THR:HG23	4:D:1536:UAG:H5'2	1.42	0.98
1:C:446:THR:HG21	1:C:481:ARG:HA	1.46	0.95
1:A:446:THR:HG21	1:A:481:ARG:HA	1.52	0.91
1:B:383:ARG:NH1	1:B:383:ARG:HG3	1.81	0.90
1:A:383:ARG:HG2	1:B:382:ASP:OD1	1.71	0.90
1:A:409:HIS:HB2	1:A:412:ARG:HH21	1.34	0.89
1:C:27:ARG:HG3	1:C:28:PRO:HD2	1.54	0.89
1:D:446:THR:HG21	1:D:481:ARG:HA	1.52	0.89
1:A:383:ARG:NH1	1:A:383:ARG:HG3	1.75	0.88
1:A:116:ARG:HH11	1:A:116:ARG:HG2	0.79	0.88
1:B:181:ILE:HD13	1:B:375:PRO:HG2	1.55	0.88
1:C:98:ARG:O	1:D:74:PRO:HG2	1.71	0.88
1:B:27:ARG:HG3	1:B:28:PRO:HD2	1.55	0.88
1:C:319:GLY:HA3	1:C:380:GLN:HE22	1.39	0.87
1:B:446:THR:HG21	1:B:481:ARG:HA	1.56	0.87
1:C:383:ARG:HH11	1:C:383:ARG:HG3	1.40	0.86
1:A:27:ARG:HG3	1:A:28:PRO:HD2	1.55	0.86
1:B:145:ARG:O	1:D:145:ARG:NH1	2.07	0.86
1:D:383:ARG:HG3	1:D:383:ARG:NH1	1.83	0.85
1:C:517:PRO:HG2	1:D:172:GLY:HA2	1.56	0.85
1:C:383:ARG:NH1	1:C:383:ARG:HG3	1.92	0.84
1:A:383:ARG:HH11	1:A:383:ARG:CG	1.90	0.84
1:A:181:ILE:HD13	1:A:375:PRO:HG2	1.60	0.84
1:D:39:LEU:HG	1:D:134:LEU:HD22	1.60	0.83
1:B:124:HIS:ND1	1:B:125:PRO:O	2.11	0.83
1:C:74:PRO:HG2	1:D:98:ARG:O	1.78	0.83
1:A:409:HIS:HB2	1:A:412:ARG:NH2	1.94	0.82
1:B:230:ARG:NH1	4:B:1536:UAG:O22	2.13	0.82
1:D:298:THR:H	1:D:307:HIS:CD2	1.98	0.82
1:C:377:ARG:NE	2:C:1533:ADP:O2A	2.12	0.81
1:D:27:ARG:HG3	1:D:28:PRO:HD2	1.60	0.81
1:D:82:THR:HG22	1:D:87:HIS:NE2	1.95	0.81
1:B:39:LEU:HG	1:B:134:LEU:HD22	1.61	0.81
1:B:383:ARG:CG	1:B:383:ARG:HH11	1.94	0.80
1:C:298:THR:H	1:C:307:HIS:CD2	1.99	0.80

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:298:THR:H	1:A:307:HIS:CD2	2.01	0.79
1:C:181:ILE:HD13	1:C:375:PRO:HG2	1.64	0.79
1:D:181:ILE:HD13	1:D:375:PRO:HG2	1.63	0.79
1:D:383:ARG:HH11	1:D:383:ARG:CG	1.96	0.78
1:B:82:THR:HG22	1:B:87:HIS:NE2	1.98	0.78
1:B:115:GLY:O	1:B:116:ARG:HG2	1.84	0.78
1:C:82:THR:HG22	1:C:87:HIS:NE2	1.98	0.78
1:B:157:LYS:HB3	1:B:220:GLU:HG2	1.63	0.78
1:D:82:THR:HG22	1:D:87:HIS:CD2	2.18	0.78
1:A:124:HIS:ND1	1:A:125:PRO:O	2.16	0.78
1:B:298:THR:H	1:B:307:HIS:CD2	2.02	0.78
1:A:409:HIS:CB	1:A:412:ARG:HH21	1.97	0.77
1:B:446:THR:HG22	1:B:447:ASP:H	1.47	0.77
1:B:429:ARG:NH1	1:B:458:ILE:HG12	1.99	0.77
1:D:157:LYS:HB3	1:D:220:GLU:HG2	1.66	0.77
1:D:299:VAL:HG22	1:D:308:TRP:HB2	1.66	0.76
1:C:299:VAL:HG22	1:C:308:TRP:HB2	1.68	0.76
1:C:493:ARG:HE	1:C:494:PRO:HD2	1.51	0.76
1:D:248:HIS:CE1	4:D:1536:UAG:H262	2.21	0.75
1:A:299:VAL:HG22	1:A:308:TRP:HB2	1.65	0.75
1:B:338:ARG:NH1	1:B:373:ARG:HG3	2.01	0.75
1:A:39:LEU:HG	1:A:134:LEU:HD22	1.69	0.75
1:B:429:ARG:HH12	1:B:458:ILE:HG12	1.50	0.75
1:A:82:THR:HG22	1:A:87:HIS:NE2	2.01	0.75
1:D:157:LYS:HB2	2:D:1534:ADP:O2B	1.87	0.75
1:C:298:THR:H	1:C:307:HIS:HD2	1.35	0.73
1:B:469:VAL:O	1:B:469:VAL:HG12	1.88	0.72
1:B:69:ALA:O	1:B:72:VAL:HG13	1.88	0.72
1:A:446:THR:HG23	1:A:478:ILE:O	1.90	0.72
1:B:297:ILE:HA	1:B:307:HIS:HD2	1.55	0.72
1:C:158:THR:HB	2:C:1533:ADP:O2A	1.91	0.71
1:B:299:VAL:HG22	1:B:308:TRP:HB2	1.72	0.71
1:D:446:THR:HG23	1:D:478:ILE:O	1.89	0.71
1:C:198:GLU:HG3	4:C:1535:UAG:O6'	1.91	0.71
1:D:248:HIS:HE1	4:D:1536:UAG:H262	1.54	0.71
1:B:446:THR:HG23	1:B:478:ILE:O	1.91	0.70
1:C:383:ARG:CG	1:C:383:ARG:HH11	2.03	0.70
1:A:116:ARG:HG2	1:A:116:ARG:O	1.92	0.70
1:D:469:VAL:HG12	1:D:471:GLY:H	1.57	0.70
1:D:69:ALA:O	1:D:72:VAL:HG13	1.92	0.70
1:C:424:ARG:HG3	1:C:424:ARG:NH1	1.91	0.69

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:124:HIS:ND1	1:D:125:PRO:O	2.25	0.69
1:A:151:ILE:HD13	1:A:160:THR:HG22	1.74	0.69
1:D:298:THR:H	1:D:307:HIS:HD2	1.41	0.69
1:C:39:LEU:HG	1:C:134:LEU:HD22	1.75	0.69
1:C:151:ILE:HD13	1:C:160:THR:HG22	1.73	0.69
1:D:96:ILE:HD11	1:D:117:ALA:HB1	1.74	0.69
4:A:1536:UAG:O1B	4:A:1536:UAG:H5'1	1.92	0.68
1:A:69:ALA:O	1:A:72:VAL:HG13	1.93	0.68
1:C:98:ARG:C	1:D:74:PRO:HG2	2.14	0.68
1:D:437:ALA:HB1	1:D:469:VAL:HG22	1.73	0.68
1:C:157:LYS:HB3	1:C:220:GLU:HG2	1.76	0.68
1:A:187:GLY:HA2	1:B:517:PRO:CA	2.23	0.68
1:B:466:ALA:O	1:B:469:VAL:HG23	1.94	0.67
1:D:335:ILE:HD12	1:D:366:VAL:HG23	1.76	0.67
1:C:74:PRO:HG2	1:D:98:ARG:C	2.13	0.67
1:D:151:ILE:HD13	1:D:160:THR:HG22	1.76	0.67
1:C:437:ALA:O	1:C:473:ALA:HB2	1.95	0.67
1:D:378:LEU:HD12	1:D:390:LEU:HD23	1.77	0.67
1:C:157:LYS:O	1:C:161:THR:HG23	1.95	0.66
1:A:298:THR:H	1:A:307:HIS:HD2	1.44	0.66
1:D:96:ILE:CD1	1:D:117:ALA:HB1	2.26	0.66
1:A:141:HIS:HB3	1:A:144:GLU:HG3	1.78	0.66
1:C:446:THR:HG23	1:C:478:ILE:O	1.96	0.66
1:C:165:GLU:OE2	1:C:169:ARG:HD3	1.94	0.66
1:D:54:ARG:HA	1:D:57:THR:HG22	1.77	0.66
1:A:404:LEU:HD21	1:A:416:VAL:HG21	1.77	0.66
1:D:43:VAL:HG13	1:D:124:HIS:CD2	2.32	0.65
1:C:469:VAL:HG23	1:C:473:ALA:HB3	1.78	0.65
1:C:424:ARG:HH11	1:C:424:ARG:CG	2.03	0.65
1:B:338:ARG:NH2	1:B:380:GLN:HG3	2.12	0.65
1:A:437:ALA:O	1:A:473:ALA:HB2	1.98	0.64
1:C:82:THR:HG22	1:C:87:HIS:CD2	2.32	0.64
1:A:392:ASP:OD1	2:A:1533:ADP:O3'	2.12	0.64
1:B:235:ARG:HD2	1:B:235:ARG:N	2.13	0.64
1:A:382:ASP:OD1	1:B:383:ARG:HG2	1.98	0.63
1:C:518:PHE:HE2	1:C:520:ASP:OD2	1.81	0.63
1:C:404:LEU:HD21	1:C:416:VAL:HG21	1.80	0.63
1:A:82:THR:HG22	1:A:87:HIS:CD2	2.34	0.63
1:B:437:ALA:O	1:B:473:ALA:HB2	1.99	0.63
1:B:263:ALA:HA	1:B:289:MET:SD	2.38	0.63
1:C:96:ILE:HD11	1:C:117:ALA:HB1	1.80	0.63

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:297:ILE:HA	1:B:307:HIS:CD2	2.33	0.62
1:A:157:LYS:O	1:A:161:THR:HG23	1.99	0.62
1:D:297:ILE:HA	1:D:307:HIS:HD2	1.65	0.62
1:A:34:VAL:HG11	1:A:39:LEU:HD13	1.80	0.62
1:B:151:ILE:HD13	1:B:160:THR:HG22	1.81	0.62
1:A:515:VAL:HG13	1:B:187:GLY:H	1.64	0.62
1:B:157:LYS:O	1:B:161:THR:HG23	1.99	0.62
1:A:116:ARG:CG	1:A:116:ARG:O	2.46	0.62
1:B:82:THR:HG22	1:B:87:HIS:CD2	2.34	0.62
1:D:367:PRO:HA	1:D:370:ARG:NH1	2.15	0.62
1:B:275:ARG:HE	1:D:235:ARG:NH2	1.97	0.62
1:A:456:THR:HB	1:C:90:ARG:HD3	1.82	0.62
1:C:69:ALA:O	1:C:72:VAL:HG13	2.00	0.62
1:B:183:ILE:HD12	1:B:192:SER:HB3	1.83	0.61
1:B:378:LEU:HD12	1:B:390:LEU:HD23	1.81	0.61
1:C:353:ALA:O	1:C:357:THR:HG23	2.00	0.61
1:B:415:ALA:HB2	1:B:491:TRP:CZ3	2.36	0.61
1:A:43:VAL:HG22	1:A:130:VAL:CG2	2.31	0.61
1:D:518:PHE:HE2	1:D:520:ASP:OD2	1.83	0.61
1:A:319:GLY:HA3	1:A:380:GLN:HE22	1.65	0.61
1:C:124:HIS:ND1	1:C:125:PRO:O	2.33	0.61
1:A:266:PHE:HB3	1:A:293:ALA:HB2	1.83	0.61
1:C:450:PRO:O	1:C:453:GLU:HB3	1.99	0.61
1:A:446:THR:HG22	1:A:447:ASP:H	1.65	0.61
1:B:516:ARG:HB3	1:B:516:ARG:CZ	2.31	0.61
1:C:68:ARG:HA	4:C:1535:UAG:O2	2.01	0.61
1:B:69:ALA:O	1:B:72:VAL:CG1	2.49	0.60
1:D:224:HIS:NE2	4:D:1536:UAG:H231	2.16	0.60
1:D:437:ALA:O	1:D:473:ALA:HB2	2.01	0.60
1:B:422:GLY:HA2	1:B:453:GLU:OE2	2.01	0.60
1:C:335:ILE:HD12	1:C:366:VAL:HG23	1.83	0.60
1:A:297:ILE:HA	1:A:307:HIS:HD2	1.64	0.60
1:C:446:THR:HG22	1:C:447:ASP:H	1.66	0.59
1:A:183:ILE:HD12	1:A:192:SER:HB3	1.83	0.59
1:B:298:THR:H	1:B:307:HIS:HD2	1.47	0.59
1:A:115:GLY:O	1:A:116:ARG:NH1	2.35	0.59
1:C:43:VAL:HG13	1:C:124:HIS:CD2	2.36	0.59
1:C:183:ILE:HD12	1:C:192:SER:HB3	1.84	0.59
1:C:517:PRO:CG	1:D:172:GLY:HA2	2.29	0.59
1:C:297:ILE:HA	1:C:307:HIS:HD2	1.68	0.59
1:B:115:GLY:O	1:B:116:ARG:CG	2.51	0.59

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:380:GLN:NE2	1:B:388:LEU:HD11	2.18	0.58
1:C:43:VAL:HG22	1:C:130:VAL:CG2	2.32	0.58
1:D:404:LEU:HD21	1:D:416:VAL:HG21	1.84	0.58
1:A:67:LEU:O	4:A:1536:UAG:O2'	2.20	0.58
1:B:149:ILE:HD11	1:B:358:VAL:HG21	1.84	0.58
1:D:337:ILE:HD13	1:D:338:ARG:H	1.67	0.58
1:A:104:LEU:HD13	1:A:127:PRO:HB3	1.84	0.58
1:D:380:GLN:NE2	1:D:388:LEU:HD11	2.17	0.58
1:C:259:PHE:CE2	1:C:289:MET:HG2	2.39	0.58
1:C:337:ILE:HD13	1:C:338:ARG:H	1.67	0.58
1:A:456:THR:CB	1:C:90:ARG:HD3	2.34	0.57
1:D:415:ALA:HB2	1:D:491:TRP:CZ3	2.40	0.57
1:B:337:ILE:HD13	1:B:338:ARG:H	1.70	0.57
1:B:467:ALA:O	1:B:469:VAL:N	2.33	0.57
1:B:327:ASP:HB2	1:B:328:PRO:CD	2.35	0.57
1:A:157:LYS:HB3	1:A:220:GLU:HG2	1.87	0.57
1:C:518:PHE:CZ	1:C:523:GLU:HG3	2.40	0.57
4:D:1536:UAG:O5B	4:D:1536:UAG:O2B	2.22	0.56
1:D:144:GLU:HG2	1:D:235:ARG:HD3	1.87	0.56
1:B:467:ALA:C	1:B:469:VAL:H	2.08	0.56
1:A:43:VAL:HG22	1:A:130:VAL:HG22	1.87	0.56
1:B:281:ILE:O	1:B:281:ILE:HG22	2.05	0.56
1:A:187:GLY:HA2	1:B:517:PRO:HA	1.86	0.56
1:B:43:VAL:HG13	1:B:124:HIS:CD2	2.40	0.56
1:C:173:ARG:HH22	1:C:358:VAL:HG13	1.71	0.56
1:A:224:HIS:O	1:A:228:LEU:HD22	2.06	0.56
1:C:267:ASP:HB3	1:C:270:SER:HB2	1.86	0.56
1:D:267:ASP:HB3	1:D:270:SER:HB2	1.88	0.56
1:D:85:THR:HB	4:D:1536:UAG:O1A	2.05	0.56
1:D:106:ASP:HB2	1:D:107:PRO:CD	2.36	0.56
1:B:181:ILE:HA	1:B:505:HIS:CD2	2.41	0.56
1:A:417:VAL:HG13	1:A:500:ILE:HD13	1.88	0.56
1:B:410:PRO:O	1:B:411:ASP:HB2	2.06	0.56
1:B:106:ASP:HB2	1:B:107:PRO:CD	2.36	0.55
1:A:33:GLY:HA3	1:A:61:THR:HG22	1.87	0.55
1:A:176:GLY:HA2	1:A:184:ARG:O	2.06	0.55
1:B:446:THR:HG22	1:B:447:ASP:N	2.19	0.55
1:A:43:VAL:HG13	1:A:124:HIS:CD2	2.41	0.55
1:A:418:PHE:HB3	1:A:501:ALA:HB3	1.88	0.55
1:A:380:GLN:NE2	1:A:388:LEU:HD11	2.22	0.55
1:C:415:ALA:HB2	1:C:491:TRP:CZ3	2.41	0.55

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:469:VAL:O	1:B:469:VAL:CG1	2.55	0.55
1:C:404:LEU:HD21	1:C:416:VAL:CG2	2.36	0.55
1:C:151:ILE:HD13	1:C:160:THR:CG2	2.37	0.55
1:B:424:ARG:O	1:B:426:PRO:HD3	2.05	0.55
1:C:327:ASP:HB2	1:C:328:PRO:CD	2.36	0.55
1:D:443:VAL:HG22	1:D:475:VAL:HB	1.88	0.55
1:A:410:PRO:O	1:A:411:ASP:HB2	2.06	0.55
1:C:34:VAL:HG11	1:C:39:LEU:HD13	1.88	0.55
1:A:338:ARG:HG2	1:A:338:ARG:O	2.07	0.55
1:A:409:HIS:HB3	1:A:412:ARG:HE	1.72	0.54
1:A:297:ILE:HA	1:A:307:HIS:CD2	2.42	0.54
1:B:259:PHE:CE2	1:B:289:MET:HG2	2.42	0.54
1:D:181:ILE:HG23	1:D:505:HIS:CD2	2.42	0.54
1:B:33:GLY:HA3	1:B:61:THR:HG22	1.90	0.54
1:B:404:LEU:HD21	1:B:416:VAL:HG21	1.90	0.54
1:B:518:PHE:HE2	1:B:520:ASP:OD2	1.89	0.54
1:D:266:PHE:HB3	1:D:293:ALA:HB2	1.88	0.54
1:C:493:ARG:NE	1:C:494:PRO:HD2	2.20	0.54
1:C:297:ILE:HA	1:C:307:HIS:CD2	2.43	0.54
1:B:317:ASP:O	1:B:318:ALA:HB3	2.08	0.54
1:D:183:ILE:HD12	1:D:192:SER:HB3	1.89	0.54
1:D:394:ALA:HB2	2:D:1534:ADP:O3'	2.08	0.54
1:C:263:ALA:HA	1:C:289:MET:SD	2.48	0.54
1:A:388:LEU:HB3	1:A:497:VAL:HB	1.90	0.53
1:B:173:ARG:HH22	1:B:358:VAL:HG13	1.72	0.53
1:D:86:THR:OG1	1:D:87:HIS:N	2.40	0.53
1:A:33:GLY:HA3	1:A:61:THR:CG2	2.39	0.53
1:C:27:ARG:HG3	1:C:28:PRO:CD	2.34	0.53
1:A:173:ARG:HH22	1:A:358:VAL:HG13	1.72	0.53
1:D:518:PHE:CZ	1:D:523:GLU:HG3	2.44	0.53
1:D:404:LEU:HD21	1:D:416:VAL:CG2	2.37	0.53
1:D:418:PHE:HB3	1:D:501:ALA:HB3	1.91	0.53
1:D:240:ALA:HB2	1:D:354:ILE:HD11	1.90	0.53
1:A:54:ARG:HA	1:A:57:THR:HG22	1.90	0.53
1:B:418:PHE:HB3	1:B:501:ALA:HB3	1.91	0.53
1:D:297:ILE:HA	1:D:307:HIS:CD2	2.43	0.53
1:D:319:GLY:HA3	1:D:380:GLN:HE22	1.73	0.53
1:A:415:ALA:HB2	1:A:491:TRP:CZ3	2.44	0.53
1:C:443:VAL:HG22	1:C:475:VAL:HB	1.91	0.52
1:A:263:ALA:HA	1:A:289:MET:SD	2.49	0.52
1:A:443:VAL:HG22	1:A:475:VAL:HB	1.92	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:298:THR:N	1:C:307:HIS:HD2	2.06	0.52
1:D:176:GLY:HA2	1:D:184:ARG:O	2.10	0.52
1:C:132:GLY:HA3	1:C:232:ASP:HB2	1.91	0.52
1:A:187:GLY:HA2	1:B:517:PRO:CB	2.40	0.52
1:A:187:GLY:HA3	1:B:515:VAL:HG22	1.91	0.52
1:B:409:HIS:CD2	1:B:410:PRO:O	2.63	0.52
1:C:266:PHE:HB3	1:C:293:ALA:HB2	1.92	0.52
1:B:104:LEU:HD13	1:B:127:PRO:HB3	1.92	0.51
1:A:518:PHE:HE2	1:A:520:ASP:OD2	1.92	0.51
1:D:157:LYS:CB	2:D:1534:ADP:O2B	2.56	0.51
1:A:187:GLY:HA2	1:B:517:PRO:HB3	1.91	0.51
1:A:399:ALA:O	1:A:403:VAL:HG23	2.11	0.51
1:A:151:ILE:HD12	1:A:161:THR:HG22	1.91	0.51
1:D:263:ALA:HA	1:D:289:MET:SD	2.50	0.51
1:B:275:ARG:HE	1:D:235:ARG:HH21	1.57	0.51
1:A:104:LEU:CD1	1:A:127:PRO:HB3	2.41	0.51
1:D:173:ARG:HH22	1:D:358:VAL:HG13	1.75	0.51
1:D:446:THR:HG22	1:D:447:ASP:H	1.75	0.51
1:B:468:GLU:C	1:B:470:GLY:H	2.14	0.51
1:C:173:ARG:HH22	1:C:358:VAL:CG1	2.23	0.51
1:D:317:ASP:O	1:D:318:ALA:HB3	2.11	0.51
1:C:158:THR:OG1	2:C:1533:ADP:O3B	2.15	0.51
1:C:33:GLY:HA3	1:C:61:THR:CG2	2.41	0.51
1:A:404:LEU:HD21	1:A:416:VAL:CG2	2.41	0.51
1:D:159:THR:HG23	1:D:374:VAL:HG11	1.92	0.50
1:A:327:ASP:HB2	1:A:328:PRO:CD	2.42	0.50
1:C:310:ALA:O	1:C:311:THR:HG23	2.11	0.50
1:C:358:VAL:CG1	1:C:358:VAL:O	2.59	0.50
1:C:317:ASP:O	1:C:318:ALA:HB3	2.11	0.50
1:D:267:ASP:O	1:D:273:ARG:HB2	2.11	0.50
1:C:104:LEU:HD13	1:C:127:PRO:HB3	1.93	0.50
1:C:149:ILE:HD11	1:C:358:VAL:HG21	1.94	0.50
1:B:259:PHE:CZ	1:B:289:MET:HG2	2.46	0.50
1:C:446:THR:CG2	1:C:481:ARG:HA	2.32	0.50
1:B:43:VAL:HG22	1:B:130:VAL:CG2	2.42	0.50
1:B:220:GLU:OE1	2:B:1534:ADP:O3B	2.30	0.50
1:A:96:ILE:HD11	1:A:117:ALA:HB1	1.92	0.50
1:C:380:GLN:NE2	1:C:388:LEU:HD11	2.27	0.50
1:B:33:GLY:HA3	1:B:61:THR:CG2	2.42	0.50
1:A:518:PHE:CZ	1:A:523:GLU:HG3	2.46	0.50
1:B:267:ASP:HB3	1:B:270:SER:HB2	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:86:THR:CG2	4:D:1536:UAG:H5'2	2.30	0.50
1:C:86:THR:OG1	1:C:87:HIS:N	2.45	0.50
1:A:404:LEU:CD2	1:A:416:VAL:HG21	2.42	0.50
1:A:260:GLU:HA	1:A:260:GLU:OE1	2.12	0.50
1:A:515:VAL:HG13	1:A:515:VAL:O	2.12	0.49
1:C:104:LEU:HD23	1:C:122:LEU:HB3	1.93	0.49
1:D:409:HIS:CD2	1:D:410:PRO:O	2.64	0.49
1:A:281:ILE:O	1:A:281:ILE:HG22	2.12	0.49
1:C:422:GLY:C	1:C:424:ARG:H	2.15	0.49
1:C:417:VAL:HB	1:C:444:VAL:HB	1.94	0.49
1:A:298:THR:N	1:A:307:HIS:HD2	2.09	0.49
4:B:1536:UAG:O1B	4:B:1536:UAG:O2A	2.31	0.49
1:A:337:ILE:HD13	1:A:338:ARG:H	1.77	0.49
1:D:358:VAL:O	1:D:358:VAL:CG1	2.60	0.49
1:C:418:PHE:HB3	1:C:501:ALA:HB3	1.95	0.49
1:B:338:ARG:CZ	1:B:373:ARG:HG3	2.42	0.49
1:A:69:ALA:O	1:A:72:VAL:CG1	2.61	0.49
1:C:69:ALA:O	1:C:72:VAL:CG1	2.61	0.48
1:A:52:ALA:C	1:A:54:ARG:N	2.66	0.48
1:B:399:ALA:O	1:B:403:VAL:HG23	2.13	0.48
1:A:409:HIS:CB	1:A:412:ARG:NH2	2.65	0.48
1:B:43:VAL:HG22	1:B:130:VAL:HG22	1.94	0.48
1:C:281:ILE:HG22	1:C:281:ILE:O	2.12	0.48
1:D:224:HIS:O	1:D:228:LEU:HD22	2.14	0.48
1:C:43:VAL:HG22	1:C:130:VAL:HG22	1.93	0.48
1:B:116:ARG:O	1:B:116:ARG:CG	2.61	0.48
1:B:362:PRO:O	1:B:366:VAL:HB	2.13	0.48
1:A:27:ARG:NH2	1:A:76:ASP:OD2	2.45	0.48
1:A:454:ASP:HA	1:A:455:PRO:HD3	1.61	0.48
1:B:298:THR:N	1:B:307:HIS:HD2	2.12	0.48
1:A:308:TRP:CE2	1:A:328:PRO:HD3	2.49	0.48
1:D:259:PHE:CE2	1:D:289:MET:HG2	2.49	0.48
1:B:266:PHE:HB3	1:B:293:ALA:HB2	1.95	0.48
1:D:33:GLY:HA3	1:D:61:THR:HG22	1.95	0.48
1:B:425:ASP:OD2	1:B:428:LYS:HB3	2.14	0.48
1:C:196:THR:HB	1:C:225:ALA:HB2	1.96	0.48
1:B:151:ILE:HD13	1:B:160:THR:CG2	2.43	0.48
1:A:409:HIS:CD2	1:A:410:PRO:O	2.67	0.47
1:B:106:ASP:HB2	1:B:107:PRO:HD2	1.96	0.47
2:D:1534:ADP:O2A	2:D:1534:ADP:O3B	2.31	0.47
1:C:33:GLY:HA3	1:C:61:THR:HG22	1.94	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:240:ALA:HA	1:B:278:VAL:O	2.14	0.47
1:A:327:ASP:HB2	1:A:328:PRO:HD2	1.96	0.47
1:D:287:ARG:HD2	1:D:304:ARG:NH1	2.29	0.47
1:D:223:SER:HG	1:D:258:TYR:HE1	1.62	0.47
1:B:64:GLY:HA3	1:B:76:ASP:OD1	2.13	0.47
1:C:72:VAL:HG23	1:C:73:SER:O	2.14	0.47
1:B:358:VAL:CG1	1:B:358:VAL:O	2.61	0.47
1:C:366:VAL:N	1:C:367:PRO:CD	2.77	0.47
1:B:518:PHE:CZ	1:B:523:GLU:HG3	2.49	0.47
1:A:27:ARG:HG3	1:A:28:PRO:CD	2.36	0.47
1:A:353:ALA:O	1:A:357:THR:HG23	2.15	0.47
1:C:82:THR:HG23	1:C:106:ASP:OD2	2.15	0.47
1:B:366:VAL:N	1:B:367:PRO:CD	2.78	0.47
1:A:250:ASP:N	1:A:250:ASP:OD2	2.48	0.47
1:C:327:ASP:OD1	1:C:331:VAL:HB	2.15	0.47
1:C:224:HIS:O	1:C:228:LEU:HD22	2.15	0.47
1:C:98:ARG:O	1:D:74:PRO:CG	2.55	0.47
1:A:358:VAL:CG1	1:A:358:VAL:O	2.62	0.47
1:A:48:ALA:HB3	1:A:121:VAL:HB	1.96	0.47
1:D:298:THR:N	1:D:307:HIS:HD2	2.08	0.46
1:A:169:ARG:HD2	1:B:517:PRO:HG2	1.96	0.46
1:C:287:ARG:HD2	1:C:304:ARG:NH1	2.30	0.46
1:A:447:ASP:OD1	1:A:459:ARG:NH1	2.47	0.46
1:C:74:PRO:HD3	1:D:74:PRO:HD3	1.97	0.46
1:D:106:ASP:HA	1:D:124:HIS:O	2.16	0.46
1:B:335:ILE:HG13	1:B:352:LEU:HD11	1.96	0.46
1:D:158:THR:OG1	2:D:1534:ADP:O3B	2.25	0.46
1:C:259:PHE:CZ	1:C:289:MET:HG2	2.51	0.46
1:D:69:ALA:O	1:D:72:VAL:CG1	2.60	0.46
1:C:399:ALA:O	1:C:403:VAL:HG23	2.15	0.46
1:C:96:ILE:CD1	1:C:117:ALA:HB1	2.46	0.46
1:A:417:VAL:HB	1:A:444:VAL:HB	1.98	0.46
1:D:72:VAL:HG23	1:D:73:SER:O	2.15	0.46
1:A:60:ARG:HG2	1:A:60:ARG:NH1	2.30	0.46
1:B:82:THR:HG23	1:B:106:ASP:OD2	2.15	0.46
1:C:327:ASP:HB2	1:C:328:PRO:HD2	1.96	0.46
1:C:335:ILE:HG13	1:C:352:LEU:HD11	1.96	0.46
1:A:421:GLY:HA2	1:A:448:ASP:O	2.16	0.46
1:C:469:VAL:CG2	1:C:473:ALA:HB3	2.45	0.46
1:A:425:ASP:O	1:A:428:LYS:HG2	2.15	0.46
1:D:335:ILE:HG13	1:D:352:LEU:HD11	1.97	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:151:ILE:HD13	1:D:160:THR:CG2	2.43	0.46
1:A:267:ASP:HB3	1:A:270:SER:HB2	1.96	0.46
1:C:249:LEU:HD12	1:C:249:LEU:HA	1.74	0.46
1:B:104:LEU:HD23	1:B:122:LEU:HB3	1.97	0.45
1:D:310:ALA:HA	1:D:324:THR:O	2.16	0.45
1:C:409:HIS:CD2	1:C:410:PRO:O	2.68	0.45
1:C:74:PRO:HG2	1:D:98:ARG:CA	2.46	0.45
1:B:86:THR:OG1	1:B:87:HIS:N	2.48	0.45
1:B:281:ILE:O	1:B:281:ILE:CG2	2.63	0.45
1:D:327:ASP:HB2	1:D:328:PRO:CD	2.46	0.45
1:A:198:GLU:OE1	4:A:1536:UAG:O6'	2.32	0.45
1:B:532:GLU:OE1	1:B:532:GLU:HA	2.16	0.45
1:A:446:THR:CG2	1:A:481:ARG:HA	2.37	0.45
1:C:125:PRO:O	1:C:126:ALA:C	2.53	0.45
1:C:43:VAL:HG22	1:C:130:VAL:HG21	1.98	0.45
1:A:72:VAL:HG23	1:A:73:SER:O	2.16	0.45
1:B:275:ARG:CZ	1:D:144:GLU:OE1	2.65	0.45
1:A:259:PHE:CE2	1:A:289:MET:HG2	2.51	0.45
1:D:104:LEU:HD13	1:D:127:PRO:HB3	1.99	0.45
1:B:248:HIS:CE1	4:B:1536:UAG:O21	2.68	0.45
1:B:281:ILE:HG12	1:B:298:THR:HB	1.97	0.45
1:D:46:ALA:O	1:D:122:LEU:HA	2.16	0.45
1:A:240:ALA:HA	1:A:278:VAL:O	2.16	0.45
1:B:106:ASP:HA	1:B:124:HIS:O	2.17	0.45
1:B:159:THR:HG23	1:B:374:VAL:HG11	1.99	0.45
1:B:447:ASP:OD1	1:B:459:ARG:NH1	2.50	0.45
1:A:159:THR:HG23	1:A:374:VAL:HG11	1.98	0.45
1:D:125:PRO:O	1:D:126:ALA:C	2.54	0.45
1:C:273:ARG:NH2	1:C:295:ASP:OD2	2.48	0.45
1:D:376:GLY:O	1:D:392:ASP:HA	2.16	0.45
1:B:240:ALA:HB2	1:B:354:ILE:HD11	1.98	0.45
1:D:250:ASP:N	1:D:250:ASP:OD2	2.48	0.45
1:A:335:ILE:HG13	1:A:352:LEU:HD11	1.98	0.45
1:D:39:LEU:HD12	1:D:39:LEU:HA	1.69	0.45
1:D:43:VAL:HG22	1:D:130:VAL:CG2	2.47	0.45
1:B:417:VAL:HB	1:B:444:VAL:HB	1.99	0.45
1:B:297:ILE:CA	1:B:307:HIS:HD2	2.27	0.45
1:B:455:PRO:HA	1:B:458:ILE:HD12	1.99	0.45
1:D:367:PRO:O	1:D:371:GLU:HG2	2.17	0.45
1:C:404:LEU:CD2	1:C:416:VAL:HG21	2.45	0.45
1:C:260:GLU:OE1	1:C:292:ARG:NH2	2.50	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:399:ALA:O	1:D:403:VAL:HG23	2.16	0.45
1:B:404:LEU:HD21	1:B:416:VAL:CG2	2.46	0.45
1:B:68:ARG:O	1:B:69:ALA:C	2.56	0.44
1:B:275:ARG:NH2	1:D:144:GLU:OE1	2.51	0.44
1:A:46:ALA:O	1:A:122:LEU:HA	2.17	0.44
1:A:106:ASP:HA	1:A:124:HIS:O	2.17	0.44
1:D:132:GLY:HA2	1:D:199:ALA:HB1	1.99	0.44
1:C:421:GLY:HA2	1:C:448:ASP:O	2.18	0.44
1:A:105:THR:O	1:A:123:VAL:HA	2.18	0.44
1:B:60:ARG:HG2	1:B:60:ARG:NH1	2.32	0.44
1:A:374:VAL:HG23	1:A:375:PRO:HD2	2.00	0.44
1:A:125:PRO:O	1:A:126:ALA:C	2.54	0.44
1:D:353:ALA:O	1:D:357:THR:HG23	2.17	0.44
1:A:412:ARG:HD2	1:A:497:VAL:HG12	1.98	0.44
1:C:74:PRO:CG	1:D:98:ARG:O	2.56	0.44
1:C:281:ILE:CG2	1:C:281:ILE:O	2.65	0.44
1:A:454:ASP:CB	1:C:86:THR:HB	2.48	0.44
1:C:455:PRO:HA	1:C:458:ILE:HD12	1.99	0.44
1:B:132:GLY:HA2	1:B:199:ALA:HB1	1.99	0.44
1:A:151:ILE:HD13	1:A:160:THR:CG2	2.43	0.44
1:C:151:ILE:HD12	1:C:161:THR:HG22	1.99	0.44
1:D:33:GLY:HA3	1:D:61:THR:CG2	2.48	0.44
1:C:429:ARG:HB2	1:C:461:GLU:HG2	1.99	0.44
1:B:145:ARG:HA	1:D:145:ARG:O	2.18	0.44
1:C:392:ASP:CG	2:C:1533:ADP:HO3'	2.20	0.44
1:C:308:TRP:CE2	1:C:328:PRO:HD3	2.53	0.44
1:C:43:VAL:CG1	1:C:124:HIS:CD2	3.01	0.44
1:D:380:GLN:HE21	1:D:388:LEU:HD11	1.83	0.44
1:D:343:TYR:CD2	1:D:406:THR:HG21	2.53	0.44
1:D:421:GLY:HA2	1:D:448:ASP:O	2.18	0.44
1:A:49:GLU:OE2	1:A:49:GLU:HA	2.17	0.44
1:C:106:ASP:HA	1:C:124:HIS:O	2.18	0.43
1:D:367:PRO:HA	1:D:370:ARG:HH12	1.82	0.43
1:A:273:ARG:NH2	1:A:295:ASP:OD2	2.48	0.43
1:C:240:ALA:HA	1:C:278:VAL:O	2.17	0.43
1:B:353:ALA:O	1:B:357:THR:HG23	2.18	0.43
1:B:54:ARG:O	1:B:55:ALA:HB3	2.19	0.43
1:A:86:THR:OG1	1:A:87:HIS:N	2.51	0.43
1:A:260:GLU:OE1	1:A:292:ARG:NH2	2.50	0.43
1:B:336:GLY:O	1:B:370:ARG:HA	2.18	0.43
1:D:281:ILE:O	1:D:281:ILE:HG22	2.17	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:380:GLN:HE21	1:A:388:LEU:HD11	1.84	0.43
1:B:27:ARG:HG3	1:B:28:PRO:CD	2.38	0.43
1:C:165:GLU:OE2	1:C:169:ARG:NH1	2.50	0.43
1:A:43:VAL:HG22	1:A:130:VAL:HG21	2.00	0.43
1:D:417:VAL:HG13	1:D:500:ILE:HD13	2.00	0.43
1:D:157:LYS:O	1:D:161:THR:HG23	2.19	0.43
1:D:308:TRP:CE2	1:D:328:PRO:HD3	2.54	0.43
1:C:127:PRO:C	1:C:129:GLY:N	2.72	0.43
1:D:374:VAL:HG23	1:D:375:PRO:HD2	2.01	0.43
1:D:366:VAL:N	1:D:367:PRO:CD	2.82	0.43
1:B:376:GLY:O	1:B:392:ASP:HA	2.19	0.43
1:D:395:HIS:N	1:D:395:HIS:ND1	2.67	0.43
1:A:154:THR:OG1	1:A:244:LEU:HA	2.18	0.43
1:B:443:VAL:HG22	1:B:475:VAL:HB	2.00	0.43
1:D:362:PRO:O	1:D:366:VAL:HB	2.19	0.42
1:C:185:VAL:HB	1:C:188:ALA:HB3	2.01	0.42
1:C:100:ALA:O	1:C:119:VAL:HG11	2.19	0.42
1:B:72:VAL:HG23	1:B:73:SER:O	2.19	0.42
1:D:240:ALA:CB	1:D:354:ILE:HD11	2.49	0.42
1:B:310:ALA:HA	1:B:324:THR:O	2.19	0.42
1:B:173:ARG:HH22	1:B:358:VAL:CG1	2.33	0.42
1:C:343:TYR:CD2	1:C:406:THR:HG21	2.55	0.42
1:A:106:ASP:HB2	1:A:107:PRO:CD	2.50	0.42
1:A:68:ARG:HA	4:A:1536:UAG:O2	2.20	0.42
1:B:30:ALA:CB	1:C:514:ARG:CB	2.98	0.42
1:A:90:ARG:HB3	1:C:456:THR:HG21	2.01	0.42
1:D:446:THR:CG2	1:D:481:ARG:HA	2.36	0.42
1:A:132:GLY:HA3	1:A:232:ASP:HB2	2.01	0.42
1:D:109:GLY:O	1:D:113:ILE:HD12	2.20	0.42
1:B:377:ARG:HE	2:B:1534:ADP:PA	2.42	0.42
1:D:149:ILE:HD11	1:D:358:VAL:HG21	2.02	0.42
1:B:287:ARG:HD2	1:B:304:ARG:NH1	2.34	0.42
1:B:273:ARG:NH2	1:B:295:ASP:OD2	2.51	0.42
1:C:272:LEU:O	1:C:273:ARG:C	2.59	0.42
1:A:196:THR:HA	1:A:197:PRO:HD3	1.79	0.42
1:C:98:ARG:CA	1:D:74:PRO:HG2	2.50	0.41
1:B:289:MET:HA	1:B:289:MET:HE3	2.02	0.41
1:A:335:ILE:HG22	1:A:336:GLY:N	2.35	0.41
1:C:447:ASP:OD1	1:C:459:ARG:NH1	2.54	0.41
1:D:260:GLU:OE1	1:D:292:ARG:NH2	2.53	0.41
1:B:238:VAL:HA	1:B:276:THR:O	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:ARG:HH11	1:B:458:ILE:HG23	1.85	0.41
1:A:293:ALA:O	1:A:295:ASP:N	2.52	0.41
1:A:428:LYS:O	1:A:432:MET:HG3	2.20	0.41
1:B:242:THR:O	1:B:280:CYS:HB3	2.20	0.41
1:D:104:LEU:HD23	1:D:122:LEU:HB3	2.01	0.41
4:A:1536:UAG:O1A	4:A:1536:UAG:O2B	2.38	0.41
1:D:388:LEU:HB3	1:D:497:VAL:HB	2.02	0.41
1:C:293:ALA:O	1:C:294:ALA:HB3	2.20	0.41
1:D:259:PHE:CZ	1:D:289:MET:HG2	2.55	0.41
1:A:238:VAL:HA	1:A:276:THR:O	2.21	0.41
1:A:335:ILE:HD12	1:A:366:VAL:HG23	2.02	0.41
1:A:287:ARG:HD2	1:A:304:ARG:NH1	2.36	0.41
1:C:250:ASP:OD2	1:C:250:ASP:N	2.52	0.41
1:A:317:ASP:O	1:A:318:ALA:HB3	2.20	0.41
1:D:466:ALA:O	1:D:469:VAL:HG23	2.20	0.41
1:A:68:ARG:O	1:A:69:ALA:C	2.59	0.41
1:D:240:ALA:HA	1:D:278:VAL:O	2.21	0.41
1:C:398:GLU:HG2	1:C:399:ALA:N	2.36	0.41
1:C:176:GLY:HA2	1:C:184:ARG:O	2.20	0.41
1:A:409:HIS:HB3	1:A:412:ARG:NE	2.35	0.41
1:B:308:TRP:CE2	1:B:328:PRO:HD3	2.56	0.41
1:D:43:VAL:HG22	1:D:130:VAL:HG22	2.03	0.41
1:B:310:ALA:O	1:B:311:THR:HG23	2.21	0.41
1:D:100:ALA:O	1:D:119:VAL:HG11	2.21	0.41
1:C:158:THR:HB	2:C:1533:ADP:PA	2.60	0.41
1:B:467:ALA:C	1:B:469:VAL:N	2.74	0.41
1:B:260:GLU:OE1	1:B:292:ARG:NH2	2.54	0.41
1:C:101:VAL:O	1:C:102:ALA:HB2	2.21	0.41
1:B:224:HIS:O	1:B:228:LEU:HD22	2.20	0.41
1:B:374:VAL:HG23	1:B:375:PRO:HD2	2.02	0.41
1:D:54:ARG:HA	1:D:57:THR:CG2	2.48	0.41
1:C:358:VAL:O	1:C:358:VAL:HG12	2.21	0.41
1:A:281:ILE:O	1:A:281:ILE:CG2	2.68	0.41
1:D:242:THR:O	1:D:280:CYS:HB3	2.21	0.41
1:D:355:LEU:HB3	1:D:360:VAL:HB	2.03	0.41
1:D:327:ASP:HB2	1:D:328:PRO:HD2	2.03	0.40
1:C:260:GLU:HA	1:C:260:GLU:OE1	2.21	0.40
1:D:157:LYS:CB	1:D:220:GLU:HG2	2.46	0.40
1:C:362:PRO:O	1:C:366:VAL:HB	2.20	0.40
1:C:289:MET:HE3	1:C:289:MET:HA	2.03	0.40
1:D:166:ALA:HA	1:D:169:ARG:NH1	2.37	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:281:ILE:HG12	1:C:298:THR:HB	2.03	0.40
1:A:157:LYS:HE2	1:A:157:LYS:HB2	1.88	0.40
1:B:358:VAL:O	1:B:358:VAL:HG12	2.19	0.40
1:B:417:VAL:HG13	1:B:500:ILE:HD13	2.04	0.40
1:C:446:THR:HG22	1:C:447:ASP:N	2.34	0.40
4:B:1536:UAG:H202	4:B:1536:UAG:O4'	2.21	0.40
1:D:335:ILE:HG22	1:D:336:GLY:N	2.37	0.40
1:A:456:THR:HB	1:C:90:ARG:CD	2.50	0.40
1:B:317:ASP:O	1:B:318:ALA:CB	2.69	0.40
1:A:149:ILE:HD11	1:A:358:VAL:HG21	2.04	0.40
1:B:366:VAL:HG12	1:B:367:PRO:HD3	2.04	0.40
1:A:366:VAL:N	1:A:367:PRO:CD	2.85	0.40
1:D:179:GLY:O	1:D:180:THR:C	2.60	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:269:ASP:O	1:D:269:ASP:O[1_554]	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	495/535 (92%)	453 (92%)	39 (8%)	3 (1%)	30	72
1	B	495/535 (92%)	442 (89%)	46 (9%)	7 (1%)	14	51
1	C	493/535 (92%)	448 (91%)	39 (8%)	6 (1%)	16	56
1	D	477/535 (89%)	439 (92%)	35 (7%)	3 (1%)	30	72
All	All	1960/2140 (92%)	1782 (91%)	159 (8%)	19 (1%)	19	61

All (19) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	423	ASP
1	B	469	VAL
1	C	116	ARG
1	B	468	GLU
1	B	514	ARG
1	C	423	ASP
1	A	246	ARG
1	D	246	ARG
1	D	394	ALA
1	A	425	ASP
1	B	116	ARG
1	C	246	ARG
1	C	425	ASP
1	C	471	GLY
1	D	130	VAL
1	A	130	VAL
1	B	425	ASP
1	C	130	VAL
1	B	471	GLY

5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	341/382 (89%)	285 (84%)	56 (16%)	3 14
1	B	340/382 (89%)	290 (85%)	50 (15%)	4 18
1	C	338/382 (88%)	283 (84%)	55 (16%)	3 14
1	D	332/382 (87%)	279 (84%)	53 (16%)	3 15
All	All	1351/1528 (88%)	1137 (84%)	214 (16%)	3 15

All (214) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	26	LEU
1	A	27	ARG
1	A	31	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	39	LEU
1	A	41	ASP
1	A	47	LEU
1	A	56	VAL
1	A	60	ARG
1	A	67	LEU
1	A	72	VAL
1	A	77	LEU
1	A	82	THR
1	A	104	LEU
1	A	106	ASP
1	A	116	ARG
1	A	138	VAL
1	A	143	SER
1	A	144	GLU
1	A	145	ARG
1	A	168	LEU
1	A	177	LEU
1	A	189	ASP
1	A	212	ARG
1	A	215	ASP
1	A	218	VAL
1	A	228	LEU
1	A	249	LEU
1	A	272	LEU
1	A	289	MET
1	A	292	ARG
1	A	303	ASP
1	A	309	ARG
1	A	337	ILE
1	A	357	THR
1	A	366	VAL
1	A	369	LEU
1	A	374	VAL
1	A	378	LEU
1	A	380	GLN
1	A	383	ARG
1	A	388	LEU
1	A	395	HIS
1	A	401	ARG
1	A	413	ARG
1	A	414	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	417	VAL
1	A	442	LEU
1	A	443	VAL
1	A	446	THR
1	A	451	ARG
1	A	456	THR
1	A	475	VAL
1	A	482	ARG
1	A	497	VAL
1	A	498	VAL
1	A	529	GLU
1	B	27	ARG
1	B	31	VAL
1	B	39	LEU
1	B	47	LEU
1	B	60	ARG
1	B	67	LEU
1	B	72	VAL
1	B	77	LEU
1	B	82	THR
1	B	104	LEU
1	B	106	ASP
1	B	130	VAL
1	B	138	VAL
1	B	143	SER
1	B	145	ARG
1	B	168	LEU
1	B	177	LEU
1	B	189	ASP
1	B	215	ASP
1	B	218	VAL
1	B	249	LEU
1	B	272	LEU
1	B	275	ARG
1	B	289	MET
1	B	309	ARG
1	B	337	ILE
1	B	357	THR
1	B	369	LEU
1	B	374	VAL
1	B	378	LEU
1	B	383	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	388	LEU
1	B	395	HIS
1	B	396	LYS
1	B	401	ARG
1	B	413	ARG
1	B	414	LEU
1	B	417	VAL
1	B	424	ARG
1	B	442	LEU
1	B	451	ARG
1	B	454	ASP
1	B	468	GLU
1	B	475	VAL
1	B	482	ARG
1	B	491	TRP
1	B	497	VAL
1	B	515	VAL
1	B	516	ARG
1	B	529	GLU
1	C	27	ARG
1	C	31	VAL
1	C	39	LEU
1	C	41	ASP
1	C	47	LEU
1	C	56	VAL
1	C	60	ARG
1	C	67	LEU
1	C	72	VAL
1	C	77	LEU
1	C	82	THR
1	C	104	LEU
1	C	130	VAL
1	C	138	VAL
1	C	143	SER
1	C	145	ARG
1	C	168	LEU
1	C	169	ARG
1	C	177	LEU
1	C	189	ASP
1	C	212	ARG
1	C	215	ASP
1	C	218	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	249	LEU
1	C	272	LEU
1	C	275	ARG
1	C	289	MET
1	C	292	ARG
1	C	337	ILE
1	C	338	ARG
1	C	357	THR
1	C	366	VAL
1	C	369	LEU
1	C	374	VAL
1	C	378	LEU
1	C	383	ARG
1	C	388	LEU
1	C	395	HIS
1	C	398	GLU
1	C	401	ARG
1	C	413	ARG
1	C	414	LEU
1	C	417	VAL
1	C	424	ARG
1	C	442	LEU
1	C	446	THR
1	C	451	ARG
1	C	468	GLU
1	C	475	VAL
1	C	482	ARG
1	C	493	ARG
1	C	497	VAL
1	C	515	VAL
1	C	516	ARG
1	C	529	GLU
1	D	27	ARG
1	D	31	VAL
1	D	39	LEU
1	D	41	ASP
1	D	47	LEU
1	D	56	VAL
1	D	60	ARG
1	D	67	LEU
1	D	72	VAL
1	D	77	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	82	THR
1	D	104	LEU
1	D	106	ASP
1	D	130	VAL
1	D	138	VAL
1	D	143	SER
1	D	145	ARG
1	D	168	LEU
1	D	169	ARG
1	D	177	LEU
1	D	189	ASP
1	D	215	ASP
1	D	249	LEU
1	D	272	LEU
1	D	275	ARG
1	D	289	MET
1	D	309	ARG
1	D	317	ASP
1	D	337	ILE
1	D	357	THR
1	D	366	VAL
1	D	369	LEU
1	D	370	ARG
1	D	371	GLU
1	D	374	VAL
1	D	378	LEU
1	D	380	GLN
1	D	383	ARG
1	D	388	LEU
1	D	395	HIS
1	D	401	ARG
1	D	406	THR
1	D	413	ARG
1	D	414	LEU
1	D	417	VAL
1	D	442	LEU
1	D	446	THR
1	D	456	THR
1	D	482	ARG
1	D	497	VAL
1	D	521	ARG
1	D	529	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	D	532	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	307	HIS
1	A	333	HIS
1	A	380	GLN
1	A	409	HIS
1	B	307	HIS
1	B	333	HIS
1	B	380	GLN
1	B	409	HIS
1	C	307	HIS
1	C	321	GLN
1	C	333	HIS
1	C	380	GLN
1	C	409	HIS
1	D	307	HIS
1	D	380	GLN
1	D	409	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

4 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	KCX	A	262	1	7,11,12	1.34	1 (14%)	7,12,14	1.37	2 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
1	KCX	B	262	1	7,11,12	0.45	0	7,12,14	1.92	1 (14%)
1	KCX	C	262	1	7,11,12	0.99	1 (14%)	7,12,14	1.24	2 (28%)
1	KCX	D	262	1	7,11,12	1.07	1 (14%)	7,12,14	1.09	1 (14%)

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	KCX	A	262	1	-	0/6/10/12	0/0/0/0
1	KCX	B	262	1	-	0/6/10/12	0/0/0/0
1	KCX	C	262	1	-	0/6/10/12	0/0/0/0
1	KCX	D	262	1	-	0/6/10/12	0/0/0/0

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	262	KCX	CB-CA	-2.02	1.51	1.53
1	D	262	KCX	CE-NZ	2.12	1.51	1.46
1	A	262	KCX	CE-NZ	2.64	1.52	1.46

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	262	KCX	CE-NZ-CX	-4.77	118.09	123.49
1	A	262	KCX	CE-NZ-CX	-2.72	120.41	123.49
1	C	262	KCX	CE-NZ-CX	-2.20	121.00	123.49
1	D	262	KCX	O-C-CA	-2.05	120.14	125.49
1	C	262	KCX	O-C-CA	-2.04	120.17	125.49
1	A	262	KCX	O-C-CA	-2.04	120.19	125.49

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)

Of 18 ligands modelled in this entry, 10 are monoatomic - leaving 8 for Mogul analysis.

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	ADP	A	1533	3	22,29,29	1.18	2 (9%)	27,45,45	2.14	6 (22%)
4	UAG	A	1536	3	45,60,60	1.80	7 (15%)	61,88,88	2.53	22 (36%)
2	ADP	B	1534	3	22,29,29	1.24	2 (9%)	27,45,45	2.48	8 (29%)
4	UAG	B	1536	3	45,60,60	1.53	5 (11%)	61,88,88	2.43	20 (32%)
2	ADP	C	1533	3	22,29,29	1.16	2 (9%)	27,45,45	2.04	5 (18%)
4	UAG	C	1535	3	45,60,60	1.44	7 (15%)	61,88,88	2.18	19 (31%)
2	ADP	D	1534	3	22,29,29	1.12	2 (9%)	27,45,45	2.05	9 (33%)
4	UAG	D	1536	3	45,60,60	1.66	4 (8%)	61,88,88	2.44	18 (29%)

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	ADP	A	1533	3	-	0/12/32/32	0/3/3/3
4	UAG	A	1536	3	-	0/45/92/92	0/3/3/3
2	ADP	B	1534	3	-	0/12/32/32	0/3/3/3
4	UAG	B	1536	3	-	0/45/92/92	0/3/3/3
2	ADP	C	1533	3	-	0/12/32/32	0/3/3/3
4	UAG	C	1535	3	-	0/45/92/92	0/3/3/3
2	ADP	D	1534	3	-	0/12/32/32	0/3/3/3
4	UAG	D	1536	3	-	0/45/92/92	0/3/3/3

All (31) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	1535	UAG	PA-O2A	2.04	1.63	1.54
4	B	1536	UAG	PA-O2A	2.15	1.64	1.54
2	D	1534	ADP	O4'-C1'	2.15	1.43	1.41
4	C	1535	UAG	PB-O2B	2.21	1.64	1.54
4	C	1535	UAG	C24-N5	2.27	1.49	1.46
2	C	1533	ADP	O4'-C1'	2.34	1.44	1.41
2	B	1534	ADP	O4'-C1'	2.48	1.44	1.41
4	A	1536	UAG	C25-C24	2.62	1.57	1.53
4	B	1536	UAG	C24-N5	2.64	1.50	1.46
4	C	1535	UAG	O5'-C1'	2.68	1.48	1.41
4	D	1536	UAG	PA-O2A	2.72	1.66	1.54
2	A	1533	ADP	O4'-C1'	2.74	1.44	1.41
4	C	1535	UAG	C4-N3	3.13	1.38	1.33
4	C	1535	UAG	C6-N1	3.17	1.40	1.35
4	A	1536	UAG	O4B-C1B	3.18	1.45	1.41
2	B	1534	ADP	C5-C4	3.39	1.48	1.40
2	A	1533	ADP	C5-C4	3.49	1.48	1.40
2	C	1533	ADP	C5-C4	3.52	1.48	1.40
4	B	1536	UAG	O4B-C1B	3.68	1.45	1.41
2	D	1534	ADP	C5-C4	3.74	1.48	1.40
4	A	1536	UAG	C24-N5	3.85	1.52	1.46
4	A	1536	UAG	PA-O1A	4.12	1.66	1.51
4	A	1536	UAG	C4-N3	4.26	1.41	1.33
4	A	1536	UAG	PB-O1B	4.46	1.67	1.51
4	C	1535	UAG	C25-C24	4.54	1.59	1.53
4	D	1536	UAG	C4-N3	4.71	1.41	1.33
4	B	1536	UAG	C4-N3	4.91	1.42	1.33
4	D	1536	UAG	C6-N1	4.92	1.42	1.35
4	B	1536	UAG	C6-N1	4.94	1.42	1.35
4	A	1536	UAG	C6-N1	5.28	1.43	1.35
4	D	1536	UAG	O4B-C1B	6.36	1.49	1.41

All (107) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	1534	ADP	N3-C2-N1	-9.02	121.98	128.89
4	B	1536	UAG	O3A-PB-O1'	-8.85	78.17	103.63
4	A	1536	UAG	O5'-C1'-O1'	-8.51	100.14	111.36
2	A	1533	ADP	N3-C2-N1	-8.20	122.62	128.89
4	A	1536	UAG	O3A-PB-O1'	-8.18	80.08	103.63
2	C	1533	ADP	N3-C2-N1	-7.98	122.78	128.89
4	B	1536	UAG	O5'-C1'-O1'	-7.94	100.89	111.36
4	D	1536	UAG	O2B-PB-O3A	-7.35	71.74	105.09

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	C	1535	UAG	O3A-PB-O1'	-6.99	83.52	103.63
4	B	1536	UAG	O5'-C5'-C6'	-5.87	91.51	106.36
4	C	1535	UAG	O2B-PB-O3A	-5.64	79.49	105.09
4	D	1536	UAG	O3'-C18-C19	-5.31	99.38	111.24
4	A	1536	UAG	C4B-O4B-C1B	-5.15	104.06	109.72
4	B	1536	UAG	O2B-PB-O3A	-5.12	81.86	105.09
2	D	1534	ADP	N3-C2-N1	-4.71	125.28	128.89
4	A	1536	UAG	O2B-PB-O3A	-4.67	83.91	105.09
4	D	1536	UAG	O4B-C1B-N1	-4.64	98.29	108.08
4	D	1536	UAG	O3A-PB-O1'	-4.60	90.38	103.63
4	C	1535	UAG	C4B-O4B-C1B	-4.46	104.82	109.72
4	D	1536	UAG	O3'-C3'-C4'	-4.37	95.88	107.17
4	D	1536	UAG	O5'-C5'-C4'	-4.32	101.57	109.68
2	B	1534	ADP	O2B-PB-O3A	-3.95	87.16	105.09
2	C	1533	ADP	C2'-C1'-N9	-3.90	108.34	114.29
4	D	1536	UAG	C1'-C2'-N2'	-3.88	103.71	111.01
2	B	1534	ADP	C1'-N9-C4	-3.71	121.34	126.94
4	A	1536	UAG	C20-C18-C19	-3.66	101.39	111.05
4	B	1536	UAG	C1'-C2'-N2'	-3.52	104.39	111.01
4	D	1536	UAG	C1'-O5'-C5'	-3.49	106.96	113.75
2	D	1534	ADP	C4-C5-N7	-3.45	106.30	109.48
4	C	1535	UAG	O3'-C3'-C4'	-3.27	98.74	107.17
2	D	1534	ADP	PA-O3A-PB	-3.17	122.05	132.67
4	A	1536	UAG	C6'-C5'-C4'	-3.16	105.22	113.02
4	D	1536	UAG	C23-C21-N4	-3.09	104.47	110.31
4	B	1536	UAG	C22-C21-N4	-2.86	104.52	111.67
4	B	1536	UAG	PB-O3A-PA	-2.81	124.84	132.73
2	A	1533	ADP	C2'-C1'-N9	-2.81	110.00	114.29
4	A	1536	UAG	O4'-C4'-C3'	-2.74	103.40	109.87
4	C	1535	UAG	O5B-PA-O1A	-2.73	99.02	109.62
2	D	1534	ADP	C1'-N9-C4	-2.71	122.85	126.94
4	C	1535	UAG	C1'-C2'-N2'	-2.64	106.05	111.01
2	D	1534	ADP	O4'-C1'-N9	-2.58	102.69	108.10
4	B	1536	UAG	O4B-C1B-N1	-2.58	102.65	108.08
4	D	1536	UAG	C21-C22-N5	-2.53	110.87	116.83
4	A	1536	UAG	O2A-PA-O1A	-2.53	98.80	112.53
2	C	1533	ADP	C1'-N9-C4	-2.52	123.15	126.94
4	A	1536	UAG	C3'-C2'-N2'	-2.50	106.71	111.07
4	D	1536	UAG	O1'-C1'-C2'	-2.48	103.86	108.42
2	D	1534	ADP	C2'-C1'-N9	-2.44	110.56	114.29
4	B	1536	UAG	O4B-C4B-C5B	-2.41	100.69	109.32
4	B	1536	UAG	C23-C21-N4	-2.39	105.80	110.31

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1533	ADP	C4-C5-N7	-2.37	107.30	109.48
4	C	1535	UAG	O1'-C1'-C2'	-2.32	104.14	108.42
4	C	1535	UAG	C20-C18-C19	-2.26	105.09	111.05
2	C	1533	ADP	C4-C5-N7	-2.24	107.41	109.48
4	B	1536	UAG	O2A-PA-O1A	-2.18	100.69	112.53
4	C	1535	UAG	O4B-C4B-C5B	-2.16	101.59	109.32
4	B	1536	UAG	C3'-C2'-N2'	-2.16	107.31	111.07
2	A	1533	ADP	O3'-C3'-C4'	-2.11	104.72	111.05
4	A	1536	UAG	PB-O3A-PA	-2.11	126.81	132.73
4	A	1536	UAG	C1'-C2'-C3'	-2.04	106.22	110.13
4	A	1536	UAG	C2'-N2'-C7'	2.04	128.35	123.10
4	C	1535	UAG	O7'-C7'-N2'	2.04	126.03	121.86
4	B	1536	UAG	O2B-PB-O1B	2.04	123.60	112.53
4	A	1536	UAG	O2B-PB-O1B	2.05	123.65	112.53
2	B	1534	ADP	O2B-PB-O1B	2.05	117.19	110.58
4	C	1535	UAG	O2B-PB-O1'	2.06	114.76	106.49
4	B	1536	UAG	C26-C25-C24	2.07	117.20	112.99
2	C	1533	ADP	C2-N1-C6	2.10	122.52	118.77
2	B	1534	ADP	C2'-C1'-N9	2.10	117.50	114.29
2	D	1534	ADP	C2-N1-C6	2.10	122.52	118.77
2	B	1534	ADP	O2A-PA-O1A	2.13	124.09	112.53
4	A	1536	UAG	C1'-O5'-C5'	2.27	118.15	113.75
4	B	1536	UAG	O5'-C1'-C2'	2.30	115.78	110.78
4	C	1535	UAG	O5'-C5'-C6'	2.30	112.17	106.36
4	B	1536	UAG	O3A-PA-O5B	2.31	109.07	102.94
2	A	1533	ADP	C2-N1-C6	2.41	123.07	118.77
4	B	1536	UAG	C3'-C4'-C5'	2.41	115.07	109.61
4	C	1535	UAG	O1'-PB-O1B	2.42	118.96	109.46
4	C	1535	UAG	C6'-C5'-C4'	2.45	119.05	113.02
2	B	1534	ADP	C2-N1-C6	2.47	123.19	118.77
2	A	1533	ADP	C4'-O4'-C1'	2.60	112.57	109.72
4	A	1536	UAG	C4-N3-C2	2.65	116.77	114.14
4	A	1536	UAG	C26-C25-C24	2.76	118.59	112.99
4	A	1536	UAG	O1'-C1'-C2'	2.81	113.59	108.42
4	D	1536	UAG	O19-C22-N5	2.96	128.73	122.93
4	D	1536	UAG	C21-N4-C19	2.97	128.07	121.27
4	C	1535	UAG	C26-C25-C24	3.02	119.12	112.99
4	C	1535	UAG	C24-N5-C22	3.02	128.14	123.43
4	A	1536	UAG	C23-C21-C22	3.07	116.25	110.19
4	B	1536	UAG	O3'-C18-C20	3.09	116.52	107.50
4	A	1536	UAG	C3'-C4'-C5'	3.16	116.77	109.61
4	D	1536	UAG	C4-N3-C2	3.16	117.27	114.14

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	1536	UAG	O2B-PB-O1B	3.26	130.18	112.53
4	A	1536	UAG	O4B-C1B-N1	3.26	114.96	108.08
4	A	1536	UAG	O5'-C5'-C4'	3.31	115.89	109.68
4	D	1536	UAG	O3'-C18-C20	3.32	117.19	107.50
4	B	1536	UAG	O1'-PB-O1B	3.33	122.55	109.46
2	D	1534	ADP	O3B-PB-O1B	3.33	121.30	110.58
4	A	1536	UAG	O2B-PB-O1'	3.37	120.03	106.49
2	B	1534	ADP	O3B-PB-O1B	3.41	121.56	110.58
4	C	1535	UAG	O5'-C1'-O1'	3.95	116.58	111.36
2	D	1534	ADP	O3B-PB-O2B	4.03	122.71	107.38
4	D	1536	UAG	O3A-PA-O5B	4.41	114.65	102.94
4	B	1536	UAG	C4-N3-C2	4.80	118.90	114.14
4	C	1535	UAG	C4-N3-C2	4.90	119.00	114.14
4	C	1535	UAG	O3A-PA-O5B	5.82	118.38	102.94
4	D	1536	UAG	C24-N5-C22	6.63	133.76	123.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

8 monomers are involved in 31 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1533	ADP	1	0
4	A	1536	UAG	5	0
2	B	1534	ADP	2	0
4	B	1536	UAG	4	0
2	C	1533	ADP	5	0
4	C	1535	UAG	2	0
2	D	1534	ADP	5	0
4	D	1536	UAG	7	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	501/535 (93%)	-0.07	2 (0%)	93	80	25, 58, 104, 128	0
1	B	499/535 (93%)	-0.18	2 (0%)	93	80	24, 53, 99, 118	0
1	C	497/535 (92%)	-0.09	8 (1%)	74	47	30, 65, 103, 137	0
1	D	487/535 (91%)	-0.14	5 (1%)	84	60	29, 60, 115, 155	0
All	All	1984/2140 (92%)	-0.12	17 (0%)	85	64	24, 59, 105, 155	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	470	GLY	4.7
1	B	186	GLY	4.0
1	D	392	ASP	3.4
1	C	57	THR	3.2
1	C	59	ASP	3.0
1	A	318	ALA	2.9
1	D	462	ILE	2.7
1	C	464	ALA	2.4
1	B	340	PRO	2.2
1	C	330	GLY	2.2
1	D	397	PRO	2.2
1	A	422	GLY	2.2
1	C	467	ALA	2.2
1	D	470	GLY	2.2
1	D	399	ALA	2.2
1	C	97	ALA	2.1
1	C	463	LEU	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	KCX	B	262	12/13	0.98	0.15	-	29,32,37,41	0
1	KCX	A	262	12/13	0.97	0.18	-	33,36,39,39	0
1	KCX	D	262	12/13	0.97	0.16	-	33,36,42,43	0
1	KCX	C	262	12/13	0.98	0.16	-	35,36,43,45	0

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
3	MG	D	1537	1/1	0.96	0.33	2.60	53,53,53,53	0
2	ADP	A	1533	27/27	0.93	0.27	0.62	56,84,93,95	0
3	MG	C	1536	1/1	0.90	0.19	0.20	43,43,43,43	0
2	ADP	B	1534	27/27	0.96	0.17	-0.30	41,60,69,71	0
4	UAG	B	1536	58/58	0.96	0.17	-0.35	39,45,52,53	0
3	MG	D	1533	1/1	0.89	0.20	-0.41	50,50,50,50	0
2	ADP	C	1533	27/27	0.97	0.17	-0.45	49,59,65,72	0
2	ADP	D	1534	27/27	0.96	0.16	-0.49	46,55,64,72	0
4	UAG	A	1536	58/58	0.95	0.17	-0.60	36,45,53,62	0
4	UAG	D	1536	58/58	0.94	0.17	-0.62	48,56,69,74	0
4	UAG	C	1535	58/58	0.95	0.17	-0.77	44,54,69,74	0
3	MG	D	1535	1/1	0.97	0.08	-2.25	51,51,51,51	0
3	MG	C	1534	1/1	0.99	0.04	-3.11	60,60,60,60	0
3	MG	B	1535	1/1	0.97	0.06	-3.12	46,46,46,46	0
3	MG	A	1534	1/1	0.94	0.07	-5.65	48,48,48,48	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
3	MG	B	1537	1/1	0.95	0.19	-	39,39,39,39	0
3	MG	B	1533	1/1	0.92	0.32	-	30,30,30,30	0
3	MG	A	1535	1/1	0.67	0.21	-	37,37,37,37	0

6.5 Other polymers (i)

There are no such residues in this entry.