W O R L D W I D E

wwPDB

PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 01:41 PM GMT

|		
PDB ID	:	3UOJ
Title	:	Aurora A in complex with RPM1715
Authors	:	Martin, M.P.; Zhu, J.-Y.; Schonbrunn, E.
Deposited on	:	2011-11-16
Resolution	:	2.90 Å(reported)

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 2.90 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.
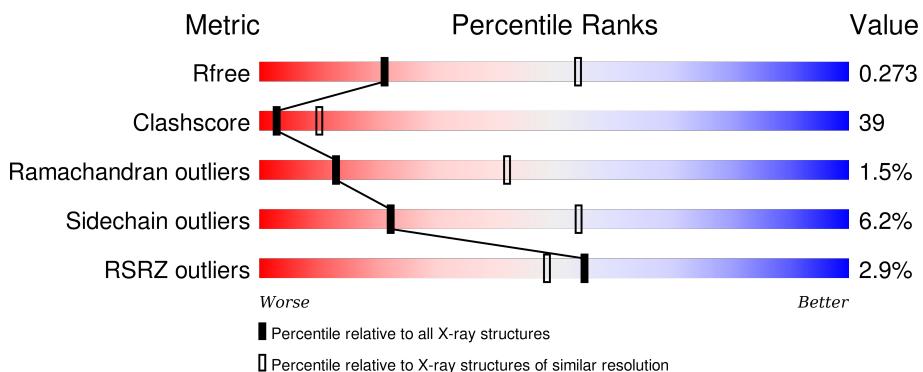
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1451 (2.90-2.90)
Clashscore	102246	1668 (2.90-2.90)
Ramachandran outliers	100387	1630 (2.90-2.90)
Sidechain outliers	100360	1632 (2.90-2.90)
RSRZ outliers	91569	1456 (2.90-2.90)

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	279	
1	B	279	

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 4394 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 Aurora kinase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	S	0	0	0
			2158	1386	380	386	6			
1	B	263	Total	C	N	O	S	0	0	0
			2158	1386	380	386	6			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	287	ASP	THR	ENGINEERED MUTATION	UNP O14965
B	287	ASP	THR	ENGINEERED MUTATION	UNP O14965

- Molecule 2 is 4-({4-[(2-CYANOPHENYL)AMINO]PYRIMIDIN-2-YL}AMINO)BENZOIC ACID (three-letter code: 0C5) (formula: $C_{18}H_{13}N_5O_2$).
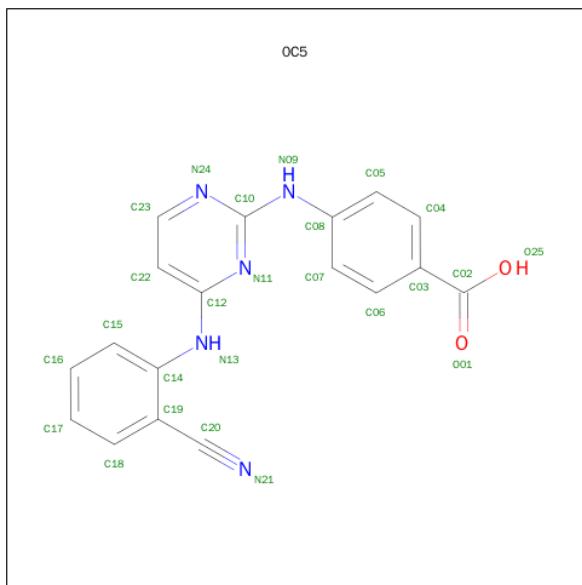
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			25	18	5	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			25	18	5	2		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	14	Total	O	0	0
			14	14		
3	B	14	Total	O	0	0
			14	14		

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: Aurora kinase A
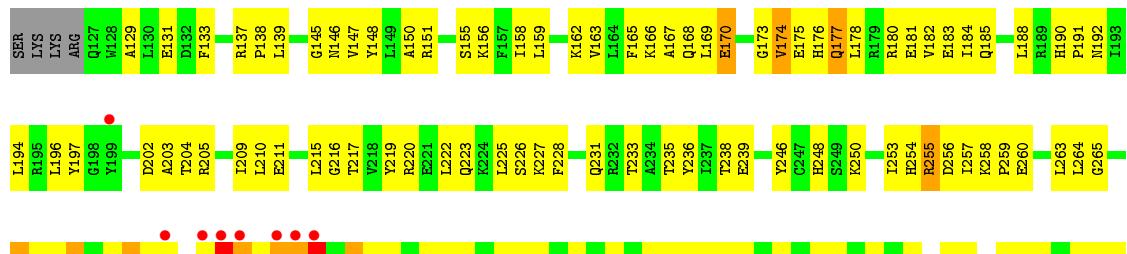
• Molecule 1: Aurora kinase A
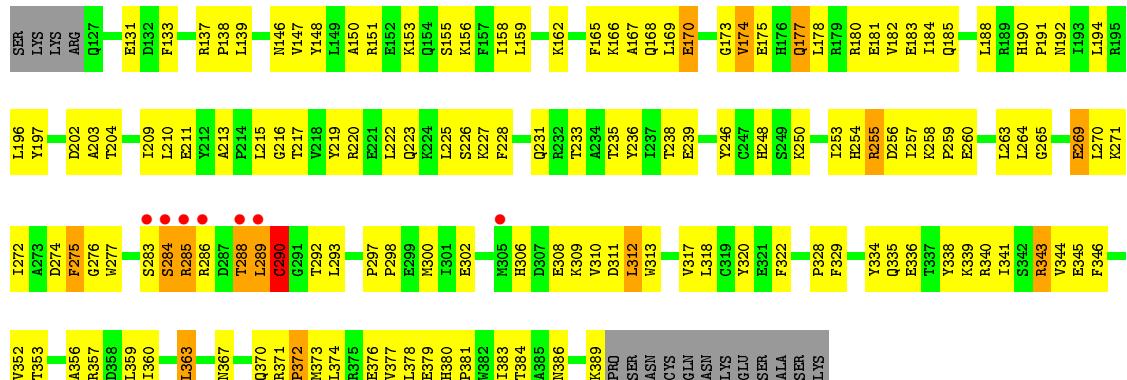
4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α, β, γ	85.71Å 85.71Å 77.08Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	18.95 – 2.90 18.95 – 2.90	Depositor EDS
% Data completeness (in resolution range)	99.4 (18.95-2.90) 99.4 (18.95-2.90)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	0.04	Depositor
$< I/\sigma(I) >$ [1]	5.25 (at 2.88Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, R_{free}	0.227 , 0.274 0.227 , 0.273	Depositor DCC
R_{free} test set	557 reflections (4.17%)	DCC
Wilson B-factor (Å^2)	65.7	Xtriage
Anisotropy	0.156	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.29 , 35.4	EDS
Estimated twinning fraction	0.028 for -h,-k,l 0.488 for h,-h-k,-l 0.029 for -k,-h,-l	Xtriage
L-test for twinning[2]	$< |L| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Outliers	0 of 13920 reflections	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	4394	wwPDB-VP
Average B, all atoms (Å^2)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.81% 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 (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: 0C5

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	0.58	0/2212	0.78	0/2990
1	B	0.58	0/2212	0.79	3/2990 (0.1%)
All	All	0.58	0/4424	0.78	3/5980 (0.1%)

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	4
1	B	0	3
All	All	0	7

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	363	LEU	CA-CB-CG	5.21	127.28	115.30
1	B	343	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	B	284	SER	C-N-CA	5.18	134.65	121.70

There are no chirality outliers.

All (7) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	285	ARG	Peptide
1	A	288	THR	Peptide
1	A	289	LEU	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
1	A	372	PRO	Peptide
1	B	288	THR	Peptide
1	B	289	LEU	Peptide
1	B	372	PRO	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	2158	0	2162	176	0
1	B	2158	0	2162	170	0
2	A	25	0	12	1	0
2	B	25	0	12	3	0
3	A	14	0	0	3	0
3	B	14	0	0	4	0
All	All	4394	0	4348	342	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 39.

All (342) 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:338:TYR:CD1	1:B:338:TYR:CD1	2.36	1.13
1:A:253:ILE:HG22	1:A:254:HIS:N	1.60	1.13
1:B:253:ILE:HG22	1:B:254:HIS:N	1.60	1.09
1:A:175:GLU:N	1:A:177:GLN:HE22	1.51	1.06
1:B:175:GLU:N	1:B:177:GLN:HE22	1.50	1.06
1:A:288:THR:HG23	1:A:289:LEU:H	1.24	1.02
1:B:288:THR:HG23	1:B:289:LEU:H	1.25	1.02
1:B:253:ILE:CG2	1:B:254:HIS:N	2.26	0.99
1:A:253:ILE:CG2	1:A:254:HIS:N	2.26	0.99
1:B:166:LYS:HA	1:B:169:LEU:HB2	1.50	0.93
1:A:253:ILE:CG2	1:A:254:HIS:H	1.83	0.91
1:A:166:LYS:HA	1:A:169:LEU:HB2	1.50	0.90
1:B:178:LEU:HD13	1:B:277:TRP:CH2	2.06	0.90

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:LEU:HD13	1:A:277:TRP:CH2	2.07	0.89
1:B:253:ILE:CG2	1:B:254:HIS:H	1.83	0.89
1:A:359:LEU:O	1:A:363:LEU:HD13	1.73	0.87
1:B:220:ARG:HB3	3:B:22:HOH:O	1.75	0.87
1:A:220:ARG:HB3	3:A:28:HOH:O	1.75	0.85
1:B:297:PRO:HG2	1:B:300:MET:HG3	1.60	0.83
1:A:344:VAL:O	1:A:344:VAL:HG12	1.78	0.82
1:B:344:VAL:O	1:B:344:VAL:HG12	1.79	0.82
1:B:178:LEU:HD13	1:B:277:TRP:HH2	1.42	0.82
1:B:340:ARG:NH1	1:B:345:GLU:OE2	2.13	0.82
1:A:297:PRO:HG2	1:A:300:MET:HG3	1.61	0.81
1:A:340:ARG:NH1	1:A:345:GLU:OE2	2.14	0.81
1:A:178:LEU:HD13	1:A:277:TRP:HH2	1.43	0.79
1:A:215:LEU:HD12	1:A:265:GLY:O	1.81	0.79
1:B:344:VAL:HG13	1:B:346:PHE:HE2	1.47	0.78
1:A:344:VAL:HG13	1:A:346:PHE:HE2	1.48	0.77
1:B:215:LEU:HD12	1:B:265:GLY:O	1.84	0.77
1:A:338:TYR:HD1	1:B:338:TYR:CE1	2.03	0.77
1:A:288:THR:HG23	1:A:289:LEU:N	1.98	0.77
1:A:338:TYR:CE1	1:B:338:TYR:HD1	2.03	0.77
1:A:288:THR:CG2	1:A:289:LEU:H	1.98	0.77
1:B:288:THR:CG2	1:B:289:LEU:H	1.98	0.74
1:B:192:ASN:ND2	1:B:239:GLU:HG2	2.01	0.74
1:A:192:ASN:ND2	1:A:239:GLU:HG2	2.02	0.74
1:A:338:TYR:CE1	1:B:338:TYR:CD1	2.75	0.74
1:B:367:ASN:HB3	1:B:370:GLN:HG3	1.69	0.73
1:A:335:GLN:HB3	3:A:29:HOH:O	1.86	0.73
1:A:367:ASN:HB3	1:A:370:GLN:HG3	1.70	0.73
1:A:253:ILE:HG22	1:A:254:HIS:H	1.38	0.72
1:B:231:GLN:HA	1:B:386:ASN:O	1.89	0.72
1:A:334:TYR:CD1	1:B:302:GLU:HG2	2.25	0.72
1:B:320:TYR:HB2	1:B:360:ILE:HD13	1.71	0.72
1:A:302:GLU:HG2	1:B:334:TYR:CD1	2.24	0.72
1:A:338:TYR:CD1	1:B:338:TYR:CE1	2.75	0.72
1:A:231:GLN:HA	1:A:386:ASN:O	1.89	0.72
1:B:288:THR:HG23	1:B:289:LEU:N	1.99	0.72
1:B:343:ARG:HD2	1:B:345:GLU:OE1	1.90	0.71
2:B:2:0C5:N11	2:B:2:0C5:H4	2.04	0.71
1:A:343:ARG:HD2	1:A:345:GLU:OE1	1.90	0.71
1:B:257:ILE:O	1:B:257:ILE:HG13	1.90	0.71
1:A:320:TYR:HB2	1:A:360:ILE:HD13	1.71	0.70

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:202:ASP:CG	1:A:203:ALA:H	1.95	0.70
1:A:257:ILE:HG13	1:A:257:ILE:O	1.90	0.70
1:B:177:GLN:HE21	1:B:178:LEU:H	1.39	0.70
1:A:373:MET:HG3	1:A:374:LEU:H	1.57	0.70
1:A:284:SER:OG	1:A:286:ARG:HB2	1.91	0.70
1:B:202:ASP:CG	1:B:203:ALA:H	1.95	0.70
1:B:197:TYR:HE2	1:B:211:GLU:HA	1.57	0.69
1:A:192:ASN:HD21	1:A:239:GLU:HG2	1.57	0.69
1:A:177:GLN:HE21	1:A:178:LEU:H	1.39	0.69
1:B:335:GLN:HB3	3:B:24:HOH:O	1.92	0.69
1:A:378:LEU:HA	1:A:383:ILE:CD1	2.23	0.69
1:A:196:LEU:HD13	1:A:210:LEU:CD2	2.23	0.68
1:B:192:ASN:HD21	1:B:239:GLU:HG2	1.56	0.68
1:B:373:MET:HG3	1:B:374:LEU:H	1.58	0.68
1:B:344:VAL:CG1	1:B:346:PHE:HE2	2.05	0.68
1:A:378:LEU:HA	1:A:383:ILE:HD11	1.77	0.67
1:A:176:HIS:HB2	3:B:8:HOH:O	1.93	0.67
1:B:196:LEU:HD13	1:B:210:LEU:CD2	2.23	0.67
1:B:378:LEU:HA	1:B:383:ILE:CD1	2.24	0.67
1:B:175:GLU:N	1:B:177:GLN:NE2	2.35	0.67
1:B:383:ILE:HG13	1:B:384:THR:N	2.10	0.67
1:B:344:VAL:HG13	1:B:346:PHE:CE2	2.29	0.67
1:A:197:TYR:HE2	1:A:211:GLU:HA	1.58	0.67
1:A:277:TRP:HE3	1:A:277:TRP:H	1.42	0.67
1:B:378:LEU:HA	1:B:383:ILE:HD11	1.76	0.66
1:A:378:LEU:C	1:A:383:ILE:HD11	2.16	0.66
1:A:344:VAL:HG13	1:A:346:PHE:CE2	2.31	0.66
1:A:344:VAL:CG1	1:A:346:PHE:HE2	2.07	0.66
1:A:383:ILE:HG13	1:A:384:THR:N	2.10	0.66
1:B:196:LEU:HD13	1:B:210:LEU:HD21	1.79	0.65
1:A:174:VAL:HG12	1:A:177:GLN:NE2	2.12	0.65
1:B:378:LEU:C	1:B:383:ILE:HD11	2.17	0.65
1:B:174:VAL:HA	1:B:177:GLN:NE2	2.12	0.65
1:B:175:GLU:H	1:B:177:GLN:HE22	1.38	0.65
1:B:277:TRP:H	1:B:277:TRP:HE3	1.42	0.65
1:A:196:LEU:HD13	1:A:210:LEU:HD21	1.79	0.64
2:A:1:0C5:N11	2:A:1:0C5:H4	2.13	0.64
1:B:228:PHE:CE2	1:B:236:TYR:HE2	2.15	0.64
1:B:256:ASP:N	1:B:274:ASP:OD1	2.31	0.64
1:A:228:PHE:CE2	1:A:236:TYR:HE2	2.16	0.64
1:A:235:THR:HG23	1:A:389:LYS:HB2	1.80	0.64

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:174:VAL:HG12	1:B:177:GLN:NE2	2.13	0.63
1:A:184:ILE:HG13	1:A:185:GLN:N	2.14	0.63
1:A:174:VAL:HA	1:A:177:GLN:NE2	2.13	0.63
1:A:196:LEU:CD1	1:A:210:LEU:HD23	2.28	0.63
1:B:196:LEU:CD1	1:B:210:LEU:HD23	2.29	0.63
1:A:175:GLU:H	1:A:177:GLN:HE22	1.38	0.63
1:B:202:ASP:OD1	1:B:203:ALA:N	2.31	0.63
1:A:202:ASP:OD1	1:A:203:ALA:N	2.31	0.62
1:A:256:ASP:N	1:A:274:ASP:OD1	2.31	0.62
1:A:170:GLU:O	1:A:173:GLY:N	2.28	0.62
1:B:312:LEU:O	1:B:363:LEU:HD12	1.99	0.62
1:A:289:LEU:O	1:A:290:CYS:HB3	2.00	0.62
1:B:235:THR:HG23	1:B:389:LYS:HB2	1.80	0.62
1:A:359:LEU:O	1:A:363:LEU:CD1	2.48	0.61
1:B:178:LEU:HD13	1:B:277:TRP:CZ3	2.35	0.61
1:A:288:THR:CG2	1:A:289:LEU:N	2.62	0.61
1:B:170:GLU:O	1:B:173:GLY:N	2.28	0.61
1:B:177:GLN:H	1:B:177:GLN:CD	2.04	0.61
1:B:184:ILE:HG13	1:B:185:GLN:N	2.14	0.61
1:A:344:VAL:CG1	1:A:344:VAL:O	2.48	0.61
1:A:177:GLN:H	1:A:177:GLN:CD	2.04	0.61
1:A:378:LEU:O	1:A:383:ILE:HD11	2.01	0.61
1:B:283:SER:O	1:B:284:SER:OG	2.15	0.61
1:B:288:THR:CG2	1:B:289:LEU:N	2.62	0.60
1:A:196:LEU:HD12	1:A:210:LEU:HD23	1.82	0.60
1:A:204:THR:HG23	1:A:205:ARG:HG3	1.82	0.60
1:A:383:ILE:HG13	1:A:384:THR:H	1.65	0.60
1:A:178:LEU:HD13	1:A:277:TRP:CZ3	2.35	0.60
1:B:289:LEU:O	1:B:290:CYS:HB3	2.01	0.60
1:B:248:HIS:HD2	1:B:374:LEU:HD11	1.65	0.60
1:B:383:ILE:HG13	1:B:384:THR:H	1.65	0.60
1:A:184:ILE:CG1	1:A:185:GLN:H	2.15	0.60
1:A:139:LEU:HD12	1:A:147:VAL:HG12	1.83	0.60
1:A:177:GLN:NE2	1:A:178:LEU:H	1.99	0.59
1:B:174:VAL:HA	1:B:177:GLN:CD	2.23	0.59
1:A:175:GLU:N	1:A:177:GLN:NE2	2.36	0.59
1:B:177:GLN:NE2	1:B:178:LEU:H	2.00	0.59
1:B:196:LEU:HD12	1:B:210:LEU:HD23	1.83	0.59
1:B:184:ILE:CG1	1:B:185:GLN:H	2.15	0.59
1:A:248:HIS:HD2	1:A:374:LEU:HD11	1.66	0.59
1:A:174:VAL:HA	1:A:177:GLN:CD	2.23	0.58

Continued on next page...

Full wwPDB X-ray Structure Validation Report

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:310:VAL:HG23	1:B:311:ASP:N	2.19	0.58
1:B:197:TYR:CE2	1:B:211:GLU:HA	2.38	0.58
1:B:378:LEU:O	1:B:383:ILE:HD11	2.02	0.58
1:B:139:LEU:HD12	1:B:147:VAL:HG12	1.84	0.58
1:B:253:ILE:HG23	1:B:254:HIS:H	1.69	0.58
1:B:226:SER:O	1:B:227:LYS:HG3	2.04	0.57
1:B:248:HIS:CD2	1:B:374:LEU:HD11	2.40	0.57
1:B:344:VAL:O	1:B:344:VAL:CG1	2.50	0.57
1:A:264:LEU:HD23	1:A:269:GLU:O	2.04	0.57
1:B:264:LEU:HD23	1:B:269:GLU:O	2.05	0.57
1:A:310:VAL:HG23	1:A:311:ASP:N	2.20	0.57
1:B:166:LYS:CA	1:B:169:LEU:HB2	2.29	0.57
1:B:297:PRO:CG	1:B:300:MET:HG3	2.34	0.56
1:A:197:TYR:CE2	1:A:211:GLU:HA	2.39	0.56
1:A:378:LEU:CA	1:A:383:ILE:HD11	2.35	0.56
1:B:184:ILE:CG1	1:B:185:GLN:N	2.67	0.56
1:A:184:ILE:CG1	1:A:185:GLN:N	2.67	0.56
1:B:253:ILE:HG22	1:B:254:HIS:H	1.38	0.56
1:B:378:LEU:CA	1:B:383:ILE:HD11	2.35	0.56
1:A:226:SER:O	1:A:227:LYS:HG3	2.06	0.56
1:A:248:HIS:CD2	1:A:374:LEU:HD11	2.40	0.55
1:B:174:VAL:CA	1:B:177:GLN:NE2	2.69	0.55
1:A:194:LEU:HD12	1:A:211:GLU:HG2	1.87	0.55
1:A:174:VAL:CA	1:A:177:GLN:NE2	2.70	0.55
1:B:338:TYR:CD2	1:B:338:TYR:C	2.80	0.55
1:A:338:TYR:C	1:A:338:TYR:CD2	2.80	0.54
1:B:174:VAL:C	1:B:177:GLN:HE22	2.11	0.54
1:B:309:LYS:HE2	1:B:372:PRO:O	2.07	0.54
1:A:194:LEU:CD1	1:A:211:GLU:HG2	2.38	0.54
1:B:184:ILE:HG13	1:B:185:GLN:H	1.72	0.54
1:A:293:LEU:HD12	1:A:334:TYR:HD1	1.73	0.54
1:B:194:LEU:HD12	1:B:211:GLU:HG2	1.88	0.54
1:A:246:TYR:CD2	1:A:246:TYR:C	2.81	0.54
1:A:309:LYS:HE2	1:A:372:PRO:O	2.07	0.53
1:A:174:VAL:C	1:A:177:GLN:HE22	2.11	0.53
1:A:220:ARG:O	1:A:223:GLN:HB2	2.08	0.53
1:A:292:THR:HA	3:A:13:HOH:O	2.08	0.53
1:A:293:LEU:HD12	1:A:334:TYR:CD1	2.44	0.52
1:B:246:TYR:CD2	1:B:246:TYR:C	2.82	0.52
1:B:293:LEU:HD12	1:B:334:TYR:HD1	1.74	0.52
1:B:188:LEU:HD22	1:B:246:TYR:HE2	1.73	0.52

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:258:LYS:HB2	1:A:259:PRO:HD2	1.92	0.52
1:B:258:LYS:HB2	1:B:259:PRO:HD2	1.92	0.52
1:A:166:LYS:CA	1:A:169:LEU:HB2	2.30	0.52
1:B:174:VAL:HG11	1:B:277:TRP:HZ2	1.74	0.52
1:A:238:THR:HG23	1:A:378:LEU:HD22	1.92	0.52
1:B:194:LEU:CD1	1:B:211:GLU:HG2	2.39	0.52
1:A:188:LEU:HD22	1:A:246:TYR:HE2	1.73	0.52
1:A:253:ILE:HG23	1:A:254:HIS:H	1.69	0.52
1:A:196:LEU:CD1	1:A:210:LEU:CD2	2.86	0.52
1:B:374:LEU:O	1:B:377:VAL:HB	2.10	0.52
1:B:238:THR:HG23	1:B:378:LEU:HD22	1.92	0.52
1:A:174:VAL:HG11	1:A:277:TRP:HZ2	1.75	0.51
1:A:297:PRO:CG	1:A:300:MET:HG3	2.36	0.51
1:B:293:LEU:HD12	1:B:334:TYR:CD1	2.45	0.51
1:A:133:PHE:HE1	1:A:159:LEU:HD21	1.76	0.51
1:B:183:GLU:OE1	1:B:183:GLU:HA	2.11	0.51
1:B:231:GLN:NE2	3:B:30:HOH:O	2.27	0.50
1:A:192:ASN:HA	1:A:270:LEU:O	2.11	0.50
1:A:215:LEU:HB2	1:A:264:LEU:HB2	1.93	0.50
1:A:217:THR:HG22	1:A:263:LEU:HD23	1.94	0.50
1:B:192:ASN:HA	1:B:270:LEU:O	2.11	0.50
1:A:196:LEU:HD22	1:A:275:PHE:HE2	1.76	0.50
1:A:151:ARG:HB3	1:A:158:ILE:HG12	1.95	0.49
1:A:253:ILE:HG22	1:A:254:HIS:CA	2.41	0.49
1:B:178:LEU:O	1:B:182:VAL:HG13	2.12	0.49
1:B:196:LEU:HD22	1:B:275:PHE:HE2	1.77	0.49
1:A:183:GLU:HA	1:A:183:GLU:OE1	2.10	0.49
1:A:180:ARG:O	1:A:183:GLU:N	2.46	0.49
1:A:275:PHE:CG	1:A:276:GLY:N	2.81	0.49
1:B:317:VAL:HG13	1:B:328:PRO:HD2	1.95	0.49
1:A:353:THR:O	1:A:356:ALA:HB3	2.13	0.49
1:A:313:TRP:CZ2	1:A:329:PHE:CE2	3.00	0.49
1:B:344:VAL:CG1	1:B:346:PHE:CE2	2.92	0.49
1:B:217:THR:HG22	1:B:263:LEU:HD23	1.94	0.49
1:A:317:VAL:HG13	1:A:328:PRO:HD2	1.95	0.49
1:B:275:PHE:CG	1:B:276:GLY:N	2.80	0.49
1:B:215:LEU:HB2	1:B:264:LEU:HB2	1.95	0.48
1:B:133:PHE:HE1	1:B:159:LEU:HD21	1.77	0.48
1:A:178:LEU:O	1:A:182:VAL:HG13	2.13	0.48
1:B:196:LEU:CD1	1:B:210:LEU:CD2	2.86	0.48
1:B:236:TYR:HA	1:B:239:GLU:OE1	2.14	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:239:GLU:HG3	1:A:389:LYS:CE	2.44	0.48
1:A:139:LEU:HD12	1:A:147:VAL:CG1	2.44	0.47
1:B:220:ARG:O	1:B:223:GLN:HB3	2.13	0.47
1:B:180:ARG:O	1:B:183:GLU:N	2.47	0.47
1:A:219:TYR:CD2	1:A:260:GLU:HG2	2.49	0.47
1:A:184:ILE:HG13	1:A:185:GLN:H	1.72	0.47
1:B:151:ARG:HB3	1:B:158:ILE:HG12	1.96	0.47
1:B:239:GLU:HG3	1:B:389:LYS:CE	2.45	0.47
1:A:253:ILE:HD13	1:A:308:GLU:N	2.29	0.47
1:A:202:ASP:CG	1:A:203:ALA:N	2.67	0.47
1:A:374:LEU:O	1:A:377:VAL:HB	2.13	0.47
1:B:220:ARG:NH1	1:B:223:GLN:HG2	2.30	0.47
1:B:236:TYR:O	1:B:239:GLU:HB2	2.15	0.47
1:B:353:THR:O	1:B:356:ALA:HB3	2.15	0.46
1:A:236:TYR:HA	1:A:239:GLU:OE1	2.15	0.46
1:B:313:TRP:CZ2	1:B:329:PHE:CE2	3.04	0.46
1:B:289:LEU:O	1:B:290:CYS:CB	2.64	0.46
1:B:233:THR:HG23	1:B:322:PHE:HD2	1.80	0.46
1:A:289:LEU:O	1:A:290:CYS:CB	2.63	0.46
1:B:202:ASP:CG	1:B:203:ALA:N	2.67	0.46
1:B:194:LEU:HD22	1:B:263:LEU:HD12	1.98	0.46
1:A:313:TRP:HZ2	1:A:329:PHE:CE2	2.33	0.46
1:B:213:ALA:O	2:B:2:0C5:N09	2.40	0.46
1:A:284:SER:OG	1:A:285:ARG:N	2.48	0.46
1:B:339:LYS:HE2	1:B:339:LYS:HB3	1.71	0.46
1:B:253:ILE:HD13	1:B:308:GLU:N	2.31	0.46
1:B:219:TYR:CD2	1:B:260:GLU:HG2	2.51	0.46
1:A:215:LEU:HB2	1:A:264:LEU:CB	2.46	0.45
1:B:284:SER:O	1:B:285:ARG:HG3	2.16	0.45
1:B:306:HIS:HB2	1:B:310:VAL:CG1	2.47	0.45
1:B:165:PHE:C	1:B:167:ALA:H	2.20	0.45
1:A:380:HIS:HA	1:A:381:PRO:HD2	1.65	0.45
1:B:139:LEU:HD12	1:B:147:VAL:CG1	2.46	0.45
1:B:215:LEU:HB2	1:B:264:LEU:CB	2.46	0.45
2:B:2:0C5:N11	2:B:2:0C5:C07	2.73	0.45
1:B:155:SER:O	1:B:156:LYS:HB2	2.17	0.45
1:A:315:LEU:HB3	1:A:363:LEU:HD23	1.97	0.45
1:A:236:TYR:O	1:A:239:GLU:HB2	2.15	0.45
1:B:376:GLU:HA	1:B:379:GLU:HB3	1.99	0.45
1:A:352:VAL:HB	1:A:357:ARG:NH1	2.32	0.45
1:B:147:VAL:HG22	1:B:162:LYS:HG3	1.99	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:138:PRO:HA	1:A:148:TYR:HA	1.99	0.45
1:A:219:TYR:O	1:A:223:GLN:HG2	2.17	0.45
1:B:131:GLU:O	1:B:153:LYS:NZ	2.40	0.44
1:A:298:PRO:O	1:A:302:GLU:HB2	2.16	0.44
1:B:275:PHE:CD1	1:B:276:GLY:N	2.85	0.44
1:A:339:LYS:HB3	1:A:339:LYS:HE2	1.72	0.44
1:A:233:THR:HG23	1:A:322:PHE:HD2	1.82	0.44
1:A:376:GLU:HA	1:A:379:GLU:HB3	2.00	0.44
1:A:165:PHE:C	1:A:167:ALA:H	2.20	0.44
1:B:190:HIS:CG	1:B:191:PRO:HD2	2.52	0.44
1:B:253:ILE:HG22	1:B:254:HIS:CA	2.40	0.44
1:A:194:LEU:HD22	1:A:263:LEU:HD12	1.98	0.44
1:B:359:LEU:O	1:B:363:LEU:CD2	2.65	0.44
1:B:181:GLU:O	1:B:184:ILE:HG12	2.18	0.44
1:B:228:PHE:CE2	1:B:236:TYR:CE2	3.03	0.44
1:B:216:GLY:O	1:B:263:LEU:HA	2.17	0.44
1:B:138:PRO:HA	1:B:148:TYR:HA	1.99	0.44
1:A:177:GLN:HE21	1:A:178:LEU:N	2.12	0.44
1:A:239:GLU:HG3	1:A:389:LYS:HE2	2.00	0.44
1:A:275:PHE:CD1	1:A:276:GLY:N	2.86	0.43
1:A:253:ILE:C	1:A:255:ARG:H	2.22	0.43
1:B:277:TRP:N	1:B:277:TRP:CE3	2.82	0.43
1:B:298:PRO:O	1:B:302:GLU:HB2	2.18	0.43
1:A:181:GLU:O	1:A:184:ILE:HG12	2.18	0.43
1:A:306:HIS:HB2	1:A:310:VAL:CG1	2.48	0.43
1:A:272:ILE:O	1:A:272:ILE:HG22	2.18	0.43
1:B:225:LEU:HD12	1:B:225:LEU:N	2.34	0.43
1:A:165:PHE:HB2	1:A:168:GLN:HB2	2.00	0.43
1:B:380:HIS:HA	1:B:381:PRO:HD2	1.65	0.43
1:B:165:PHE:HB2	1:B:168:GLN:HB2	1.99	0.43
1:B:196:LEU:HD22	1:B:275:PHE:CE2	2.54	0.43
1:B:225:LEU:N	1:B:225:LEU:CD1	2.82	0.43
1:B:238:THR:HG23	1:B:378:LEU:CD2	2.49	0.43
1:B:352:VAL:HB	1:B:357:ARG:NH1	2.34	0.43
1:A:277:TRP:N	1:A:277:TRP:CE3	2.82	0.43
1:A:315:LEU:HD23	1:A:315:LEU:HA	1.84	0.43
1:A:216:GLY:O	1:A:263:LEU:HA	2.18	0.43
1:A:150:ALA:HB3	1:A:159:LEU:HD12	2.00	0.43
1:A:147:VAL:HG22	1:A:162:LYS:HG3	2.01	0.43
1:B:253:ILE:C	1:B:255:ARG:H	2.22	0.42
1:A:190:HIS:CG	1:A:191:PRO:HD2	2.54	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:239:GLU:HG3	1:B:389:LYS:HE2	2.01	0.42
1:A:286:ARG:HB3	1:A:287:ASP:H	1.56	0.42
1:A:225:LEU:N	1:A:225:LEU:HD12	2.34	0.42
1:A:238:THR:HG23	1:A:378:LEU:CD2	2.49	0.42
1:A:196:LEU:HD22	1:A:275:PHE:CE2	2.53	0.42
1:B:371:ARG:HA	1:B:372:PRO:HD3	1.89	0.42
1:B:250:LYS:HD2	1:B:250:LYS:HA	1.59	0.42
1:A:155:SER:O	1:A:156:LYS:HB2	2.19	0.42
1:A:159:LEU:HD22	1:A:209:ILE:HG23	2.02	0.42
1:B:150:ALA:HB3	1:B:159:LEU:HD12	2.02	0.42
1:A:250:LYS:HD2	1:A:250:LYS:HA	1.59	0.42
1:A:340:ARG:HD2	1:A:345:GLU:HB2	2.01	0.41
1:A:225:LEU:CD1	1:A:225:LEU:N	2.83	0.41
1:A:216:GLY:O	1:A:264:LEU:N	2.51	0.41
1:B:275:PHE:CD1	1:B:275:PHE:C	2.93	0.41
1:B:313:TRP:HZ2	1:B:329:PHE:CE2	2.37	0.41
1:B:177:GLN:HE21	1:B:178:LEU:N	2.12	0.41
1:A:166:LYS:HA	1:A:169:LEU:CB	2.37	0.41
1:A:231:GLN:HG2	1:A:386:ASN:O	2.20	0.41
1:B:310:VAL:HG23	1:B:311:ASP:H	1.83	0.41
1:A:180:ARG:HD3	1:A:180:ARG:HA	1.81	0.41
1:B:159:LEU:HD22	1:B:209:ILE:HG23	2.03	0.41
1:B:192:ASN:O	1:B:271:LYS:HA	2.20	0.41
1:A:371:ARG:HA	1:A:372:PRO:HD3	1.88	0.41
1:B:131:GLU:O	1:B:153:LYS:HD2	2.21	0.41
1:B:272:ILE:HG22	1:B:272:ILE:O	2.21	0.41
1:A:174:VAL:HG12	1:A:177:GLN:HE21	1.82	0.41
1:A:275:PHE:C	1:A:275:PHE:CD1	2.94	0.41
1:B:174:VAL:HG12	1:B:177:GLN:HE21	1.83	0.41
1:B:310:VAL:CG2	1:B:311:ASP:N	2.84	0.41
1:A:129:ALA:C	1:A:131:GLU:H	2.24	0.41
1:A:318:LEU:HD23	1:A:318:LEU:HA	1.79	0.41
1:A:192:ASN:O	1:A:271:LYS:HA	2.20	0.41
1:A:296:LEU:HB3	1:A:301:ILE:HG23	2.03	0.40
1:A:344:VAL:CG1	1:A:346:PHE:CE2	2.94	0.40
1:B:340:ARG:HD2	1:B:345:GLU:HB2	2.02	0.40
1:A:196:LEU:HD12	1:A:209:ILE:O	2.20	0.40
1:B:191:PRO:O	1:B:271:LYS:CE	2.70	0.40
1:B:165:PHE:O	1:B:204:THR:O	2.39	0.40
1:A:181:GLU:HG3	1:A:181:GLU:O	2.21	0.40
1:B:318:LEU:HD23	1:B:318:LEU:HA	1.78	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:145:GLY:HA3	1:A:163:VAL:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	261/279 (94%)	225 (86%)	32 (12%)	4 (2%)	13	42
1	B	261/279 (94%)	225 (86%)	32 (12%)	4 (2%)	13	42
All	All	522/558 (94%)	450 (86%)	64 (12%)	8 (2%)	13	42

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	285	ARG
1	B	286	ARG
1	A	285	ARG
1	A	286	ARG
1	A	290	CYS
1	B	290	CYS
1	A	341	ILE
1	B	341	ILE

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	232/247 (94%)	216 (93%)	16 (7%)	19	48
1	B	232/247 (94%)	219 (94%)	13 (6%)	26	60
All	All	464/494 (94%)	435 (94%)	29 (6%)	22	54

All (29) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	ARG
1	A	146	ASN
1	A	170	GLU
1	A	174	VAL
1	A	177	GLN
1	A	222	LEU
1	A	255	ARG
1	A	269	GLU
1	A	272	ILE
1	A	275	PHE
1	A	290	CYS
1	A	292	THR
1	A	294	ASP
1	A	304	ARG
1	A	312	LEU
1	A	336	GLU
1	B	137	ARG
1	B	146	ASN
1	B	170	GLU
1	B	174	VAL
1	B	177	GLN
1	B	222	LEU
1	B	255	ARG
1	B	269	GLU
1	B	275	PHE
1	B	290	CYS
1	B	292	THR
1	B	312	LEU
1	B	336	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	177	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	248	HIS
1	B	177	GLN
1	B	248	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)

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

2 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	0C5	A	1	-	24,27,27	2.26	4 (16%)	32,36,36	1.94	7 (21%)
2	0C5	B	2	-	24,27,27	2.30	4 (16%)	32,36,36	1.90	7 (21%)

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	0C5	A	1	-	-	0/10/14/14	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	0C5	B	2	-	-	0/10/14/14	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1	0C5	C20-N21	-2.60	1.08	1.14
2	B	2	0C5	C20-N21	-2.55	1.08	1.14
2	A	1	0C5	C10-N09	4.45	1.44	1.36
2	B	2	0C5	C10-N09	4.53	1.44	1.36
2	A	1	0C5	C19-C20	4.79	1.51	1.44
2	B	2	0C5	C19-C20	5.06	1.52	1.44
2	A	1	0C5	C12-N13	7.89	1.52	1.38
2	B	2	0C5	C12-N13	7.97	1.52	1.38

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2	0C5	C22-C23-N24	-4.94	118.26	123.90
2	A	1	0C5	C22-C23-N24	-4.71	118.52	123.90
2	A	1	0C5	N24-C10-N11	-3.87	122.54	126.67
2	B	2	0C5	N24-C10-N11	-3.54	122.90	126.67
2	B	2	0C5	C22-C12-N11	-3.43	117.10	123.24
2	A	1	0C5	C22-C12-N11	-3.34	117.27	123.24
2	B	2	0C5	C08-N09-C10	-2.44	122.73	129.19
2	A	1	0C5	C04-C03-C02	-2.31	117.35	120.45
2	A	1	0C5	C19-C14-N13	2.18	120.87	118.30
2	B	2	0C5	C10-N11-C12	2.18	120.44	116.61
2	B	2	0C5	C19-C14-N13	2.42	121.15	118.30
2	A	1	0C5	C10-N11-C12	2.47	120.95	116.61
2	A	1	0C5	C23-N24-C10	5.23	120.03	115.49
2	B	2	0C5	C23-N24-C10	5.29	120.09	115.49

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1	0C5	1	0
2	B	2	0C5	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 (i)

6.1 Protein, DNA and RNA chains (i)

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å^2)	Q<0.9
1	A	263/279 (94%)	-0.12	8 (3%) 54	47	33, 62, 113, 171	0
1	B	263/279 (94%)	-0.10	7 (2%) 58	52	33, 62, 112, 171	0
All	All	526/558 (94%)	-0.11	15 (2%) 55	49	33, 62, 113, 171	0

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	286	ARG	7.6
1	B	284	SER	7.1
1	A	284	SER	6.5
1	B	285	ARG	6.2
1	B	286	ARG	5.8
1	A	289	LEU	3.8
1	A	288	THR	3.5
1	B	288	THR	3.2
1	A	285	ARG	3.2
1	A	277	TRP	2.8
1	A	290	CYS	2.5
1	B	305	MET	2.3
1	B	289	LEU	2.2
1	B	283	SER	2.2
1	A	199	TYR	2.1

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, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	0C5	A	1	25/25	0.97	0.19	0.19	26,44,53,62	0
2	0C5	B	2	25/25	0.97	0.19	0.12	28,43,52,60	0

6.5 Other polymers (i)

There are no such residues in this entry.