



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 01:42 PM GMT

PDB ID : 3UOK  
Title : Aurora A in complex with YL5-81-1  
Authors : Martin, M.P.; Zhu, J.-Y.; Schonbrunn, E.  
Deposited on : 2011-11-16  
Resolution : 2.95 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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) 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

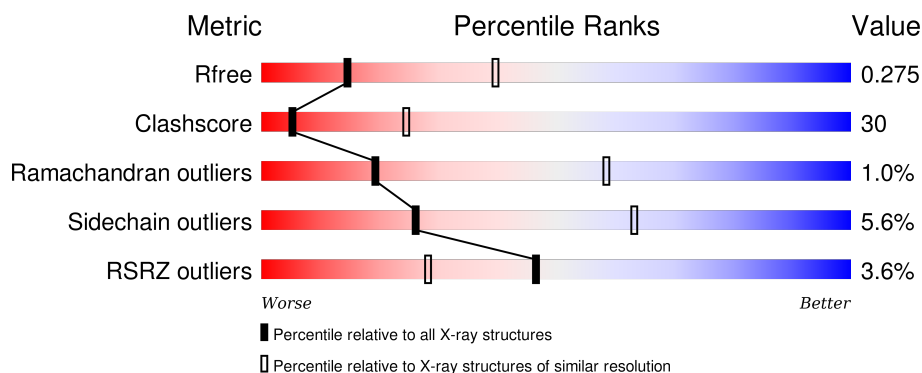
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.95 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	2184 (3.00-2.92)
Clashscore	102246	2552 (3.00-2.92)
Ramachandran outliers	100387	2468 (3.00-2.92)
Sidechain outliers	100360	2471 (3.00-2.92)
RSRZ outliers	91569	2201 (3.00-2.92)

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  $\geq 3$ , 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  $\leq 5\%$ . 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 4423 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.

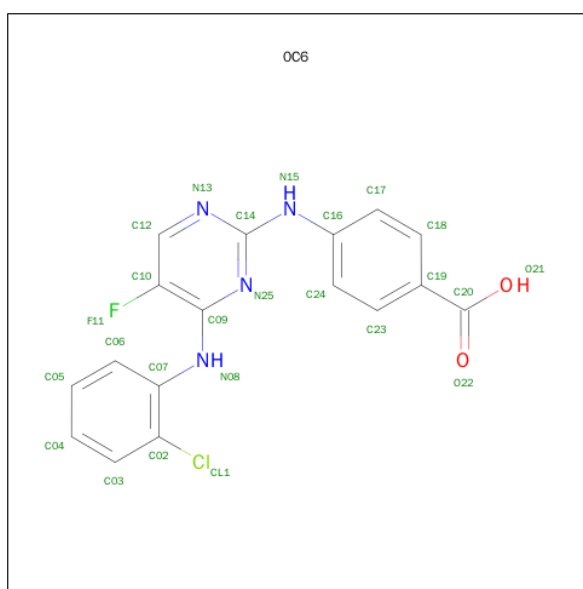
- Molecule 1 is a protein called Aurora kinase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	265	Total	C	N	O	S	0	0	0
			2178	1398	386	388	6			
1	B	265	Total	C	N	O	S	0	0	0
			2178	1398	386	388	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-CHLOROPHENYL)AMINO]-5-FLUOROPYRIMIDIN-2-YL}AMINO)BENZOIC ACID (three-letter code: 0C6) (formula: C<sub>17</sub>H<sub>12</sub>ClFN<sub>4</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	A	1	Total	C	Cl	F	N	O	0	0
			25	17	1	1	4	2		

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Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
2	B	1	Total	C	Cl	F	N	O	0	0
			25	17	1	1	4	2		

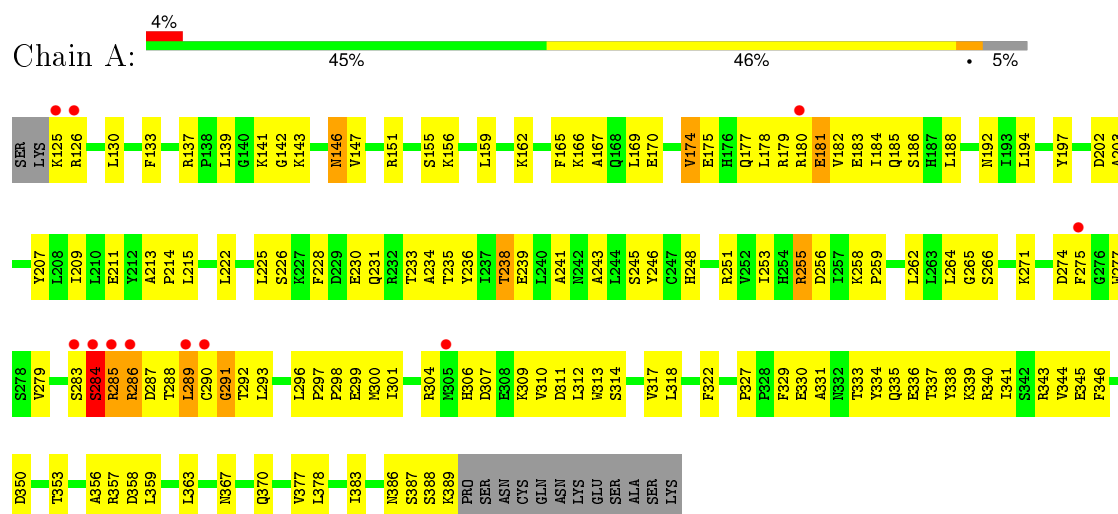
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	8	Total	O	0	0
			8	8		
3	B	9	Total	O	0	0
			9	9		

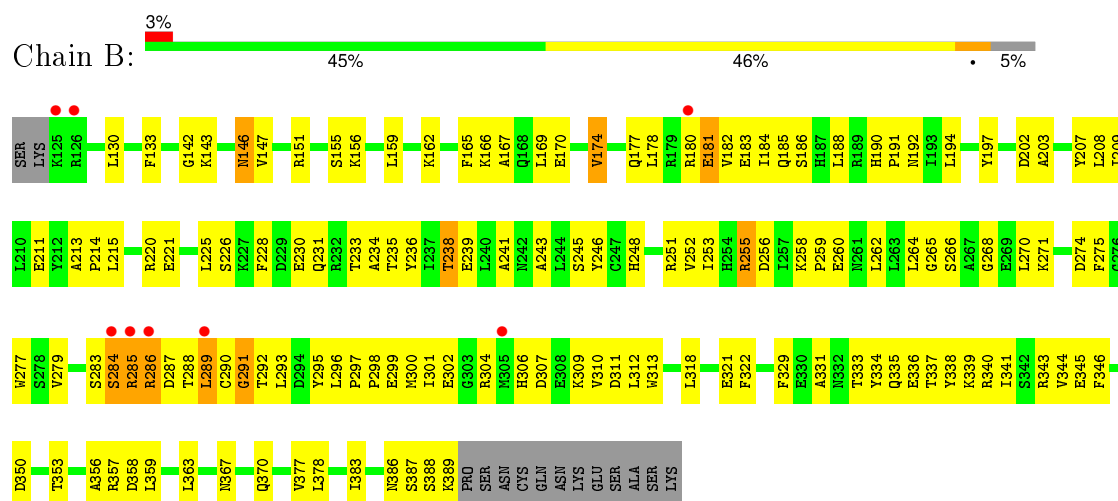
### 3 Residue-property plots

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

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.75Å 85.75Å 76.70Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	19.89 – 2.95 19.89 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (19.89-2.95) 99.8 (19.89-2.95)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.01 (at 2.93Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.7_650)	Depositor
R, $R_{free}$	0.223 , 0.276 0.221 , 0.275	Depositor DCC
$R_{free}$ test set	527 reflections (4.17%)	DCC
Wilson B-factor (Å <sup>2</sup> )	55.7	Xtriage
Anisotropy	0.036	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 25.9	EDS
Estimated twinning fraction	0.032 for -h,-k,l 0.487 for h,-h-k,-l 0.035 for -k,-h,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 13174 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	4423	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.84% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  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: 0C6

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	0.53	0/2232	0.73	0/3015
1	B	0.54	0/2232	0.73	0/3015
All	All	0.54	0/4464	0.73	0/6030

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	5
1	B	0	4
All	All	0	9

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	284	SER	Mainchain
1	A	285	ARG	Peptide
1	A	288	THR	Peptide
1	A	289	LEU	Peptide
1	A	291	GLY	Peptide
1	B	268	GLY	Peptide
1	B	288	THR	Peptide
1	B	289	LEU	Peptide
1	B	291	GLY	Peptide

## 5.2 Too-close contacts ⓘ

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	2178	0	2188	136	0
1	B	2178	0	2188	138	0
2	A	25	0	11	3	0
2	B	25	0	11	4	0
3	A	8	0	0	0	0
3	B	9	0	0	2	0
All	All	4423	0	4398	267	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 30.

All (267) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:339:LYS:HE3	3:B:8:HOH:O	1.49	1.12
1:B:252:VAL:HG11	1:B:255:ARG:HH21	1.19	1.08
1:B:252:VAL:HG11	1:B:255:ARG:NH2	1.75	1.02
1:A:289:LEU:HB3	1:A:292:THR:CG2	1.94	0.97
1:B:289:LEU:HB3	1:B:292:THR:CG2	1.95	0.97
1:A:235:THR:HG22	1:A:388:SER:H	1.30	0.96
1:A:289:LEU:HB3	1:A:292:THR:HG23	1.46	0.96
1:B:289:LEU:HB3	1:B:292:THR:HG23	1.46	0.95
1:B:252:VAL:CG1	1:B:255:ARG:HH21	1.79	0.95
1:A:185:GLN:HA	1:A:188:LEU:HD12	1.48	0.94
1:B:235:THR:HG22	1:B:388:SER:H	1.32	0.93
1:A:180:ARG:HG3	1:B:180:ARG:HG3	1.50	0.93
1:B:185:GLN:HA	1:B:188:LEU:HD12	1.50	0.93
1:A:166:LYS:HA	1:A:169:LEU:HB2	1.49	0.92
1:B:234:ALA:O	1:B:238:THR:HG22	1.70	0.91
1:A:139:LEU:HB2	1:A:147:VAL:HG23	1.52	0.91
1:B:166:LYS:HA	1:B:169:LEU:HB2	1.50	0.91
1:A:234:ALA:O	1:A:238:THR:HG22	1.70	0.90
1:B:166:LYS:H	1:B:169:LEU:HD13	1.43	0.84
1:A:166:LYS:H	1:A:169:LEU:HD13	1.45	0.82
1:A:340:ARG:HD2	1:A:345:GLU:HB2	1.62	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:340:ARG:HD2	1:B:345:GLU:HB2	1.62	0.81
1:A:344:VAL:O	1:A:344:VAL:HG12	1.82	0.80
1:B:344:VAL:O	1:B:344:VAL:HG12	1.81	0.79
1:B:147:VAL:HG22	1:B:162:LYS:HG3	1.65	0.78
1:A:147:VAL:HG12	1:A:162:LYS:HG3	1.65	0.78
1:A:335:GLN:HA	1:B:338:TYR:HE2	1.50	0.77
1:A:235:THR:CG2	1:A:388:SER:H	1.98	0.77
1:A:338:TYR:HE2	1:B:335:GLN:HA	1.51	0.76
1:B:220:ARG:NH2	1:B:221:GLU:OE2	2.19	0.76
1:B:185:GLN:HE21	1:B:255:ARG:NH1	1.85	0.75
1:B:235:THR:CG2	1:B:388:SER:H	2.00	0.75
2:B:1:0C6:N25	2:B:1:0C6:H8	2.04	0.72
1:A:289:LEU:HD13	1:A:292:THR:HG22	1.71	0.72
1:A:197:TYR:CE2	1:A:211:GLU:HA	2.25	0.71
2:A:2:0C6:N25	2:A:2:0C6:H8	2.05	0.71
1:A:197:TYR:HB2	1:A:209:ILE:HG22	1.73	0.70
1:B:197:TYR:HB2	1:B:209:ILE:HG22	1.72	0.70
1:B:197:TYR:CE2	1:B:211:GLU:HA	2.26	0.70
1:B:252:VAL:CG1	1:B:255:ARG:NH2	2.46	0.69
1:B:367:ASN:HB3	1:B:370:GLN:HG3	1.75	0.69
1:A:174:VAL:HG23	1:A:177:GLN:HB3	1.74	0.69
1:A:367:ASN:HB3	1:A:370:GLN:HG3	1.74	0.69
1:B:289:LEU:HD13	1:B:292:THR:HG22	1.73	0.69
1:B:174:VAL:HG23	1:B:177:GLN:HB3	1.75	0.68
1:A:336:GLU:HA	1:A:339:LYS:HD2	1.77	0.67
1:B:336:GLU:HA	1:B:339:LYS:HD2	1.77	0.67
1:A:283:SER:O	1:A:284:SER:O	2.13	0.66
1:B:340:ARG:NH1	1:B:345:GLU:OE2	2.29	0.66
1:A:139:LEU:HB2	1:A:147:VAL:CG2	2.25	0.66
1:B:181:GLU:HB3	1:B:275:PHE:HE1	1.60	0.65
1:A:340:ARG:NH1	1:A:345:GLU:OE2	2.29	0.65
1:A:181:GLU:HB3	1:A:275:PHE:HE1	1.61	0.64
1:A:215:LEU:HD12	1:A:265:GLY:O	1.97	0.64
1:B:215:LEU:HD12	1:B:265:GLY:O	1.97	0.64
1:A:335:GLN:HA	1:B:338:TYR:CE2	2.33	0.63
1:A:184:ILE:HG13	1:A:185:GLN:H	1.64	0.63
1:B:230:GLU:OE1	1:B:353:THR:HG21	1.99	0.63
1:A:174:VAL:HG22	1:A:174:VAL:O	1.98	0.63
1:A:125:LYS:O	1:A:126:ARG:HB2	1.99	0.62
1:B:184:ILE:HG13	1:B:185:GLN:H	1.63	0.62
1:B:174:VAL:O	1:B:174:VAL:HG22	1.98	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:VAL:CG1	1:A:162:LYS:HG3	2.31	0.61
1:B:289:LEU:HA	1:B:291:GLY:H	1.66	0.61
1:A:230:GLU:OE1	1:A:353:THR:HG21	2.00	0.60
1:A:231:GLN:HA	1:A:386:ASN:O	2.02	0.60
1:B:230:GLU:OE2	1:B:353:THR:OG1	2.18	0.60
1:A:289:LEU:HA	1:A:291:GLY:H	1.66	0.60
1:B:335:GLN:O	1:B:339:LYS:HG3	2.02	0.60
1:A:225:LEU:O	1:A:226:SER:HB2	2.01	0.60
1:A:185:GLN:HE21	1:A:255:ARG:HH21	1.50	0.59
1:A:125:LYS:O	1:A:125:LYS:HG2	2.03	0.59
1:B:256:ASP:N	1:B:274:ASP:OD1	2.33	0.59
1:B:231:GLN:HA	1:B:386:ASN:O	2.03	0.59
1:B:307:ASP:OD1	1:B:309:LYS:HB2	2.03	0.59
1:A:202:ASP:CG	1:A:203:ALA:H	2.06	0.58
1:A:307:ASP:OD1	1:A:309:LYS:HB2	2.03	0.58
1:A:338:TYR:CE2	1:B:335:GLN:HA	2.34	0.58
1:B:230:GLU:OE2	1:B:353:THR:CG2	2.52	0.58
1:B:202:ASP:CG	1:B:203:ALA:H	2.06	0.58
1:A:230:GLU:OE2	1:A:353:THR:CG2	2.51	0.58
1:B:225:LEU:O	1:B:226:SER:HB2	2.02	0.58
1:B:225:LEU:N	1:B:225:LEU:HD23	2.17	0.58
1:B:192:ASN:O	1:B:271:LYS:HA	2.04	0.57
1:B:174:VAL:HB	1:B:177:GLN:HE21	1.69	0.57
1:A:335:GLN:O	1:A:339:LYS:HG3	2.03	0.57
1:A:147:VAL:O	1:A:147:VAL:HG23	2.05	0.57
1:B:181:GLU:O	1:B:184:ILE:HG13	2.04	0.57
1:A:181:GLU:O	1:A:184:ILE:HG13	2.05	0.57
1:B:214:PRO:HG2	1:B:266:SER:HA	1.87	0.56
1:A:225:LEU:N	1:A:225:LEU:HD23	2.20	0.55
1:A:339:LYS:HE2	1:B:339:LYS:HE2	1.88	0.55
1:B:184:ILE:HG13	1:B:185:GLN:N	2.22	0.55
1:A:289:LEU:HB3	1:A:292:THR:HG22	1.86	0.55
1:A:343:ARG:HB3	1:A:345:GLU:OE1	2.07	0.55
1:A:214:PRO:HG2	1:A:266:SER:HA	1.88	0.55
1:A:344:VAL:CG1	1:A:344:VAL:O	2.54	0.54
1:A:194:LEU:HD11	1:A:211:GLU:O	2.07	0.54
1:A:178:LEU:O	1:A:182:VAL:HG13	2.07	0.54
1:B:343:ARG:HB3	1:B:345:GLU:OE1	2.07	0.54
1:A:192:ASN:O	1:A:271:LYS:HA	2.08	0.54
1:A:184:ILE:HG13	1:A:185:GLN:N	2.23	0.54
1:B:289:LEU:HB3	1:B:292:THR:HG22	1.86	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:230:GLU:OE2	1:A:353:THR:OG1	2.19	0.54
1:A:306:HIS:HB2	1:A:310:VAL:CG1	2.37	0.54
1:B:130:LEU:HD13	1:B:207:TYR:CE2	2.43	0.54
1:A:130:LEU:HD13	1:A:207:TYR:CE2	2.43	0.54
1:A:174:VAL:HG21	1:A:277:TRP:CZ2	2.43	0.53
1:B:194:LEU:HD11	1:B:211:GLU:O	2.08	0.53
1:B:220:ARG:CZ	1:B:221:GLU:OE2	2.57	0.53
1:B:306:HIS:HB2	1:B:310:VAL:CG1	2.38	0.53
1:B:178:LEU:O	1:B:182:VAL:HG13	2.08	0.53
1:A:331:ALA:HB1	1:A:336:GLU:HG2	1.91	0.53
1:A:243:ALA:O	1:A:246:TYR:HB3	2.09	0.53
1:B:331:ALA:HB1	1:B:336:GLU:HG2	1.90	0.52
1:A:297:PRO:HG2	1:A:300:MET:HG3	1.90	0.52
1:B:297:PRO:HG2	1:B:300:MET:HG3	1.91	0.52
1:B:174:VAL:HG21	1:B:277:TRP:CZ2	2.43	0.52
1:B:230:GLU:CD	1:B:353:THR:HG21	2.29	0.52
1:B:146:ASN:OD1	1:B:146:ASN:N	2.42	0.52
1:B:215:LEU:HB2	1:B:264:LEU:O	2.10	0.52
1:A:234:ALA:O	1:A:238:THR:CG2	2.52	0.52
1:A:146:ASN:OD1	1:A:146:ASN:N	2.41	0.52
1:A:377:VAL:O	1:A:383:ILE:HG13	2.10	0.52
1:A:215:LEU:HB2	1:A:264:LEU:O	2.10	0.52
1:A:230:GLU:CD	1:A:353:THR:HG21	2.31	0.52
1:A:333:THR:OG1	1:A:336:GLU:HB3	2.09	0.52
1:B:344:VAL:O	1:B:344:VAL:CG1	2.52	0.52
1:A:256:ASP:N	1:A:274:ASP:OD1	2.35	0.51
1:B:233:THR:HG23	1:B:322:PHE:HD2	1.75	0.51
1:B:333:THR:OG1	1:B:336:GLU:HB3	2.10	0.51
1:B:377:VAL:O	1:B:383:ILE:HG13	2.09	0.51
1:B:243:ALA:O	1:B:246:TYR:HB3	2.09	0.51
1:B:277:TRP:H	1:B:277:TRP:HE3	1.56	0.51
1:B:230:GLU:OE2	1:B:353:THR:HG21	2.11	0.51
1:A:233:THR:HG23	1:A:322:PHE:HD2	1.75	0.51
1:B:147:VAL:CG2	1:B:162:LYS:HG3	2.38	0.50
1:B:339:LYS:CE	3:B:8:HOH:O	2.26	0.50
1:A:230:GLU:OE2	1:A:353:THR:HG21	2.11	0.50
1:B:289:LEU:HA	1:B:291:GLY:N	2.27	0.50
1:B:166:LYS:N	1:B:169:LEU:HD13	2.19	0.50
1:A:329:PHE:CE1	1:A:346:PHE:HB3	2.46	0.49
1:B:241:ALA:HB3	1:B:378:LEU:HD21	1.93	0.49
1:B:239:GLU:HG2	1:B:389:LYS:HZ2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:ALA:O	1:B:238:THR:CG2	2.52	0.49
1:A:353:THR:O	1:A:356:ALA:HB3	2.12	0.49
1:B:142:GLY:N	1:B:279:VAL:HG12	2.27	0.49
1:A:241:ALA:HB3	1:A:378:LEU:HD21	1.93	0.49
1:B:335:GLN:H	1:B:335:GLN:CD	2.16	0.49
1:A:367:ASN:HB3	1:A:370:GLN:CG	2.42	0.49
1:A:285:ARG:O	1:A:286:ARG:C	2.50	0.49
1:A:287:ASP:HA	1:A:290:CYS:HB2	1.94	0.49
1:B:331:ALA:HB1	1:B:336:GLU:CG	2.43	0.49
1:A:289:LEU:HA	1:A:291:GLY:N	2.27	0.49
1:B:310:VAL:HG23	1:B:311:ASP:N	2.27	0.49
1:B:166:LYS:HA	1:B:169:LEU:CB	2.35	0.48
1:B:238:THR:HG21	1:B:387:SER:OG	2.13	0.48
1:B:353:THR:O	1:B:356:ALA:HB3	2.13	0.48
1:A:334:TYR:HB3	1:B:338:TYR:OH	2.14	0.48
1:A:238:THR:HG21	1:A:387:SER:OG	2.13	0.48
1:A:262:LEU:HD11	1:A:318:LEU:HD11	1.96	0.48
1:A:142:GLY:N	1:A:279:VAL:HG12	2.28	0.48
1:A:335:GLN:CD	1:A:335:GLN:H	2.18	0.48
1:B:248:HIS:CE1	1:B:253:ILE:HG22	2.49	0.48
1:A:239:GLU:HG2	1:A:389:LYS:HZ2	1.78	0.48
1:A:228:PHE:CE2	1:A:236:TYR:HE2	2.31	0.47
1:A:297:PRO:HB3	1:A:313:TRP:CG	2.49	0.47
1:A:310:VAL:HG23	1:A:311:ASP:N	2.29	0.47
2:B:1:0C6:C17	2:B:1:0C6:N25	2.76	0.47
1:A:166:LYS:N	1:A:169:LEU:HD13	2.21	0.47
1:A:338:TYR:OH	1:B:334:TYR:HB3	2.14	0.47
1:B:343:ARG:CB	1:B:345:GLU:OE1	2.63	0.47
1:B:228:PHE:CE2	1:B:236:TYR:HE2	2.33	0.47
1:B:329:PHE:CE1	1:B:346:PHE:HB3	2.50	0.47
1:A:170:GLU:HG2	1:B:251:ARG:NH2	2.29	0.47
1:B:297:PRO:HB3	1:B:313:TRP:CG	2.50	0.47
1:B:213:ALA:O	2:B:1:0C6:N15	2.43	0.46
1:B:133:PHE:HE2	1:B:159:LEU:HD21	1.79	0.46
1:A:331:ALA:HB1	1:A:336:GLU:CG	2.46	0.46
1:A:235:THR:O	1:A:238:THR:HG23	2.15	0.46
1:A:343:ARG:CB	1:A:345:GLU:OE1	2.64	0.46
1:B:367:ASN:HB3	1:B:370:GLN:CG	2.42	0.46
1:A:318:LEU:HD23	1:A:318:LEU:HA	1.77	0.46
1:A:251:ARG:NH2	1:B:170:GLU:HG2	2.31	0.46
1:A:248:HIS:CE1	1:A:253:ILE:HG22	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:133:PHE:HE2	1:A:159:LEU:HD21	1.80	0.46
1:B:285:ARG:O	1:B:286:ARG:C	2.54	0.46
1:B:262:LEU:HD11	1:B:318:LEU:HD11	1.96	0.45
1:B:337:THR:O	1:B:341:ILE:HG13	2.16	0.45
1:A:256:ASP:OD2	1:A:258:LYS:HG2	2.16	0.45
1:A:337:THR:O	1:A:341:ILE:HG13	2.16	0.45
1:A:277:TRP:HE3	1:A:277:TRP:H	1.57	0.45
1:B:142:GLY:CA	1:B:279:VAL:HG12	2.46	0.45
1:A:259:PRO:HA	1:A:262:LEU:HD12	1.97	0.45
1:A:166:LYS:HA	1:A:169:LEU:CB	2.35	0.45
1:B:357:ARG:O	1:B:358:ASP:C	2.55	0.45
1:B:184:ILE:CG1	1:B:185:GLN:N	2.80	0.45
1:B:235:THR:O	1:B:238:THR:HG23	2.16	0.45
1:A:359:LEU:HG	1:A:363:LEU:HD12	1.99	0.45
1:A:142:GLY:CA	1:A:279:VAL:HG12	2.47	0.45
1:A:179:ARG:HA	1:A:179:ARG:HD3	1.77	0.45
1:B:359:LEU:HG	1:B:363:LEU:HD12	1.99	0.44
1:B:287:ASP:HA	1:B:290:CYS:HB2	1.98	0.44
1:B:293:LEU:HA	1:B:296:LEU:HD12	2.00	0.44
1:A:184:ILE:CG1	1:A:185:GLN:N	2.80	0.44
1:A:310:VAL:O	1:A:313:TRP:HB3	2.18	0.44
1:A:185:GLN:HE21	1:A:255:ARG:NH2	2.13	0.44
1:A:357:ARG:O	1:A:358:ASP:C	2.55	0.44
1:A:255:ARG:HD2	1:A:255:ARG:HA	1.46	0.44
1:B:299:GLU:HA	1:B:304:ARG:HH21	1.83	0.44
1:B:259:PRO:HA	1:B:262:LEU:HD12	2.00	0.44
1:A:175:GLU:OE2	1:B:251:ARG:NH2	2.51	0.43
1:B:256:ASP:OD2	1:B:258:LYS:HG2	2.18	0.43
1:A:293:LEU:HA	1:A:296:LEU:HD12	2.00	0.43
1:B:283:SER:O	1:B:284:SER:O	2.35	0.43
1:B:255:ARG:HA	1:B:255:ARG:HD2	1.49	0.43
2:A:2:OC6:C17	2:A:2:OC6:N25	2.76	0.43
1:B:208:LEU:HD13	1:B:275:PHE:CE2	2.54	0.43
1:A:174:VAL:HG21	1:A:277:TRP:CH2	2.54	0.43
1:B:310:VAL:O	1:B:313:TRP:HB3	2.18	0.43
1:A:165:PHE:C	1:A:167:ALA:H	2.22	0.43
1:B:318:LEU:HD23	1:B:318:LEU:HA	1.77	0.43
1:B:301:ILE:CD1	1:B:341:ILE:HG21	2.49	0.42
1:B:165:PHE:C	1:B:167:ALA:H	2.21	0.42
1:B:213:ALA:O	2:B:1:OC6:H12	2.19	0.42
1:B:174:VAL:HG21	1:B:277:TRP:CH2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:289:LEU:CD1	1:A:292:THR:HG22	2.47	0.42
1:B:202:ASP:OD1	1:B:203:ALA:N	2.52	0.42
1:B:298:PRO:O	1:B:302:GLU:HB2	2.18	0.42
1:B:331:ALA:CB	1:B:336:GLU:HG3	2.49	0.42
1:B:299:GLU:CD	1:B:299:GLU:H	2.23	0.42
1:A:202:ASP:OD1	1:A:203:ALA:N	2.53	0.42
1:A:383:ILE:HA	1:A:383:ILE:HD13	1.93	0.42
1:B:383:ILE:HD13	1:B:383:ILE:HA	1.94	0.42
1:A:248:HIS:ND1	1:A:253:ILE:HG22	2.35	0.42
1:B:197:TYR:HE2	1:B:211:GLU:HA	1.81	0.42
1:B:258:LYS:HB2	1:B:259:PRO:HD2	2.02	0.42
1:B:155:SER:O	1:B:156:LYS:HB2	2.21	0.41
1:A:297:PRO:HA	1:A:298:PRO:HD3	1.97	0.41
1:A:147:VAL:O	1:A:147:VAL:CG2	2.68	0.41
1:A:213:ALA:O	2:A:2:OC6:H12	2.20	0.41
1:A:125:LYS:O	1:A:126:ARG:CB	2.66	0.41
1:B:295:TYR:OH	1:B:321:GLU:OE1	2.26	0.41
1:A:331:ALA:CB	1:A:336:GLU:HG3	2.51	0.41
1:A:222:LEU:HA	1:A:228:PHE:CE1	2.55	0.41
1:B:231:GLN:O	1:B:235:THR:HG23	2.20	0.41
1:A:141:LYS:HE2	1:A:146:ASN:ND2	2.36	0.41
1:B:248:HIS:ND1	1:B:253:ILE:HG22	2.35	0.41
1:A:299:GLU:HA	1:A:304:ARG:HH21	1.84	0.41
1:B:190:HIS:HA	1:B:191:PRO:HD2	1.86	0.41
1:A:289:LEU:CA	1:A:291:GLY:H	2.33	0.41
1:A:231:GLN:O	1:A:235:THR:HG23	2.21	0.41
1:A:213:ALA:HA	1:A:214:PRO:HD3	1.66	0.41
1:B:142:GLY:HA3	1:B:279:VAL:HG12	2.03	0.41
1:A:287:ASP:HA	1:A:290:CYS:CB	2.51	0.41
1:A:301:ILE:CD1	1:A:341:ILE:HG21	2.51	0.41
1:A:314:SER:O	1:A:317:VAL:N	2.54	0.41
1:A:327:PRO:HG2	1:A:330:GLU:HB2	2.03	0.41
1:B:256:ASP:HB3	1:B:274:ASP:OD1	2.21	0.41
1:B:202:ASP:CG	1:B:203:ALA:N	2.74	0.41
1:A:258:LYS:HB2	1:A:259:PRO:HD2	2.03	0.41
1:A:197:TYR:HE2	1:A:211:GLU:HA	1.80	0.40
1:B:262:LEU:HD22	1:B:270:LEU:HD21	2.04	0.40
1:A:299:GLU:CD	1:A:299:GLU:H	2.24	0.40
1:A:155:SER:O	1:A:156:LYS:HB2	2.21	0.40
1:B:235:THR:HA	1:B:238:THR:HG23	2.04	0.40
1:B:236:TYR:CD1	1:B:270:LEU:HD12	2.56	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	263/279 (94%)	233 (89%)	28 (11%)	2 (1%)	24	64
1	B	263/279 (94%)	234 (89%)	26 (10%)	3 (1%)	17	56
All	All	526/558 (94%)	467 (89%)	54 (10%)	5 (1%)	19	58

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	284	SER
1	B	284	SER
1	B	285	ARG
1	A	286	ARG
1	B	286	ARG

### 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	234/247 (95%)	221 (94%)	13 (6%)	26	63
1	B	234/247 (95%)	221 (94%)	13 (6%)	26	63
All	All	468/494 (95%)	442 (94%)	26 (6%)	26	63

All (26) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	137	ARG
1	A	143	LYS
1	A	146	ASN
1	A	151	ARG
1	A	174	VAL
1	A	181	GLU
1	A	183	GLU
1	A	186	SER
1	A	238	THR
1	A	245	SER
1	A	255	ARG
1	A	312	LEU
1	A	350	ASP
1	B	143	LYS
1	B	146	ASN
1	B	151	ARG
1	B	174	VAL
1	B	181	GLU
1	B	183	GLU
1	B	186	SER
1	B	238	THR
1	B	245	SER
1	B	255	ARG
1	B	260	GLU
1	B	312	LEU
1	B	350	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	177	GLN
1	A	185	GLN
1	A	192	ASN
1	A	261	ASN
1	A	370	GLN
1	B	177	GLN
1	B	185	GLN
1	B	192	ASN
1	B	261	ASN
1	B	370	GLN



### 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	0C6	A	2	-	22,27,27	1.80	4 (18%)	29,37,37	1.55	6 (20%)
2	0C6	B	1	-	22,27,27	1.77	4 (18%)	29,37,37	1.45	5 (17%)

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	0C6	A	2	-	-	0/8/12/12	0/3/3/3
2	0C6	B	1	-	-	0/8/12/12	0/3/3/3

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	0C6	C07-N08	2.24	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	2	OC6	C07-N08	2.27	1.46	1.39
2	A	2	OC6	C14-N15	4.14	1.43	1.36
2	B	1	OC6	C14-N15	4.19	1.43	1.36
2	B	1	OC6	C09-N08	4.44	1.44	1.36
2	B	1	OC6	C16-N15	4.64	1.50	1.40
2	A	2	OC6	C09-N08	4.69	1.45	1.36
2	A	2	OC6	C16-N15	4.77	1.50	1.40

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	OC6	N13-C14-N25	-3.52	122.92	126.67
2	A	2	OC6	N13-C14-N25	-3.48	122.96	126.67
2	B	1	OC6	C12-C10-C09	-3.23	118.22	121.51
2	A	2	OC6	C12-C10-C09	-3.21	118.25	121.51
2	B	1	OC6	C16-N15-C14	-2.53	122.50	129.19
2	A	2	OC6	C16-N15-C14	-2.51	122.53	129.19
2	B	1	OC6	C07-N08-C09	-2.25	124.26	129.36
2	A	2	OC6	C07-N08-C09	-2.11	124.58	129.36
2	B	1	OC6	F11-C10-C09	2.11	121.39	119.73
2	A	2	OC6	C07-C02-CL1	2.64	122.92	119.45
2	A	2	OC6	F11-C10-C09	2.88	121.98	119.73

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2	OC6	3	0
2	B	1	OC6	4	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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	265/279 (94%)	-0.03	11 (4%) 40 23	21, 49, 95, 167	0
1	B	265/279 (94%)	-0.02	8 (3%) 54 33	21, 49, 96, 166	0
All	All	530/558 (94%)	-0.02	19 (3%) 46 28	21, 49, 97, 167	0

All (19) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	284	SER	10.4
1	A	284	SER	9.5
1	B	125	LYS	7.4
1	B	286	ARG	5.6
1	A	286	ARG	4.9
1	A	126	ARG	4.7
1	A	125	LYS	3.9
1	B	126	ARG	3.9
1	A	290	CYS	3.4
1	A	285	ARG	3.1
1	B	180	ARG	3.1
1	A	180	ARG	3.0
1	B	285	ARG	2.8
1	A	275	PHE	2.8
1	B	305	MET	2.7
1	B	289	LEU	2.6
1	A	289	LEU	2.4
1	A	283	SER	2.4
1	A	305	MET	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<sup>th</sup> 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( $\text{\AA}^2$ )	Q<0.9
2	0C6	A	2	25/25	0.97	0.18	0.12	16,32,43,45	0
2	0C6	B	1	25/25	0.98	0.17	-0.04	16,32,42,46	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.