WORLDWIDE PDB PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 03:47 PM GMT

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PDB ID	:	4DHF
Title	:	Structure of Aurora A mutant bound to Biogenidec cpd 15
Authors	:	Silvian, L.; Marcotte, D.J.
Deposited on	:	2012-01-27
Resolution	:	2.80 Å(reported)

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION
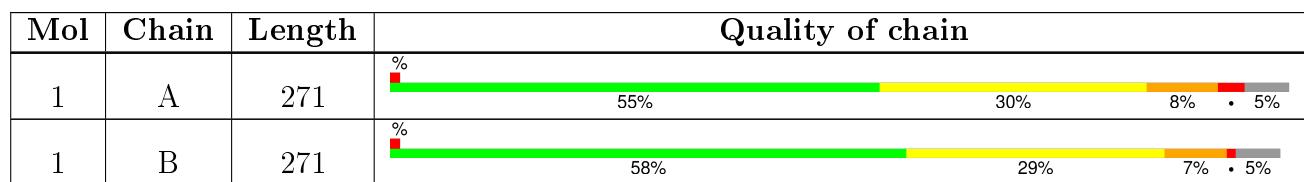
The reported resolution of this entry is 2.80 Å.

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

Metric	Percentile Ranks	Value
Rfree		0.298
Clashscore		25
Ramachandran outliers		5.3%
Sidechain outliers		11.9%
RSRZ outliers		1.2%

Worse ← → *Better*

■ Percentile relative to all X-ray structures
▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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

Mol	Chain	Length	Quality of chain
1	A	271	% 55% 30% 8% · 5%
1	B	271	% 58% 29% 7% · 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 4300 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.
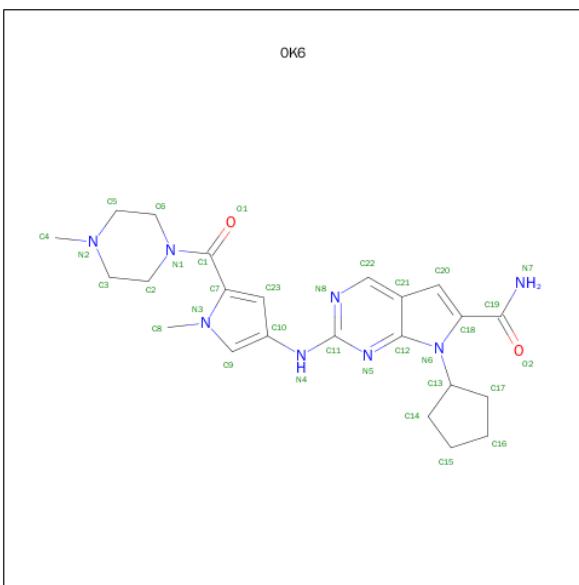
- Molecule 1 is a protein called Aurora kinase A.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	258	Total 2111	C 1358	N 370	O 377	S 6	0	0	0
1	B	258	Total 2111	C 1358	N 370	O 377	S 6	0	0	0

There are 14 discrepancies between the modelled and reference sequences:
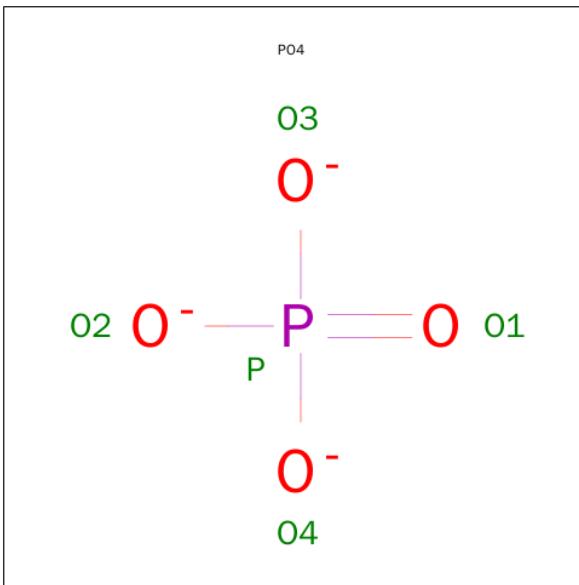
Chain	Residue	Modelled	Actual	Comment	Reference
A	121	GLY	-	EXPRESSION TAG	UNP O14965
A	122	PRO	-	EXPRESSION TAG	UNP O14965
A	123	LEU	-	EXPRESSION TAG	UNP O14965
A	124	GLY	-	EXPRESSION TAG	UNP O14965
A	125	SER	-	EXPRESSION TAG	UNP O14965
A	287	ASP	THR	ENGINEERED MUTATION	UNP O14965
A	288	ASP	THR	ENGINEERED MUTATION	UNP O14965
B	121	GLY	-	EXPRESSION TAG	UNP O14965
B	122	PRO	-	EXPRESSION TAG	UNP O14965
B	123	LEU	-	EXPRESSION TAG	UNP O14965
B	124	GLY	-	EXPRESSION TAG	UNP O14965
B	125	SER	-	EXPRESSION TAG	UNP O14965
B	287	ASP	THR	ENGINEERED MUTATION	UNP O14965
B	288	ASP	THR	ENGINEERED MUTATION	UNP O14965

- Molecule 2 is 7-CYCLOPENTYL-2-({1-METHYL-5-[(4-METHYLPIPERAZIN-1-YL)CARBONYL]-1H-PYRROL-3-YL}AMINO)-7H-PYRROLO[2,3-D]PYRIMIDINE-6-CARBOXAMIDE (three-letter code: 0K6) (formula: $C_{23}H_{30}N_8O_2$).

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total 33	C 23	N 8	O 2	0	0
2	B	1	Total 33	C 23	N 8	O 2	0	0

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O_4P).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 5	O 4	P 1	0	0
3	B	1	Total 5	O 4	P 1	0	0
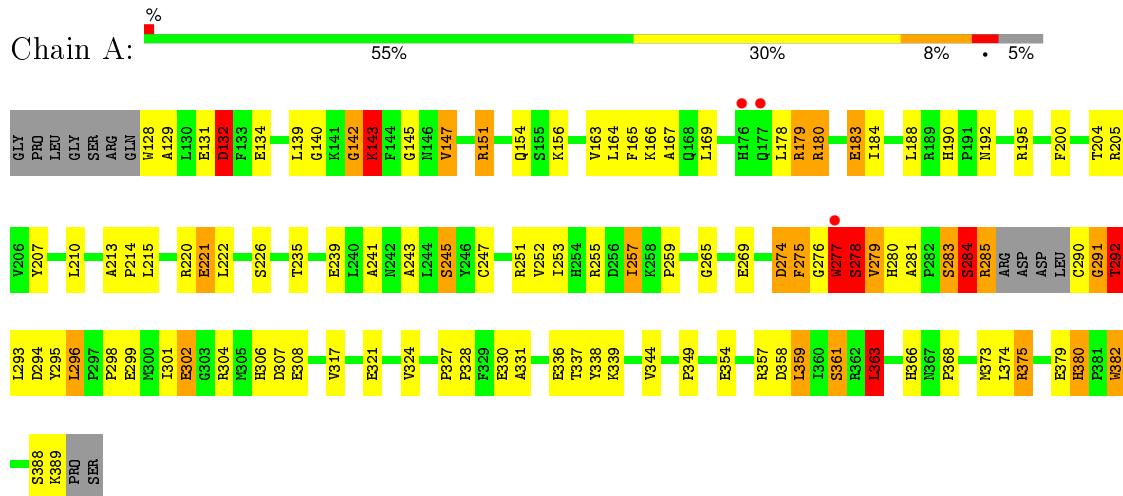
• Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total 1	Mg 1	0	0
4	A	1	Total 1	Mg 1	0	0
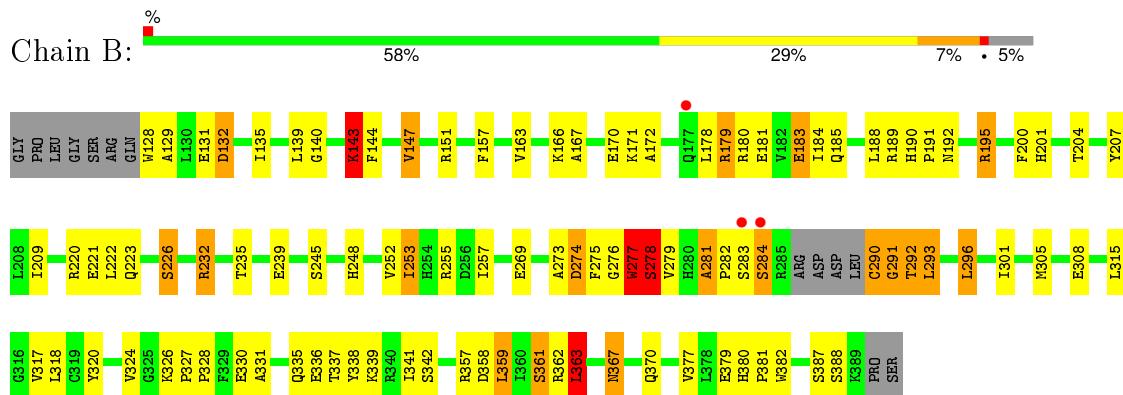
3 Residue-property plots ⓘ

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 (i)

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α, β, γ	81.59Å 81.59Å 166.06Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	27.68 – 2.80 27.68 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.6 (27.68-2.80) 99.6 (27.68-2.80)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	4.12 (at 2.80Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.206 , 0.299 0.205 , 0.298	Depositor DCC
R_{free} test set	766 reflections (5.25%)	DCC
Wilson B-factor (Å^2)	65.8	Xtriage
Anisotropy	0.169	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.37 , 39.6	EDS
Estimated twinning fraction	0.489 for h,-h-k,-l	Xtriage
L-test for twinning [2]	$<|L|> = 0.52$, $<L^2> = 0.36$	Xtriage
Outliers	0 of 15345 reflections	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	4300	wwPDB-VP
Average B, all atoms (Å^2)	59.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.90% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: PO4, 0K6, MG

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	0.68	3/2164 (0.1%)	0.82	1/2925 (0.0%)
1	B	0.66	3/2164 (0.1%)	0.84	2/2925 (0.1%)
All	All	0.67	6/4328 (0.1%)	0.83	3/5850 (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	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	382	TRP	CD2-CE2	5.92	1.48	1.41
1	A	128	TRP	CD2-CE2	5.79	1.48	1.41
1	A	277	TRP	CD2-CE2	5.59	1.48	1.41
1	B	382	TRP	CD2-CE2	5.46	1.47	1.41
1	B	128	TRP	CD2-CE2	5.16	1.47	1.41
1	B	277	TRP	CD2-CE2	5.06	1.47	1.41

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	278	SER	N-CA-C	6.22	127.81	111.00
1	A	363	LEU	CA-CB-CG	5.65	128.30	115.30
1	B	363	LEU	CA-CB-CG	5.00	126.80	115.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	278	SER	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	2111	0	2107	109	0
1	B	2111	0	2107	106	0
2	A	33	0	30	9	0
2	B	33	0	30	7	0
3	A	5	0	0	1	0
3	B	5	0	0	0	0
4	A	1	0	0	0	0
4	B	1	0	0	0	0
All	All	4300	0	4274	211	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 25.

All (211) 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:283:SER:HA	1:B:284:SER:HB3	1.28	1.15
1:A:183:GLU:CD	1:A:183:GLU:H	1.45	1.12
1:A:375:ARG:H	1:A:375:ARG:HD2	1.15	1.12
1:A:183:GLU:N	1:A:183:GLU:CD	2.14	0.98
1:B:183:GLU:CD	1:B:183:GLU:N	2.17	0.95
1:A:336:GLU:OE2	1:B:336:GLU:OE1	1.85	0.95
1:A:190:HIS:HD2	1:A:192:ASN:H	1.12	0.93
1:B:183:GLU:CD	1:B:183:GLU:H	1.72	0.92
1:B:283:SER:HA	1:B:284:SER:CB	2.00	0.91
1:A:283:SER:OG	1:A:284:SER:HB2	1.69	0.91
1:B:220:ARG:NH1	1:B:223:GLN:HB3	1.85	0.90
1:A:339:LYS:HZ1	1:B:339:LYS:HZ1	1.12	0.90
1:A:339:LYS:NZ	1:B:339:LYS:HZ1	1.70	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:375:ARG:N	1:A:375:ARG:HD2	1.91	0.86
1:B:140:GLY:HA3	2:B:401:0K6:H6	1.57	0.86
1:B:277:TRP:HA	1:B:278:SER:O	1.75	0.86
1:B:281:ALA:HB1	1:B:282:PRO:CD	2.08	0.83
1:A:283:SER:CB	1:A:284:SER:HB2	2.10	0.82
1:B:147:VAL:HG11	2:B:401:0K6:H2	1.43	0.81
1:B:184:ILE:O	1:B:188:LEU:HG	1.80	0.81
1:A:129:ALA:O	1:A:132:ASP:HB2	1.80	0.80
1:A:339:LYS:NZ	1:B:339:LYS:NZ	2.30	0.80
1:B:195:ARG:HH11	1:B:195:ARG:HG2	1.45	0.80
1:B:129:ALA:O	1:B:132:ASP:HB2	1.82	0.80
1:A:301:ILE:HG23	1:A:338:TYR:CE2	2.18	0.79
1:B:367:ASN:ND2	1:B:370:GLN:HG3	1.98	0.78
1:A:183:GLU:N	1:A:183:GLU:OE1	2.17	0.78
1:B:301:ILE:HG23	1:B:338:TYR:CE2	2.19	0.78
1:B:220:ARG:HH12	1:B:223:GLN:HB3	1.48	0.76
1:A:252:VAL:HB	1:A:279:VAL:HG11	1.67	0.76
1:B:283:SER:CA	1:B:284:SER:HB3	2.12	0.76
1:A:339:LYS:HZ1	1:B:339:LYS:NZ	1.83	0.75
1:A:147:VAL:HG11	2:A:401:0K6:H2	1.53	0.73
1:B:232:ARG:HG3	1:B:232:ARG:HH11	1.54	0.73
1:A:291:GLY:O	1:A:293:LEU:N	2.21	0.73
1:B:281:ALA:HB1	1:B:282:PRO:HD2	1.69	0.72
1:B:277:TRP:N	1:B:277:TRP:CD1	2.56	0.72
1:A:252:VAL:HB	1:A:279:VAL:CG1	2.22	0.70
1:A:388:SER:O	1:A:389:LYS:HB2	1.90	0.70
1:B:189:ARG:HD3	1:B:195:ARG:HD2	1.75	0.68
1:A:375:ARG:CD	1:A:375:ARG:H	1.98	0.68
1:B:195:ARG:HG2	1:B:195:ARG:NH1	2.07	0.67
1:A:296:LEU:HB3	1:A:301:ILE:CD1	2.24	0.67
1:B:290:CYS:HB2	1:B:291:GLY:HA2	1.76	0.67
1:B:181:GLU:HG3	1:B:185:GLN:HE21	1.59	0.67
1:B:357:ARG:O	1:B:361:SER:HB2	1.94	0.67
1:A:302:GLU:HG3	1:A:304:ARG:NE	2.10	0.67
1:B:296:LEU:HB3	1:B:301:ILE:CD1	2.25	0.66
1:A:331:ALA:HB1	1:A:336:GLU:CD	2.18	0.64
2:A:401:0K6:N7	2:A:401:0K6:H3	2.11	0.64
1:A:139:LEU:O	2:A:401:0K6:H17	1.98	0.64
1:A:131:GLU:O	1:A:132:ASP:HB2	1.96	0.64
1:B:232:ARG:NH1	1:B:232:ARG:HG3	2.12	0.63
1:A:255:ARG:HH21	1:A:277:TRP:HB2	1.61	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:357:ARG:O	1:A:361:SER:HB2	1.98	0.63
1:A:190:HIS:CD2	1:A:192:ASN:H	2.04	0.63
1:A:373:MET:HB3	1:A:375:ARG:HH21	1.63	0.62
1:B:359:LEU:HD22	1:B:363:LEU:HD22	1.81	0.62
1:B:274:ASP:O	1:B:275:PHE:HB2	1.99	0.61
1:A:235:THR:O	1:A:239:GLU:HG3	2.00	0.61
1:B:139:LEU:O	2:B:401:0K6:H17	2.01	0.61
1:A:359:LEU:HD22	1:A:363:LEU:HD22	1.81	0.61
1:B:190:HIS:HD2	1:B:192:ASN:H	1.47	0.61
1:B:292:THR:OG1	1:B:293:LEU:N	2.33	0.61
1:A:140:GLY:HA3	2:A:401:0K6:C16	2.31	0.60
1:A:291:GLY:C	1:A:293:LEU:H	2.05	0.60
1:B:331:ALA:HB1	1:B:336:GLU:OE1	2.01	0.59
1:A:142:GLY:HA2	1:A:145:GLY:O	2.02	0.59
1:B:331:ALA:HB1	1:B:336:GLU:CD	2.22	0.59
1:B:180:ARG:NH2	1:B:183:GLU:HG2	2.17	0.59
1:A:180:ARG:O	1:A:183:GLU:OE1	2.21	0.58
1:A:200:PHE:CE2	1:A:207:TYR:CD2	2.92	0.58
1:B:143:LYS:CE	1:B:143:LYS:H	2.17	0.58
1:B:367:ASN:HD22	1:B:370:GLN:HG3	1.70	0.57
1:A:339:LYS:HZ2	1:B:339:LYS:NZ	2.02	0.57
1:A:180:ARG:C	1:A:183:GLU:OE1	2.43	0.57
1:B:232:ARG:CG	1:B:232:ARG:HH11	2.18	0.57
1:B:163:VAL:HG22	1:B:207:TYR:HD1	1.70	0.57
1:A:131:GLU:O	1:A:132:ASP:CB	2.53	0.56
1:A:296:LEU:HB3	1:A:301:ILE:HD13	1.88	0.56
1:A:163:VAL:HG22	1:A:207:TYR:HD1	1.71	0.56
1:A:302:GLU:OE1	1:A:304:ARG:NH2	2.29	0.56
1:B:222:LEU:O	1:B:226:SER:N	2.39	0.55
1:B:200:PHE:CE2	1:B:207:TYR:CD2	2.95	0.55
1:A:317:VAL:HG13	1:A:328:PRO:HD2	1.89	0.55
2:B:401:0K6:H15	2:B:401:0K6:N5	2.22	0.55
1:A:259:PRO:HD3	1:A:295:TYR:CZ	2.41	0.55
1:B:358:ASP:OD2	1:B:380:HIS:HE1	1.90	0.54
1:B:140:GLY:HA3	2:B:401:0K6:C16	2.32	0.54
1:B:317:VAL:HG13	1:B:328:PRO:HD2	1.90	0.54
1:B:257:ILE:HG22	1:B:318:LEU:HD11	1.90	0.53
1:A:296:LEU:HB3	1:A:301:ILE:HD11	1.90	0.53
1:A:151:ARG:HD3	1:A:156:LYS:HA	1.90	0.53
1:A:336:GLU:CD	1:B:336:GLU:CD	2.67	0.53
2:A:401:0K6:H15	2:A:401:0K6:N5	2.24	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:166:LYS:HA	1:A:169:LEU:HD12	1.91	0.53
1:A:295:TYR:OH	1:A:321:GLU:OE2	2.25	0.52
1:A:210:LEU:HD13	2:A:401:0K6:H12	1.91	0.52
1:B:190:HIS:CD2	1:B:191:PRO:HD2	2.45	0.52
1:A:179:ARG:C	1:A:183:GLU:OE2	2.47	0.52
1:B:183:GLU:OE1	1:B:184:ILE:N	2.37	0.52
1:A:302:GLU:HG3	1:A:304:ARG:HE	1.72	0.51
1:B:143:LYS:HG2	1:B:144:PHE:H	1.76	0.50
1:B:143:LYS:H	1:B:143:LYS:NZ	2.08	0.50
1:A:358:ASP:OD2	1:A:380:HIS:HE1	1.94	0.50
1:B:326:LYS:HD3	1:B:330:GLU:OE1	2.12	0.49
1:A:277:TRP:HE3	1:A:277:TRP:H	1.58	0.49
1:A:302:GLU:HG3	1:A:304:ARG:CZ	2.42	0.49
1:B:180:ARG:CZ	1:B:183:GLU:HG2	2.41	0.49
1:A:251:ARG:NH1	1:A:308:GLU:OE1	2.46	0.49
1:A:301:ILE:HG23	1:A:338:TYR:CD2	2.46	0.49
1:A:166:LYS:O	1:A:167:ALA:C	2.49	0.49
1:B:296:LEU:CB	1:B:301:ILE:HD11	2.43	0.49
1:A:147:VAL:HG11	2:A:401:0K6:N7	2.26	0.49
1:A:296:LEU:HD23	1:A:301:ILE:HD11	1.95	0.49
1:A:247:CYS:O	1:A:252:VAL:HG22	2.12	0.48
1:B:179:ARG:C	1:B:183:GLU:OE2	2.52	0.48
1:A:252:VAL:HA	1:A:279:VAL:HB	1.95	0.48
1:A:163:VAL:HG22	1:A:207:TYR:CD1	2.49	0.47
1:B:253:ILE:HG21	1:B:308:GLU:HA	1.95	0.47
1:B:380:HIS:O	1:B:381:PRO:C	2.53	0.47
1:A:180:ARG:HG3	1:A:184:ILE:HD11	1.97	0.47
1:A:184:ILE:O	1:A:188:LEU:HG	2.14	0.47
1:B:147:VAL:HG11	2:B:401:0K6:N7	2.22	0.47
1:A:274:ASP:O	1:A:275:PHE:HB2	2.14	0.47
1:B:200:PHE:HE1	1:B:209:ILE:HD11	1.80	0.47
1:B:255:ARG:HH21	1:B:277:TRP:HB3	1.79	0.47
1:A:259:PRO:HD3	1:A:295:TYR:CE2	2.50	0.47
1:A:192:ASN:HB2	1:A:243:ALA:HB2	1.97	0.46
1:B:292:THR:O	1:B:293:LEU:HB2	2.15	0.46
1:B:284:SER:HB2	1:B:305:MET:HG3	1.97	0.46
1:A:379:GLU:O	1:A:380:HIS:C	2.54	0.46
1:B:183:GLU:OE1	1:B:183:GLU:N	2.49	0.46
2:B:401:0K6:C9	2:B:401:0K6:N5	2.76	0.46
1:B:143:LYS:HE3	1:B:143:LYS:H	1.79	0.46
1:B:166:LYS:O	1:B:167:ALA:C	2.53	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:221:GLU:O	1:A:221:GLU:HG3	2.15	0.46
1:A:278:SER:HB3	1:A:279:VAL:H	1.61	0.46
1:A:269:GLU:H	1:A:269:GLU:HG2	1.35	0.46
1:B:170:GLU:C	1:B:172:ALA:H	2.18	0.46
1:A:307:ASP:HB2	1:A:308:GLU:OE2	2.16	0.45
1:B:337:THR:O	1:B:341:ILE:HG13	2.16	0.45
1:A:290:CYS:O	1:A:292:THR:N	2.48	0.45
1:B:135:ILE:N	1:B:135:ILE:HD13	2.32	0.45
1:A:257:ILE:H	1:A:257:ILE:HD13	1.81	0.45
1:A:301:ILE:CG2	1:A:338:TYR:CE2	2.94	0.45
2:A:401:0K6:H2	2:A:401:0K6:H3	1.81	0.45
1:B:269:GLU:HG2	1:B:269:GLU:H	1.56	0.45
1:B:387:SER:OG	1:B:388:SER:N	2.49	0.45
1:B:290:CYS:CB	1:B:291:GLY:HA2	2.43	0.45
1:A:143:LYS:HD2	3:A:402:PO4:O4	2.17	0.45
1:A:284:SER:HB3	1:A:285:ARG:H	1.49	0.45
1:A:380:HIS:CD2	1:A:382:TRP:H	2.34	0.44
1:A:293:LEU:O	1:A:296:LEU:HB2	2.17	0.44
1:B:359:LEU:HD21	1:B:377:VAL:HG22	1.99	0.44
1:A:222:LEU:O	1:A:226:SER:N	2.51	0.44
1:A:374:LEU:H	1:A:375:ARG:HH21	1.65	0.44
1:A:336:GLU:OE2	1:B:336:GLU:CD	2.55	0.44
1:A:339:LYS:HZ2	1:B:339:LYS:HZ2	1.65	0.44
1:A:253:ILE:HG21	1:A:308:GLU:HA	2.00	0.44
1:A:252:VAL:HB	1:A:279:VAL:CB	2.48	0.44
1:B:315:LEU:HA	1:B:315:LEU:HD12	1.68	0.44
1:B:358:ASP:O	1:B:362:ARG:HG3	2.18	0.44
1:B:296:LEU:CB	1:B:301:ILE:CD1	2.96	0.43
1:A:366:HIS:O	1:A:368:PRO:HD3	2.18	0.43
1:A:374:LEU:H	1:A:375:ARG:NH2	2.16	0.43
1:A:373:MET:HB3	1:A:375:ARG:NH2	2.31	0.43
1:A:283:SER:HG	1:A:306:HIS:CD2	2.36	0.43
1:B:131:GLU:O	1:B:132:ASP:CB	2.66	0.43
1:B:170:GLU:O	1:B:172:ALA:N	2.51	0.43
1:B:180:ARG:C	1:B:183:GLU:OE1	2.57	0.43
1:B:277:TRP:HA	1:B:278:SER:C	2.36	0.43
1:B:320:TYR:O	1:B:324:VAL:HG23	2.19	0.43
1:B:255:ARG:NH2	1:B:277:TRP:HB3	2.34	0.43
1:B:131:GLU:CD	1:B:131:GLU:H	2.22	0.43
1:B:379:GLU:O	1:B:380:HIS:C	2.57	0.43
1:A:265:GLY:HA3	1:A:269:GLU:HG3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:241:ALA:O	1:A:245:SER:HB2	2.19	0.43
1:A:298:PRO:O	1:A:302:GLU:HG2	2.19	0.43
1:B:253:ILE:O	1:B:278:SER:HA	2.19	0.43
1:B:235:THR:O	1:B:239:GLU:HG3	2.17	0.43
1:A:131:GLU:CD	1:A:131:GLU:H	2.22	0.42
1:B:179:ARG:O	1:B:183:GLU:OE2	2.36	0.42
1:B:326:LYS:HA	1:B:327:PRO:HD3	1.94	0.42
1:A:324:VAL:HG13	1:A:349:PRO:HG2	2.02	0.42
1:B:163:VAL:HG22	1:B:207:TYR:CD1	2.51	0.42
1:A:331:ALA:HB3	1:A:337:THR:OG1	2.20	0.42
1:A:140:GLY:HA3	2:A:401:0K6:H7	1.99	0.42
1:A:291:GLY:C	1:A:293:LEU:N	2.69	0.42
1:A:327:PRO:HG2	1:A:330:GLU:HB2	2.02	0.42
1:A:278:SER:OG	1:A:279:VAL:HG13	2.20	0.42
1:A:380:HIS:HD2	1:A:382:TRP:H	1.66	0.42
1:B:151:ARG:HA	1:B:157:PHE:O	2.20	0.41
1:B:273:ALA:O	1:B:274:ASP:HB3	2.20	0.41
1:A:213:ALA:HA	1:A:214:PRO:HD3	1.88	0.41
1:A:165:PHE:CE1	1:A:205:ARG:HD3	2.55	0.41
1:A:299:GLU:N	1:A:299:GLU:OE1	2.48	0.41
1:A:180:ARG:HG3	1:A:184:ILE:CD1	2.51	0.41
1:B:248:HIS:CE1	1:B:308:GLU:HB2	2.55	0.41
1:B:255:ARG:NE	1:B:279:VAL:HG22	2.36	0.41
1:B:301:ILE:CG2	1:B:338:TYR:CE2	2.98	0.41
1:A:253:ILE:CG2	1:A:308:GLU:HA	2.50	0.41
1:A:143:LYS:HB3	1:A:143:LYS:HE2	1.86	0.41
1:B:283:SER:CA	1:B:284:SER:CB	2.82	0.41
1:A:308:GLU:CD	1:A:308:GLU:H	2.22	0.41
1:B:367:ASN:ND2	1:B:370:GLN:CG	2.79	0.41
1:B:139:LEU:HB2	1:B:147:VAL:HG22	2.04	0.40
1:B:281:ALA:CB	1:B:282:PRO:CD	2.82	0.40
1:B:131:GLU:O	1:B:132:ASP:HB2	2.21	0.40
1:B:222:LEU:O	1:B:226:SER:HA	2.22	0.40
1:B:170:GLU:C	1:B:172:ALA:N	2.75	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	254/271 (94%)	214 (84%)	25 (10%)	15 (6%)	2	5
1	B	254/271 (94%)	215 (85%)	27 (11%)	12 (5%)	3	9
All	All	508/542 (94%)	429 (84%)	52 (10%)	27 (5%)	2	7

All (27) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	281	ALA
1	A	284	SER
1	A	292	THR
1	B	278	SER
1	B	284	SER
1	A	132	ASP
1	A	291	GLY
1	B	132	ASP
1	B	276	GLY
1	B	281	ALA
1	A	142	GLY
1	A	276	GLY
1	A	294	ASP
1	B	226	SER
1	B	293	LEU
1	A	143	LYS
1	A	278	SER
1	A	280	HIS
1	B	274	ASP
1	B	292	THR
1	A	274	ASP
1	A	275	PHE
1	A	380	HIS
1	B	143	LYS
1	B	171	LYS

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Mol	Chain	Res	Type
1	B	291	GLY
1	A	279	VAL

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	226/238 (95%)	194 (86%)	32 (14%)	4	12
1	B	226/238 (95%)	204 (90%)	22 (10%)	10	29
All	All	452/476 (95%)	398 (88%)	54 (12%)	6	19

All (54) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	132	ASP
1	A	134	GLU
1	A	143	LYS
1	A	147	VAL
1	A	151	ARG
1	A	154	GLN
1	A	164	LEU
1	A	178	LEU
1	A	179	ARG
1	A	180	ARG
1	A	183	GLU
1	A	195	ARG
1	A	204	THR
1	A	215	LEU
1	A	220	ARG
1	A	221	GLU
1	A	245	SER
1	A	257	ILE
1	A	277	TRP
1	A	278	SER
1	A	283	SER

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Mol	Chain	Res	Type
1	A	284	SER
1	A	285	ARG
1	A	292	THR
1	A	296	LEU
1	A	302	GLU
1	A	344	VAL
1	A	354	GLU
1	A	359	LEU
1	A	361	SER
1	A	363	LEU
1	A	375	ARG
1	B	143	LYS
1	B	147	VAL
1	B	178	LEU
1	B	179	ARG
1	B	183	GLU
1	B	195	ARG
1	B	201	HIS
1	B	204	THR
1	B	221	GLU
1	B	232	ARG
1	B	245	SER
1	B	252	VAL
1	B	253	ILE
1	B	277	TRP
1	B	290	CYS
1	B	296	LEU
1	B	335	GLN
1	B	342	SER
1	B	359	LEU
1	B	361	SER
1	B	363	LEU
1	B	367	ASN

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	146	ASN
1	A	177	GLN
1	A	185	GLN
1	A	190	HIS
1	A	192	ASN

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Mol	Chain	Res	Type
1	A	201	HIS
1	A	335	GLN
1	A	367	ASN
1	A	380	HIS
1	B	177	GLN
1	B	185	GLN
1	B	190	HIS
1	B	335	GLN
1	B	367	ASN
1	B	370	GLN
1	B	380	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)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 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	0K6	A	401	-	34,37,37	1.00	3 (8%)	39,54,54	3.23	18 (46%)
3	PO4	A	402	4	4,4,4	0.16	0	6,6,6	0.28	0

Mol	Type	Chain	Res	Link	Bond lengths				Bond angles			
					Counts	RMSZ	#|Z| > 2		Counts	RMSZ	#|Z| > 2	
2	0K6	B	401	-	34,37,37	1.00	3 (8%)		39,54,54	3.12	18 (46%)	
3	PO4	B	402	4	4,4,4	0.22	0		6,6,6	0.30	0	

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	0K6	A	401	-	-	0/7/37/37	0/5/5/5
3	PO4	A	402	4	-	0/0/0/0	0/0/0/0
2	0K6	B	401	-	-	0/7/37/37	0/5/5/5
3	PO4	B	402	4	-	0/0/0/0	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	0K6	C9-N3	-2.48	1.34	1.38
2	A	401	0K6	C10-N4	-2.39	1.35	1.40
2	B	401	0K6	C10-N4	-2.29	1.35	1.40
2	A	401	0K6	C9-N3	-2.19	1.35	1.38
2	A	401	0K6	C20-C18	2.42	1.40	1.38
2	B	401	0K6	C20-C18	2.92	1.40	1.38

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	401	0K6	C2-C3-N2	-7.07	103.32	110.79
2	A	401	0K6	C2-C3-N2	-6.96	103.43	110.79
2	A	401	0K6	N8-C11-N5	-5.61	120.41	126.62
2	B	401	0K6	N8-C11-N5	-5.12	120.95	126.62
2	A	401	0K6	O1-C1-C7	-5.11	111.63	118.42
2	A	401	0K6	C6-C5-N2	-5.05	105.46	110.79
2	B	401	0K6	C18-C20-C21	-4.71	100.67	106.55
2	B	401	0K6	O1-C1-C7	-4.41	112.56	118.42
2	B	401	0K6	C6-C5-N2	-4.39	106.16	110.79
2	A	401	0K6	C21-C22-N8	-4.26	116.24	124.06
2	B	401	0K6	C21-C22-N8	-3.70	117.26	124.06
2	A	401	0K6	C18-C20-C21	-3.54	102.14	106.55
2	B	401	0K6	C20-C21-C22	-2.60	127.32	136.55
2	A	401	0K6	C20-C21-C22	-2.51	127.65	136.55
2	A	401	0K6	O2-C19-C18	-2.48	117.13	119.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	0K6	C18-N6-C13	-2.34	121.28	126.24
2	B	401	0K6	C20-C18-C19	-2.28	123.87	129.77
2	B	401	0K6	C18-N6-C13	-2.07	121.84	126.24
2	A	401	0K6	C20-C18-C19	-2.05	124.46	129.77
2	B	401	0K6	C7-C1-N1	2.25	127.62	119.69
2	B	401	0K6	C20-C21-C12	2.39	111.92	105.18
2	A	401	0K6	C7-C1-N1	2.54	128.61	119.69
2	B	401	0K6	C18-C19-N7	2.60	119.15	116.30
2	B	401	0K6	C2-N1-C6	3.10	118.31	112.56
2	A	401	0K6	C18-C19-N7	3.21	119.82	116.30
2	B	401	0K6	C22-N8-C11	3.24	122.00	115.97
2	A	401	0K6	C11-N5-C12	3.48	119.28	115.09
2	A	401	0K6	C3-N2-C5	3.62	114.28	109.53
2	B	401	0K6	C11-N5-C12	3.62	119.45	115.09
2	B	401	0K6	C3-N2-C5	3.65	114.32	109.53
2	A	401	0K6	C22-N8-C11	3.70	122.84	115.97
2	A	401	0K6	C2-N1-C6	3.87	119.74	112.56
2	A	401	0K6	C4-N2-C5	6.32	120.47	110.63
2	B	401	0K6	C4-N2-C5	7.24	121.91	110.63
2	B	401	0K6	C4-N2-C3	8.42	123.75	110.63
2	A	401	0K6	C4-N2-C3	9.36	125.22	110.63

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 17 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	401	0K6	9	0
3	A	402	PO4	1	0
2	B	401	0K6	7	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	258/271 (95%)	-0.06	3 (1%)	81	73	33, 56, 91, 114	0
1	B	258/271 (95%)	-0.08	3 (1%)	81	73	33, 56, 88, 106	0
All	All	516/542 (95%)	-0.07	6 (1%)	81	73	33, 56, 90, 114	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	283	SER	4.2
1	A	277	TRP	2.6
1	B	284	SER	2.5
1	A	176	HIS	2.3
1	B	177	GLN	2.1
1	A	177	GLN	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(Å²)	Q<0.9
2	0K6	B	401	33/33	0.95	0.24	1.94	38,60,74,82	0
2	0K6	A	401	33/33	0.95	0.25	1.57	41,57,73,83	0
3	PO4	B	402	5/5	0.72	0.21	0.80	93,100,116,117	0
3	PO4	A	402	5/5	0.89	0.09	-3.07	114,120,120,120	0
4	MG	A	403	1/1	0.97	0.10	-	79,79,79,79	0
4	MG	B	403	1/1	0.95	0.10	-	68,68,68,68	0

6.5 Other polymers (i)

There are no such residues in this entry.