



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 10:43 AM GMT

PDB ID : 3MVL
Title : P38 Alpha Map Kinase complexed with pyrrolotriazine inhibitor 7K
Authors : Sack, J.S.
Deposited on : 2010-05-04
Resolution : 2.80 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 ⓘ symbol.

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

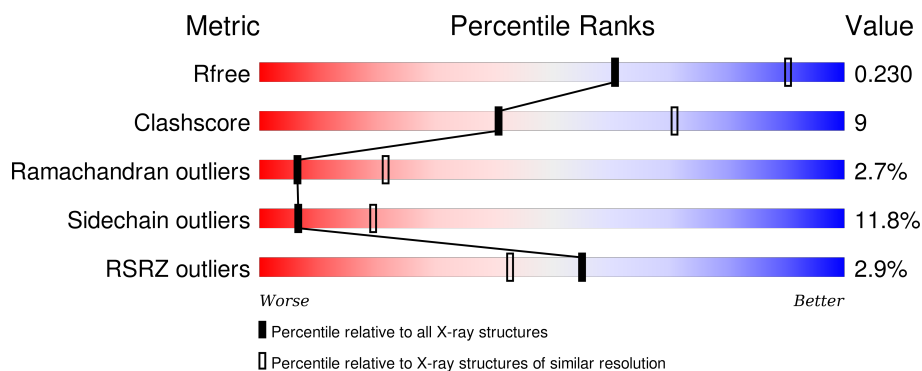
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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	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 $\leq 5\%$. 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	366	<div> <div>2%</div> <div>64%</div> <div>25%</div> <div>7%</div> </div>
1	B	366	<div> <div>3%</div> <div>63%</div> <div>27%</div> <div>7%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5667 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.

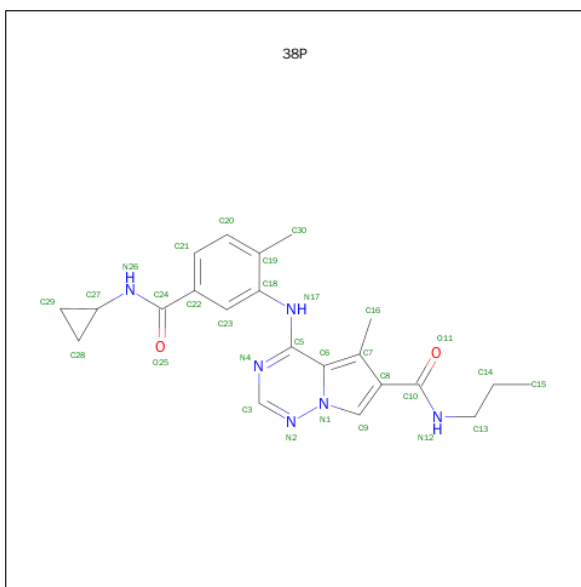
- Molecule 1 is a protein called Mitogen-activated protein kinase 14.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	0	0
			2741	1759	471	499	12			
1	B	339	Total	C	N	O	S	0	0	0
			2741	1759	471	499	12			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-5	MET	-	EXPRESSION TAG	UNP Q16539
A	-4	ALA	-	EXPRESSION TAG	UNP Q16539
A	-3	HIS	-	EXPRESSION TAG	UNP Q16539
A	-2	HIS	-	EXPRESSION TAG	UNP Q16539
A	-1	HIS	-	EXPRESSION TAG	UNP Q16539
A	0	HIS	-	EXPRESSION TAG	UNP Q16539
A	1	HIS	-	EXPRESSION TAG	UNP Q16539
B	-5	MET	-	EXPRESSION TAG	UNP Q16539
B	-4	ALA	-	EXPRESSION TAG	UNP Q16539
B	-3	HIS	-	EXPRESSION TAG	UNP Q16539
B	-2	HIS	-	EXPRESSION TAG	UNP Q16539
B	-1	HIS	-	EXPRESSION TAG	UNP Q16539
B	0	HIS	-	EXPRESSION TAG	UNP Q16539
B	1	HIS	-	EXPRESSION TAG	UNP Q16539

- Molecule 2 is 4-{{5-(CYCLOPROPYLCARBAMOYL)-2-METHYLPHENYL}AMINO}-5-METHYL-N-PROPYLPYRROLO[2,1-F][1,2,4]TRIAZINE-6-CARBOXAMIDE (three-letter code: 38P) (formula: C₂₂H₂₆N₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			30	22	6	2		
2	B	1	Total	C	N	O	0	0
			30	22	6	2		

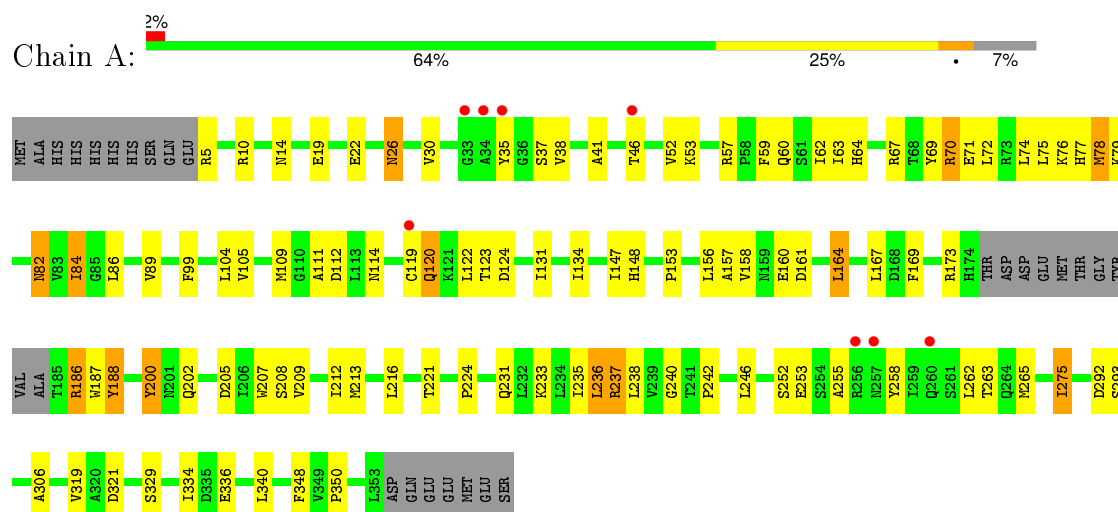
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	58	Total	O	0	0
			58	58		
3	B	67	Total	O	0	0
			67	67		

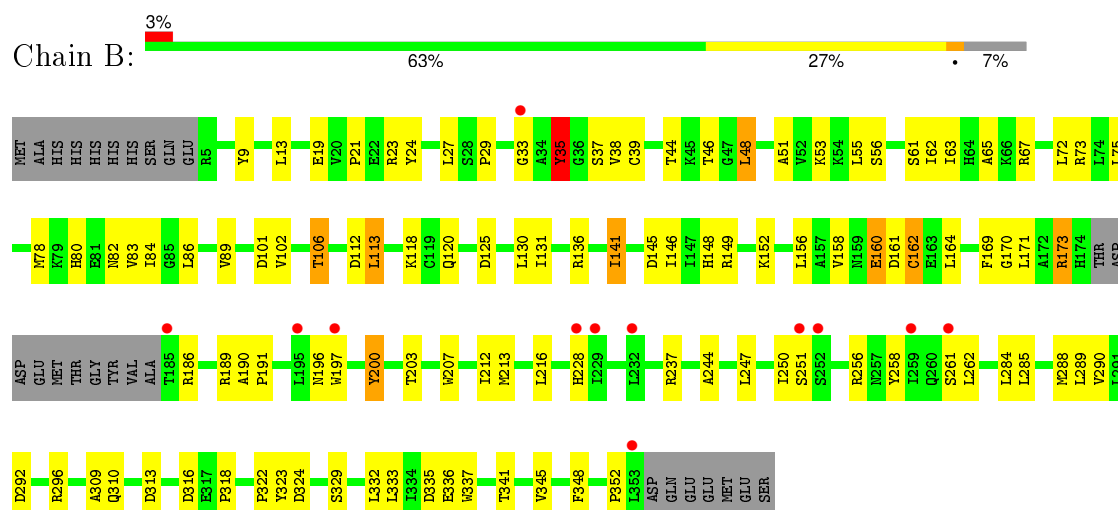
3 Residue-property plots [i](#)

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: Mitogen-activated protein kinase 14



- Molecule 1: Mitogen-activated protein kinase 14



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	67.54Å 71.68Å 72.82Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	33.77 – 2.80 33.77 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (33.77-2.80) 99.5 (33.77-2.80)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	9.33 (at 2.81Å)	Xtriage
Refinement program	BUSTER 2.9.4	Depositor
R, R_{free}	0.227 , 0.335 0.180 , 0.230	Depositor DCC
R_{free} test set	871 reflections (5.34%)	DCC
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.592	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 20.6	EDS
Estimated twinning fraction	0.106 for -h,l,k 0.105 for -h,-l,-k 0.477 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.38$, $\langle L^2 \rangle = 0.21$	Xtriage
Outliers	0 of 17201 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	5667	wwPDB-VP
Average B, all atoms (Å ²)	30.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.14% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: 38P

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	0.59	0/2805	0.82	0/3807
1	B	0.57	0/2805	0.80	0/3807
All	All	0.58	0/5610	0.81	0/7614

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	2741	0	2747	49	0
1	B	2741	0	2747	47	0
2	A	30	0	26	5	0
2	B	30	0	26	4	0
3	A	58	0	0	2	0
3	B	67	0	0	3	0
All	All	5667	0	5546	95	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 9.

All (95) 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:71:GLU:HG3	2:A:361:38P:H29	1.54	0.87
1:B:75:LEU:HB3	1:B:86:LEU:HB2	1.61	0.82
1:A:22:GLU:HG2	3:A:380:HOH:O	1.86	0.75
1:B:203:THR:HB	1:B:296:ARG:HD2	1.74	0.70
1:A:84:ILE:HG13	1:A:167:LEU:HD23	1.74	0.69
1:B:82:ASN:OD1	1:B:136:ARG:NH1	2.27	0.67
1:A:111:ALA:HA	2:A:361:38P:H14A	1.76	0.67
1:B:67:ARG:HB2	3:B:416:HOH:O	1.94	0.66
1:A:131:ILE:HG13	1:A:213:MET:HG3	1.83	0.60
1:B:55:LEU:HD12	1:B:102:VAL:HB	1.85	0.59
1:A:76:LYS:HE3	1:A:348:PHE:HB2	1.84	0.59
1:A:57:ARG:HB3	1:A:60:GLN:HB2	1.84	0.59
1:A:153:PRO:HD3	1:A:212:ILE:HG12	1.84	0.58
1:A:319:VAL:HG23	1:B:237:ARG:HH12	1.67	0.58
1:A:109:MET:HG3	1:A:157:ALA:HB1	1.85	0.57
1:B:38:VAL:HG22	1:B:53:LYS:HG3	1.86	0.57
1:A:221:THR:HB	1:A:224:PRO:HG3	1.87	0.57
1:B:113:LEU:HD21	1:B:216:LEU:HD21	1.87	0.56
1:B:146:ILE:HD11	1:B:323:TYR:CD2	2.42	0.55
1:A:64:HIS:HA	1:A:67:ARG:HG2	1.89	0.54
1:A:63:ILE:HG22	1:A:67:ARG:HD3	1.90	0.53
1:B:80:HIS:HB3	1:B:83:VAL:HB	1.90	0.53
1:A:187:TRP:HD1	1:A:231:GLN:NE2	2.07	0.53
1:A:147:ILE:HG12	1:A:202:GLN:HA	1.91	0.53
1:A:72:LEU:HD13	1:A:89:VAL:HG21	1.90	0.52
1:B:75:LEU:HD13	1:B:86:LEU:HD23	1.91	0.52
1:A:169:PHE:O	2:A:361:38P:H28	2.08	0.52
1:A:134:ILE:HG12	1:A:156:LEU:HD22	1.92	0.51
1:A:148:HIS:CD2	1:A:169:PHE:HB3	2.45	0.51
1:B:73:ARG:NH2	1:B:324:ASP:O	2.44	0.51
1:B:169:PHE:O	2:B:361:38P:H28	2.12	0.50
1:B:190:ALA:HA	1:B:207:TRP:CD1	2.46	0.50
1:A:52:VAL:HG13	1:A:105:VAL:HG22	1.93	0.50
1:B:13:LEU:HD22	1:B:29:PRO:HD3	1.94	0.50
1:B:244:ALA:HA	1:B:247:LEU:HD12	1.92	0.50
1:B:106:THR:HG21	2:B:361:38P:HN17	1.75	0.50
1:A:10:ARG:HG3	1:A:19:GLU:HG2	1.95	0.49
1:B:310:GLN:HB3	3:B:426:HOH:O	2.12	0.48
1:B:207:TRP:HB2	1:B:296:ARG:NH1	2.28	0.48
1:A:255:ALA:HA	1:A:258:TYR:HB3	1.95	0.48
1:B:72:LEU:HD11	1:B:89:VAL:HG11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:LYS:HE3	2:A:361:38P:C20	2.43	0.47
1:B:86:LEU:HD12	1:B:348:PHE:CE1	2.49	0.47
1:A:82:ASN:HA	1:A:164:LEU:O	2.15	0.47
1:A:69:TYR:CE1	1:A:340:LEU:HB3	2.49	0.47
1:B:51:ALA:HB3	1:B:106:THR:HG22	1.96	0.47
1:B:149:ARG:HD2	1:B:173:ARG:HA	1.97	0.47
1:B:78:MET:HE3	1:B:141:ILE:HG13	1.97	0.47
1:B:148:HIS:HA	1:B:170:GLY:H	1.79	0.46
1:B:33:GLY:HA3	2:B:361:38P:H3	1.97	0.46
1:A:112:ASP:OD1	1:A:114:ASN:HB3	2.15	0.46
1:B:309:ALA:HA	3:B:382:HOH:O	2.17	0.45
1:B:250:ILE:HB	1:B:256:ARG:HD3	1.97	0.45
1:B:290:VAL:HG12	1:B:292:ASP:H	1.82	0.45
1:B:316:ASP:C	1:B:318:PRO:HD3	2.37	0.45
1:A:71:GLU:HG2	1:A:75:LEU:HD11	1.99	0.45
1:A:186:ARG:HD3	1:A:186:ARG:H	1.81	0.45
1:A:329:SER:HB3	3:A:375:HOH:O	2.17	0.45
1:B:9:TYR:OH	1:B:27:LEU:HD23	2.17	0.44
1:A:205:ASP:O	1:A:209:VAL:HG23	2.17	0.44
1:A:208:SER:O	1:A:212:ILE:HG13	2.18	0.44
1:A:187:TRP:HD1	1:A:231:GLN:HE22	1.66	0.43
1:A:122:LEU:HD13	1:A:216:LEU:HD22	1.99	0.43
1:B:65:ALA:O	1:B:337:TRP:HB3	2.19	0.43
1:B:258:TYR:CZ	1:B:262:LEU:HD11	2.52	0.43
1:A:160:GLU:H	1:A:160:GLU:CD	2.19	0.43
1:B:75:LEU:HD11	2:B:361:38P:H21	2.01	0.43
1:A:38:VAL:HG22	1:A:53:LYS:HG3	2.01	0.43
1:A:275:ILE:HG13	1:A:275:ILE:H	1.46	0.43
1:B:160:GLU:C	1:B:162:CYS:H	2.22	0.42
1:A:236:LEU:C	1:A:238:LEU:H	2.21	0.42
1:B:21:PRO:HD2	1:B:24:TYR:HD2	1.84	0.42
1:A:59:PHE:O	1:A:334:ILE:HG21	2.19	0.42
1:B:131:ILE:HG13	1:B:213:MET:HG3	2.00	0.42
1:A:153:PRO:HA	1:A:156:LEU:HD12	2.02	0.42
1:A:233:LYS:HE2	1:A:237:ARG:HH21	1.85	0.42
1:A:74:LEU:O	1:A:78:MET:HG2	2.19	0.42
1:A:188:TYR:CD2	1:A:188:TYR:N	2.87	0.42
1:B:191:PRO:HD3	1:B:207:TRP:CE2	2.55	0.42
1:A:67:ARG:HA	1:A:70:ARG:HH11	1.85	0.42
1:B:341:THR:O	1:B:345:VAL:HG23	2.20	0.42
1:B:284:LEU:HA	1:B:284:LEU:HD12	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:156:LEU:HD11	1:B:212:ILE:HD13	2.02	0.41
1:B:23:ARG:HA	1:B:44:THR:OG1	2.20	0.41
1:B:113:LEU:HD11	1:B:130:LEU:HD13	2.01	0.41
1:B:46:THR:OG1	1:B:48:LEU:HB2	2.20	0.41
1:A:242:PRO:HB3	1:A:246:LEU:HD23	2.02	0.41
1:A:169:PHE:N	2:A:361:38P:H28	2.35	0.41
1:B:213:MET:SD	1:B:288:MET:HE1	2.61	0.41
1:A:26:ASN:O	1:A:41:ALA:HA	2.21	0.41
1:B:35:TYR:CE2	1:B:171:LEU:HD13	2.56	0.41
1:A:207:TRP:HZ2	1:A:235:ILE:HG12	1.86	0.41
1:B:288:MET:HB2	1:B:288:MET:HE2	1.89	0.41
1:A:233:LYS:O	1:A:237:ARG:HB2	2.21	0.40
1:A:77:HIS:NE2	1:A:321:ASP:O	2.50	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	335/366 (92%)	283 (84%)	42 (12%)	10 (3%)	5	18
1	B	335/366 (92%)	288 (86%)	39 (12%)	8 (2%)	7	25
All	All	670/732 (92%)	571 (85%)	81 (12%)	18 (3%)	6	21

All (18) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	26	ASN
1	A	99	PHE
1	A	252	SER
1	A	306	ALA
1	B	261	SER

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Mol	Chain	Res	Type
1	B	322	PRO
1	A	200	TYR
1	A	237	ARG
1	B	173	ARG
1	B	352	PRO
1	A	35	TYR
1	A	120	GLN
1	B	200	TYR
1	B	35	TYR
1	B	196	ASN
1	A	350	PRO
1	B	313	ASP
1	A	240	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	301/325 (93%)	268 (89%)	33 (11%)	8	23
1	B	301/325 (93%)	263 (87%)	38 (13%)	5	17
All	All	602/650 (93%)	531 (88%)	71 (12%)	6	19

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	14	ASN
1	A	30	VAL
1	A	37	SER
1	A	46	THR
1	A	62	ILE
1	A	70	ARG
1	A	78	MET
1	A	79	LYS
1	A	82	ASN

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Mol	Chain	Res	Type
1	A	84	ILE
1	A	86	LEU
1	A	104	LEU
1	A	119	CYS
1	A	120	GLN
1	A	123	THR
1	A	124	ASP
1	A	158	VAL
1	A	161	ASP
1	A	164	LEU
1	A	173	ARG
1	A	186	ARG
1	A	188	TYR
1	A	200	TYR
1	A	236	LEU
1	A	253	GLU
1	A	262	LEU
1	A	263	THR
1	A	265	MET
1	A	275	ILE
1	A	292	ASP
1	A	293	SER
1	A	336	GLU
1	B	19	GLU
1	B	35	TYR
1	B	37	SER
1	B	39	CYS
1	B	48	LEU
1	B	56	SER
1	B	61	SER
1	B	62	ILE
1	B	63	ILE
1	B	84	ILE
1	B	101	ASP
1	B	106	THR
1	B	112	ASP
1	B	113	LEU
1	B	118	LYS
1	B	120	GLN
1	B	125	ASP
1	B	141	ILE
1	B	145	ASP

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Mol	Chain	Res	Type
1	B	152	LYS
1	B	158	VAL
1	B	160	GLU
1	B	161	ASP
1	B	162	CYS
1	B	164	LEU
1	B	186	ARG
1	B	189	ARG
1	B	197	TRP
1	B	200	TYR
1	B	228	HIS
1	B	251	SER
1	B	285	LEU
1	B	289	LEU
1	B	329	SER
1	B	332	LEU
1	B	333	LEU
1	B	335	ASP
1	B	336	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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	38P	A	361	-	27,33,33	2.05	7 (25%)	32,47,47	3.60	8 (25%)
2	38P	B	361	-	27,33,33	2.03	6 (22%)	32,47,47	3.58	8 (25%)

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	38P	A	361	-	-	0/18/22/22	0/3/4/4
2	38P	B	361	-	-	0/18/22/22	0/3/4/4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	361	38P	C18-C19	2.06	1.44	1.40
2	B	361	38P	C21-C22	2.11	1.42	1.39
2	A	361	38P	C23-C18	2.25	1.43	1.39
2	A	361	38P	C21-C22	2.25	1.43	1.39
2	A	361	38P	C20-C21	2.26	1.42	1.38
2	B	361	38P	C3-N4	2.37	1.38	1.33
2	A	361	38P	C3-N4	2.37	1.38	1.33
2	B	361	38P	C20-C21	2.38	1.43	1.38
2	B	361	38P	C23-C18	2.39	1.43	1.39
2	A	361	38P	C5-N4	3.27	1.39	1.34
2	B	361	38P	C5-N4	3.30	1.39	1.34
2	B	361	38P	C8-C7	7.54	1.50	1.40
2	A	361	38P	C8-C7	7.73	1.50	1.40

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	361	38P	C28-C27-N26	-16.77	92.78	118.71
2	B	361	38P	C28-C27-N26	-16.70	92.88	118.71
2	A	361	38P	N2-C3-N4	-4.33	121.33	128.66
2	B	361	38P	N2-C3-N4	-4.29	121.41	128.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	361	38P	C27-N26-C24	-3.63	118.00	122.52
2	A	361	38P	C27-N26-C24	-3.48	118.18	122.52
2	A	361	38P	C18-N17-C5	-2.99	121.40	129.04
2	B	361	38P	C18-N17-C5	-2.96	121.48	129.04
2	A	361	38P	N17-C5-N4	-2.81	116.19	118.85
2	B	361	38P	N17-C5-N4	-2.58	116.41	118.85
2	A	361	38P	C29-C28-C27	-2.30	57.40	59.78
2	B	361	38P	C29-C28-C27	-2.30	57.40	59.78
2	A	361	38P	C28-C29-C27	2.22	62.08	59.78
2	B	361	38P	C28-C29-C27	2.26	62.12	59.78
2	A	361	38P	C3-N4-C5	7.55	121.92	116.48
2	B	361	38P	C3-N4-C5	7.59	121.95	116.48

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	361	38P	5	0
2	B	361	38P	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

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, 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	339/366 (92%)	-0.48	8 (2%) 62 50	4, 24, 61, 95	0
1	B	339/366 (92%)	-0.33	12 (3%) 48 35	5, 28, 76, 97	0
All	All	678/732 (92%)	-0.40	20 (2%) 55 43	4, 26, 67, 97	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	35	TYR	5.8
1	A	34	ALA	5.7
1	B	259	ILE	4.6
1	A	257	ASN	4.5
1	B	251	SER	3.9
1	B	197	TRP	3.5
1	A	256	ARG	3.0
1	A	33	GLY	2.9
1	B	252	SER	2.7
1	B	232	LEU	2.7
1	B	353	LEU	2.7
1	A	119	CYS	2.6
1	B	229	ILE	2.5
1	B	185	THR	2.4
1	B	261	SER	2.2
1	A	46	THR	2.2
1	A	260	GLN	2.1
1	B	33	GLY	2.1
1	B	228	HIS	2.1
1	B	195	LEU	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, 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(\AA^2)	Q<0.9
2	38P	B	361	30/30	0.94	0.15	0.03	4,23,30,31	0
2	38P	A	361	30/30	0.95	0.13	-0.21	3,19,23,29	0

6.5 Other polymers [i](#)

There are no such residues in this entry.