Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:33 PM GMT

PDB ID	:	1U54
Title	:	Crystal Structures of the Phosphorylated and Unphosphorylated Kinase Domains of the CDC42-associated Tyrosine Kinase ACK1 bound to AMP-PCP
Authors	:	Lougheed, J.C.; Chen, R.H.; Mak, P.; Stout, T.J.
Deposited on	:	2004-07-26
Resolution	:	2.80 Å(reported)

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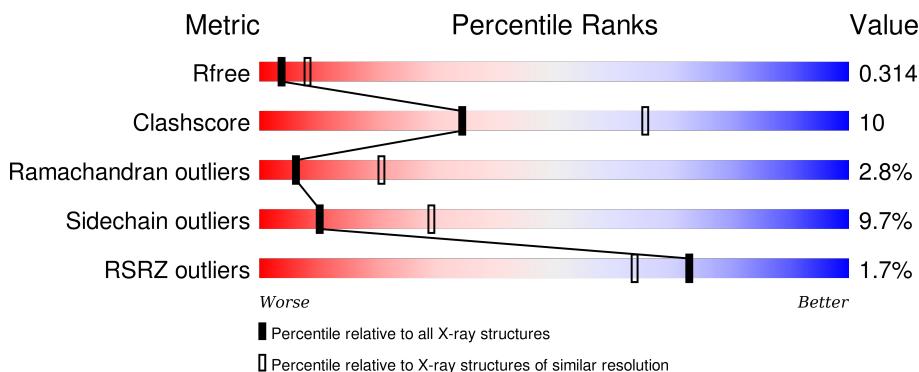
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	2393 (2.80-2.80)
Clashscore	102246	2827 (2.80-2.80)
Ramachandran outliers	100387	2782 (2.80-2.80)
Sidechain outliers	100360	2784 (2.80-2.80)
RSRZ outliers	91569	2404 (2.80-2.80)

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	291	
2	B	291	
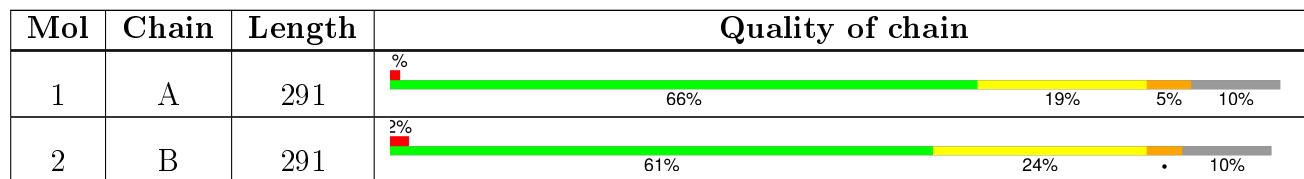
2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 4293 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 Activated CDC42 kinase 1.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	263	Total	C	N	O	P	S	0	0	0
			2117	1345	377	379	1	15			

There are 5 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	GLY	-	CLONING ARTIFACT	UNP Q07912
A	108	SER	-	CLONING ARTIFACT	UNP Q07912
A	284	PTR	TYR	MODIFIED RESIDUE	UNP Q07912
A	396	GLU	-	CLONING ARTIFACT	UNP Q07912
A	397	PHE	-	CLONING ARTIFACT	UNP Q07912

- Molecule 2 is a protein called Activated CDC42 kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	261	Total	C	N	O	S	0	0	0
			2100	1338	374	373	15			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	107	GLY	-	CLONING ARTIFACT	UNP Q07912
B	108	SER	-	CLONING ARTIFACT	UNP Q07912
B	396	GLU	-	CLONING ARTIFACT	UNP Q07912
B	397	PHE	-	CLONING ARTIFACT	UNP Q07912

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

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

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

- Molecule 4 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: $C_{11}H_{18}N_5O_{12}P_3$).
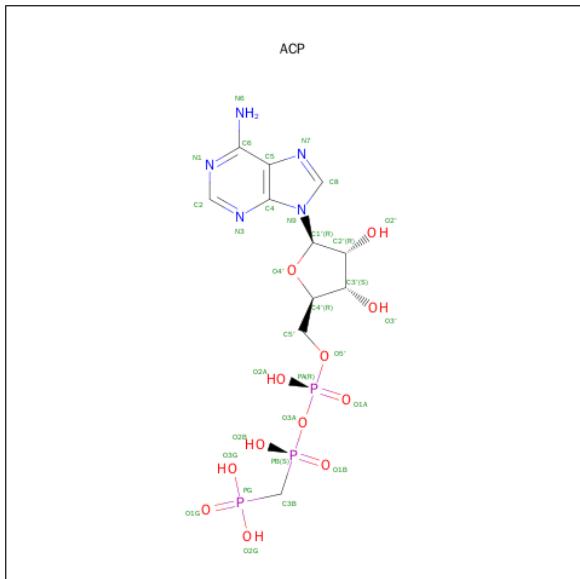
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 31	C 11	N 5	O 12	P 3	0	0
4	B	1	Total 31	C 11	N 5	O 12	P 3	0	0

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	6	Total 6	O 6	0	0
5	B	4	Total 4	O 4	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: Activated CDC42 kinase 1
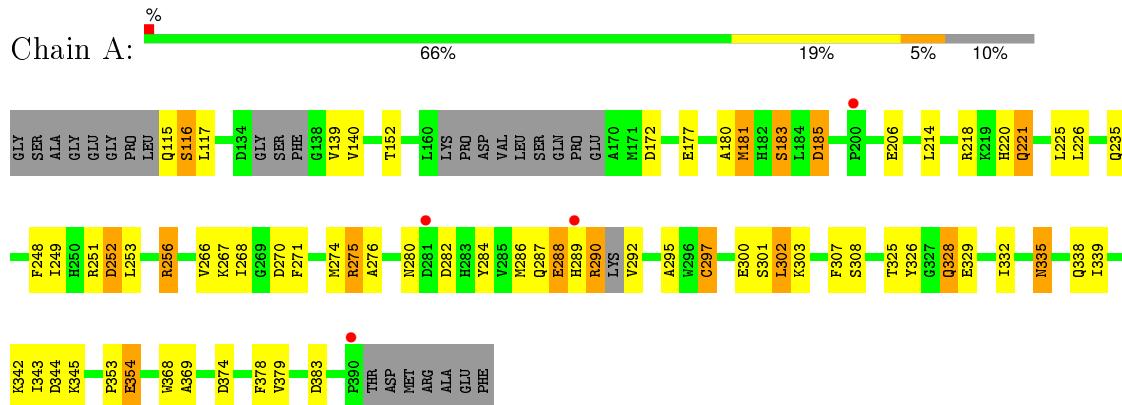
- Molecule 2: Activated CDC42 kinase 1
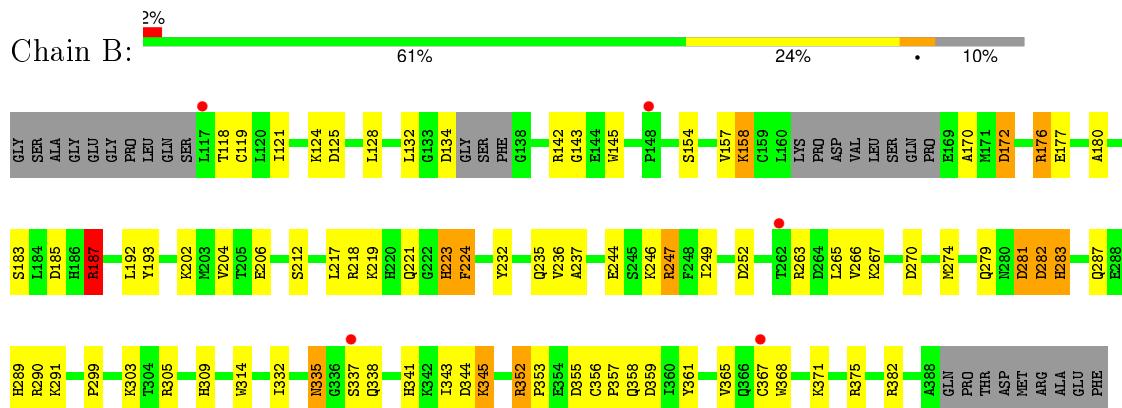
4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	200.38Å 42.33Å 70.85Å 90.00° 96.28° 90.00°	Depositor
Resolution (Å)	38.71 – 2.80 35.69 – 2.80	Depositor EDS
% Data completeness (in resolution range)	98.3 (38.71-2.80) 98.3 (35.69-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$<I/\sigma(I)>$ [1]	3.13 (at 2.81Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.222 , 0.322 0.226 , 0.314	Depositor DCC
R_{free} test set	684 reflections (4.88%)	DCC
Wilson B-factor (Å^2)	63.2	Xtriage
Anisotropy	0.260	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.25 , 55.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$<|L|>$ = 0.49, $<L^2>$ = 0.32	Xtriage
Outliers	0 of 14697 reflections	Xtriage
F_o,F_c correlation	0.92	EDS
Total number of atoms	4293	wwPDB-VP
Average B, all atoms (Å^2)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.27% 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: MG, ACP, PTR

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	0.80	0/2147	1.04	7/2900 (0.2%)
2	B	0.84	0/2148	1.03	11/2903 (0.4%)
All	All	0.82	0/4295	1.04	18/5803 (0.3%)

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

There are no bond length outliers.

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	256	ARG	NE-CZ-NH1	11.01	125.81	120.30
1	A	256	ARG	NE-CZ-NH2	-10.60	115.00	120.30
2	B	185	ASP	CB-CG-OD2	9.83	127.15	118.30
1	A	252	ASP	CB-CG-OD2	8.55	125.99	118.30
2	B	344	ASP	CB-CG-OD2	8.28	125.75	118.30
1	A	270	ASP	CB-CG-OD2	8.23	125.71	118.30
2	B	172	ASP	CB-CG-OD2	7.48	125.03	118.30
1	A	282	ASP	CB-CG-OD2	7.04	124.63	118.30
2	B	252	ASP	CB-CG-OD2	6.69	124.32	118.30
2	B	359	ASP	CB-CG-OD2	6.62	124.25	118.30
2	B	187	ARG	NE-CZ-NH1	6.43	123.52	120.30
1	A	185	ASP	CB-CG-OD2	6.33	123.99	118.30
2	B	355	ASP	CB-CG-OD2	6.02	123.72	118.30
2	B	125	ASP	CB-CG-OD2	5.68	123.42	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	281	ASP	CB-CG-OD2	5.35	123.12	118.30
1	A	383	ASP	CB-CG-OD2	5.30	123.07	118.30
2	B	134	ASP	CB-CG-OD2	5.26	123.04	118.30
2	B	247	ARG	NE-CZ-NH1	5.13	122.87	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	268	ILE	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	2117	0	2105	40	0
2	B	2100	0	2099	39	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
4	A	31	0	14	1	0
4	B	31	0	14	3	0
5	A	6	0	0	0	0
5	B	4	0	0	1	0
All	All	4293	0	4232	80	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 10.

All (80) 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:284:PTR:HE2	1:A:286:MET:HB2	1.40	1.03
2:B:180:ALA:HB1	2:B:274:MET:HE2	1.50	0.91
2:B:235:GLN:HE21	2:B:266:VAL:HG12	1.42	0.84
2:B:232:TYR:OH	2:B:263:ARG:O	1.99	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:A:101:ACP:O3A	4:A:101:ACP:O1G	2.02	0.76
1:A:284:PTR:CE2	1:A:286:MET:HB2	2.20	0.67
1:A:288:GLU:O	1:A:290:ARG:N	2.31	0.63
1:A:206:GLU:OE2	1:A:267:LYS:NZ	2.26	0.62
2:B:282:ASP:OD1	2:B:283:HIS:HB3	2.00	0.60
2:B:223:HIS:O	2:B:224:PHE:C	2.39	0.59
2:B:361:TYR:O	2:B:365:VAL:HG23	2.04	0.57
2:B:244:GLU:HG3	2:B:309:HIS:ND1	2.18	0.57
2:B:299:PRO:HG3	2:B:343:ILE:HD12	1.87	0.56
1:A:185:ASP:C	1:A:185:ASP:OD1	2.46	0.53
1:A:248:PHE:CE1	1:A:276:ALA:HB2	2.44	0.53
1:A:275:ARG:NE	1:A:284:PTR:O3P	2.43	0.52
1:A:214:LEU:HD21	1:A:218:ARG:NH2	2.25	0.52
2:B:128:LEU:HD21	2:B:157:VAL:HG11	1.93	0.51
1:A:221:GLN:NE2	1:A:326:TYR:CB	2.74	0.50
2:B:158:LYS:HE3	4:B:400:ACP:O3A	2.12	0.49
2:B:367:CYS:O	2:B:375:ARG:HD3	2.11	0.49
1:A:307:PHE:N	1:A:307:PHE:CD2	2.81	0.49
2:B:358:GLN:HG3	5:B:1:HOH:O	2.12	0.49
1:A:286:MET:HG2	1:A:287:GLN:N	2.29	0.48
2:B:217:LEU:HA	2:B:224:PHE:CE2	2.49	0.48
2:B:121:ILE:HG12	2:B:145:TRP:NE1	2.29	0.47
1:A:368:TRP:O	1:A:369:ALA:C	2.50	0.47
1:A:253:LEU:HA	1:A:253:LEU:HD12	1.73	0.47
1:A:353:PRO:O	1:A:354:GLU:C	2.51	0.47
2:B:341:HIS:HA	2:B:345:LYS:HB2	1.96	0.47
1:A:339:ILE:O	1:A:342:LYS:HB2	2.15	0.47
1:A:235:GLN:OE1	1:A:266:VAL:HG12	2.15	0.46
1:A:300:GLU:HG2	1:A:301:SER:N	2.30	0.46
2:B:192:LEU:HD12	2:B:204:VAL:O	2.15	0.46
2:B:121:ILE:HD13	2:B:204:VAL:HG21	1.98	0.46
2:B:265:LEU:HD21	2:B:267:LYS:HE2	1.97	0.46
2:B:287:GLN:O	2:B:305:ARG:NH1	2.49	0.46
1:A:328:GLN:HA	2:B:303:LYS:O	2.16	0.46
1:A:335:ASN:HB2	1:A:338:GLN:HG3	1.96	0.46
2:B:172:ASP:O	2:B:176:ARG:HB2	2.16	0.46
1:A:252:ASP:OD1	1:A:256:ARG:NH2	2.49	0.45
1:A:115:GLN:O	1:A:116:SER:CB	2.63	0.45
2:B:223:HIS:ND1	2:B:224:PHE:N	2.64	0.45
2:B:244:GLU:HA	2:B:309:HIS:CE1	2.52	0.45
2:B:193:TYR:HE1	2:B:206:GLU:HA	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:274:MET:O	1:A:275:ARG:NH1	2.48	0.45
1:A:221:GLN:NE2	1:A:326:TYR:HB2	2.32	0.45
1:A:177:GLU:O	1:A:181:MET:HE3	2.16	0.45
1:A:221:GLN:O	1:A:326:TYR:CE1	2.70	0.45
2:B:314:TRP:CE3	2:B:368:TRP:HA	2.52	0.44
1:A:180:ALA:O	1:A:183:SER:OG	2.35	0.44
2:B:180:ALA:HB1	2:B:274:MET:CE	2.36	0.43
1:A:325:THR:HB	1:A:328:GLN:CB	2.49	0.43
2:B:142:ARG:HG2	2:B:143:GLY:N	2.33	0.43
1:A:325:THR:CB	1:A:328:GLN:HB3	2.49	0.43
1:A:139:VAL:CG1	1:A:140:VAL:N	2.82	0.43
1:A:221:GLN:NE2	1:A:326:TYR:HB3	2.34	0.43
2:B:290:ARG:C	2:B:291:LYS:HG2	2.39	0.42
2:B:352:ARG:HB2	2:B:361:TYR:CD2	2.53	0.42
2:B:177:GLU:O	2:B:180:ALA:HB3	2.20	0.42
2:B:235:GLN:NE2	2:B:266:VAL:HG12	2.22	0.42
2:B:132:LEU:HD13	4:B:400:ACP:C2	2.50	0.42
2:B:236:VAL:O	2:B:237:ALA:C	2.58	0.42
1:A:286:MET:HG2	1:A:287:GLN:H	1.85	0.41
1:A:328:GLN:HE21	1:A:328:GLN:HB2	1.64	0.41
1:A:344:ASP:O	1:A:345:LYS:C	2.59	0.41
4:B:400:ACP:O2B	4:B:400:ACP:O1G	2.39	0.41
1:A:325:THR:OG1	1:A:328:GLN:HB3	2.20	0.41
1:A:181:MET:CE	1:A:271:PHE:HB2	2.51	0.41
2:B:287:GLN:OE1	2:B:289:HIS:HE1	2.03	0.41
1:A:302:LEU:CD1	1:A:343:ILE:HD11	2.51	0.41
2:B:335:ASN:ND2	2:B:338:GLN:H	2.19	0.41
1:A:225:LEU:HG	1:A:226:LEU:N	2.35	0.41
1:A:297:CYS:HB2	1:A:301:SER:HB2	2.03	0.40
2:B:187:ARG:HH11	2:B:187:ARG:HG3	1.86	0.40
2:B:352:ARG:HA	2:B:353:PRO:HD2	1.90	0.40
1:A:378:PHE:O	1:A:379:VAL:C	2.59	0.40
2:B:249:ILE:HG21	2:B:249:ILE:HD13	1.85	0.40
1:A:220:HIS:O	1:A:221:GLN:C	2.59	0.40
2:B:314:TRP:C	2:B:314:TRP:CD1	2.95	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	254/291 (87%)	221 (87%)	25 (10%)	8 (3%)	5	17
2	B	255/291 (88%)	232 (91%)	17 (7%)	6 (2%)	7	25
All	All	509/582 (88%)	453 (89%)	42 (8%)	14 (3%)	6	21

All (14) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	289	HIS
1	A	354	GLU
2	B	170	ALA
1	A	116	SER
1	A	221	GLN
1	A	332	ILE
2	B	270	ASP
1	A	288	GLU
1	A	295	ALA
1	A	335	ASN
2	B	219	LYS
2	B	224	PHE
2	B	332	ILE
2	B	357	PRO

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	227/249 (91%)	209 (92%)	18 (8%)	15	40
2	B	226/250 (90%)	200 (88%)	26 (12%)	7	21
All	All	453/499 (91%)	409 (90%)	44 (10%)	10	29

All (44) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	117	LEU
1	A	152	THR
1	A	172	ASP
1	A	181	MET
1	A	183	SER
1	A	249	ILE
1	A	251	ARG
1	A	275	ARG
1	A	280	ASN
1	A	290	ARG
1	A	292	VAL
1	A	297	CYS
1	A	302	LEU
1	A	303	LYS
1	A	308	SER
1	A	328	GLN
1	A	329	GLU
1	A	374	ASP
2	B	118	THR
2	B	119	CYS
2	B	124	LYS
2	B	154	SER
2	B	158	LYS
2	B	176	ARG
2	B	183	SER
2	B	187	ARG
2	B	202	LYS
2	B	212	SER
2	B	218	ARG
2	B	221	GLN
2	B	223	HIS
2	B	246	LYS
2	B	247	ARG
2	B	279	GLN
2	B	281	ASP

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Mol	Chain	Res	Type
2	B	282	ASP
2	B	283	HIS
2	B	335	ASN
2	B	337	SER
2	B	345	LYS
2	B	352	ARG
2	B	356	CYS
2	B	371	LYS
2	B	382	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	188	ASN
1	A	221	GLN
1	A	309	HIS
1	A	328	GLN
2	B	235	GLN
2	B	289	HIS
2	B	335	ASN
2	B	341	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)

1 non-standard protein/DNA/RNA residue is modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
1	PTR	A	284	1	14,16,17	1.81	1 (7%)	18,22,24	1.01	1 (5%)

Full wwPDB X-ray Structure Validation Report

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	PTR	A	284	1	-	0/9/11/13	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	284	PTR	OH-CZ	-6.58	1.24	1.40

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	284	PTR	CG-CB-CA	-2.04	109.59	114.21

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	284	PTR	3	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 6 ligands modelled in this entry, 4 are monoatomic - leaving 2 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
4	ACP	A	101	3	25,33,33	2.17	8 (32%)	31,52,52	3.57	11 (35%)
4	ACP	B	400	3	25,33,33	2.52	7 (28%)	31,52,52	2.01	9 (29%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ACP	A	101	3	-	0/15/38/38	0/3/3/3
4	ACP	B	400	3	-	0/15/38/38	0/3/3/3

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	400	ACP	O4'-C1'	2.05	1.43	1.41
4	A	101	ACP	C5'-C4'	2.07	1.58	1.51
4	B	400	ACP	C5-C4	2.16	1.45	1.40
4	A	101	ACP	C2-N3	2.35	1.36	1.32
4	B	400	ACP	C2-N3	2.44	1.36	1.32
4	B	400	ACP	PB-O1B	2.70	1.58	1.51
4	A	101	ACP	C5-C4	3.09	1.47	1.40
4	A	101	ACP	PG-O1G	3.23	1.57	1.50
4	A	101	ACP	O4'-C1'	3.74	1.45	1.41
4	A	101	ACP	C8-N7	3.93	1.42	1.34
4	A	101	ACP	C4-N3	4.30	1.42	1.35
4	B	400	ACP	PG-O1G	4.30	1.60	1.50
4	A	101	ACP	PB-O3A	5.33	1.64	1.58
4	B	400	ACP	C4-N3	6.23	1.44	1.35
4	B	400	ACP	PB-O3A	7.94	1.67	1.58

All (20) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	101	ACP	C2'-C1'-N9	-13.43	93.78	114.29
4	A	101	ACP	O1G-PG-C3B	-6.48	96.36	111.13
4	A	101	ACP	N3-C2-N1	-6.33	124.05	128.89
4	B	400	ACP	N3-C2-N1	-5.63	124.58	128.89
4	B	400	ACP	PA-O3A-PB	-4.53	120.00	132.73
4	B	400	ACP	C2'-C1'-N9	-3.86	108.39	114.29
4	A	101	ACP	PA-O3A-PB	-3.78	122.11	132.73
4	A	101	ACP	C4-C5-N7	-3.37	106.38	109.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	400	ACP	O5'-PA-O1A	-2.44	100.15	109.62
4	B	400	ACP	O2'-C2'-C3'	-2.09	105.03	111.83
4	B	400	ACP	O3'-C3'-C4'	2.02	117.10	111.05
4	A	101	ACP	O2G-PG-O1G	2.02	117.58	112.40
4	A	101	ACP	C2'-C3'-C4'	2.12	106.97	102.61
4	B	400	ACP	O2B-PB-O1B	2.14	116.86	110.12
4	B	400	ACP	C2-N1-C6	2.38	123.03	118.77
4	A	101	ACP	C2-N1-C6	2.60	123.41	118.77
4	B	400	ACP	N6-C6-N1	2.80	125.20	119.20
4	A	101	ACP	O4'-C4'-C5'	2.89	119.67	109.32
4	A	101	ACP	O4'-C1'-N9	5.63	119.88	108.10
4	A	101	ACP	O2B-PB-O1B	5.75	128.20	110.12

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
4	A	101	ACP	1	0
4	B	400	ACP	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	262/291 (90%)	-0.24	4 (1%)	76	68	23, 28, 32, 36	29 (11%)
2	B	261/291 (89%)	-0.23	5 (1%)	70	59	21, 27, 31, 40	21 (8%)
All	All	523/582 (89%)	-0.23	9 (1%)	73	63	21, 27, 32, 40	50 (9%)

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	390	PRO	3.4
2	B	262	THR	3.3
1	A	281	ASP	3.0
1	A	200	PRO	2.8
2	B	148	PRO	2.6
1	A	289	HIS	2.1
2	B	117	LEU	2.1
2	B	367	CYS	2.1
2	B	337	SER	2.0

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

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 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
1	PTR	A	284	16/17	0.94	0.20	-	31,32,37,38	5

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
4	ACP	B	400	31/31	0.93	0.17	0.50	42,48,58,59	0
4	ACP	A	101	31/31	0.93	0.17	-0.08	43,51,56,57	0
3	MG	B	398	1/1	0.96	0.16	-	57,57,57,57	0
3	MG	A	398	1/1	0.72	0.16	-	48,48,48,48	0
3	MG	B	399	1/1	0.76	0.15	-	55,55,55,55	0
3	MG	A	399	1/1	0.73	0.27	-	48,48,48,48	0

6.5 Other polymers (i)

There are no such residues in this entry.