



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:35 PM GMT

PDB ID : 3ZXT
Title : Dimeric structure of DAPK-1 catalytic domain in complex with AMPPCP-Mg
Authors : De Diego, I.; Lehmann, F.; Wilmanns, M.
Deposited on : 2011-08-15
Resolution : 2.65 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

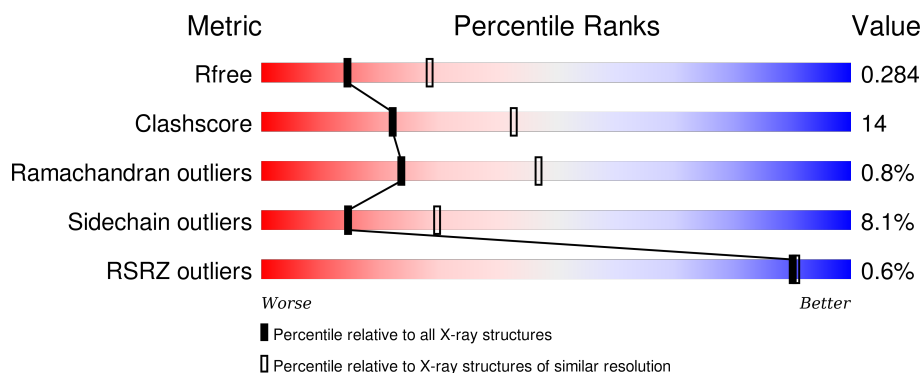
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.65 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	3152 (2.70-2.62)
Clashscore	102246	3524 (2.70-2.62)
Ramachandran outliers	100387	3469 (2.70-2.62)
Sidechain outliers	100360	3469 (2.70-2.62)
RSRZ outliers	91569	3161 (2.70-2.62)

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	285	<div> <div>65%</div> <div>19%</div> <div>•</div> <div>13%</div> </div>
1	B	285	<div> <div>67%</div> <div>19%</div> <div>•</div> <div>11%</div> </div>
1	C	285	<div> <div>67%</div> <div>22%</div> <div>•</div> <div>9%</div> </div>
1	D	285	<div> <div>65%</div> <div>20%</div> <div>•</div> <div>14%</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACP	A	1277	-	-	X	-
2	ACP	B	1279	-	-	X	-
2	ACP	C	1278	-	-	-	X

2 Entry composition [i](#)

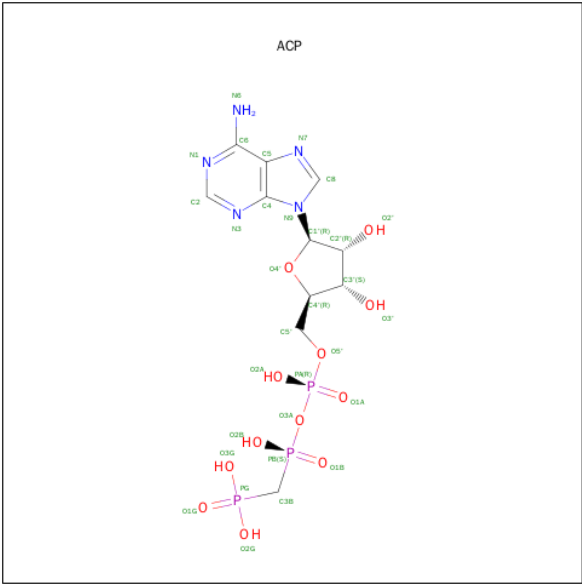
There are 4 unique types of molecules in this entry. The entry contains 7932 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 DEATH-ASSOCIATED PROTEIN KINASE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	249	Total	C	N	O	S	0	0	0
			1918	1243	306	365	4			
1	B	253	Total	C	N	O	S	0	0	0
			1955	1265	313	373	4			
1	C	259	Total	C	N	O	S	0	0	0
			1949	1252	328	365	4			
1	D	245	Total	C	N	O	S	0	0	0
			1852	1194	298	356	4			

- Molecule 2 is PHOSPHOMETHYLPHOSPHONIC ACID ADENYLATE ESTER (three-letter code: ACP) (formula: C₁₁H₁₈N₅O₁₂P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	B	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	P	0	0
			31	11	5	12	3		
2	D	1	Total	C	N	O	P	0	0
			31	11	5	12	3		

- 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		
3	A	2	Total	Mg	0	0
			2	2		
3	D	1	Total	Mg	0	0
			1	1		
3	C	1	Total	Mg	0	0
			1	1		

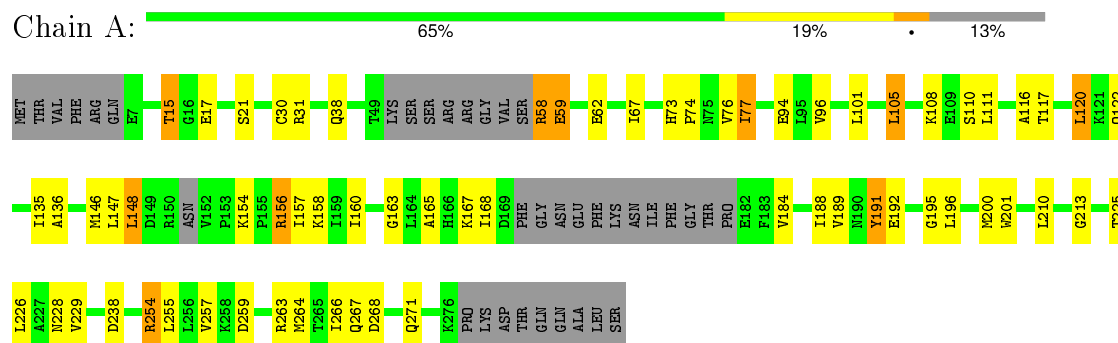
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	31	Total	O	0	0
			31	31		
4	B	24	Total	O	0	0
			24	24		
4	C	35	Total	O	0	0
			35	35		
4	D	38	Total	O	0	0
			38	38		

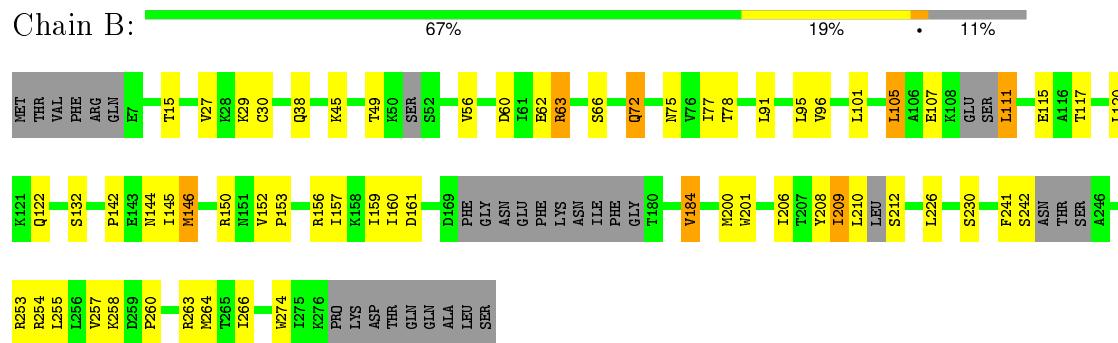
3 Residue-property plots

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.

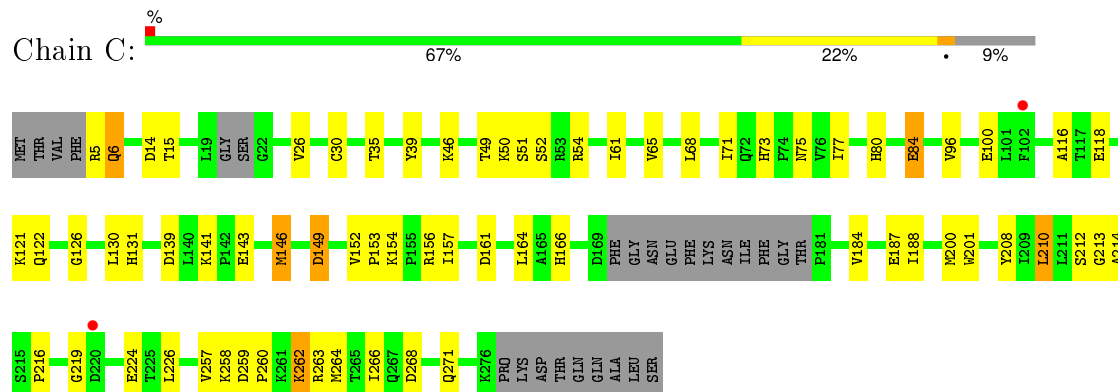
• Molecule 1: DEATH-ASSOCIATED PROTEIN KINASE 1



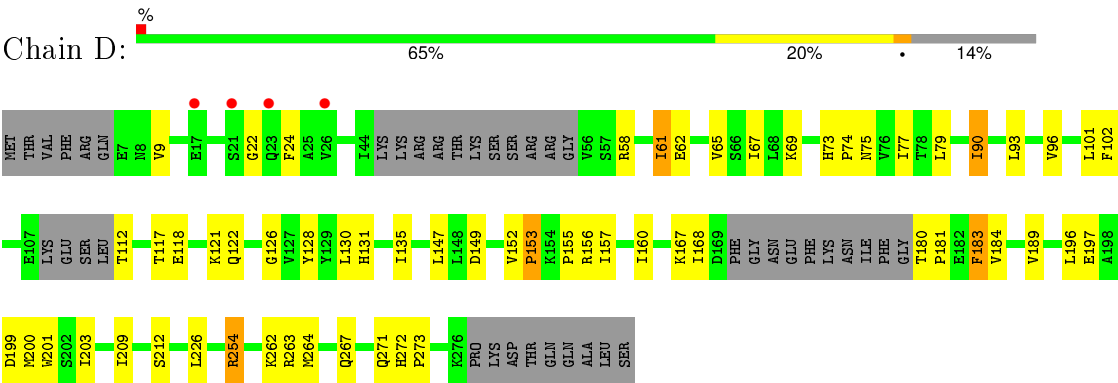
• Molecule 1: DEATH-ASSOCIATED PROTEIN KINASE 1



• Molecule 1: DEATH-ASSOCIATED PROTEIN KINASE 1



● Molecule 1: DEATH-ASSOCIATED PROTEIN KINASE 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.41Å 76.58Å 106.89Å 90.00° 92.01° 90.00°	Depositor
Resolution (Å)	106.83 – 2.65 45.71 – 2.65	Depositor EDS
% Data completeness (in resolution range)	99.8 (106.83-2.65) 99.8 (45.71-2.65)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.47 (at 2.65Å)	Xtriage
Refinement program	REFMAC 5.6.0117	Depositor
R, R_{free}	0.216 , 0.285 0.216 , 0.284	Depositor DCC
R_{free} test set	1976 reflections (5.29%)	DCC
Wilson B-factor (Å ²)	53.5	Xtriage
Anisotropy	0.722	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 48.4	EDS
Estimated twinning fraction	0.031 for h,-k,-l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 39308 reflections	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	7932	wwPDB-VP
Average B, all atoms (Å ²)	60.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.39% 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: MG, ACP

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	0.77	1/1955 (0.1%)	0.88	0/2654
1	B	0.72	2/1991 (0.1%)	0.79	0/2698
1	C	0.63	1/1985 (0.1%)	0.73	1/2698 (0.0%)
1	D	0.66	2/1888 (0.1%)	0.76	1/2570 (0.0%)
All	All	0.70	6/7819 (0.1%)	0.79	2/10620 (0.0%)

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	3
1	D	0	1
All	All	0	4

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	201	TRP	CD2-CE2	6.59	1.49	1.41
1	C	201	TRP	CD2-CE2	5.67	1.48	1.41
1	B	201	TRP	CD2-CE2	5.46	1.48	1.41
1	D	201	TRP	CD2-CE2	5.25	1.47	1.41
1	D	183	PHE	CE2-CZ	5.08	1.47	1.37
1	B	274	TRP	CD2-CE2	5.07	1.47	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	139	ASP	CB-CG-OD1	5.55	123.29	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	199	ASP	CB-CG-OD1	5.05	122.84	118.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	163	GLY	Peptide
1	A	213	GLY	Peptide
1	A	58	ARG	Peptide
1	D	183	PHE	Mainchain

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	1918	0	1827	48	0
1	B	1955	0	1873	47	0
1	C	1949	0	1823	48	0
1	D	1852	0	1726	52	0
2	A	31	0	14	14	0
2	B	31	0	14	9	0
2	C	31	0	14	5	0
2	D	31	0	14	6	0
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
4	A	31	0	0	5	0
4	B	24	0	0	5	0
4	C	35	0	0	2	0
4	D	38	0	0	6	0
All	All	7932	0	7305	209	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 14.

All (209) 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:D:79:LEU:HA	4:D:2009:HOH:O	1.26	1.29
4:A:2018:HOH:O	1:B:230:SER:HB2	1.37	1.21
1:B:210:LEU:HD21	4:B:2016:HOH:O	1.47	1.12
1:D:152:VAL:HG12	1:D:153:PRO:HD2	1.16	1.12
1:B:210:LEU:CD2	4:B:2016:HOH:O	1.99	1.06
1:A:254:ARG:HG2	1:A:254:ARG:HH11	1.24	1.02
1:D:152:VAL:HG12	1:D:153:PRO:CD	1.97	0.94
1:D:77:ILE:HD11	2:D:1277:ACP:N6	1.87	0.90
1:A:160:ILE:HD12	2:A:1277:ACP:H5'2	1.56	0.88
1:C:122:GLN:HE22	1:C:156:ARG:HA	1.37	0.88
1:B:60:ASP:OD1	1:B:63:ARG:NH2	2.07	0.88
1:A:148:LEU:HD13	1:A:156:ARG:HB3	1.56	0.87
1:C:61:ILE:O	1:C:65:VAL:HG23	1.76	0.85
2:B:1279:ACP:O5'	2:B:1279:ACP:H8	1.77	0.84
1:B:152:VAL:HG13	1:B:153:PRO:HD2	1.60	0.83
1:D:152:VAL:CG1	1:D:153:PRO:HD2	2.05	0.83
1:C:149:ASP:OD2	1:C:152:VAL:HG23	1.79	0.82
2:A:1277:ACP:H5'2	2:A:1277:ACP:C8	2.10	0.80
1:D:112:THR:N	4:D:2017:HOH:O	2.13	0.80
2:C:1278:ACP:H3B2	4:C:2005:HOH:O	1.81	0.80
1:B:77:ILE:HD12	1:B:160:ILE:HG22	1.64	0.80
1:D:200:MET:HE1	1:D:203:ILE:HD12	1.62	0.80
1:C:200:MET:HE1	1:C:266:ILE:HB	1.65	0.79
1:D:93:LEU:HD23	4:D:2009:HOH:O	1.83	0.78
1:C:6:GLN:HE22	1:C:84:GLU:HG2	1.48	0.78
1:A:271:GLN:NE2	4:A:2029:HOH:O	2.16	0.78
1:C:200:MET:CE	1:C:266:ILE:HB	2.14	0.77
1:B:152:VAL:CG1	1:B:153:PRO:HD2	2.14	0.77
2:A:1277:ACP:C5'	2:A:1277:ACP:H8	2.15	0.77
1:D:58:ARG:O	1:D:62:GLU:HG2	1.85	0.76
1:D:93:LEU:HA	4:D:2009:HOH:O	1.87	0.74
1:A:105:LEU:O	1:A:108:LYS:O	2.07	0.72
1:A:122:GLN:HE22	1:A:156:ARG:HA	1.52	0.72
1:C:116:ALA:HB1	1:C:210:LEU:CD2	2.19	0.71
2:D:1277:ACP:O1G	4:D:2035:HOH:O	2.09	0.70
1:A:160:ILE:HD12	2:A:1277:ACP:C5'	2.20	0.70
2:A:1277:ACP:O3G	4:A:2015:HOH:O	2.10	0.70
1:B:200:MET:CE	1:B:266:ILE:HB	2.22	0.70
1:C:6:GLN:NE2	1:C:84:GLU:HG2	2.05	0.69
1:A:58:ARG:O	1:A:59:GLU:HB3	1.91	0.69
1:D:209:ILE:O	1:D:212:SER:O	2.11	0.69
1:A:160:ILE:CD1	2:A:1277:ACP:H5'2	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:C:1278:ACP:O1A	2:C:1278:ACP:H3'	1.93	0.67
1:A:254:ARG:HH11	1:A:254:ARG:CG	2.03	0.67
1:C:100:GLU:HG2	1:C:143:GLU:HA	1.76	0.66
1:B:200:MET:HE1	1:B:266:ILE:HB	1.77	0.66
1:A:77:ILE:HD11	1:A:96:VAL:CG2	2.27	0.65
1:A:254:ARG:HG2	1:A:254:ARG:NH1	2.01	0.65
1:D:22:GLY:HA3	2:D:1277:ACP:H3B2	1.79	0.65
1:A:77:ILE:HG13	1:A:94:GLU:HB3	1.78	0.65
1:C:212:SER:O	1:C:214:ALA:N	2.30	0.65
1:B:77:ILE:CD1	2:B:1279:ACP:N6	2.60	0.64
1:B:96:VAL:HB	1:B:146:MET:HG2	1.77	0.64
1:D:77:ILE:HD11	2:D:1277:ACP:HN62	1.63	0.64
1:C:131:HIS:CE1	1:C:200:MET:CE	2.81	0.64
2:A:1277:ACP:C5'	2:A:1277:ACP:C8	2.75	0.64
1:D:122:GLN:HE22	1:D:157:ILE:H	1.45	0.64
1:D:122:GLN:NE2	1:D:157:ILE:H	1.95	0.63
1:A:200:MET:HE1	1:A:266:ILE:HD13	1.81	0.63
1:B:122:GLN:HE22	1:B:156:ARG:HA	1.62	0.63
1:A:200:MET:O	1:A:255:LEU:HD22	1.99	0.63
1:C:152:VAL:HG13	1:C:153:PRO:HD2	1.79	0.62
1:D:102:PHE:HE2	1:D:209:ILE:CG2	2.13	0.62
1:C:39:TYR:CZ	1:C:80:HIS:HD2	2.17	0.62
1:D:122:GLN:HE22	1:D:156:ARG:HA	1.65	0.62
1:A:136:ALA:O	1:A:165:ALA:HA	2.00	0.62
1:C:208:TYR:CD1	1:C:216:PRO:HD3	2.35	0.61
1:C:15:THR:HA	1:C:30:CYS:HB3	1.82	0.61
1:D:254:ARG:HB3	1:D:264:MET:HG3	1.84	0.60
1:B:257:VAL:HB	1:B:263:ARG:HG2	1.83	0.60
1:D:152:VAL:CG1	1:D:153:PRO:CD	2.73	0.60
1:D:147:LEU:HD22	1:D:155:PRO:HB2	1.84	0.60
1:D:77:ILE:HD12	1:D:160:ILE:HG22	1.84	0.59
1:C:39:TYR:CZ	1:C:80:HIS:CD2	2.90	0.59
1:A:257:VAL:O	1:A:263:ARG:NH1	2.36	0.59
1:A:184:VAL:HG23	1:A:189:VAL:HG23	1.84	0.59
1:A:157:ILE:O	1:A:157:ILE:HD12	2.01	0.59
1:D:167:LYS:O	1:D:168:ILE:HD12	2.02	0.59
2:B:1279:ACP:H8	2:B:1279:ACP:C5'	2.32	0.59
1:C:122:GLN:NE2	1:C:157:ILE:H	2.01	0.58
1:A:67:ILE:HG23	1:A:135:ILE:HD13	1.83	0.58
1:D:77:ILE:CD1	2:D:1277:ACP:N6	2.64	0.57
1:B:210:LEU:HD22	4:B:2016:HOH:O	1.82	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:ASP:HB2	2:B:1279:ACP:O1A	2.05	0.57
1:B:27:VAL:HG21	2:B:1279:ACP:H5'1	1.84	0.57
1:A:77:ILE:CD1	1:A:96:VAL:CG2	2.82	0.57
1:C:116:ALA:HB1	1:C:210:LEU:HD23	1.85	0.57
1:D:101:LEU:HD23	1:D:102:PHE:HE1	1.68	0.57
1:A:111:LEU:HD12	1:A:210:LEU:HG	1.86	0.57
1:A:116:ALA:O	1:A:120:LEU:HB2	2.06	0.56
1:B:27:VAL:CG2	2:B:1279:ACP:H5'1	2.36	0.56
1:C:68:LEU:HD23	1:C:71:ILE:HD11	1.88	0.55
1:C:131:HIS:CE1	1:C:200:MET:HE2	2.42	0.55
1:C:152:VAL:HG12	1:C:154:LYS:H	1.72	0.55
1:C:5:ARG:N	4:C:2001:HOH:O	2.40	0.55
1:D:73:HIS:HE1	1:D:75:ASN:HD22	1.56	0.54
1:B:209:ILE:O	1:B:209:ILE:HG22	2.06	0.54
1:B:77:ILE:HD11	2:B:1279:ACP:N6	2.21	0.54
1:C:77:ILE:HD13	1:C:96:VAL:CG2	2.38	0.54
1:B:208:TYR:C	1:B:210:LEU:H	2.12	0.53
1:B:77:ILE:HD13	2:B:1279:ACP:N6	2.22	0.53
1:D:149:ASP:CG	1:D:152:VAL:HG23	2.29	0.53
2:D:1277:ACP:H8	2:D:1277:ACP:O2A	2.09	0.53
1:A:96:VAL:HG12	1:A:147:LEU:O	2.09	0.53
1:A:160:ILE:HD11	2:A:1277:ACP:H3'	1.91	0.53
1:B:15:THR:HA	1:B:30:CYS:SG	2.49	0.53
1:C:122:GLN:NE2	1:C:156:ARG:HA	2.16	0.53
1:D:90:ILE:H	1:D:90:ILE:HD12	1.73	0.52
1:C:258:LYS:O	1:C:260:PRO:HD3	2.09	0.52
1:B:241:PHE:O	1:B:242:SER:CB	2.56	0.52
1:D:73:HIS:CE1	1:D:75:ASN:HB2	2.45	0.52
1:B:258:LYS:O	1:B:260:PRO:HD3	2.10	0.52
2:A:1277:ACP:O5'	2:A:1277:ACP:H8	2.09	0.52
1:D:180:THR:N	1:D:181:PRO:CD	2.73	0.52
1:B:72:GLN:HG3	4:B:2004:HOH:O	2.11	0.51
2:A:1277:ACP:O2A	2:A:1277:ACP:C4'	2.57	0.51
1:C:73:HIS:CE1	1:C:75:ASN:HB2	2.45	0.51
1:C:264:MET:HG3	1:C:268:ASP:HB3	1.93	0.51
1:A:264:MET:HG3	1:A:268:ASP:HB2	1.93	0.51
1:C:131:HIS:CE1	1:C:200:MET:HE3	2.45	0.51
1:A:157:ILE:C	1:A:157:ILE:HD12	2.31	0.51
2:A:1277:ACP:O1A	2:A:1277:ACP:O1B	2.27	0.51
1:B:77:ILE:HD11	2:B:1279:ACP:HN62	1.75	0.50
1:A:264:MET:HG3	1:A:268:ASP:CB	2.41	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:67:ILE:HG23	1:D:135:ILE:HD13	1.92	0.50
1:C:161:ASP:OD2	2:C:1278:ACP:O1B	2.29	0.50
1:D:101:LEU:HD23	1:D:102:PHE:CE1	2.47	0.50
2:A:1277:ACP:H5'2	2:A:1277:ACP:H8	1.79	0.50
1:B:122:GLN:HE22	1:B:157:ILE:H	1.59	0.50
1:D:96:VAL:HG12	1:D:147:LEU:O	2.12	0.50
1:C:187:GLU:OE2	1:D:263:ARG:NH2	2.45	0.50
1:A:31:ARG:CB	4:A:2002:HOH:O	2.60	0.50
1:A:77:ILE:HD13	1:A:160:ILE:HG22	1.94	0.49
1:D:272:HIS:ND1	1:D:273:PRO:HD2	2.27	0.49
1:C:39:TYR:OH	1:C:80:HIS:HD2	1.95	0.49
1:D:131:HIS:CE1	1:D:196:LEU:HB3	2.48	0.49
1:C:39:TYR:OH	1:C:80:HIS:CD2	2.66	0.49
1:D:61:ILE:O	1:D:65:VAL:HG23	2.13	0.49
1:B:75:ASN:O	1:B:159:ILE:N	2.38	0.48
1:B:241:PHE:O	1:B:242:SER:HB3	2.14	0.48
1:A:200:MET:HE1	1:A:266:ILE:HB	1.96	0.48
1:C:96:VAL:HG11	1:C:146:MET:HB3	1.94	0.48
1:A:154:LYS:O	1:A:156:ARG:NH1	2.46	0.48
1:B:230:SER:O	1:B:258:LYS:HE3	2.14	0.47
1:B:122:GLN:NE2	1:B:157:ILE:H	2.11	0.47
1:D:149:ASP:OD1	1:D:152:VAL:HG23	2.14	0.47
1:B:144:ASN:O	1:B:145:ILE:HD13	2.14	0.47
1:C:131:HIS:HE1	1:C:200:MET:HE2	1.78	0.47
1:B:255:LEU:O	1:B:263:ARG:HD3	2.14	0.47
1:C:49:THR:HB	1:C:52:SER:HB2	1.96	0.47
1:A:74:PRO:O	1:A:158:LYS:NZ	2.41	0.47
1:B:200:MET:HE3	1:B:266:ILE:HB	1.96	0.47
1:D:272:HIS:CG	1:D:273:PRO:HD2	2.50	0.47
1:D:102:PHE:HE2	1:D:209:ILE:HG22	1.80	0.46
1:B:56:VAL:HG12	1:B:60:ASP:HB2	1.98	0.46
1:D:128:TYR:HE1	1:D:267:GLN:HG3	1.81	0.46
1:C:184:VAL:HG11	1:C:188:ILE:CG2	2.46	0.46
1:C:122:GLN:HE22	1:C:157:ILE:H	1.64	0.46
1:D:90:ILE:HD12	1:D:90:ILE:N	2.30	0.46
1:A:229:VAL:HG11	1:B:184:VAL:O	2.15	0.46
1:B:152:VAL:CG1	1:B:153:PRO:CD	2.91	0.46
1:D:102:PHE:CE2	1:D:209:ILE:HG22	2.51	0.46
1:B:254:ARG:O	1:B:264:MET:HB2	2.15	0.46
2:C:1278:ACP:H3'	2:C:1278:ACP:PA	2.56	0.46
1:D:122:GLN:HE22	1:D:157:ILE:N	2.12	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:164:LEU:O	1:C:166:HIS:ND1	2.43	0.45
1:A:200:MET:CE	1:A:266:ILE:HB	2.47	0.45
1:A:168:ILE:HG12	1:A:195:GLY:HA2	1.97	0.45
1:B:210:LEU:O	1:B:212:SER:N	2.49	0.45
1:B:111:LEU:HD13	1:B:115:GLU:HB3	1.98	0.45
1:A:136:ALA:HB2	1:A:196:LEU:HD23	1.99	0.45
1:C:116:ALA:HB1	1:C:210:LEU:HD21	1.97	0.45
2:A:1277:ACP:H4'	2:A:1277:ACP:O2A	2.17	0.44
1:C:257:VAL:HB	1:C:263:ARG:HG3	1.99	0.44
1:B:206:ILE:O	1:B:210:LEU:HG	2.17	0.44
1:C:219:GLY:HA3	1:C:224:GLU:HB3	2.00	0.44
1:A:160:ILE:CD1	2:A:1277:ACP:C5'	2.89	0.44
1:A:167:LYS:HB2	4:A:2016:HOH:O	2.17	0.43
1:A:96:VAL:HB	1:A:146:MET:HG2	1.99	0.43
1:D:126:GLY:O	1:D:130:LEU:HG	2.18	0.43
1:D:102:PHE:CE2	1:D:209:ILE:CG2	2.98	0.43
1:A:73:HIS:HB3	1:A:76:VAL:HG22	2.00	0.43
1:C:141:LYS:HE3	1:C:143:GLU:OE2	2.19	0.43
1:C:184:VAL:HG11	1:C:188:ILE:HG21	2.01	0.43
1:C:259:ASP:HB3	1:C:262:LYS:HG3	2.00	0.43
1:B:101:LEU:HG	1:B:105:LEU:HD22	2.00	0.42
2:C:1278:ACP:O2B	2:C:1278:ACP:H5'2	2.19	0.42
1:A:264:MET:CG	1:A:268:ASP:HB2	2.49	0.42
1:A:122:GLN:NE2	1:A:157:ILE:H	2.18	0.42
1:C:184:VAL:HG12	1:C:188:ILE:HB	2.00	0.42
1:D:184:VAL:HG12	1:D:189:VAL:HG23	2.02	0.42
1:B:142:PRO:HG3	4:B:2015:HOH:O	2.20	0.42
1:D:267:GLN:CD	1:D:267:GLN:H	2.22	0.42
1:C:126:GLY:O	1:C:130:LEU:HG	2.20	0.42
1:C:46:LYS:NZ	1:C:84:GLU:OE2	2.38	0.41
1:D:73:HIS:CG	1:D:74:PRO:HD2	2.55	0.41
1:D:197:GLU:N	1:D:197:GLU:OE1	2.41	0.41
1:D:200:MET:HE1	1:D:203:ILE:CD1	2.43	0.41
1:C:187:GLU:CD	1:D:263:ARG:HH22	2.23	0.41
1:A:225:THR:O	1:A:228:ASN:HB2	2.20	0.41
1:A:188:ILE:O	1:A:191:TYR:N	2.52	0.41
1:B:29:LYS:HE3	1:B:95:LEU:HD21	2.02	0.41
1:B:122:GLN:HE22	1:B:156:ARG:CA	2.33	0.41
1:A:15:THR:HG22	1:A:30:CYS:SG	2.60	0.41
1:D:79:LEU:HD12	4:D:2009:HOH:O	2.20	0.41
1:A:101:LEU:O	1:A:105:LEU:HB2	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:56:VAL:CG1	1:B:60:ASP:HB2	2.51	0.41
1:A:59:GLU:HA	1:A:62:GLU:OE1	2.22	0.40
1:B:264:MET:HE2	1:B:264:MET:HB3	2.00	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	241/285 (85%)	225 (93%)	13 (5%)	3 (1%)	16	35
1	B	241/285 (85%)	225 (93%)	15 (6%)	1 (0%)	39	65
1	C	253/285 (89%)	235 (93%)	16 (6%)	2 (1%)	24	47
1	D	237/285 (83%)	218 (92%)	17 (7%)	2 (1%)	24	47
All	All	972/1140 (85%)	903 (93%)	61 (6%)	8 (1%)	24	47

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	213	GLY
1	A	59	GLU
1	A	191	TYR
1	B	209	ILE
1	C	35	THR
1	D	24	PHE
1	A	192	GLU
1	D	153	PRO

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	195/254 (77%)	179 (92%)	16 (8%)	14	29
1	B	201/254 (79%)	181 (90%)	20 (10%)	9	19
1	C	188/254 (74%)	173 (92%)	15 (8%)	15	31
1	D	184/254 (72%)	173 (94%)	11 (6%)	24	47
All	All	768/1016 (76%)	706 (92%)	62 (8%)	15	30

All (62) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	15	THR
1	A	17	GLU
1	A	21	SER
1	A	38	GLN
1	A	77	ILE
1	A	105	LEU
1	A	110	SER
1	A	117	THR
1	A	120	LEU
1	A	148	LEU
1	A	156	ARG
1	A	226	LEU
1	A	238	ASP
1	A	254	ARG
1	A	259	ASP
1	A	267	GLN
1	B	38	GLN
1	B	45	LYS
1	B	49	THR
1	B	62	GLU
1	B	63	ARG
1	B	66	SER
1	B	72	GLN
1	B	78	THR

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Mol	Chain	Res	Type
1	B	91	LEU
1	B	105	LEU
1	B	107	GLU
1	B	111	LEU
1	B	117	THR
1	B	120	LEU
1	B	132	SER
1	B	146	MET
1	B	150	ARG
1	B	184	VAL
1	B	226	LEU
1	B	253	ARG
1	C	6	GLN
1	C	14	ASP
1	C	26	VAL
1	C	50	LYS
1	C	51	SER
1	C	54	ARG
1	C	84	GLU
1	C	118	GLU
1	C	121	LYS
1	C	146	MET
1	C	149	ASP
1	C	210	LEU
1	C	226	LEU
1	C	262	LYS
1	C	271	GLN
1	D	9	VAL
1	D	61	ILE
1	D	69	LYS
1	D	90	ILE
1	D	117	THR
1	D	118	GLU
1	D	121	LYS
1	D	226	LEU
1	D	254	ARG
1	D	262	LYS
1	D	271	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	75	ASN
1	A	122	GLN
1	B	72	GLN
1	B	75	ASN
1	B	80	HIS
1	B	122	GLN
1	B	131	HIS
1	B	144	ASN
1	C	6	GLN
1	C	80	HIS
1	C	122	GLN
1	C	131	HIS
1	C	144	ASN
1	C	151	ASN
1	D	75	ASN
1	D	80	HIS
1	D	122	GLN
1	D	144	ASN
1	D	190	ASN

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 10 ligands modelled in this entry, 6 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	ACP	A	1277	3	25,33,33	2.20	8 (32%)	31,52,52	3.14	12 (38%)
2	ACP	B	1279	3	25,33,33	2.30	6 (24%)	31,52,52	3.06	11 (35%)
2	ACP	C	1278	3	25,33,33	1.80	6 (24%)	31,52,52	1.99	6 (19%)
2	ACP	D	1277	3	25,33,33	1.87	8 (32%)	31,52,52	1.89	3 (9%)

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	ACP	A	1277	3	-	0/15/38/38	0/3/3/3
2	ACP	B	1279	3	-	0/15/38/38	0/3/3/3
2	ACP	C	1278	3	-	0/15/38/38	0/3/3/3
2	ACP	D	1277	3	-	0/15/38/38	0/3/3/3

All (28) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1278	ACP	PG-O3G	-3.03	1.47	1.54
2	D	1277	ACP	PG-O3G	-2.04	1.49	1.54
2	A	1277	ACP	C5'-C4'	2.03	1.58	1.51
2	B	1279	ACP	O4'-C1'	2.06	1.43	1.41
2	D	1277	ACP	O4'-C1'	2.14	1.43	1.41
2	C	1278	ACP	PB-O2B	2.30	1.61	1.56
2	C	1278	ACP	O4'-C1'	2.31	1.44	1.41
2	D	1277	ACP	PB-O2B	2.51	1.62	1.56
2	D	1277	ACP	C5-C4	2.71	1.46	1.40
2	D	1277	ACP	C2-N3	2.77	1.37	1.32
2	B	1279	ACP	PG-O2G	2.79	1.61	1.54
2	D	1277	ACP	PG-O2G	2.88	1.61	1.54
2	A	1277	ACP	C2-N3	2.99	1.37	1.32
2	A	1277	ACP	PB-O3A	2.99	1.61	1.58
2	B	1279	ACP	C5-C4	3.09	1.47	1.40
2	B	1279	ACP	PB-O2B	3.10	1.63	1.56
2	A	1277	ACP	PB-O2B	3.11	1.63	1.56
2	C	1278	ACP	C5-C4	3.13	1.47	1.40
2	C	1278	ACP	PG-O2G	3.20	1.62	1.54
2	A	1277	ACP	PG-O2G	3.29	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1277	ACP	PB-O3A	3.42	1.62	1.58
2	A	1277	ACP	C5-C4	3.52	1.48	1.40
2	A	1277	ACP	O4'-C1'	4.33	1.46	1.41
2	C	1278	ACP	PG-O1G	5.24	1.62	1.50
2	A	1277	ACP	PG-O1G	5.53	1.62	1.50
2	B	1279	ACP	PG-O1G	5.53	1.62	1.50
2	D	1277	ACP	PG-O1G	5.54	1.62	1.50
2	B	1279	ACP	PB-O3A	7.44	1.66	1.58

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1279	ACP	N3-C2-N1	-10.07	121.18	128.89
2	A	1277	ACP	N3-C2-N1	-8.66	122.26	128.89
2	A	1277	ACP	PA-O3A-PB	-8.62	108.52	132.73
2	A	1277	ACP	C2'-C1'-N9	-8.15	101.83	114.29
2	D	1277	ACP	N3-C2-N1	-7.46	123.18	128.89
2	C	1278	ACP	N3-C2-N1	-6.21	124.14	128.89
2	C	1278	ACP	C2'-C1'-N9	-6.06	105.03	114.29
2	B	1279	ACP	PA-O3A-PB	-6.03	115.80	132.73
2	D	1277	ACP	PA-O3A-PB	-3.79	122.09	132.73
2	C	1278	ACP	PA-O3A-PB	-3.74	122.23	132.73
2	B	1279	ACP	C2'-C1'-N9	-3.62	108.77	114.29
2	D	1277	ACP	C2'-C1'-N9	-3.36	109.16	114.29
2	B	1279	ACP	O2A-PA-O3A	-3.28	90.20	105.09
2	B	1279	ACP	O2A-PA-O5'	-3.23	92.17	108.46
2	B	1279	ACP	O2B-PB-O1B	-3.21	100.02	110.12
2	C	1278	ACP	C4-C5-N7	-3.01	106.71	109.48
2	B	1279	ACP	C4-C5-N7	-2.11	107.54	109.48
2	A	1277	ACP	C5'-C4'-C3'	-2.07	106.98	115.21
2	C	1278	ACP	O1G-PG-C3B	-2.03	106.51	111.13
2	A	1277	ACP	C1'-N9-C4	2.04	130.02	126.94
2	A	1277	ACP	O4'-C1'-N9	2.12	112.53	108.10
2	A	1277	ACP	C2'-C3'-C4'	2.14	107.02	102.61
2	A	1277	ACP	O2G-PG-C3B	2.15	111.61	106.40
2	B	1279	ACP	O3G-PG-C3B	2.41	112.26	106.40
2	A	1277	ACP	N6-C6-N1	2.42	124.41	119.20
2	A	1277	ACP	O3'-C3'-C4'	2.59	118.82	111.05
2	B	1279	ACP	C4'-O4'-C1'	2.76	112.75	109.72
2	C	1278	ACP	O2G-PG-C3B	2.79	113.16	106.40
2	B	1279	ACP	O5'-C5'-C4'	3.56	122.24	109.12
2	A	1277	ACP	O3A-PA-O5'	3.80	113.03	102.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1277	ACP	O5'-C5'-C4'	4.30	124.96	109.12
2	B	1279	ACP	O3A-PA-O5'	7.22	122.08	102.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 34 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1277	ACP	14	0
2	B	1279	ACP	9	0
2	C	1278	ACP	5	0
2	D	1277	ACP	6	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	249/285 (87%)	-0.06	0	100 100	27, 51, 83, 106	0
1	B	253/285 (88%)	-0.07	0	100 100	36, 54, 77, 93	0
1	C	259/285 (90%)	-0.03	2 (0%)	87 87	43, 64, 89, 105	0
1	D	245/285 (85%)	0.07	4 (1%)	74 74	42, 63, 107, 141	0
All	All	1006/1140 (88%)	-0.02	6 (0%)	90 91	27, 59, 91, 141	0

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	21	SER	4.2
1	D	23	GLN	2.6
1	C	220	ASP	2.2
1	C	102	PHE	2.1
1	D	26	VAL	2.1
1	D	17	GLU	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(Å ²)	Q<0.9
2	ACP	C	1278	31/31	0.90	0.32	4.16	42,46,51,55	31
2	ACP	A	1277	31/31	0.94	0.16	-0.44	43,47,56,63	0
2	ACP	D	1277	31/31	0.88	0.18	-0.45	42,61,74,85	31
2	ACP	B	1279	31/31	0.95	0.14	-1.49	39,44,55,59	0
3	MG	A	1279	1/1	0.79	0.19	-	51,51,51,51	0
3	MG	A	1278	1/1	0.86	0.20	-	42,42,42,42	0
3	MG	B	1278	1/1	0.93	0.40	-	58,58,58,58	0
3	MG	C	1277	1/1	0.88	0.50	-	41,41,41,41	1
3	MG	D	1278	1/1	0.95	0.14	-	58,58,58,58	1
3	MG	B	1277	1/1	0.91	0.25	-	44,44,44,44	0

6.5 Other polymers [i](#)

There are no such residues in this entry.