



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 14, 2017 – 08:40 pm GMT

PDB ID : 1SQ5
Title : Crystal Structure of E. coli Pantothenate kinase
Authors : Ivey, R.A.; Zhang, Y.-M.; Virga, K.G.; Hevener, K.; Lee, R.E.; Rock, C.O.;
Jackowski, S.; Park, H.-W.
Deposited on : 2004-03-17
Resolution : 2.20 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 : 1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix) : 1.9-1692
EDS : trunk28620
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
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) : recalc28949

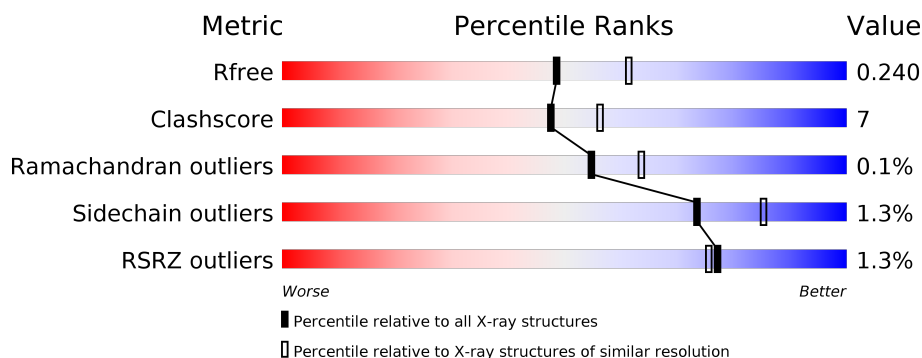
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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}	100719	4002 (2.20-2.20)
Clashscore	112137	4730 (2.20-2.20)
Ramachandran outliers	110173	4656 (2.20-2.20)
Sidechain outliers	110143	4657 (2.20-2.20)
RSRZ outliers	101464	4033 (2.20-2.20)

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	308	<div> <div>2%</div> <div>79%</div> <div>19%</div> <div>••</div> </div>
1	B	308	<div> <div>2%</div> <div>81%</div> <div>16%</div> <div>•</div> </div>
1	C	308	<div> <div>2%</div> <div>81%</div> <div>15%</div> <div>•</div> </div>
1	D	308	<div> <div>2%</div> <div>81%</div> <div>17%</div> <div>•</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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	PAU	B	6003	-	-	-	X
2	PAU	C	6002	-	-	-	X
2	PAU	D	6004	-	-	-	X

2 Entry composition [i](#)

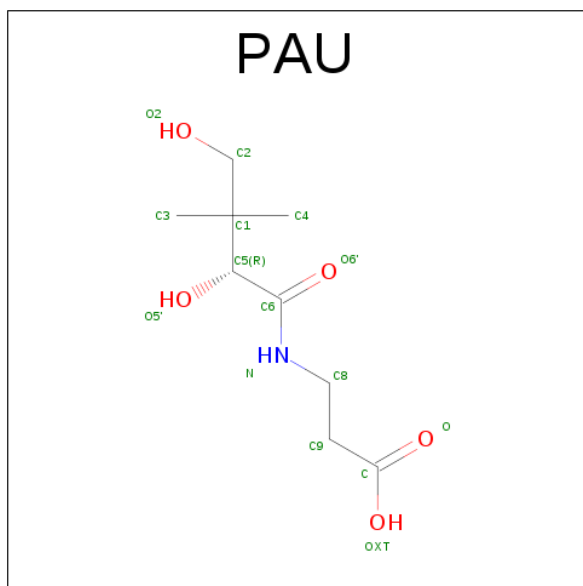
There are 4 unique types of molecules in this entry. The entry contains 10703 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Pantothenate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	302	Total	C	N	O	S	0	0	0
			2414	1555	411	442	6			
1	B	302	Total	C	N	O	S	0	0	0
			2418	1558	411	444	5			
1	C	298	Total	C	N	O	S	0	0	0
			2391	1541	404	440	6			
1	D	304	Total	C	N	O	S	0	0	0
			2427	1564	412	445	6			

- Molecule 2 is PANTOTHENOIC ACID (three-letter code: PAU) (formula: C₉H₁₇NO₅).



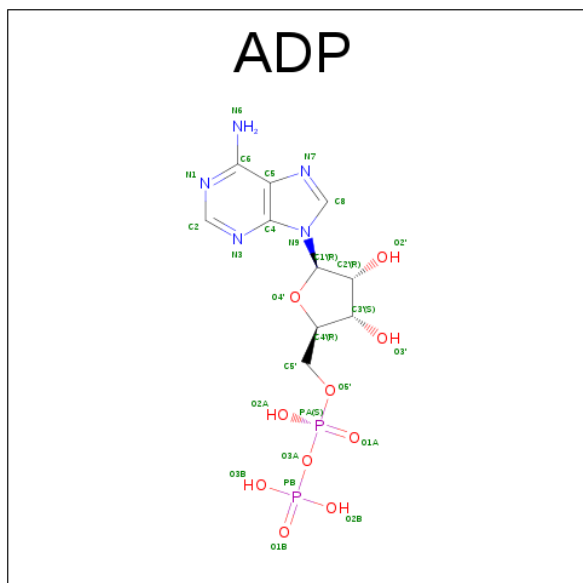
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			15	9	1	5		
2	C	1	Total	C	N	O	0	0
			15	9	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			15	9	1	5		
2	D	1	Total	C	N	O	0	0
			15	9	1	5		

- Molecule 3 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	B	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	C	1	Total	C	N	O	P	0	0
			27	10	5	10	2		
3	D	1	Total	C	N	O	P	0	0
			27	10	5	10	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	235	Total	O	0	0
			235	235		
4	B	191	Total	O	0	0
			191	191		
4	C	230	Total	O	0	0
			230	230		

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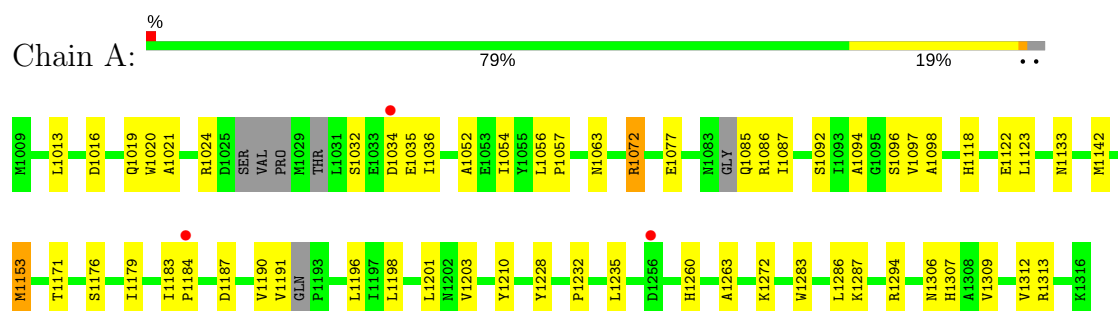
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	229	Total 229	O 229	0	0

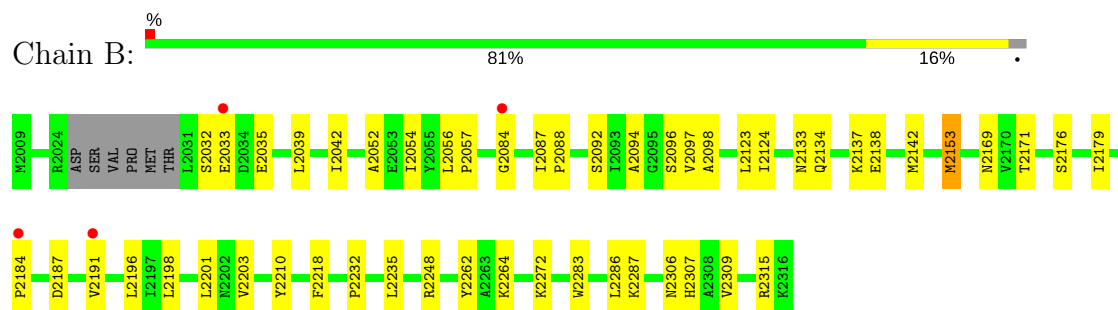
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

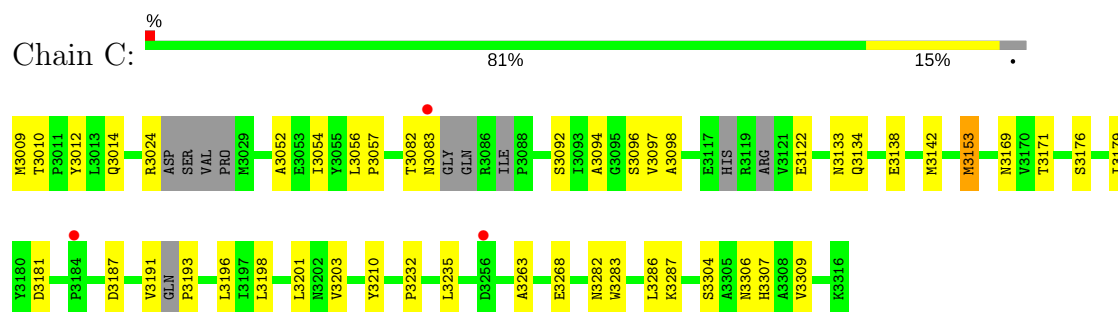
• Molecule 1: Pantothenate kinase



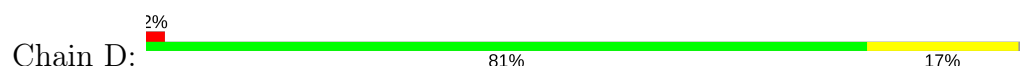
• Molecule 1: Pantothenate kinase

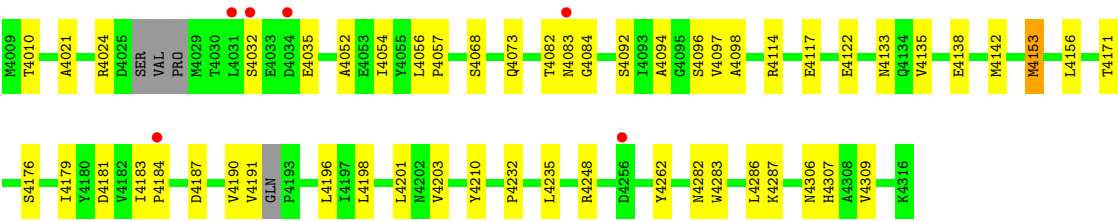


• Molecule 1: Pantothenate kinase



• Molecule 1: Pantothenate kinase





4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	181.20Å 181.66Å 47.42Å 90.00° 104.79° 90.00°	Depositor
Resolution (Å)	20.00 – 2.20 40.82 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.2 (20.00-2.20) 88.7 (40.82-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.75 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.187 , 0.225 0.202 , 0.240	Depositor DCC
R_{free} test set	7076 reflections (10.07%)	DCC
Wilson B-factor (Å ²)	22.3	Xtriage
Anisotropy	0.579	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 45.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k+l,h+l,-l 0.000 for -k+l,-h-l,-l 0.024 for -h-2*l,-k,l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10703	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 7.64% 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, 0.333 respectively for untwinned datasets, and 0.375, 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: PAU, ADP

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	0.34	0/2468	0.58	0/3349
1	B	0.33	0/2475	0.57	0/3364
1	C	0.35	0/2442	0.57	0/3309
1	D	0.33	0/2483	0.57	0/3374
All	All	0.34	0/9868	0.57	0/13396

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 [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	2414	0	2381	39	0
1	B	2418	0	2392	32	0
1	C	2391	0	2370	35	1
1	D	2427	0	2400	33	0
2	A	15	0	16	0	0
2	B	15	0	16	0	0
2	C	15	0	16	1	0
2	D	15	0	16	1	0
3	A	27	0	12	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	27	0	12	0	0
3	C	27	0	12	0	0
3	D	27	0	12	0	0
4	A	235	0	0	6	0
4	B	191	0	0	5	0
4	C	230	0	0	8	0
4	D	229	0	0	5	0
All	All	10703	0	9655	136	1

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 7.

All (136) 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:C:3263:ALA:HB2	4:C:7336:HOH:O	1.89	0.72
1:C:3010:THR:HG22	1:C:3012:TYR:H	1.55	0.72
1:A:1263:ALA:HB2	4:A:7647:HOH:O	1.89	0.71
1:C:3009:MET:HB3	4:C:7474:HOH:O	1.93	0.68
1:D:4021:ALA:O	1:D:4024:ARG:HG2	1.95	0.66
1:D:4032:SER:HB3	1:D:4035:GLU:HG3	1.79	0.65
1:A:1032:SER:OG	1:A:1035:GLU:HG3	1.98	0.64
1:D:4024:ARG:HD2	4:D:7663:HOH:O	1.98	0.63
1:C:3010:THR:HB	4:C:7358:HOH:O	2.00	0.61
1:D:4133:ASN:O	1:D:4142:MET:HE1	2.00	0.61
1:C:3282:ASN:OD1	2:C:6002:PAU:H81	2.02	0.60
1:B:2176:SER:HB3	1:B:2179:ILE:HG12	1.83	0.59
1:C:3304:SER:HB2	4:C:7615:HOH:O	2.01	0.59
1:A:1153:MET:HG3	1:A:1210:TYR:CZ	2.38	0.59
1:B:2191:VAL:HG22	4:B:7864:HOH:O	2.02	0.59
1:A:1072:ARG:HG3	1:D:4068:SER:OG	2.02	0.58
1:B:2248:ARG:HD2	1:B:2262:TYR:O	2.03	0.58
1:A:1133:ASN:O	1:A:1142:MET:HE1	2.03	0.58
1:C:3232:PRO:HD2	1:C:3235:LEU:HD12	1.86	0.58
1:B:2153:MET:HG3	1:B:2210:TYR:CZ	2.38	0.58
1:A:1077:GLU:HB2	4:A:7483:HOH:O	2.05	0.57
1:A:1032:SER:O	1:A:1036:ILE:HG13	2.05	0.57
1:A:1232:PRO:HD2	1:A:1235:LEU:HD12	1.87	0.57
1:A:1313:ARG:NH2	4:A:7478:HOH:O	2.38	0.56
1:C:3153:MET:HG3	1:C:3210:TYR:CZ	2.40	0.56
1:B:2171:THR:CG2	1:B:2187:ASP:HB3	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:2232:PRO:HD2	1:B:2235:LEU:HD12	1.87	0.56
1:D:4135:VAL:O	1:D:4138:GLU:HG2	2.06	0.55
1:D:4282:ASN:OD1	2:D:6004:PAU:H81	2.06	0.55
1:D:4153:MET:HG3	1:D:4210:TYR:CZ	2.41	0.55
1:D:4232:PRO:HD2	1:D:4235:LEU:HD12	1.86	0.55
1:D:4283:TRP:CE2	1:D:4287:LYS:HD2	2.42	0.54
1:B:2133:ASN:O	1:B:2142:MET:HE1	2.08	0.54
1:B:2184:PRO:HG2	4:B:7531:HOH:O	2.06	0.54
1:D:4122:GLU:HG3	1:D:4190:VAL:HG13	1.88	0.54
1:B:2283:TRP:CE2	1:B:2287:LYS:HD2	2.43	0.54
1:A:1191:VAL:HG22	4:A:7715:HOH:O	2.07	0.54
1:B:2134:GLN:O	1:B:2138:GLU:HG3	2.08	0.54
1:A:1283:TRP:CE2	1:A:1287:LYS:HD2	2.42	0.54
1:C:3283:TRP:CE2	1:C:3287:LYS:HD2	2.43	0.54
1:B:2272:LYS:HD2	4:B:7597:HOH:O	2.09	0.53
1:B:2032:SER:OG	1:B:2035:GLU:HG3	2.08	0.53
1:C:3134:GLN:O	1:C:3138:GLU:HG3	2.08	0.53
1:C:3082:THR:HB	4:C:7724:HOH:O	2.07	0.52
1:B:2054:ILE:HG21	1:B:2309:VAL:HG21	1.92	0.52
1:D:4156:LEU:HG	4:D:7352:HOH:O	2.09	0.52
1:A:1272:LYS:HD2	4:A:7409:HOH:O	2.09	0.52
1:D:4133:ASN:ND2	1:D:4181:ASP:HB2	2.25	0.52
1:A:1096:SER:HB2	1:A:1286:LEU:HD13	1.92	0.51
1:B:2039:LEU:HD23	1:B:2042:ILE:HD12	1.92	0.51
1:C:3010:THR:HG21	4:C:7458:HOH:O	2.08	0.51
1:D:4248:ARG:HD2	1:D:4262:TYR:O	2.11	0.51
1:B:2033:GLU:HG3	4:B:7442:HOH:O	2.10	0.51
1:B:2123:LEU:HD23	1:B:2124:ILE:N	2.26	0.51
1:A:1176:SER:HB3	1:A:1179:ILE:HG12	1.92	0.51
1:C:3056:LEU:HB2	1:C:3057:PRO:HD3	1.93	0.51
1:A:1056:LEU:HB2	1:A:1057:PRO:HD3	1.93	0.50
1:B:2056:LEU:HB2	1:B:2057:PRO:HD3	1.94	0.50
1:C:3191:VAL:O	1:C:3191:VAL:HG23	2.12	0.50
1:D:4056:LEU:HB2	1:D:4057:PRO:HD3	1.94	0.49
1:A:1021:ALA:O	1:A:1024:ARG:HD3	2.13	0.49
1:A:1016:ASP:H	1:A:1019:GLN:NE2	2.11	0.49
1:A:1260:HIS:HE1	1:B:2264:LYS:NZ	2.09	0.49
1:D:4176:SER:HB3	1:D:4179:ILE:HG12	1.95	0.49
1:A:1171:THR:CG2	1:A:1187:ASP:HB3	2.43	0.49
1:C:3096:SER:HB2	1:C:3286:LEU:HD13	1.94	0.49
1:B:2315:ARG:HG3	4:B:7470:HOH:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3082:THR:HG22	1:C:3083:ASN:N	2.29	0.48
1:D:4201:LEU:C	1:D:4201:LEU:HD12	2.34	0.48
1:A:1092:SER:HA	1:A:1198:LEU:O	2.14	0.47
1:A:1054:ILE:HG21	1:A:1309:VAL:HG21	1.96	0.47
1:C:3171:THR:CG2	1:C:3187:ASP:HB3	2.44	0.47
1:C:3268:GLU:HB2	4:C:7146:HOH:O	2.14	0.47
1:C:3024:ARG:HD3	1:C:3052:ALA:O	2.15	0.47
1:C:3176:SER:HB3	1:C:3179:ILE:HG12	1.95	0.47
1:C:3201:LEU:HD12	1:C:3201:LEU:C	2.35	0.47
1:C:3133:ASN:ND2	1:C:3181:ASP:HB2	2.29	0.47
1:D:4054:ILE:HG21	1:D:4309:VAL:HG21	1.96	0.47
1:B:2191:VAL:HG23	1:B:2191:VAL:O	2.13	0.47
1:B:2092:SER:HA	1:B:2198:LEU:O	2.15	0.46
1:A:1201:LEU:C	1:A:1201:LEU:HD12	2.35	0.46
1:B:2096:SER:HB2	1:B:2286:LEU:HD13	1.97	0.46
1:C:3092:SER:HA	1:C:3198:LEU:O	2.14	0.46
1:B:2094:ALA:HB2	1:B:2203:VAL:CG2	2.46	0.46
1:D:4153:MET:HG3	1:D:4210:TYR:CE2	2.50	0.46
1:B:2201:LEU:C	1:B:2201:LEU:HD12	2.37	0.46
1:D:4306:ASN:O	1:D:4307:HIS:HB2	2.16	0.46
1:B:2306:ASN:O	1:B:2307:HIS:HB2	2.16	0.45
1:A:1016:ASP:OD1	1:A:1019:GLN:HG3	2.16	0.45
1:A:1085:GLN:HB3	4:A:7245:HOH:O	2.16	0.45
1:B:2137:LYS:HB2	1:B:2142:MET:CE	2.46	0.45
1:A:1191:VAL:O	1:A:1191:VAL:HG23	2.16	0.45
1:D:4092:SER:HA	1:D:4198:LEU:O	2.16	0.45
1:B:2153:MET:HG3	1:B:2210:TYR:CE2	2.52	0.45
1:D:4096:SER:HB2	1:D:4286:LEU:HD13	1.97	0.45
1:D:4191:VAL:O	1:D:4191:VAL:HG23	2.16	0.44
1:A:1153:MET:HG3	1:A:1210:TYR:CE2	2.52	0.44
1:D:4114:ARG:HD3	4:D:7833:HOH:O	2.18	0.44
1:C:3094:ALA:HB2	1:C:3203:VAL:CG2	2.46	0.44
1:C:3153:MET:HG3	1:C:3210:TYR:CE2	2.51	0.44
1:C:3122:GLU:HG3	1:C:3193:PRO:HG3	2.00	0.44
1:D:4117:GLU:HB3	4:D:7802:HOH:O	2.18	0.44
1:D:4094:ALA:HB2	1:D:4203:VAL:CG2	2.47	0.44
1:A:1086:ARG:C	1:A:1087:ILE:HD12	2.38	0.43
1:A:1183:ILE:HA	1:A:1184:PRO:HD2	1.83	0.43
1:C:3054:ILE:HG21	1:C:3309:VAL:HG21	2.00	0.43
1:D:4082:THR:C	1:D:4084:GLY:H	2.22	0.43
1:B:2123:LEU:HD23	1:B:2123:LEU:C	2.38	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1063:ASN:ND2	1:A:1118:HIS:NE2	2.66	0.43
1:D:4171:THR:CG2	1:D:4187:ASP:HB3	2.49	0.43
1:B:2052:ALA:HA	1:B:2056:LEU:HD12	2.01	0.43
1:C:3010:THR:HG22	1:C:3012:TYR:N	2.29	0.43
1:A:1052:ALA:HA	1:A:1056:LEU:HD12	2.01	0.42
1:A:1306:ASN:O	1:A:1307:HIS:HB2	2.18	0.42
1:C:3306:ASN:O	1:C:3307:HIS:HB2	2.19	0.42
1:A:1020:TRP:CZ3	1:A:1312:VAL:HG11	2.54	0.42
1:A:1013:LEU:HD22	1:D:4082:THR:HG21	2.02	0.42
1:A:1097:VAL:O	1:A:1098:ALA:HB3	2.21	0.41
1:A:1122:GLU:HG3	1:A:1190:VAL:HG13	2.01	0.41
1:D:4052:ALA:HA	1:D:4056:LEU:HD12	2.02	0.41
1:A:1094:ALA:HB2	1:A:1203:VAL:CG2	2.50	0.41
1:A:1228:TYR:CD2	1:A:1294:ARG:HG3	2.56	0.41
1:D:4073:GLN:NE2	4:D:7460:HOH:O	2.49	0.41
1:D:4183:ILE:HA	1:D:4184:PRO:HD2	1.82	0.41
1:A:1016:ASP:H	1:A:1019:GLN:HE21	1.69	0.41
1:B:2169:ASN:OD1	1:B:2191:VAL:HG12	2.21	0.41
1:C:3094:ALA:HB2	1:C:3203:VAL:HG22	2.03	0.41
1:D:4097:VAL:O	1:D:4098:ALA:HB3	2.20	0.41
1:B:2097:VAL:O	1:B:2098:ALA:HB3	2.20	0.40
1:C:3097:VAL:O	1:C:3098:ALA:HB3	2.21	0.40
1:B:2087:ILE:HA	1:B:2088:PRO:HD3	1.94	0.40
1:C:3052:ALA:HA	1:C:3056:LEU:HD12	2.03	0.40
1:A:1176:SER:HB2	1:A:1183:ILE:HD11	2.02	0.40
1:C:3009:MET:HE2	4:C:7474:HOH:O	2.21	0.40
1:C:3133:ASN:O	1:C:3142:MET:HE1	2.21	0.40
1:C:3169:ASN:OD1	1:C:3191:VAL:HG12	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:3014:GLN:NE2	1:C:3014:GLN:NE2[2_555]	2.13	0.07

5.3 Torsion angles

5.3.1 Protein backbone

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	293/308 (95%)	287 (98%)	6 (2%)	0	100	100
1	B	298/308 (97%)	288 (97%)	9 (3%)	1 (0%)	44	49
1	C	286/308 (93%)	282 (99%)	4 (1%)	0	100	100
1	D	298/308 (97%)	292 (98%)	6 (2%)	0	100	100
All	All	1175/1232 (95%)	1149 (98%)	25 (2%)	1 (0%)	55	63

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	2084	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	260/277 (94%)	255 (98%)	5 (2%)	62	76
1	B	261/277 (94%)	258 (99%)	3 (1%)	78	88
1	C	260/277 (94%)	258 (99%)	2 (1%)	85	92
1	D	262/277 (95%)	258 (98%)	4 (2%)	70	82
All	All	1043/1108 (94%)	1029 (99%)	14 (1%)	73	85

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1034	ASP
1	A	1072	ARG
1	A	1123	LEU
1	A	1153	MET
1	A	1196	LEU
1	B	2153	MET
1	B	2196	LEU
1	B	2218	PHE
1	C	3153	MET
1	C	3196	LEU
1	D	4010	THR
1	D	4083	ASN
1	D	4153	MET
1	D	4196	LEU

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	1018	ASN
1	A	1019	GLN
1	A	1063	ASN
1	A	1085	GLN
1	A	1260	HIS
1	D	4018	ASN
1	D	4063	ASN
1	D	4177	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry

8 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
3	ADP	A	5001	-	25,29,29	0.88	1 (4%)	24,45,45	1.94	4 (16%)
2	PAU	A	6001	-	8,14,14	2.40	3 (37%)	11,19,19	1.22	2 (18%)
3	ADP	B	5002	-	25,29,29	0.83	1 (4%)	24,45,45	1.94	4 (16%)
2	PAU	B	6003	-	8,14,14	2.38	3 (37%)	11,19,19	1.33	2 (18%)
3	ADP	C	5003	-	25,29,29	1.09	1 (4%)	24,45,45	1.98	6 (25%)
2	PAU	C	6002	-	8,14,14	2.24	3 (37%)	11,19,19	1.43	1 (9%)
3	ADP	D	5004	-	25,29,29	0.93	1 (4%)	24,45,45	1.92	4 (16%)
2	PAU	D	6004	-	8,14,14	2.29	3 (37%)	11,19,19	1.34	3 (27%)

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
3	ADP	A	5001	-	-	0/12/32/32	0/3/3/3
2	PAU	A	6001	-	-	0/17/19/19	0/0/0/0
3	ADP	B	5002	-	-	0/12/32/32	0/3/3/3
2	PAU	B	6003	-	-	1/17/19/19	0/0/0/0
3	ADP	C	5003	-	-	0/12/32/32	0/3/3/3
2	PAU	C	6002	-	-	1/17/19/19	0/0/0/0
3	ADP	D	5004	-	-	0/12/32/32	0/3/3/3
2	PAU	D	6004	-	-	1/17/19/19	0/0/0/0

All (16) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	6002	PAU	O5'-C5	2.11	1.46	1.42
2	A	6001	PAU	O5'-C5	2.26	1.46	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	6004	PAU	C3-C1	2.28	1.59	1.53
2	B	6003	PAU	C3-C1	2.35	1.59	1.53
2	B	6003	PAU	O5'-C5	2.42	1.47	1.42
2	A	6001	PAU	C3-C1	2.43	1.59	1.53
2	C	6002	PAU	C3-C1	2.46	1.59	1.53
2	D	6004	PAU	O5'-C5	2.54	1.47	1.42
3	B	5002	ADP	C2-N1	3.02	1.39	1.33
3	A	5001	ADP	C2-N1	3.08	1.39	1.33
3	D	5004	ADP	C2-N1	3.25	1.40	1.33
3	C	5003	ADP	C2-N1	3.48	1.40	1.33
2	D	6004	PAU	O6'-C6	4.94	1.33	1.23
2	C	6002	PAU	O6'-C6	5.07	1.33	1.23
2	B	6003	PAU	O6'-C6	5.32	1.33	1.23
2	A	6001	PAU	O6'-C6	5.43	1.34	1.23

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	5004	ADP	N3-C2-N1	-6.62	123.09	128.86
3	A	5001	ADP	N3-C2-N1	-6.58	123.13	128.86
3	C	5003	ADP	N3-C2-N1	-6.50	123.20	128.86
3	B	5002	ADP	N3-C2-N1	-6.42	123.27	128.86
2	C	6002	PAU	C4-C1-C2	-2.62	104.23	109.06
2	D	6004	PAU	C4-C1-C2	-2.40	104.63	109.06
2	B	6003	PAU	C4-C1-C2	-2.37	104.68	109.06
3	C	5003	ADP	O3A-PB-O1B	-2.33	97.13	111.44
2	A	6001	PAU	C4-C1-C2	-2.27	104.86	109.06
3	C	5003	ADP	O3B-PB-O2B	2.03	115.80	107.61
2	D	6004	PAU	C4-C1-C5	2.05	112.37	108.82
2	D	6004	PAU	C5-C6-N	2.09	120.94	116.58
2	A	6001	PAU	C4-C1-C5	2.21	112.65	108.82
2	B	6003	PAU	C4-C1-C5	2.41	113.00	108.82
3	D	5004	ADP	C5-C6-N6	2.62	125.81	120.47
3	C	5003	ADP	C4'-O4'-C1'	2.63	112.57	109.77
3	A	5001	ADP	C5-C6-N6	2.66	125.90	120.47
3	C	5003	ADP	C2-N1-C6	2.67	123.43	118.77
3	A	5001	ADP	C2-N1-C6	2.68	123.46	118.77
3	B	5002	ADP	C4'-O4'-C1'	2.68	112.62	109.77
3	A	5001	ADP	C4'-O4'-C1'	2.71	112.65	109.77
3	D	5004	ADP	C2-N1-C6	2.73	123.54	118.77
3	B	5002	ADP	C2-N1-C6	2.78	123.63	118.77
3	D	5004	ADP	C4'-O4'-C1'	2.89	112.84	109.77

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
3	C	5003	ADP	C5-C6-N6	2.89	126.36	120.47
3	B	5002	ADP	C5-C6-N6	2.96	126.51	120.47

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	6002	PAU	C5-C6-N-C8
2	B	6003	PAU	C5-C6-N-C8
2	D	6004	PAU	C5-C6-N-C8

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	6002	PAU	1	0
2	D	6004	PAU	1	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	302/308 (98%)	-0.30	3 (0%) 82 81	15, 26, 47, 63	0
1	B	302/308 (98%)	-0.29	4 (1%) 77 75	16, 27, 47, 54	0
1	C	298/308 (96%)	-0.32	3 (1%) 82 81	14, 25, 45, 57	0
1	D	304/308 (98%)	-0.34	6 (1%) 65 63	17, 27, 49, 67	0
All	All	1206/1232 (97%)	-0.31	16 (1%) 77 75	14, 26, 48, 67	0

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	4184	PRO	4.0
1	C	3083	ASN	3.6
1	D	4256	ASP	2.9
1	B	2184	PRO	2.8
1	A	1034	ASP	2.7
1	D	4083	ASN	2.7
1	D	4032	SER	2.7
1	C	3256	ASP	2.6
1	A	1184	PRO	2.6
1	D	4031	LEU	2.5
1	A	1256	ASP	2.3
1	C	3184	PRO	2.3
1	D	4034	ASP	2.3
1	B	2191	VAL	2.2
1	B	2033	GLU	2.1
1	B	2084	GLY	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(\AA^2)	Q<0.9
2	PAU	C	6002	15/15	0.92	0.15	3.11	23,24,26,29	0
2	PAU	B	6003	15/15	0.85	0.18	2.61	30,32,34,35	0
2	PAU	D	6004	15/15	0.88	0.15	2.49	30,32,34,35	0
2	PAU	A	6001	15/15	0.93	0.14	1.47	22,24,29,29	0
3	ADP	C	5003	27/27	0.95	0.13	1.37	21,25,27,31	0
3	ADP	D	5004	27/27	0.96	0.10	-0.40	21,28,33,35	0
3	ADP	B	5002	27/27	0.97	0.09	-0.92	16,21,26,26	0
3	ADP	A	5001	27/27	0.97	0.10	-0.95	15,23,29,31	0

6.5 Other polymers [i](#)

There are no such residues in this entry.