



# Full wwPDB X-ray Structure Validation Report ⓘ

May 23, 2020 – 10:22 pm BST

PDB ID : 6AY1  
Title : Crystal structure of a nucleoside diphosphate kinase NDK from *Helicobacter pylori*  
Authors : Edwards, T.E.; Seattle Structural Genomics Center for Infectious Disease (SS-GCID)  
Deposited on : 2017-09-07  
Resolution : 2.05 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.11
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.11

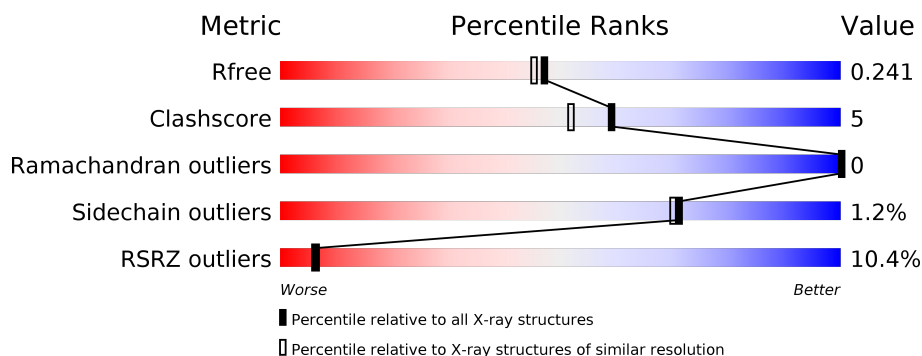
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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))
$R_{free}$	130704	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. 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	145	<div> <div>2%</div> <div> <div></div> <div>86%</div> <div>10%</div> <div>5%</div> </div> </div>
1	B	145	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>•</div> <div>6%</div> </div> </div>
1	C	145	<div> <div>%</div> <div> <div></div> <div>86%</div> <div>8%</div> <div>6%</div> </div> </div>
1	D	145	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>17%</div> <div>6%</div> </div> </div>
1	E	145	<div> <div>11%</div> <div> <div></div> <div>81%</div> <div>11%</div> <div>8%</div> </div> </div>
1	F	145	<div> <div>25%</div> <div> <div></div> <div>62%</div> <div>10%</div> <div>•</div> <div>27%</div> </div> </div>

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Mol	Chain	Length	Quality of chain
1	G	145	<div><div></div><div>34%</div><div></div><div>75%</div><div></div><div>13%</div><div></div><div>11%</div></div>
1	H	145	<div>%<div><div></div><div>82%</div><div></div><div>12%</div><div></div><div>6%</div></div></div>

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8136 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 Nucleoside diphosphate kinase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	138	Total	C	N	O	S	0	0	0
			1055	669	187	195	4			
1	B	137	Total	C	N	O	S	0	1	0
			1062	674	187	197	4			
1	C	137	Total	C	N	O	S	0	1	0
			1049	671	183	191	4			
1	D	137	Total	C	N	O	S	0	1	0
			1037	661	180	192	4			
1	E	134	Total	C	N	O	S	0	0	0
			949	605	164	176	4			
1	F	106	Total	C	N	O	S	0	0	0
			685	427	125	130	3			
1	G	129	Total	C	N	O	S	0	0	0
			888	558	157	169	4			
1	H	137	Total	C	N	O	S	0	1	0
			1044	663	182	195	4			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	expression tag	UNP B5Z9W9
A	-6	ALA	-	expression tag	UNP B5Z9W9
A	-5	HIS	-	expression tag	UNP B5Z9W9
A	-4	HIS	-	expression tag	UNP B5Z9W9
A	-3	HIS	-	expression tag	UNP B5Z9W9
A	-2	HIS	-	expression tag	UNP B5Z9W9
A	-1	HIS	-	expression tag	UNP B5Z9W9
A	0	HIS	-	expression tag	UNP B5Z9W9
B	-7	MET	-	expression tag	UNP B5Z9W9
B	-6	ALA	-	expression tag	UNP B5Z9W9
B	-5	HIS	-	expression tag	UNP B5Z9W9
B	-4	HIS	-	expression tag	UNP B5Z9W9
B	-3	HIS	-	expression tag	UNP B5Z9W9

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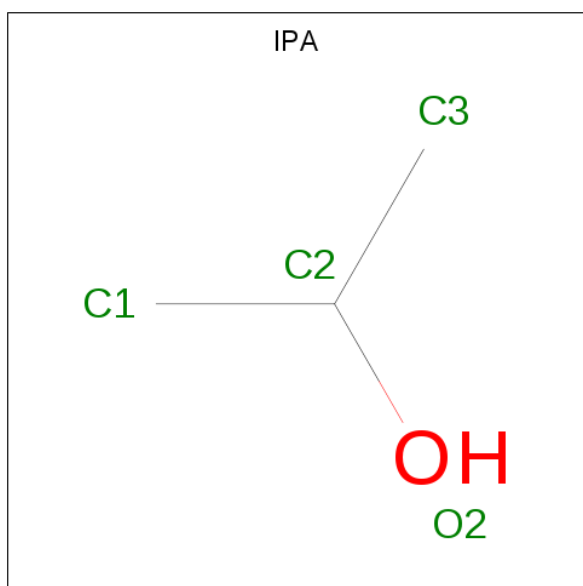
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	HIS	-	expression tag	UNP B5Z9W9
B	-1	HIS	-	expression tag	UNP B5Z9W9
B	0	HIS	-	expression tag	UNP B5Z9W9
C	-7	MET	-	expression tag	UNP B5Z9W9
C	-6	ALA	-	expression tag	UNP B5Z9W9
C	-5	HIS	-	expression tag	UNP B5Z9W9
C	-4	HIS	-	expression tag	UNP B5Z9W9
C	-3	HIS	-	expression tag	UNP B5Z9W9
C	-2	HIS	-	expression tag	UNP B5Z9W9
C	-1	HIS	-	expression tag	UNP B5Z9W9
C	0	HIS	-	expression tag	UNP B5Z9W9
D	-7	MET	-	expression tag	UNP B5Z9W9
D	-6	ALA	-	expression tag	UNP B5Z9W9
D	-5	HIS	-	expression tag	UNP B5Z9W9
D	-4	HIS	-	expression tag	UNP B5Z9W9
D	-3	HIS	-	expression tag	UNP B5Z9W9
D	-2	HIS	-	expression tag	UNP B5Z9W9
D	-1	HIS	-	expression tag	UNP B5Z9W9
D	0	HIS	-	expression tag	UNP B5Z9W9
E	-7	MET	-	expression tag	UNP B5Z9W9
E	-6	ALA	-	expression tag	UNP B5Z9W9
E	-5	HIS	-	expression tag	UNP B5Z9W9
E	-4	HIS	-	expression tag	UNP B5Z9W9
E	-3	HIS	-	expression tag	UNP B5Z9W9
E	-2	HIS	-	expression tag	UNP B5Z9W9
E	-1	HIS	-	expression tag	UNP B5Z9W9
E	0	HIS	-	expression tag	UNP B5Z9W9
F	-7	MET	-	expression tag	UNP B5Z9W9
F	-6	ALA	-	expression tag	UNP B5Z9W9
F	-5	HIS	-	expression tag	UNP B5Z9W9
F	-4	HIS	-	expression tag	UNP B5Z9W9
F	-3	HIS	-	expression tag	UNP B5Z9W9
F	-2	HIS	-	expression tag	UNP B5Z9W9
F	-1	HIS	-	expression tag	UNP B5Z9W9
F	0	HIS	-	expression tag	UNP B5Z9W9
G	-7	MET	-	expression tag	UNP B5Z9W9
G	-6	ALA	-	expression tag	UNP B5Z9W9
G	-5	HIS	-	expression tag	UNP B5Z9W9
G	-4	HIS	-	expression tag	UNP B5Z9W9
G	-3	HIS	-	expression tag	UNP B5Z9W9
G	-2	HIS	-	expression tag	UNP B5Z9W9
G	-1	HIS	-	expression tag	UNP B5Z9W9

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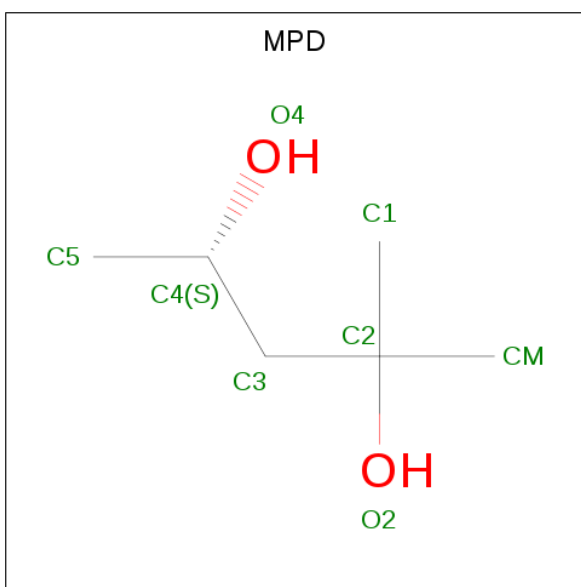
Chain	Residue	Modelled	Actual	Comment	Reference
G	0	HIS	-	expression tag	UNP B5Z9W9
H	-7	MET	-	expression tag	UNP B5Z9W9
H	-6	ALA	-	expression tag	UNP B5Z9W9
H	-5	HIS	-	expression tag	UNP B5Z9W9
H	-4	HIS	-	expression tag	UNP B5Z9W9
H	-3	HIS	-	expression tag	UNP B5Z9W9
H	-2	HIS	-	expression tag	UNP B5Z9W9
H	-1	HIS	-	expression tag	UNP B5Z9W9
H	0	HIS	-	expression tag	UNP B5Z9W9

- Molecule 2 is ISOPROPYL ALCOHOL (three-letter code: IPA) (formula: C<sub>3</sub>H<sub>8</sub>O).



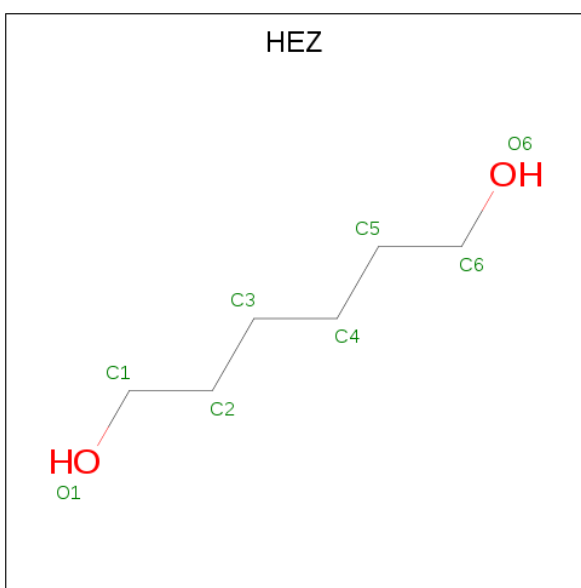
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			4	3	1		
2	B	1	Total	C	O	0	0
			4	3	1		

- Molecule 3 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			8	6	2		
3	D	1	Total	C	O	0	0
			8	6	2		

- Molecule 4 is HEXANE-1,6-DIOL (three-letter code: HEZ) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			8	6	2		
4	H	1	Total	C	O	0	0
			8	6	2		

- Molecule 5 is water.

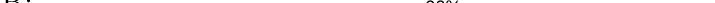
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	75	Total 75	O 75	0	0
5	B	96	Total 96	O 96	0	0
5	C	48	Total 48	O 48	0	0
5	D	42	Total 42	O 42	0	0
5	E	2	Total 2	O 2	0	0
5	G	8	Total 8	O 8	0	0
5	H	56	Total 56	O 56	0	0






- Molecule 1: Nucleoside diphosphate kinase

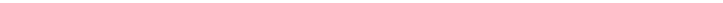


Chain B:  90% 6%




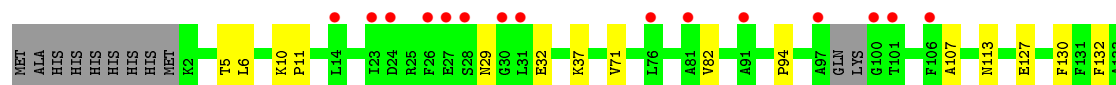
Chain C:  %



Chain D:  78% 17% 6%

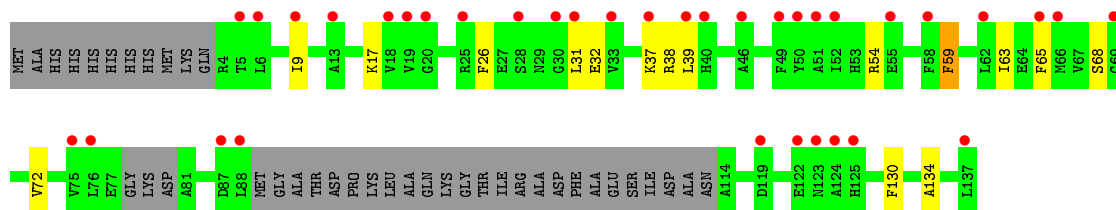


Chain E: 

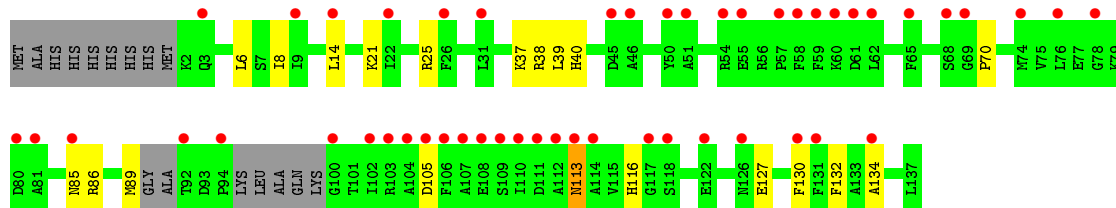
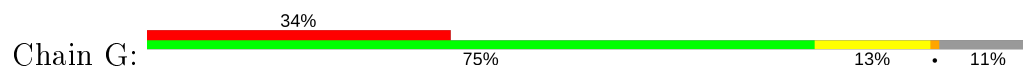




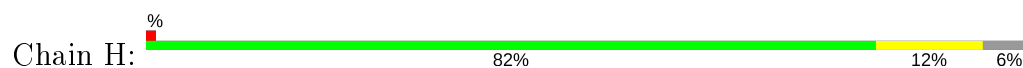
- Molecule 1: Nucleoside diphosphate kinase



- Molecule 1: Nucleoside diphosphate kinase



- Molecule 1: Nucleoside diphosphate kinase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.19 Å 93.40 Å 208.49 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	45.57 – 2.05 46.77 – 2.05	Depositor EDS
% Data completeness (in resolution range)	99.7 (45.57-2.05) 99.8 (46.77-2.05)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.96 (at 2.05 Å)	Xtriage
Refinement program	PHENIX	Depositor
R, $R_{free}$	0.206 , 0.241 0.206 , 0.241	Depositor DCC
$R_{free}$ test set	1998 reflections (2.56%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.5	Xtriage
Anisotropy	0.732	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 64.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.46$ , $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	8136	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.63% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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: MPD, IPA, HEZ

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	0.45	0/1072	0.62	0/1443
1	B	0.51	0/1082	0.64	0/1456
1	C	0.39	0/1069	0.52	0/1438
1	D	0.36	0/1058	0.51	0/1429
1	E	0.29	0/965	0.46	0/1311
1	F	0.27	0/693	0.44	0/941
1	G	0.28	0/899	0.44	0/1219
1	H	0.35	0/1064	0.54	0/1436
All	All	0.38	0/7902	0.53	0/10673

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	1055	0	1046	10	0
1	B	1062	0	1063	4	0
1	C	1049	0	1057	7	0
1	D	1037	0	1014	12	0
1	E	949	0	863	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	F	685	0	545	8	0
1	G	888	0	776	15	0
1	H	1044	0	1026	13	0
2	A	4	0	8	0	0
2	B	4	0	8	0	0
3	B	8	0	14	1	0
3	D	8	0	14	0	0
4	C	8	0	14	1	0
4	H	8	0	14	0	0
5	A	75	0	0	3	0
5	B	96	0	0	0	0
5	C	48	0	0	1	0
5	D	42	0	0	3	0
5	E	2	0	0	0	0
5	G	8	0	0	2	0
5	H	56	0	0	1	0
All	All	8136	0	7462	72	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 5.

All (72) 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:122:GLU:OE1	1:H:3:GLN:NE2	2.18	0.77
1:G:113:ASN:HD22	1:G:113:ASN:H	1.39	0.70
1:A:16:LYS:NZ	5:A:302:HOH:O	2.21	0.69
1:A:136:ASP:OD2	5:A:301:HOH:O	2.15	0.64
1:E:11:PRO:HD3	1:E:71:VAL:HG12	1.81	0.61
1:F:134:ALA:HB3	1:G:130:PHE:HA	1.82	0.61
1:F:130:PHE:HA	1:G:134:ALA:HB3	1.82	0.60
1:A:107:ALA:HB1	1:A:113:ASN:HA	1.84	0.59
1:H:135:ARG:NH2	5:H:303:HOH:O	2.36	0.58
1:D:74:MET:HE3	1:D:76:LEU:HD21	1.86	0.57
1:H:95:LYS:NZ	1:H:108:GLU:O	2.39	0.56
1:A:119:ASP:OD1	1:A:123:ASN:ND2	2.38	0.54
1:E:130:PHE:HA	1:H:134:ALA:HB3	1.90	0.54
1:F:9:ILE:HB	1:F:72:VAL:HB	1.91	0.53
1:D:119:ASP:OD1	1:D:123:ASN:ND2	2.38	0.52
1:C:37:LYS:HE2	1:C:132:PHE:CE1	2.45	0.52
1:D:25:ARG:NH2	1:D:105:ASP:OD2	2.37	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:37:LYS:HG3	1:F:39:LEU:HD23	1.92	0.51
1:D:37:LYS:HG3	1:D:39:LEU:HD23	1.91	0.51
1:G:8:ILE:HB	1:G:116:HIS:HB3	1.92	0.51
1:E:6:LEU:HD22	1:E:127:GLU:HB3	1.93	0.51
1:E:32:GLU:HB2	1:F:17:LYS:HE3	1.94	0.49
1:F:26:PHE:O	1:F:31:LEU:HB2	2.12	0.49
1:B:6:LEU:HD22	1:B:127:GLU:HB3	1.93	0.49
1:G:6:LEU:HD22	1:G:127:GLU:HB3	1.93	0.49
1:H:11:PRO:HD3	1:H:71:VAL:HG12	1.95	0.49
1:B:134:ALA:HB3	1:C:130:PHE:HA	1.94	0.49
1:E:107:ALA:HB1	1:E:113:ASN:HA	1.96	0.48
1:B:37:LYS:HE2	1:B:132:PHE:CE1	2.49	0.48
1:G:37:LYS:HG3	1:G:39:LEU:HD23	1.96	0.47
1:C:50:TYR:HE2	1:C:66:MET:HG3	1.80	0.47
1:E:94:PRO:HB3	1:E:107:ALA:HB3	1.97	0.47
1:G:37:LYS:HE3	1:G:132:PHE:CE1	2.50	0.47
1:C:11:PRO:HD3	1:C:71:VAL:HG12	1.97	0.46
1:D:3:GLN:HG3	1:D:81:ALA:HB3	1.96	0.46
1:D:135:ARG:HD3	5:D:305:HOH:O	2.15	0.46
1:E:37:LYS:HE3	1:E:132:PHE:CE1	2.51	0.46
1:H:10:LYS:HB3	1:H:11:PRO:HD2	1.97	0.46
1:H:8:ILE:HB	1:H:116:HIS:HB3	1.97	0.46
1:C:10:LYS:HB3	1:C:11:PRO:HD2	1.98	0.46
1:A:135:ARG:HD3	5:D:327:HOH:O	2.17	0.45
1:D:8:ILE:HB	1:D:116:HIS:HB3	1.98	0.45
1:G:38:ARG:NH2	5:G:201:HOH:O	2.22	0.45
1:G:113:ASN:H	1:G:113:ASN:ND2	2.12	0.45
4:C:201:HEZ:H21	4:C:201:HEZ:H51	1.57	0.45
1:G:85:ASN:O	1:G:89:MET:HG3	2.16	0.45
1:F:65:PHE:O	1:F:68:SER:OG	2.23	0.45
1:G:40:HIS:HB2	5:G:207:HOH:O	2.18	0.44
1:G:21:LYS:NZ	1:H:24:ASP:OD1	2.48	0.44
1:H:12:ASP:N	1:H:12:ASP:OD1	2.51	0.44
1:E:10:LYS:HB3	1:E:11:PRO:HD2	1.99	0.44
1:E:134:ALA:HB3	1:H:130:PHE:HA	2.00	0.43
1:A:130:PHE:HA	1:D:134:ALA:HB3	2.00	0.43
1:G:86:ARG:HA	1:G:89:MET:HE2	2.01	0.43
1:B:135:ARG:HD3	5:C:314:HOH:O	2.18	0.43
1:H:3:GLN:O	1:H:77:GLU:HA	2.20	0.42
1:H:14:LEU:HD11	1:H:72:VAL:HG23	2.01	0.42
1:D:85:ASN:O	1:D:89:MET:HG3	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:5:THR:HB	1:E:82:VAL:HG22	2.02	0.42
1:C:14:LEU:HD22	1:C:70:PRO:O	2.20	0.42
1:D:136:ASP:OD2	5:D:301:HOH:O	2.22	0.42
1:H:107:ALA:HB1	1:H:113:ASN:HA	2.02	0.41
1:D:11:PRO:O	1:D:15:LYS:HG3	2.20	0.41
1:A:15:LYS:NZ	5:A:311:HOH:O	2.53	0.41
1:G:14:LEU:HD22	1:G:70:PRO:O	2.21	0.41
1:A:8:ILE:HB	1:A:116:HIS:HB3	2.03	0.41
1:A:11:PRO:HD3	1:A:71:VAL:HG12	2.02	0.41
1:F:54:ARG:HA	1:F:59:PHE:CZ	2.55	0.41
1:G:25:ARG:NH2	1:G:105:ASP:OD2	2.32	0.41
1:C:6:LEU:HD22	1:C:127:GLU:HB3	2.03	0.41
1:D:107:ALA:HB1	1:D:113:ASN:HA	2.01	0.40
3:B:202:MPD:H11	3:B:202:MPD:H4	1.92	0.40

There are no symmetry-related clashes.

## 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	136/145 (94%)	134 (98%)	2 (2%)	0	100	100
1	B	136/145 (94%)	134 (98%)	2 (2%)	0	100	100
1	C	136/145 (94%)	135 (99%)	1 (1%)	0	100	100
1	D	136/145 (94%)	135 (99%)	1 (1%)	0	100	100
1	E	130/145 (90%)	129 (99%)	1 (1%)	0	100	100
1	F	100/145 (69%)	97 (97%)	3 (3%)	0	100	100
1	G	123/145 (85%)	122 (99%)	1 (1%)	0	100	100
1	H	136/145 (94%)	135 (99%)	1 (1%)	0	100	100
All	All	1033/1160 (89%)	1021 (99%)	12 (1%)	0	100	100

There are no Ramachandran outliers to report.

### 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	107/121 (88%)	107 (100%)	0	100	100
1	B	110/121 (91%)	110 (100%)	0	100	100
1	C	107/121 (88%)	107 (100%)	0	100	100
1	D	104/121 (86%)	101 (97%)	3 (3%)	42	35
1	E	85/121 (70%)	84 (99%)	1 (1%)	71	70
1	F	47/121 (39%)	43 (92%)	4 (8%)	10	4
1	G	75/121 (62%)	74 (99%)	1 (1%)	69	67
1	H	106/121 (88%)	106 (100%)	0	100	100
All	All	741/968 (76%)	732 (99%)	9 (1%)	71	70

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	80	ASP
1	D	86	ARG
1	D	110	ILE
1	E	29	ASN
1	F	32	GLU
1	F	38	ARG
1	F	59	PHE
1	F	63	ILE
1	G	113	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	113	ASN



### 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 ⓘ

6 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	MPD	B	202	-	7,7,7	0.32	0	9,10,10	0.31	0
4	HEZ	H	201	-	7,7,7	0.38	0	6,6,6	0.53	0
3	MPD	D	201	-	7,7,7	0.24	0	9,10,10	0.38	0
2	IPA	A	201	-	3,3,3	0.61	0	3,3,3	0.23	0
4	HEZ	C	201	-	7,7,7	0.35	0	6,6,6	0.55	0
2	IPA	B	201	-	3,3,3	0.50	0	3,3,3	0.44	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	MPD	B	202	-	-	1/5/5/5	-
4	HEZ	H	201	-	-	2/5/5/5	-
4	HEZ	C	201	-	-	3/5/5/5	-
3	MPD	D	201	-	-	4/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	201	HEZ	O1-C1-C2-C3
4	C	201	HEZ	C3-C4-C5-C6
4	H	201	HEZ	C1-C2-C3-C4
4	H	201	HEZ	C4-C5-C6-O6
4	C	201	HEZ	C2-C3-C4-C5
3	D	201	MPD	C2-C3-C4-C5
3	D	201	MPD	C1-C2-C3-C4
3	D	201	MPD	O2-C2-C3-C4
3	B	202	MPD	C2-C3-C4-C5
3	D	201	MPD	C2-C3-C4-O4

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	202	MPD	1	0
4	C	201	HEZ	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 ⓘ

### 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, 95<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	138/145 (95%)	0.49	3 (2%) 62 66	26, 38, 69, 118	0
1	B	137/145 (94%)	0.25	1 (0%) 87 89	27, 37, 62, 82	0
1	C	137/145 (94%)	0.12	1 (0%) 87 89	36, 49, 82, 115	0
1	D	137/145 (94%)	0.11	1 (0%) 87 89	34, 54, 89, 111	0
1	E	134/145 (92%)	0.71	16 (11%) 4 4	48, 82, 109, 123	0
1	F	106/145 (73%)	1.55	36 (33%) 0 0	87, 107, 131, 139	0
1	G	129/145 (88%)	1.79	50 (38%) 0 0	70, 93, 123, 149	0
1	H	137/145 (94%)	0.27	2 (1%) 73 76	33, 54, 74, 88	0
All	All	1055/1160 (90%)	0.63	110 (10%) 6 6	26, 59, 114, 149	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	112	ALA	8.4
1	G	81	ALA	6.8
1	G	78	GLY	6.8
1	E	106	PHE	6.2
1	G	107	ALA	6.0
1	G	106	PHE	5.9
1	G	113	ASN	5.3
1	G	108	GLU	5.3
1	G	109	SER	5.2
1	G	55	GLU	5.0
1	F	124	ALA	4.6
1	G	58	PHE	4.5
1	F	52	ILE	4.4
1	E	31	LEU	4.3
1	E	28	SER	4.3
1	E	97	ALA	4.2

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Mol	Chain	Res	Type	RSRZ
1	F	62	LEU	4.1
1	F	65	PHE	4.0
1	G	59	PHE	4.0
1	F	5	THR	4.0
1	G	105	ASP	4.0
1	G	111	ASP	4.0
1	G	57	PRO	3.9
1	G	26	PHE	3.8
1	F	49	PHE	3.8
1	G	74	MET	3.7
1	F	76	LEU	3.7
1	E	23	ILE	3.7
1	G	9	ILE	3.6
1	F	13	ALA	3.6
1	G	117	GLY	3.6
1	G	114	ALA	3.5
1	D	1	MET	3.5
1	E	30	GLY	3.5
1	G	85	ASN	3.3
1	F	75	VAL	3.3
1	E	100	GLY	3.2
1	G	104	ALA	3.2
1	G	100	GLY	3.2
1	G	134	ALA	3.2
1	F	51	ALA	3.1
1	A	0	HIS	3.1
1	G	80	ASP	3.0
1	E	81	ALA	3.0
1	F	28	SER	2.9
1	G	126	ASN	2.9
1	G	65	PHE	2.9
1	G	103	ARG	2.9
1	E	24	ASP	2.9
1	G	31	LEU	2.9
1	G	69	GLY	2.8
1	F	31	LEU	2.8
1	F	9	ILE	2.8
1	E	76	LEU	2.8
1	G	62	LEU	2.8
1	E	27	GLU	2.8
1	F	18	VAL	2.8
1	G	94	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	119	ASP	2.7
1	F	55	GLU	2.7
1	F	40	HIS	2.7
1	E	137	LEU	2.7
1	F	123	ASN	2.7
1	G	45	ASP	2.6
1	G	68	SER	2.6
1	F	33	VAL	2.6
1	G	61	ASP	2.6
1	F	66	MET	2.6
1	F	125	HIS	2.6
1	G	92	THR	2.6
1	F	46	ALA	2.5
1	F	20	GLY	2.5
1	G	60	LYS	2.5
1	F	69	GLY	2.4
1	G	110	ILE	2.4
1	G	131	PHE	2.4
1	G	102	ILE	2.4
1	H	1	MET	2.4
1	F	39	LEU	2.4
1	E	101	THR	2.4
1	E	26	PHE	2.3
1	B	12[A]	ASP	2.3
1	F	50	TYR	2.3
1	F	6	LEU	2.3
1	G	22	ILE	2.3
1	G	14	LEU	2.3
1	G	3	GLN	2.3
1	G	46	ALA	2.3
1	G	118	SER	2.3
1	A	52	ILE	2.2
1	G	51	ALA	2.2
1	F	137	LEU	2.2
1	F	58	PHE	2.2
1	F	122	GLU	2.2
1	G	76	LEU	2.2
1	G	122	GLU	2.2
1	F	30	GLY	2.2
1	F	87	ASP	2.1
1	G	130	PHE	2.1
1	F	37	LYS	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	58	PHE	2.1
1	H	52	ILE	2.1
1	E	14	LEU	2.1
1	G	50	TYR	2.1
1	F	88	LEU	2.0
1	F	19	VAL	2.0
1	A	50	TYR	2.0
1	F	25	ARG	2.0
1	G	54	ARG	2.0
1	E	91	ALA	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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	B-factors(Å <sup>2</sup> )	Q<0.9
4	HEZ	C	201	8/8	0.55	0.17	77,79,83,85	0
4	HEZ	H	201	8/8	0.73	0.17	53,64,69,71	0
2	IPA	A	201	4/4	0.75	0.22	52,54,55,55	0
2	IPA	B	201	4/4	0.76	0.20	62,68,68,73	0
3	MPD	B	202	8/8	0.79	0.22	62,70,75,79	0
3	MPD	D	201	8/8	0.90	0.09	66,76,82,84	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.