



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 6, 2020 – 01:07 PM BST

PDB ID : 1LDP  
Title : CRYSTAL STRUCTURE OF MURINE MHC CLASS I H-2LD WITH A MIX-  
TURE OF BOUND PEPTIDES  
Authors : Speir, J.A.; Wilson, I.A.  
Deposited on : 1998-03-15  
Resolution : 3.10 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) : **NOT EXECUTED**  
EDS : **NOT EXECUTED**  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

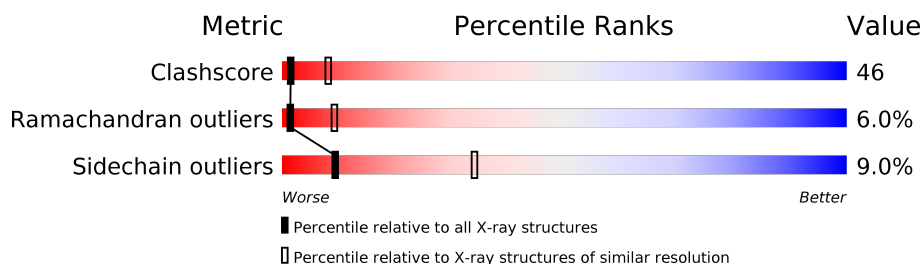
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 3.10 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))
Clashscore	141614	1184 (3.10-3.10)
Ramachandran outliers	138981	1141 (3.10-3.10)
Sidechain outliers	138945	1141 (3.10-3.10)

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  $\leq 5\%$ .

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	H	272	
2	L	99	
3	P	9	
4	Q	9	
5	A	2	

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
5	NAG	A	1	X	-	-	-
6	NAG	H	273	X	-	-	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3205 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 MHC CLASS I H-2LD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	H	272	Total	C	N	O	S	0	0	0
			2215	1402	385	418	10			

- Molecule 2 is a protein called MHC CLASS I H-2LD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	L	99	Total	C	N	O	S	0	0	0
			821	524	138	152	7			

- Molecule 3 is a protein called PEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	P	9	Total	C	N	O	S	0	0	0
			51	31	9	10	1			

- Molecule 4 is a protein called PEPTIDE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	Q	9	Total	C	N	O		0	0	0
			76	52	10	14				

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-alpha-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
5	A	2	Total	C	N	O		0	0	0
			28	16	2	10				

- Molecule 6 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



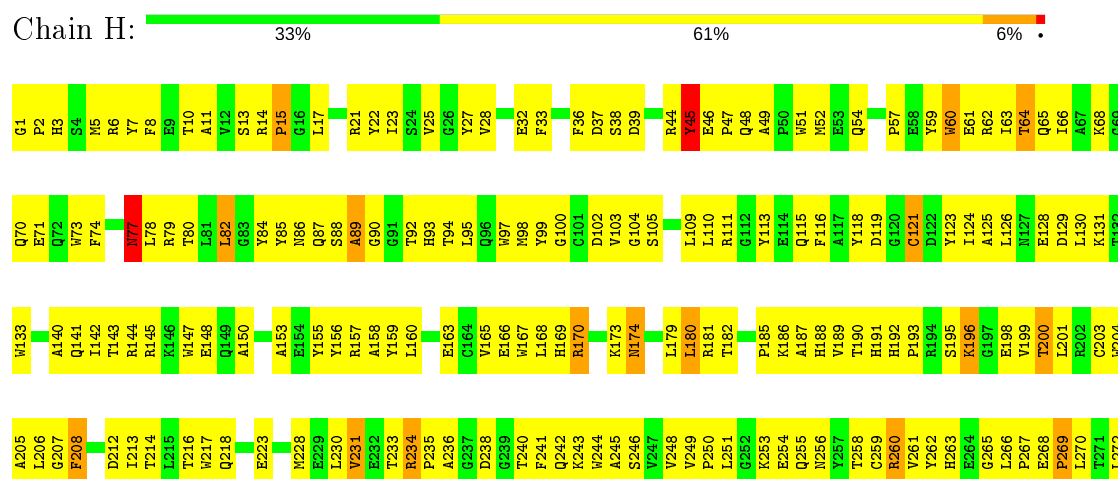
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
6	H	1	14	8	1	5	0	0

### 3 Residue-property plots

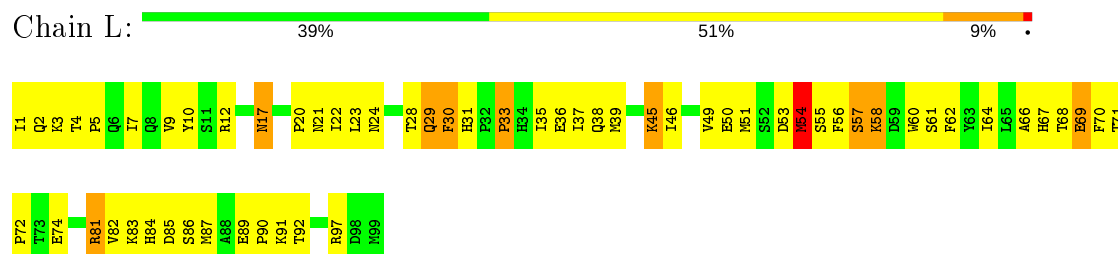
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded 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. 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.

Note EDS was not executed.

#### • Molecule 1: MHC CLASS I H-2LD



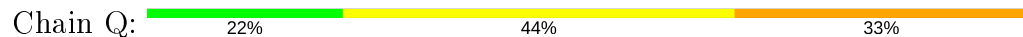
#### • Molecule 2: MHC CLASS I H-2LD



#### • Molecule 3: PEPTIDE



#### • Molecule 4: PEPTIDE



Q1	L2	S3	P4	F5	P6	F7	D8	L9
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- Molecule 5: 2-acetamido-2-deoxy- $\alpha$ -D-glucopyranose-(1-4)-2-acetamido-2-deoxy- $\beta$ -D-glucopyranose

Chain A: 

MAC1	MD2
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## 4 Data and refinement statistics

Xtriage (Phenix) and EDS were not executed - this section is therefore incomplete.

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	72.40 Å 48.98 Å 84.06 Å 90.00° 97.95° 90.00°	Depositor
Resolution (Å)	6.00 – 3.10	Depositor
% Data completeness (in resolution range)	85.0 (6.00-3.10)	Depositor
$R_{merge}$	0.11	Depositor
$R_{sym}$	0.11	Depositor
Refinement program	X-PLOR 3.825	Depositor
R, $R_{free}$	0.221 , 0.371	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3205	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP



## 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: NAG, NDG

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	H	0.69	0/2280	0.89	2/3100 (0.1%)
2	L	0.66	0/847	0.84	0/1148
3	P	0.79	0/51	0.86	0/68
4	Q	0.80	0/79	0.82	0/106
All	All	0.69	0/3257	0.87	2/4422 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	45	TYR	CA-CB-CG	5.47	123.80	113.40
1	H	82	LEU	CA-CB-CG	5.09	127.00	115.30

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	H	2215	0	2079	219	0
2	L	821	0	796	65	0
3	P	51	0	50	16	0
4	Q	76	0	69	49	0
5	A	28	0	24	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	H	14	0	13	2	0
All	All	3205	0	3031	288	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 46.

All (288) 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:H:62:ARG:NH2	4:Q:1:GLN:OE1	1.84	1.09
1:H:156:TYR:OH	4:Q:5:PHE:CZ	2.08	1.06
1:H:73:TRP:CZ2	4:Q:5:PHE:HD2	1.75	1.04
3:P:5:ALA:HB2	4:Q:5:PHE:CD1	1.29	1.00
3:P:5:ALA:HB1	4:Q:5:PHE:CD2	1.03	0.99
1:H:73:TRP:CZ2	4:Q:5:PHE:CD2	2.50	0.99
2:L:49:VAL:HG12	2:L:50:GLU:H	1.28	0.98
1:H:187:ALA:HB1	1:H:272:LEU:HD11	1.46	0.96
2:L:12:ARG:HE	2:L:22:ILE:HD12	1.34	0.91
2:L:23:LEU:HB2	2:L:70:PHE:CD1	2.06	0.90
1:H:156:TYR:CZ	4:Q:5:PHE:CZ	2.58	0.90
1:H:111:ARG:HH21	1:H:128:GLU:HG3	1.37	0.89
1:H:123:TYR:HD1	1:H:124:ILE:HG22	1.39	0.88
1:H:45:TYR:OH	4:Q:2:LEU:HD13	1.72	0.87
3:P:2:PRO:HD3	4:Q:1:GLN:H2	1.41	0.84
1:H:156:TYR:CE1	4:Q:5:PHE:CE1	2.65	0.83
1:H:170:ARG:HH11	1:H:170:ARG:HG3	1.44	0.83
1:H:191:HIS:HB2	1:H:199:VAL:HG12	1.60	0.83
1:H:190:THR:O	1:H:201:LEU:HA	1.80	0.82
1:H:5:MET:HB2	1:H:168:LEU:HD13	1.62	0.81
1:H:49:ALA:HB1	1:H:51:TRP:NE1	1.94	0.81
1:H:73:TRP:CE2	4:Q:5:PHE:HD2	1.99	0.80
1:H:191:HIS:HB2	1:H:199:VAL:CG1	2.11	0.80
2:L:12:ARG:NE	2:L:22:ILE:HD12	1.95	0.80
1:H:143:THR:HG21	4:Q:9:LEU:HD12	1.64	0.80
2:L:21:ASN:HB3	2:L:70:PHE:CE1	2.17	0.79
1:H:62:ARG:NH2	4:Q:1:GLN:CD	2.35	0.79
1:H:47:PRO:HG3	1:H:60:TRP:CZ2	2.18	0.78
1:H:82:LEU:HG	1:H:93:HIS:HE1	1.48	0.78
2:L:36:GLU:HB3	2:L:83:LYS:HB2	1.67	0.77
1:H:214:THR:HB	1:H:262:TYR:HB2	1.67	0.76
1:H:131:LYS:HA	1:H:153:ALA:HB1	1.67	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:170:ARG:O	1:H:174:ASN:ND2	2.19	0.74
1:H:185:PRO:HD2	1:H:266:LEU:HD21	1.69	0.73
1:H:234:ARG:NE	1:H:242:GLN:HG3	2.03	0.73
1:H:47:PRO:HG3	1:H:60:TRP:HZ2	1.52	0.71
1:H:60:TRP:HA	1:H:60:TRP:CE3	2.25	0.71
1:H:228:MET:HA	1:H:246:SER:O	1.91	0.71
1:H:187:ALA:CB	1:H:272:LEU:HD11	2.20	0.70
1:H:74:PHE:CE1	1:H:95:LEU:HD22	2.27	0.70
1:H:28:VAL:HG23	1:H:28:VAL:O	1.91	0.70
3:P:9:MET:OXT	4:Q:9:LEU:HG	1.91	0.70
1:H:73:TRP:O	1:H:77:ASN:HB2	1.92	0.70
1:H:123:TYR:O	1:H:140:ALA:HB1	1.92	0.70
1:H:116:PHE:HZ	4:Q:5:PHE:CZ	2.10	0.69
1:H:233:THR:HG23	1:H:243:LYS:HE2	1.74	0.69
1:H:74:PHE:HE1	1:H:95:LEU:HD22	1.56	0.68
1:H:250:PRO:HD2	1:H:253:LYS:HE2	1.76	0.68
3:P:9:MET:OXT	4:Q:9:LEU:CG	2.38	0.68
1:H:10:THR:HG21	2:L:62:PHE:CE2	2.29	0.67
2:L:30:PHE:CE2	2:L:35:ILE:HG21	2.30	0.67
1:H:60:TRP:HE3	1:H:60:TRP:HA	1.60	0.66
2:L:4:THR:HG23	2:L:5:PRO:HD2	1.76	0.66
1:H:156:TYR:CZ	4:Q:5:PHE:CE1	2.83	0.66
2:L:2:GLN:HB3	2:L:86:SER:HB3	1.76	0.66
1:H:206:LEU:HD22	1:H:242:GLN:NE2	2.11	0.66
1:H:234:ARG:HD3	1:H:234:ARG:O	1.96	0.65
2:L:70:PHE:CE2	2:L:72:PRO:HD3	2.31	0.65
1:H:45:TYR:OH	4:Q:2:LEU:CD1	2.44	0.65
1:H:156:TYR:OH	4:Q:5:PHE:CE2	2.42	0.65
2:L:83:LYS:HG2	2:L:90:PRO:HB3	1.77	0.65
1:H:192:HIS:HB2	1:H:200:THR:OG1	1.97	0.64
1:H:63:ILE:HG23	4:Q:2:LEU:HD21	1.80	0.64
1:H:14:ARG:HB3	1:H:17:LEU:HB2	1.80	0.64
1:H:198:GLU:HA	1:H:250:PRO:HA	1.79	0.64
1:H:198:GLU:HG2	1:H:250:PRO:HG3	1.79	0.64
1:H:111:ARG:NH2	1:H:128:GLU:HG3	2.11	0.64
1:H:6:ARG:HD3	1:H:113:TYR:OH	1.98	0.63
1:H:82:LEU:HG	1:H:93:HIS:CE1	2.32	0.63
1:H:218:GLN:OE1	1:H:223:GLU:HB3	1.99	0.62
1:H:170:ARG:HG3	1:H:170:ARG:NH1	2.08	0.62
1:H:174:ASN:H	1:H:174:ASN:HD22	1.47	0.61
1:H:217:TRP:HE3	1:H:258:THR:O	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:155:TYR:OH	4:Q:6:PRO:HD3	2.00	0.61
1:H:191:HIS:HA	1:H:200:THR:O	2.00	0.61
1:H:68:LYS:O	1:H:71:GLU:HB3	1.99	0.61
1:H:73:TRP:CZ2	4:Q:5:PHE:CE2	2.87	0.61
1:H:124:ILE:HD11	1:H:133:TRP:CE3	2.36	0.61
1:H:2:PRO:HD3	1:H:105:SER:OG	2.01	0.60
1:H:109:LEU:HD12	1:H:110:LEU:H	1.67	0.60
1:H:187:ALA:HB1	1:H:272:LEU:CD1	2.29	0.59
2:L:89:GLU:HB3	2:L:90:PRO:HD2	1.85	0.59
1:H:249:VAL:HG23	1:H:253:LYS:HE3	1.84	0.58
1:H:8:PHE:CE2	1:H:98:MET:SD	2.96	0.58
2:L:24:ASN:OD1	2:L:67:HIS:HB3	2.02	0.58
2:L:49:VAL:HG12	2:L:50:GLU:N	2.09	0.58
1:H:77:ASN:ND2	4:Q:9:LEU:HB3	2.17	0.58
1:H:250:PRO:HD2	1:H:253:LYS:CE	2.33	0.58
1:H:130:LEU:HB2	1:H:157:ARG:HD3	1.84	0.58
1:H:47:PRO:HB3	1:H:52:MET:HB3	1.86	0.57
1:H:163:GLU:HA	1:H:166:GLU:HB2	1.86	0.57
2:L:28:THR:O	2:L:29:GLN:HB2	2.05	0.57
3:P:2:PRO:HD3	4:Q:1:GLN:N	2.10	0.57
1:H:188:HIS:ND1	1:H:204:TRP:HB2	2.20	0.57
1:H:238:ASP:HB3	2:L:12:ARG:HH12	1.70	0.57
1:H:236:ALA:HB3	1:H:240:THR:O	2.05	0.57
1:H:21:ARG:CZ	1:H:23:ILE:HD11	2.34	0.56
1:H:144:ARG:HH21	1:H:145:ARG:HD3	1.70	0.56
1:H:192:HIS:HB2	1:H:200:THR:HG1	1.70	0.56
1:H:2:PRO:HG3	1:H:105:SER:H	1.70	0.56
1:H:126:LEU:HD21	1:H:130:LEU:HA	1.86	0.56
1:H:8:PHE:CZ	1:H:98:MET:SD	2.99	0.56
1:H:208:PHE:HE1	1:H:241:PHE:HB2	1.70	0.56
2:L:49:VAL:CG1	2:L:50:GLU:H	2.09	0.56
1:H:45:TYR:CZ	4:Q:2:LEU:HD22	2.41	0.56
1:H:21:ARG:NH1	1:H:23:ILE:HD11	2.21	0.55
1:H:155:TYR:CD2	4:Q:7:PHE:CE2	2.94	0.55
1:H:57:PRO:O	1:H:61:GLU:HG2	2.06	0.55
1:H:82:LEU:CD2	1:H:89:ALA:HA	2.37	0.55
2:L:38:GLN:HB3	2:L:81:ARG:HB3	1.88	0.55
2:L:46:ILE:HD12	2:L:68:THR:HG21	1.86	0.55
2:L:33:PRO:HG3	2:L:62:PHE:CG	2.41	0.55
1:H:51:TRP:CZ2	1:H:179:LEU:HD21	2.42	0.55
2:L:39:MET:CE	2:L:68:THR:HG22	2.37	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:155:TYR:CD2	4:Q:7:PHE:HE2	2.25	0.55
1:H:45:TYR:HH	4:Q:2:LEU:HD13	1.70	0.55
1:H:217:TRP:HD1	1:H:228:MET:HB3	1.72	0.55
1:H:216:THR:HA	1:H:228:MET:CE	2.37	0.54
1:H:150:ALA:HB1	4:Q:7:PHE:HE1	1.72	0.54
2:L:37:ILE:HD13	2:L:82:VAL:HB	1.87	0.54
1:H:104:GLY:HA3	1:H:110:LEU:HD21	1.90	0.54
2:L:56:PHE:HD1	2:L:57:SER:O	1.91	0.54
3:P:9:MET:O	4:Q:9:LEU:O	0.54	0.54
1:H:207:GLY:HA2	1:H:240:THR:HB	1.89	0.54
1:H:77:ASN:O	1:H:79:ARG:N	2.41	0.54
2:L:23:LEU:HB2	2:L:70:PHE:CG	2.43	0.53
1:H:27:TYR:CE1	1:H:32:GLU:HB2	2.43	0.53
1:H:7:TYR:OH	3:P:2:PRO:HD3	2.08	0.53
2:L:17:ASN:HA	2:L:72:PRO:HG2	1.91	0.53
2:L:30:PHE:CE1	2:L:62:PHE:O	2.61	0.53
2:L:3:LYS:HB3	2:L:29:GLN:O	2.09	0.53
5:A:2:NDG:O7	5:A:2:NDG:H3	2.07	0.53
1:H:49:ALA:HB1	1:H:51:TRP:CD1	2.43	0.52
1:H:186:LYS:O	1:H:186:LYS:HG3	2.09	0.52
1:H:70:GLN:NE2	4:Q:3:SER:O	2.42	0.52
1:H:93:HIS:O	1:H:94:THR:HG23	2.09	0.52
1:H:244:TRP:HZ3	1:H:246:SER:HB2	1.73	0.52
1:H:259:CYS:SG	1:H:260:ARG:N	2.83	0.52
2:L:87:MET:SD	2:L:91:LYS:HG3	2.49	0.52
1:H:203:CYS:HB3	1:H:245:ALA:HB3	1.92	0.52
1:H:123:TYR:CD1	1:H:124:ILE:HG22	2.31	0.51
1:H:7:TYR:CZ	3:P:2:PRO:HG3	2.45	0.51
1:H:262:TYR:CE1	1:H:269:PRO:HB3	2.45	0.51
2:L:30:PHE:CD2	2:L:35:ILE:HD12	2.45	0.51
1:H:10:THR:HG21	2:L:62:PHE:HE2	1.74	0.51
1:H:150:ALA:HB1	4:Q:7:PHE:CE1	2.45	0.51
1:H:205:ALA:O	1:H:206:LEU:HD23	2.10	0.51
1:H:233:THR:CG2	1:H:243:LYS:HE2	2.38	0.51
2:L:39:MET:HE1	2:L:67:HIS:HA	1.93	0.51
1:H:180:LEU:N	1:H:180:LEU:HD23	2.25	0.51
1:H:187:ALA:HB2	1:H:270:LEU:HD21	1.94	0.50
1:H:238:ASP:H	2:L:12:ARG:NH1	2.09	0.50
1:H:70:GLN:NE2	3:P:4:ALA:HA	2.26	0.50
1:H:208:PHE:CE1	1:H:241:PHE:HB2	2.46	0.50
1:H:70:GLN:NE2	3:P:3:ALA:O	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:5:MET:O	1:H:100:GLY:HA3	2.12	0.50
1:H:62:ARG:NH2	4:Q:1:GLN:NE2	2.60	0.50
1:H:121:CYS:SG	2:L:1:ILE:HD12	2.51	0.50
1:H:188:HIS:HB3	1:H:204:TRP:O	2.11	0.50
1:H:217:TRP:CE3	1:H:258:THR:O	2.63	0.50
1:H:218:GLN:HB2	1:H:258:THR:OG1	2.12	0.50
1:H:141:GLN:HB3	1:H:144:ARG:CZ	2.41	0.49
1:H:13:SER:C	1:H:15:PRO:HD3	2.33	0.49
2:L:39:MET:HE3	2:L:68:THR:HG22	1.94	0.49
1:H:201:LEU:HB3	1:H:217:TRP:CH2	2.46	0.49
1:H:95:LEU:HD21	3:P:9:MET:SD	2.52	0.49
2:L:55:SER:OG	2:L:56:PHE:N	2.44	0.49
1:H:73:TRP:CH2	4:Q:5:PHE:CD2	3.00	0.49
1:H:103:VAL:HG11	1:H:165:VAL:HG13	1.94	0.49
1:H:116:PHE:CZ	4:Q:5:PHE:CZ	2.95	0.49
1:H:97:TRP:CZ2	4:Q:5:PHE:CE1	3.01	0.49
1:H:10:THR:HG21	2:L:62:PHE:CZ	2.48	0.49
1:H:5:MET:CB	1:H:168:LEU:HD13	2.39	0.49
2:L:54:MET:O	2:L:54:MET:HG3	2.13	0.49
6:H:273:NAG:C3	6:H:273:NAG:O7	2.60	0.48
1:H:251:LEU:HD12	1:H:251:LEU:H	1.78	0.48
1:H:6:ARG:HA	1:H:99:TYR:O	2.13	0.48
2:L:28:THR:HG22	2:L:29:GLN:OE1	2.13	0.48
3:P:8:ALA:C	4:Q:7:PHE:O	2.48	0.48
2:L:30:PHE:CZ	2:L:35:ILE:HG21	2.49	0.48
2:L:33:PRO:HG3	2:L:62:PHE:CD2	2.49	0.48
1:H:129:ASP:O	1:H:131:LYS:HG3	2.14	0.47
1:H:45:TYR:OH	4:Q:2:LEU:HD22	2.14	0.47
2:L:53:ASP:O	2:L:55:SER:N	2.47	0.47
1:H:167:TRP:CD1	4:Q:1:GLN:HG2	2.49	0.47
1:H:204:TRP:CE3	1:H:206:LEU:HD21	2.49	0.47
1:H:267:PRO:O	1:H:268:GLU:HG3	2.14	0.47
2:L:30:PHE:HE1	2:L:62:PHE:HB2	1.79	0.47
2:L:4:THR:CG2	2:L:5:PRO:HD2	2.42	0.47
1:H:261:VAL:HG13	1:H:270:LEU:HB3	1.96	0.47
1:H:203:CYS:HB2	1:H:217:TRP:CZ2	2.49	0.47
2:L:17:ASN:H	2:L:17:ASN:ND2	2.13	0.47
1:H:59:TYR:CZ	1:H:63:ILE:HD11	2.50	0.47
1:H:11:ALA:O	1:H:94:THR:HA	2.15	0.47
2:L:30:PHE:CE1	2:L:62:PHE:HB2	2.50	0.47
1:H:181:ARG:HD2	1:H:181:ARG:HA	1.70	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:62:ARG:HH22	4:Q:1:GLN:CD	2.17	0.46
1:H:231:VAL:CG2	1:H:244:TRP:H	2.27	0.46
1:H:124:ILE:HG12	1:H:125:ALA:N	2.31	0.46
1:H:116:PHE:CZ	4:Q:5:PHE:CE2	3.04	0.46
1:H:109:LEU:HD12	1:H:110:LEU:N	2.28	0.46
1:H:150:ALA:CB	4:Q:7:PHE:CE1	2.98	0.46
1:H:181:ARG:HH11	1:H:182:THR:H	1.64	0.46
1:H:13:SER:HB2	1:H:93:HIS:H	1.80	0.46
2:L:58:LYS:C	2:L:60:TRP:H	2.19	0.46
1:H:14:ARG:HD3	1:H:17:LEU:HD12	1.98	0.46
2:L:84:HIS:ND1	2:L:86:SER:OG	2.46	0.46
1:H:208:PHE:HE2	1:H:213:ILE:HD13	1.81	0.46
1:H:236:ALA:H	1:H:241:PHE:HA	1.80	0.46
1:H:73:TRP:CD1	4:Q:5:PHE:O	2.69	0.46
1:H:121:CYS:SG	2:L:1:ILE:CD1	3.03	0.45
1:H:10:THR:HG22	1:H:11:ALA:N	2.31	0.45
1:H:118:TYR:O	1:H:119:ASP:HB2	2.15	0.45
2:L:2:GLN:HA	2:L:31:HIS:O	2.16	0.45
1:H:234:ARG:CD	1:H:242:GLN:HG3	2.46	0.45
1:H:7:TYR:O	1:H:98:MET:HA	2.16	0.45
2:L:12:ARG:HD3	2:L:22:ILE:HB	1.98	0.45
1:H:13:SER:O	1:H:92:THR:HG22	2.16	0.45
2:L:30:PHE:HB2	2:L:84:HIS:CD2	2.51	0.45
1:H:196:LYS:NZ	1:H:198:GLU:OE1	2.49	0.45
2:L:71:THR:HA	2:L:72:PRO:HD2	1.81	0.45
1:H:165:VAL:HG12	1:H:169:HIS:CE1	2.52	0.45
1:H:33:PHE:HA	1:H:48:GLN:HB2	1.99	0.45
2:L:81:ARG:HD2	2:L:90:PRO:HB2	1.99	0.45
1:H:111:ARG:NH1	1:H:113:TYR:CD2	2.85	0.44
1:H:14:ARG:N	1:H:15:PRO:HD3	2.31	0.44
1:H:73:TRP:CD1	3:P:5:ALA:O	2.71	0.44
1:H:249:VAL:HG21	1:H:254:GLU:HA	1.98	0.44
2:L:81:ARG:HD3	2:L:92:THR:OG1	2.17	0.44
1:H:45:TYR:CZ	4:Q:2:LEU:CD2	3.00	0.44
1:H:235:PRO:HA	1:H:241:PHE:CD2	2.52	0.44
1:H:208:PHE:CE2	1:H:213:ILE:HD13	2.53	0.44
1:H:65:GLN:O	1:H:66:ILE:C	2.55	0.44
1:H:141:GLN:OE1	1:H:144:ARG:NH1	2.51	0.44
1:H:155:TYR:O	1:H:158:ALA:HB3	2.18	0.44
2:L:45:LYS:HG3	2:L:45:LYS:O	2.16	0.44
1:H:131:LYS:HA	1:H:153:ALA:CB	2.42	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:192:HIS:HA	1:H:193:PRO:HD3	1.80	0.43
1:H:133:TRP:CH2	1:H:147:TRP:CZ3	3.06	0.43
1:H:21:ARG:O	1:H:23:ILE:HG13	2.17	0.43
1:H:1:GLY:O	1:H:3:HIS:NE2	2.52	0.43
1:H:57:PRO:HA	1:H:60:TRP:HB2	2.01	0.43
1:H:159:TYR:CE1	3:P:3:ALA:HB2	2.53	0.43
1:H:130:LEU:CB	1:H:157:ARG:HD3	2.48	0.43
1:H:206:LEU:HD22	1:H:242:GLN:HE21	1.82	0.43
1:H:64:THR:HG22	1:H:64:THR:O	2.17	0.43
1:H:77:ASN:HD21	4:Q:9:LEU:N	2.17	0.43
1:H:111:ARG:NH1	1:H:113:TYR:HD2	2.17	0.43
1:H:216:THR:HA	1:H:228:MET:HE3	1.99	0.43
2:L:62:PHE:CD1	2:L:62:PHE:N	2.86	0.43
1:H:179:LEU:C	1:H:180:LEU:HD23	2.39	0.43
1:H:185:PRO:HD3	1:H:263:HIS:HD2	1.83	0.43
1:H:142:ILE:HA	1:H:145:ARG:HH21	1.85	0.42
1:H:77:ASN:HD21	4:Q:9:LEU:CA	2.31	0.42
1:H:199:VAL:N	1:H:249:VAL:O	2.50	0.42
2:L:30:PHE:C	2:L:30:PHE:CD1	2.91	0.42
3:P:2:PRO:HG3	4:Q:2:LEU:HB3	1.45	0.42
2:L:68:THR:OG1	2:L:69:GLU:N	2.51	0.42
1:H:169:HIS:O	1:H:173:LYS:HG3	2.18	0.42
1:H:254:GLU:O	1:H:256:ASN:N	2.53	0.42
2:L:28:THR:HG22	2:L:29:GLN:CD	2.40	0.42
2:L:29:GLN:HA	2:L:61:SER:HB3	2.02	0.42
1:H:235:PRO:HG3	1:H:241:PHE:CE2	2.55	0.42
1:H:267:PRO:C	1:H:268:GLU:HG3	2.40	0.42
1:H:234:ARG:HA	1:H:235:PRO:HD3	1.73	0.42
2:L:35:ILE:HD11	2:L:82:VAL:HG21	2.02	0.42
1:H:191:HIS:HB2	1:H:199:VAL:HG11	1.99	0.42
1:H:97:TRP:HA	1:H:115:GLN:O	2.20	0.41
2:L:9:VAL:HG12	2:L:10:TYR:N	2.35	0.41
1:H:200:THR:CG2	1:H:248:VAL:HG22	2.50	0.41
1:H:80:THR:O	1:H:84:TYR:HD1	2.03	0.41
1:H:36:PHE:CD1	1:H:37:ASP:N	2.88	0.41
1:H:102:ASP:O	1:H:109:LEU:HD12	2.21	0.41
1:H:49:ALA:HB1	1:H:51:TRP:CE2	2.55	0.41
2:L:51:MET:HE2	2:L:66:ALA:HB2	2.03	0.41
1:H:97:TRP:CH2	4:Q:5:PHE:CD1	3.09	0.41
1:H:63:ILE:HG23	4:Q:2:LEU:CD2	2.50	0.41
1:H:262:TYR:HE1	1:H:269:PRO:HB3	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:85:TYR:O	1:H:87:GLN:HG3	2.21	0.41
1:H:231:VAL:HG13	1:H:244:TRP:CE2	2.56	0.41
2:L:5:PRO:HG3	2:L:30:PHE:HB3	2.02	0.41
1:H:37:ASP:O	1:H:39:ASP:N	2.51	0.40
1:H:46:GLU:HA	1:H:47:PRO:HD3	1.93	0.40
1:H:217:TRP:HD1	1:H:228:MET:CB	2.34	0.40
1:H:86:ASN:OD1	6:H:273:NAG:N2	2.55	0.40
1:H:188:HIS:ND1	1:H:204:TRP:CB	2.84	0.40
1:H:10:THR:O	1:H:22:TYR:HA	2.21	0.40
1:H:45:TYR:CD1	1:H:63:ILE:HG22	2.57	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	H	270/272 (99%)	215 (80%)	41 (15%)	14 (5%)	2	12
2	L	97/99 (98%)	73 (75%)	17 (18%)	7 (7%)	1	6
3	P	7/9 (78%)	5 (71%)	2 (29%)	0	100	100
4	Q	7/9 (78%)	5 (71%)	0	2 (29%)	0	0
All	All	381/389 (98%)	298 (78%)	60 (16%)	23 (6%)	1	9

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	H	89	ALA
1	H	38	SER
1	H	78	LEU
1	H	195	SER
1	H	255	GLN

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Mol	Chain	Res	Type
2	L	54	MET
2	L	74	GLU
2	L	85	ASP
1	H	64	THR
1	H	77	ASN
1	H	212	ASP
4	Q	6	PRO
4	Q	7	PHE
1	H	54	GLN
1	H	160	LEU
2	L	97	ARG
2	L	17	ASN
1	H	15	PRO
1	H	265	GLY
1	H	90	GLY
2	L	33	PRO
1	H	269	PRO
2	L	20	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	H	227/227 (100%)	208 (92%)	19 (8%)	11	38
2	L	94/94 (100%)	84 (89%)	10 (11%)	6	26
3	P	2/2 (100%)	2 (100%)	0	100	100
4	Q	9/9 (100%)	8 (89%)	1 (11%)	6	24
All	All	332/332 (100%)	302 (91%)	30 (9%)	9	34

All (30) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	H	25	VAL
1	H	44	ARG
1	H	45	TYR

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Mol	Chain	Res	Type
1	H	60	TRP
1	H	77	ASN
1	H	88	SER
1	H	121	CYS
1	H	148	GLU
1	H	170	ARG
1	H	174	ASN
1	H	180	LEU
1	H	189	VAL
1	H	196	LYS
1	H	200	THR
1	H	208	PHE
1	H	230	LEU
1	H	231	VAL
1	H	234	ARG
1	H	260	ARG
2	L	7	ILE
2	L	29	GLN
2	L	30	PHE
2	L	45	LYS
2	L	54	MET
2	L	57	SER
2	L	58	LYS
2	L	64	ILE
2	L	69	GLU
2	L	81	ARG
4	Q	5	PHE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	H	127	ASN
1	H	169	HIS
1	H	174	ASN
1	H	226	GLN
1	H	242	GLN
1	H	263	HIS
2	L	2	GLN

### 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 ⓘ

2 monosaccharides 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$
5	NAG	A	1	1,5	14,14,15	1.35	2 (14%)	17,19,21	0.84	0
5	NDG	A	2	5	14,14,15	1.34	2 (14%)	17,19,21	1.00	1 (5%)

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
5	NAG	A	1	1,5	1/1/5/7	0/6/23/26	0/1/1/1
5	NDG	A	2	5	-	1/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	2	NDG	C1-C2	3.61	1.57	1.52
5	A	1	NAG	O4-C4	3.20	1.50	1.43
5	A	1	NAG	O5-C5	2.26	1.48	1.43
5	A	2	NDG	O5-C1	2.10	1.47	1.43

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	2	NDG	C1-O5-C5	2.27	115.27	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
5	A	1	NAG	C1

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	A	2	NDG	C3-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	2	NDG	1	0

## 5.6 Ligand geometry

1 ligand 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
6	NAG	H	273	1	14,14,15	1.19	1 (7%)	17,19,21	1.05	1 (5%)

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
6	NAG	H	273	1	1/1/5/7	2/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	H	273	NAG	C1-C2	3.48	1.57	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	H	273	NAG	C2-N2-C7	-2.32	119.61	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	H	273	NAG	C1

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	H	273	NAG	C3-C2-N2-C7
6	H	273	NAG	C1-C2-N2-C7

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	H	273	NAG	2	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 ⓘ

EDS was not executed - this section is therefore empty.

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

EDS was not executed - this section is therefore empty.

### 6.3 Carbohydrates ⓘ

EDS was not executed - this section is therefore empty.

### 6.4 Ligands ⓘ

EDS was not executed - this section is therefore empty.

### 6.5 Other polymers ⓘ

EDS was not executed - this section is therefore empty.