



# Full wwPDB X-ray Structure Validation Report ⓘ

May 13, 2020 – 03:52 pm BST

PDB ID : 1DDH  
Title : MHC CLASS I H-2DD HEAVY CHAIN COMPLEXED WITH BETA-2 MICROGLOBULIN AND AN IMMUNODOMINANT PEPTIDE P18-I10 FROM THE HUMAN IMMUNODEFICIENCY VIRUS ENVELOPE GLYCOPROTEIN 120  
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Deposited on : 1998-06-22  
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
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

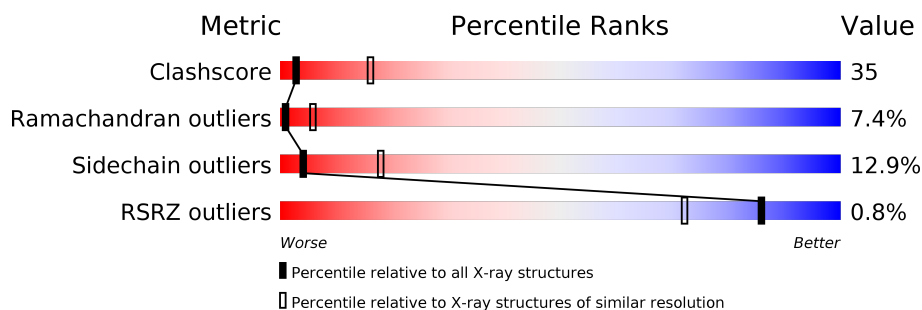
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 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)
RSRZ outliers	127900	1067 (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  $\leq 5\%$ . 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	274	<div> <div></div> <div> <div></div> <div>43%</div> <div>47%</div> <div>9%</div> </div> </div>
2	B	99	<div> <div></div> <div> <div></div> <div>37%</div> <div>54%</div> <div>8%</div> </div> </div>
3	P	10	<div> <div></div> <div> <div></div> <div>40%</div> <div>60%</div> </div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 3051 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-2DD HEAVY CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	274	Total	C	N	O	S	8	0	0
			2185	1364	394	417	10			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	68	ASN	LYS	CONFLICT	UNP P01900
A	181	ALA	ARG	CONFLICT	UNP P01900
A	212	GLU	ASP	CONFLICT	UNP P01900
A	254	GLN	GLU	CONFLICT	UNP P01900

- Molecule 2 is a protein called BETA-2 MICROGLOBULIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	99	Total	C	N	O	S	0	0	0
			786	499	133	146	8			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	85	ALA	ASP	CONFLICT	UNP P01887

- Molecule 3 is a protein called HUMAN IMMUNODEFICIENCY VIRUS ENVELOPE GLYCOPROTEIN 120.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	P	10	Total	C	N	O	0	0	0
			76	48	16	12			

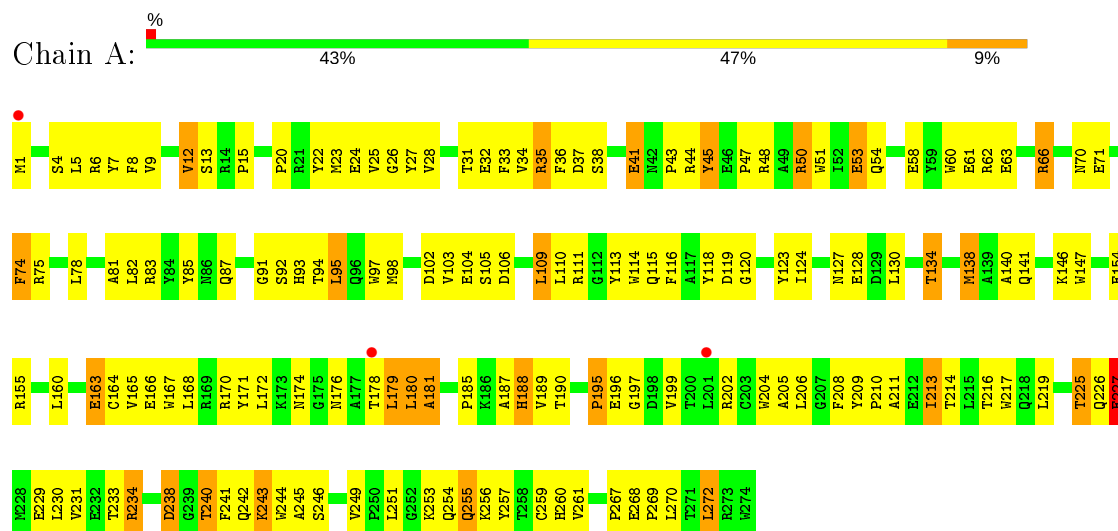
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	O	0	0
			4	4		

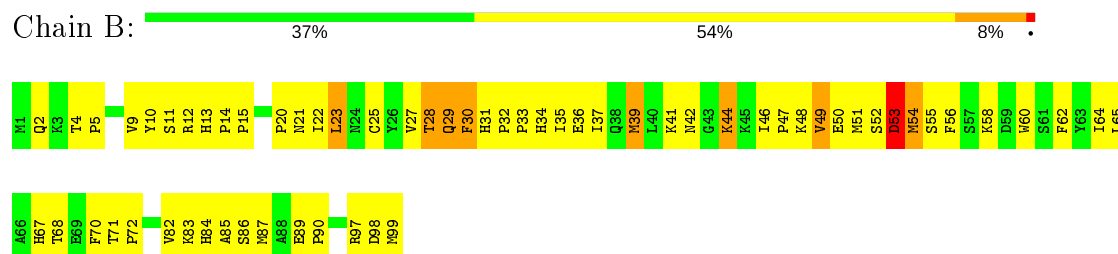
### 3 Residue-property plots [i](#)

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.

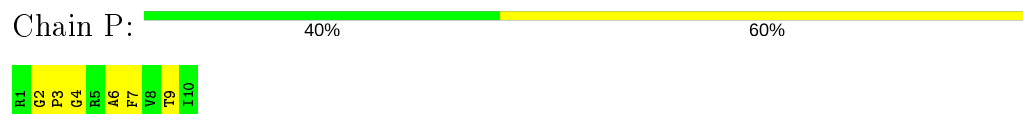
#### • Molecule 1: MHC CLASS I H-2DD HEAVY CHAIN



#### • Molecule 2: BETA-2 MICROGLOBULIN



#### • Molecule 3: HUMAN IMMUNODEFICIENCY VIRUS ENVELOPE GLYCOPROTEIN 120



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	51.33Å 91.35Å 108.20Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 3.10 91.35 – 3.00	Depositor EDS
% Data completeness (in resolution range)	86.4 (8.00-3.10) 85.5 (91.35-3.00)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.01 (at 3.01Å)	Xtriage
Refinement program	X-PLOR 3.1	Depositor
R, $R_{free}$	0.229 , 0.337 0.259 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	62.5	Xtriage
Anisotropy	0.425	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 84.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.86	EDS
Total number of atoms	3051	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.57% 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](#)

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	0.46	0/2246	0.73	0/3050
2	B	0.51	0/812	0.75	0/1102
3	P	0.48	0/77	0.92	0/101
All	All	0.47	0/3135	0.74	0/4253

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	2185	0	1990	149	0
2	B	786	0	731	59	0
3	P	76	0	82	7	0
4	A	4	0	0	0	0
All	All	3051	0	2803	205	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 35.

All (205) 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:103:VAL:HA	1:A:109:LEU:HA	1.44	0.99
1:A:35:ARG:HG3	1:A:35:ARG:HH11	1.31	0.95
1:A:9:VAL:HB	1:A:97:TRP:HB3	1.54	0.90
2:B:83:LYS:HG2	2:B:90:PRO:HB3	1.55	0.87
1:A:213:ILE:HG12	1:A:214:THR:H	1.40	0.84
1:A:45:TYR:CD2	1:A:63:GLU:HB3	2.13	0.84
2:B:13:HIS:HB2	2:B:21:ASN:HD21	1.45	0.81
2:B:30:PHE:HE2	2:B:35:ILE:HB	1.47	0.79
2:B:39:MET:CE	2:B:68:THR:HG22	2.13	0.79
1:A:111:ARG:HG3	1:A:111:ARG:HH11	1.48	0.78
1:A:12:VAL:HG13	1:A:94:THR:HG22	1.65	0.77
1:A:1:MET:HA	1:A:110:LEU:HD13	1.66	0.76
2:B:37:ILE:HG12	2:B:82:VAL:HG22	1.69	0.74
1:A:176:ASN:HB2	1:A:180:LEU:HD12	1.71	0.73
1:A:202:ARG:HG3	1:A:246:SER:OG	1.89	0.72
1:A:213:ILE:HG12	1:A:214:THR:N	2.04	0.72
1:A:8:PHE:CE2	1:A:98:MET:SD	2.83	0.72
1:A:23:MET:HG3	1:A:37:ASP:HA	1.71	0.71
1:A:71:GLU:O	1:A:75:ARG:HG2	1.90	0.71
2:B:52:SER:O	2:B:53:ASP:HB2	1.90	0.70
1:A:35:ARG:HG3	1:A:35:ARG:NH1	2.02	0.68
1:A:4:SER:O	1:A:28:VAL:HA	1.92	0.68
2:B:13:HIS:HB2	2:B:21:ASN:ND2	2.10	0.67
1:A:116:PHE:CE2	1:A:147:TRP:HH2	2.13	0.67
1:A:13:SER:HB3	1:A:78:LEU:HD13	1.77	0.66
1:A:94:THR:OG1	1:A:119:ASP:HA	1.95	0.66
2:B:46:ILE:HD13	2:B:68:THR:HG21	1.77	0.65
1:A:7:TYR:CE2	3:P:2:GLY:HA2	2.31	0.65
1:A:259:CYS:HB3	1:A:272:LEU:CD1	2.27	0.65
2:B:28:THR:OG1	2:B:29:GLN:N	2.29	0.65
1:A:209:TYR:CD1	1:A:210:PRO:HA	2.32	0.64
1:A:124:ILE:HG13	1:A:134:THR:O	1.97	0.64
2:B:5:PRO:CA	2:B:30:PHE:HB3	2.27	0.64
1:A:103:VAL:HG22	1:A:109:LEU:HB3	1.81	0.63
1:A:111:ARG:HD3	1:A:113:TYR:OH	1.98	0.63
2:B:5:PRO:HA	2:B:30:PHE:HB3	1.80	0.63
1:A:204:TRP:CE3	1:A:206:LEU:HD21	2.34	0.63
1:A:13:SER:O	1:A:15:PRO:HD3	2.00	0.61
1:A:185:PRO:HA	1:A:206:LEU:O	2.00	0.61
1:A:22:TYR:HD2	1:A:36:PHE:HE2	1.49	0.61
1:A:242:GLN:O	1:A:243:LYS:HB2	2.01	0.61
1:A:205:ALA:C	1:A:206:LEU:HD23	2.22	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:SER:O	1:A:92:SER:HA	2.02	0.59
1:A:138:MET:O	1:A:141:GLN:HB2	2.02	0.59
1:A:230:LEU:HD12	1:A:243:LYS:NZ	2.18	0.59
1:A:26:GLY:HA3	1:A:34:VAL:HG23	1.85	0.59
1:A:5:LEU:HA	1:A:27:TYR:O	2.03	0.59
1:A:111:ARG:HG3	1:A:111:ARG:NH1	2.15	0.58
1:A:70:ASN:OD1	3:P:4:GLY:HA2	2.04	0.58
1:A:123:TYR:CE1	1:A:140:ALA:HA	2.38	0.58
1:A:261:VAL:HB	1:A:270:LEU:HB3	1.84	0.58
1:A:74:PHE:HE1	1:A:95:LEU:HD13	1.69	0.58
1:A:199:VAL:O	1:A:249:VAL:HG22	2.04	0.58
2:B:12:ARG:NH1	2:B:13:HIS:NE2	2.51	0.57
1:A:35:ARG:HB2	1:A:48:ARG:HG3	1.86	0.57
2:B:25:CYS:O	2:B:27:VAL:HG23	2.05	0.57
1:A:23:MET:HA	1:A:36:PHE:O	2.05	0.57
2:B:30:PHE:CE2	2:B:35:ILE:HB	2.33	0.56
1:A:204:TRP:HE3	1:A:206:LEU:HD21	1.69	0.56
1:A:44:ARG:NH1	1:A:61:GLU:HA	2.20	0.56
2:B:34:HIS:O	2:B:84:HIS:HD2	1.88	0.56
2:B:46:ILE:O	2:B:49:VAL:HG22	2.05	0.56
1:A:35:ARG:CG	1:A:35:ARG:HH11	2.12	0.56
1:A:116:PHE:HE2	1:A:147:TRP:HH2	1.51	0.56
2:B:30:PHE:HE2	2:B:35:ILE:CB	2.18	0.56
1:A:26:GLY:HA3	1:A:34:VAL:CG2	2.35	0.55
1:A:1:MET:HA	1:A:110:LEU:CD1	2.35	0.55
1:A:204:TRP:HH2	1:A:234:ARG:NH2	2.04	0.55
1:A:58:GLU:O	1:A:62:ARG:HB2	2.07	0.55
1:A:167:TRP:HB3	1:A:171:TYR:CE2	2.42	0.54
1:A:75:ARG:NH1	1:A:75:ARG:HG3	2.21	0.54
1:A:47:PRO:HB3	1:A:60:TRP:CZ2	2.42	0.54
1:A:24:GLU:HB2	1:A:36:PHE:HB3	1.90	0.54
2:B:35:ILE:HG12	2:B:36:GLU:N	2.23	0.54
2:B:44:LYS:HB2	2:B:44:LYS:NZ	2.23	0.54
1:A:5:LEU:HB2	1:A:168:LEU:HD13	1.91	0.53
1:A:22:TYR:HE1	1:A:74:PHE:CD2	2.25	0.53
1:A:98:MET:HG2	1:A:115:GLN:HE21	1.72	0.53
1:A:9:VAL:HG21	1:A:97:TRP:HE3	1.74	0.53
1:A:13:SER:HA	1:A:20:PRO:HG3	1.90	0.53
1:A:74:PHE:HZ	1:A:97:TRP:HB2	1.73	0.53
1:A:202:ARG:HH12	2:B:99:MET:HG2	1.73	0.53
1:A:22:TYR:CD2	1:A:36:PHE:HE2	2.27	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:111:ARG:HD3	1:A:113:TYR:CZ	2.44	0.52
1:A:130:LEU:HD11	1:A:160:LEU:HD12	1.91	0.52
1:A:93:HIS:HD2	1:A:119:ASP:OD2	1.91	0.52
1:A:231:VAL:HG13	1:A:244:TRP:CZ2	2.45	0.51
2:B:39:MET:HE1	2:B:68:THR:HG22	1.89	0.51
1:A:187:ALA:O	1:A:188:HIS:HB3	2.10	0.51
1:A:75:ARG:HH11	1:A:75:ARG:HG3	1.74	0.51
1:A:211:ALA:HB2	1:A:241:PHE:CZ	2.46	0.51
1:A:33:PHE:O	1:A:48:ARG:N	2.43	0.51
1:A:118:TYR:O	1:A:119:ASP:HB2	2.11	0.51
2:B:23:LEU:O	2:B:67:HIS:HA	2.10	0.51
2:B:41:LYS:O	2:B:42:ASN:HB2	2.11	0.51
2:B:2:GLN:NE2	2:B:85:ALA:HB1	2.25	0.50
1:A:66:ARG:NH2	3:P:2:GLY:HA3	2.26	0.50
1:A:20:PRO:HG2	1:A:78:LEU:HD12	1.94	0.50
1:A:116:PHE:HE2	1:A:147:TRP:CH2	2.30	0.50
1:A:22:TYR:CE1	1:A:74:PHE:HD2	2.30	0.50
1:A:111:ARG:HH12	1:A:128:GLU:HA	1.77	0.50
1:A:50:ARG:O	1:A:53:GLU:HB2	2.11	0.50
1:A:205:ALA:O	1:A:206:LEU:HD23	2.11	0.49
1:A:4:SER:HB2	1:A:6:ARG:HD3	1.94	0.49
2:B:44:LYS:HB2	2:B:44:LYS:HZ3	1.77	0.49
1:A:66:ARG:NH1	1:A:66:ARG:HB3	2.27	0.49
2:B:32:PRO:HB2	2:B:33:PRO:HD2	1.93	0.49
1:A:102:ASP:O	1:A:110:LEU:N	2.39	0.49
1:A:47:PRO:HB2	1:A:53:GLU:HG3	1.94	0.49
1:A:163:GLU:O	1:A:167:TRP:HB2	2.13	0.49
1:A:179:LEU:O	1:A:181:ALA:N	2.46	0.49
1:A:9:VAL:HG11	1:A:74:PHE:HE2	1.78	0.48
2:B:70:PHE:CE2	2:B:72:PRO:HG3	2.48	0.48
1:A:213:ILE:CG1	1:A:214:THR:H	2.18	0.48
1:A:22:TYR:HB3	1:A:38:SER:OG	2.14	0.48
1:A:225:THR:O	1:A:227:GLU:N	2.46	0.48
1:A:85:TYR:HE2	1:A:118:TYR:CD2	2.31	0.47
1:A:97:TRP:CH2	3:P:3:PRO:HG2	2.49	0.47
1:A:97:TRP:HZ2	1:A:114:TRP:CZ2	2.32	0.47
1:A:15:PRO:HD3	1:A:92:SER:HA	1.94	0.47
1:A:204:TRP:HA	1:A:244:TRP:HB3	1.95	0.47
2:B:12:ARG:HD3	2:B:22:ILE:HD13	1.96	0.47
1:A:255:GLN:CA	1:A:255:GLN:HE21	2.28	0.47
1:A:22:TYR:CE1	1:A:74:PHE:CD2	3.02	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:30:PHE:CE2	2:B:35:ILE:HD12	2.49	0.47
1:A:44:ARG:HH12	1:A:61:GLU:HA	1.80	0.47
2:B:9:VAL:CG1	2:B:23:LEU:HD21	2.45	0.47
2:B:5:PRO:HB3	2:B:30:PHE:HB3	1.97	0.46
2:B:30:PHE:O	2:B:62:PHE:HB2	2.15	0.46
1:A:189:VAL:HA	1:A:202:ARG:O	2.15	0.46
1:A:243:LYS:HG2	1:A:244:TRP:N	2.30	0.46
1:A:243:LYS:HG2	1:A:244:TRP:H	1.80	0.46
2:B:5:PRO:HA	2:B:28:THR:O	2.15	0.46
1:A:205:ALA:O	1:A:208:PHE:HE1	1.99	0.46
1:A:25:VAL:HG13	1:A:35:ARG:NH1	2.31	0.46
2:B:64:ILE:HG12	2:B:65:LEU:N	2.31	0.46
1:A:104:GLU:HG3	1:A:105:SER:N	2.30	0.46
1:A:51:TRP:CH2	1:A:171:TYR:HB3	2.50	0.46
2:B:14:PRO:HA	2:B:15:PRO:HD2	1.78	0.46
1:A:238:ASP:C	1:A:240:THR:H	2.19	0.45
1:A:230:LEU:HD12	1:A:243:LYS:HZ1	1.80	0.45
1:A:253:LYS:O	1:A:255:GLN:N	2.50	0.45
1:A:103:VAL:HG21	1:A:165:VAL:HG13	1.97	0.45
1:A:219:LEU:HA	1:A:256:LYS:O	2.16	0.45
2:B:39:MET:O	2:B:46:ILE:HG13	2.16	0.45
1:A:216:THR:OG1	1:A:260:HIS:HB2	2.16	0.45
2:B:12:ARG:O	2:B:13:HIS:HD2	1.99	0.45
2:B:12:ARG:C	2:B:13:HIS:HD2	2.20	0.45
1:A:234:ARG:HG3	2:B:10:TYR:CZ	2.52	0.45
2:B:67:HIS:ND1	2:B:67:HIS:O	2.50	0.45
1:A:146:LYS:HD3	1:A:147:TRP:CD1	2.51	0.45
1:A:167:TRP:O	1:A:171:TYR:CD2	2.70	0.45
1:A:238:ASP:OD1	1:A:240:THR:OG1	2.34	0.45
1:A:7:TYR:CD2	3:P:2:GLY:HA2	2.51	0.45
1:A:204:TRP:HE3	1:A:206:LEU:CD2	2.31	0.44
1:A:259:CYS:HB3	1:A:272:LEU:HD11	1.98	0.44
1:A:45:TYR:HE2	1:A:66:ARG:HH12	1.63	0.44
2:B:33:PRO:HB3	2:B:62:PHE:CE2	2.52	0.44
1:A:217:TRP:HE1	1:A:245:ALA:C	2.21	0.44
2:B:12:ARG:HB3	2:B:22:ILE:HB	2.00	0.44
2:B:46:ILE:CD1	2:B:68:THR:HG21	2.47	0.44
1:A:202:ARG:NH1	2:B:99:MET:CE	2.81	0.44
1:A:103:VAL:CG2	1:A:168:LEU:HD23	2.47	0.44
2:B:53:ASP:HB3	2:B:54:MET:H	1.57	0.44
1:A:28:VAL:HG13	1:A:179:LEU:HD11	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:P:7:PHE:N	3:P:7:PHE:CD1	2.86	0.43
1:A:15:PRO:HG2	1:A:91:GLY:C	2.38	0.43
1:A:95:LEU:HD23	1:A:95:LEU:HA	1.57	0.43
1:A:147:TRP:CD1	1:A:147:TRP:N	2.87	0.43
1:A:172:LEU:O	1:A:176:ASN:N	2.52	0.43
2:B:35:ILE:HD11	2:B:82:VAL:HG13	2.01	0.43
1:A:85:TYR:CE2	1:A:118:TYR:CD2	3.06	0.43
1:A:195:PRO:O	1:A:197:GLY:N	2.51	0.43
1:A:119:ASP:O	2:B:31:HIS:NE2	2.51	0.43
2:B:83:LYS:CG	2:B:90:PRO:HB3	2.39	0.43
1:A:166:GLU:O	1:A:170:ARG:HG3	2.19	0.42
1:A:130:LEU:CD1	1:A:160:LEU:HD12	2.49	0.42
1:A:219:LEU:HD13	1:A:257:TYR:CE1	2.55	0.42
1:A:85:TYR:CB	1:A:87:GLN:HG3	2.49	0.42
2:B:51:MET:CE	2:B:64:ILE:HD11	2.49	0.42
1:A:229:GLU:O	1:A:245:ALA:HA	2.19	0.42
1:A:20:PRO:HG2	1:A:78:LEU:CD1	2.50	0.42
1:A:97:TRP:CZ3	3:P:3:PRO:HG2	2.54	0.42
2:B:31:HIS:O	2:B:84:HIS:HE1	2.03	0.42
1:A:27:TYR:CE2	1:A:32:GLU:HB2	2.55	0.42
2:B:5:PRO:CB	2:B:30:PHE:HB3	2.48	0.42
1:A:28:VAL:O	1:A:28:VAL:HG13	2.20	0.42
2:B:9:VAL:HG13	2:B:23:LEU:HD21	2.01	0.42
1:A:81:ALA:HB1	1:A:118:TYR:CZ	2.55	0.41
2:B:30:PHE:H	2:B:30:PHE:HD1	1.68	0.41
2:B:44:LYS:CB	2:B:44:LYS:NZ	2.83	0.41
2:B:53:ASP:O	2:B:54:MET:CB	2.69	0.41
2:B:56:PHE:CE2	2:B:60:TRP:CE3	3.09	0.41
1:A:160:LEU:O	1:A:164:CYS:HB3	2.20	0.41
1:A:22:TYR:CD2	1:A:71:GLU:HB2	2.56	0.41
1:A:6:ARG:HB3	1:A:98:MET:CE	2.51	0.41
1:A:82:LEU:CD1	1:A:82:LEU:H	2.34	0.41
1:A:204:TRP:CH2	1:A:234:ARG:NH2	2.87	0.41
1:A:41:GLU:O	1:A:43:PRO:HD3	2.20	0.41
2:B:48:LYS:O	2:B:50:GLU:N	2.54	0.41
1:A:111:ARG:CG	1:A:111:ARG:NH1	2.84	0.40
1:A:268:GLU:HB3	1:A:269:PRO:HD2	2.03	0.40
2:B:56:PHE:HB2	2:B:60:TRP:O	2.21	0.40
1:A:6:ARG:NH2	1:A:113:TYR:CD2	2.90	0.40
2:B:84:HIS:ND1	2:B:86:SER:OG	2.50	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	272/274 (99%)	215 (79%)	38 (14%)	19 (7%)	1	7
2	B	97/99 (98%)	73 (75%)	17 (18%)	7 (7%)	1	6
3	P	8/10 (80%)	4 (50%)	2 (25%)	2 (25%)	0	0
All	All	377/383 (98%)	292 (78%)	57 (15%)	28 (7%)	1	6

All (28) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	180	LEU
1	A	181	ALA
1	A	195	PRO
1	A	196	GLU
1	A	227	GLU
1	A	254	GLN
2	B	53	ASP
2	B	54	MET
3	P	9	THR
1	A	188	HIS
1	A	251	LEU
1	A	41	GLU
1	A	179	LEU
1	A	226	GLN
1	A	243	LYS
2	B	29	GLN
2	B	98	ASP
1	A	163	GLU
1	A	127	ASN
1	A	233	THR
2	B	20	PRO
2	B	49	VAL
1	A	53	GLU
1	A	267	PRO

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Mol	Chain	Res	Type
2	B	47	PRO
3	P	6	ALA
1	A	120	GLY
1	A	213	ILE

### 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	216/229 (94%)	190 (88%)	26 (12%)	5	20
2	B	86/93 (92%)	72 (84%)	14 (16%)	2	10
3	P	7/7 (100%)	7 (100%)	0	100	100
All	All	309/329 (94%)	269 (87%)	40 (13%)	4	18

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	12	VAL
1	A	31	THR
1	A	35	ARG
1	A	45	TYR
1	A	50	ARG
1	A	54	GLN
1	A	66	ARG
1	A	74	PHE
1	A	83	ARG
1	A	95	LEU
1	A	106	ASP
1	A	109	LEU
1	A	134	THR
1	A	138	MET
1	A	154	GLU
1	A	155	ARG
1	A	174	ASN
1	A	178	THR

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Mol	Chain	Res	Type
1	A	190	THR
1	A	225	THR
1	A	227	GLU
1	A	234	ARG
1	A	238	ASP
1	A	240	THR
1	A	255	GLN
1	A	272	LEU
2	B	4	THR
2	B	11	SER
2	B	23	LEU
2	B	28	THR
2	B	30	PHE
2	B	39	MET
2	B	44	LYS
2	B	53	ASP
2	B	55	SER
2	B	58	LYS
2	B	71	THR
2	B	87	MET
2	B	89	GLU
2	B	97	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	ASN
1	A	68	ASN
1	A	115	GLN
1	A	149	GLN
1	A	255	GLN
2	B	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 [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

There are no ligands in this entry.

## 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, 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	274/274 (100%)	0.10	3 (1%) 80 64	5, 36, 82, 142	2 (0%)
2	B	99/99 (100%)	-0.05	0 100 100	5, 26, 74, 99	0
3	P	10/10 (100%)	0.41	0 100 100	11, 57, 113, 119	0
All	All	383/383 (100%)	0.07	3 (0%) 86 72	5, 34, 80, 142	2 (0%)

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	1	MET	9.3
1	A	201	LEU	2.4
1	A	178	THR	2.4

### 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](#)

There are no ligands in this entry.

### 6.5 Other polymers [i](#)

There are no such residues in this entry.