



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 09:11 AM BST

PDB ID : 1IAO  
Title : CLASS II MHC I-AD IN COMPLEX WITH OVALBUMIN PEPTIDE 323-339  
Authors : Scott, C.A.; Peterson, P.A.; Teyton, L.; Wilson, I.A.  
Deposited on : 1998-03-13  
Resolution : 2.60 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

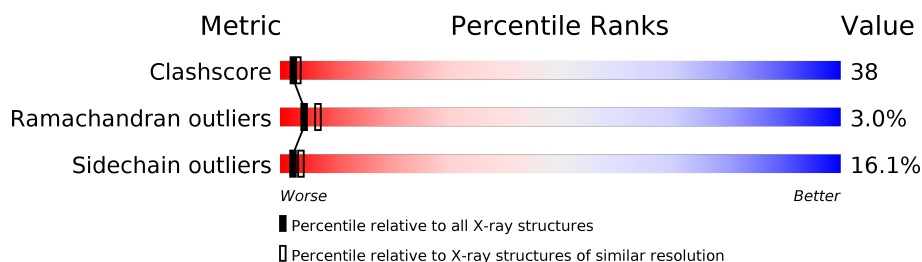
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.60 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	3518 (2.60-2.60)
Ramachandran outliers	138981	3455 (2.60-2.60)
Sidechain outliers	138945	3455 (2.60-2.60)

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	A	194	
2	B	222	

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 3035 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 II I-AD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	0	0
			1417	918	233	264	2			

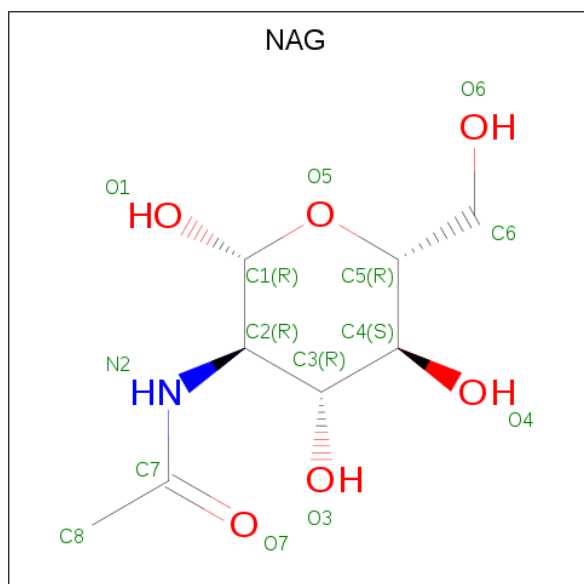
- Molecule 2 is a protein called MHC CLASS II I-AD.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	200	Total	C	N	O	S	0	0	0
			1596	997	286	307	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	69	ASP	GLU	conflict	UNP P04228

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is water.

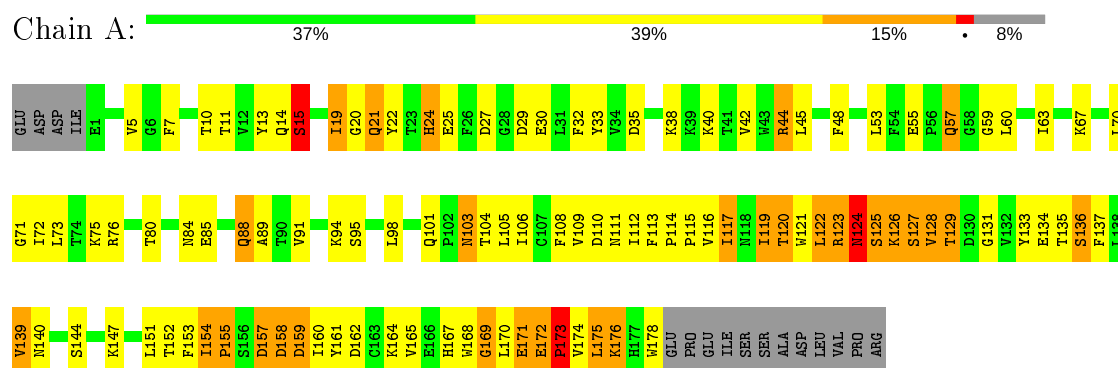
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	4	Total	O	0	0
			4	4		
4	B	4	Total	O	0	0
			4	4		

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

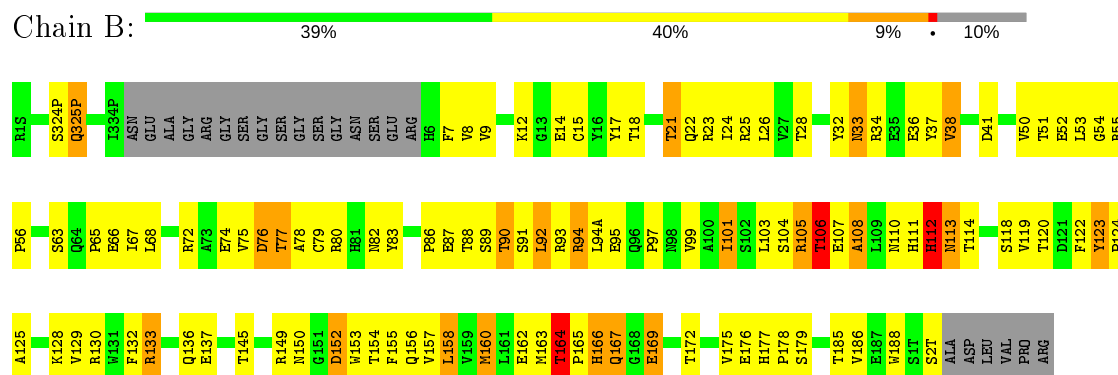
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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



- Molecule 2: MHC CLASS II I-AD



## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 41 21 2	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.30 Å   101.30 Å   92.60 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	27.00 – 2.60	Depositor
% Data completeness (in resolution range)	99.0 (27.00-2.60)	Depositor
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
Refinement program	X-PLOR 3.8	Depositor
R, $R_{free}$	0.255 , 0.320	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	3035	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	54.0	wwPDB-VP

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

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	0.57	0/1462	1.06	10/1997 (0.5%)
2	B	0.53	0/1634	0.85	6/2225 (0.3%)
All	All	0.55	0/3096	0.96	16/4222 (0.4%)

There are no bond length outliers.

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	15	SER	C-N-CD	10.70	150.87	128.40
1	A	155	PRO	N-CA-C	10.06	138.25	112.10
1	A	169	GLY	N-CA-C	-8.82	91.05	113.10
2	B	166	HIS	N-CA-C	7.01	129.94	111.00
1	A	173	PRO	N-CA-C	-6.22	95.92	112.10
1	A	15	SER	C-N-CA	-6.18	96.03	122.00
2	B	108	ALA	N-CA-C	-6.06	94.64	111.00
1	A	172	GLU	C-N-CD	5.75	140.48	128.40
2	B	106	THR	N-CA-C	5.74	126.51	111.00
2	B	124	PRO	CA-N-CD	-5.71	103.51	111.50
2	B	164	THR	N-CA-C	-5.54	96.05	111.00
2	B	123	TYR	N-CA-C	-5.50	96.16	111.00
1	A	126	LYS	N-CA-C	-5.49	96.19	111.00
1	A	171	GLU	N-CA-C	5.20	125.04	111.00
1	A	127	SER	N-CA-C	5.18	124.98	111.00
1	A	172	GLU	N-CA-C	-5.08	97.27	111.00

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1417	0	1338	119	0
2	B	1596	0	1490	118	0
3	B	14	0	13	1	0
4	A	4	0	0	1	0
4	B	4	0	0	1	0
All	All	3035	0	2841	224	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 38.

All (224) 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)
2:B:21:THR:CG2	2:B:24:ILE:HD11	1.80	1.10
1:A:164:LYS:HE3	1:A:173:PRO:HG2	1.37	1.06
2:B:21:THR:HG22	2:B:24:ILE:CD1	1.87	1.04
2:B:169:GLU:OE1	2:B:169:GLU:HA	1.56	1.04
1:A:157:ASP:C	1:A:159:ASP:H	1.57	1.02
1:A:157:ASP:O	1:A:159:ASP:N	1.94	1.01
2:B:21:THR:HG22	2:B:24:ILE:HD11	1.00	0.99
2:B:101:ILE:H	2:B:101:ILE:HD13	1.29	0.97
1:A:161:TYR:HB2	1:A:178:TRP:O	1.66	0.96
1:A:164:LYS:HE3	1:A:173:PRO:CG	1.98	0.93
1:A:158:ASP:O	1:A:160:ILE:N	2.02	0.92
2:B:50:VAL:HG23	2:B:51:THR:HG23	1.51	0.91
1:A:123:ARG:HA	1:A:160:ILE:O	1.73	0.88
1:A:35:ASP:OD2	1:A:38:LYS:HB2	1.74	0.88
1:A:172:GLU:C	1:A:173:PRO:O	2.09	0.86
1:A:103:ASN:HD22	1:A:104:THR:H	1.21	0.85
1:A:57:GLN:HA	1:A:60:LEU:HD12	1.56	0.85
1:A:157:ASP:C	1:A:159:ASP:N	2.27	0.84
1:A:11:THR:HG23	1:A:63:ILE:HD13	1.60	0.84
2:B:87:GLU:OE1	2:B:87:GLU:HA	1.75	0.83
2:B:108:ALA:HB1	2:B:113:ASN:CG	2.01	0.80
2:B:63:SER:O	2:B:65:PRO:HD3	1.82	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:151:LEU:HD22	1:A:152:THR:H	1.46	0.80
2:B:101:ILE:CD1	2:B:101:ILE:H	1.95	0.80
2:B:133:ARG:HH11	2:B:133:ARG:HG3	1.47	0.79
1:A:168:TRP:C	1:A:170:LEU:H	1.84	0.79
2:B:90:THR:HG22	2:B:91:SER:N	2.00	0.77
2:B:101:ILE:HG12	2:B:188:TRP:CE3	2.20	0.76
2:B:101:ILE:HD12	2:B:186:VAL:HG11	1.68	0.75
1:A:164:LYS:CE	1:A:173:PRO:HG2	2.16	0.74
1:A:109:VAL:HG21	1:A:119:ILE:HG21	1.69	0.73
2:B:110:ASN:O	4:B:1043:HOH:O	2.05	0.73
1:A:164:LYS:CE	1:A:173:PRO:CG	2.69	0.70
2:B:177:HIS:CD2	2:B:178:PRO:HD2	2.26	0.70
1:A:112:ILE:HD13	1:A:117:ILE:HD12	1.73	0.70
1:A:55:GLU:HB3	1:A:57:GLN:OE1	1.91	0.70
1:A:104:THR:HA	1:A:151:LEU:O	1.92	0.70
2:B:90:THR:HG22	2:B:91:SER:H	1.57	0.70
2:B:68:LEU:O	2:B:72:ARG:HG3	1.92	0.70
2:B:108:ALA:HB1	2:B:113:ASN:ND2	2.05	0.70
1:A:122:LEU:HD22	1:A:126:LYS:N	2.06	0.69
2:B:37:TYR:C	2:B:50:VAL:HG22	2.13	0.69
1:A:167:HIS:CD2	1:A:169:GLY:H	2.12	0.68
2:B:169:GLU:OE1	2:B:169:GLU:CA	2.40	0.68
1:A:167:HIS:O	1:A:170:LEU:HB3	1.93	0.68
1:A:124:ASN:ND2	1:A:126:LYS:O	2.24	0.68
1:A:174:VAL:HG13	1:A:176:LYS:HE3	1.76	0.68
2:B:110:ASN:O	2:B:111:HIS:HB3	1.92	0.68
1:A:168:TRP:C	1:A:170:LEU:N	2.47	0.68
2:B:166:HIS:CD2	2:B:166:HIS:C	2.67	0.67
2:B:22:GLN:OE1	3:B:495:NAG:C1	2.42	0.67
2:B:129:VAL:HG13	2:B:175:VAL:HG22	1.77	0.67
2:B:133:ARG:O	2:B:136:GLN:HG2	1.94	0.66
1:A:48:PHE:CZ	2:B:90:THR:HG23	2.32	0.65
1:A:14:GLN:HB2	1:A:19:ILE:HG22	1.79	0.65
2:B:36:GLU:O	2:B:50:VAL:CG2	2.45	0.65
2:B:101:ILE:HD12	2:B:186:VAL:CG1	2.27	0.64
2:B:90:THR:CG2	2:B:91:SER:N	2.59	0.64
1:A:167:HIS:HB3	1:A:170:LEU:HD23	1.79	0.64
1:A:139:VAL:HG22	2:B:12:LYS:NZ	2.13	0.63
2:B:120:THR:HG22	2:B:156:GLN:HB2	1.80	0.63
2:B:78:ALA:O	2:B:82:ASN:HB2	1.98	0.63
1:A:120:THR:O	1:A:164:LYS:N	2.20	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:118:SER:HA	2:B:158:LEU:HD12	1.80	0.63
1:A:30:GLU:OE2	1:A:136:SER:OG	2.18	0.62
1:A:164:LYS:HG3	1:A:173:PRO:HB2	1.82	0.62
1:A:174:VAL:HG13	1:A:176:LYS:CE	2.29	0.62
1:A:98:LEU:HB3	1:A:101:GLN:HB2	1.81	0.62
2:B:99:VAL:CG1	2:B:175:VAL:HG21	2.30	0.62
1:A:70:LEU:HD13	2:B:9:VAL:HG13	1.82	0.60
1:A:172:GLU:O	1:A:173:PRO:C	2.29	0.60
1:A:131:GLY:HA3	1:A:152:THR:OG1	2.01	0.60
1:A:48:PHE:CE2	2:B:90:THR:HG23	2.37	0.60
1:A:45:LEU:O	1:A:48:PHE:HB2	2.01	0.59
1:A:29:ASP:HB3	2:B:153:TRP:CE2	2.37	0.59
2:B:112:HIS:CE1	2:B:164:THR:HG23	2.38	0.59
2:B:82:ASN:HA	2:B:86:PRO:HD2	1.85	0.59
1:A:154:ILE:O	1:A:154:ILE:CG1	2.51	0.59
1:A:89:ALA:HA	1:A:108:PHE:O	2.03	0.58
1:A:105:LEU:N	1:A:151:LEU:O	2.31	0.58
2:B:32:TYR:O	2:B:33:ASN:HB2	2.03	0.58
2:B:157:VAL:C	2:B:158:LEU:HD13	2.24	0.58
2:B:108:ALA:HB1	2:B:113:ASN:OD1	2.03	0.57
1:A:112:ILE:HG21	1:A:137:PHE:HE1	1.70	0.57
1:A:105:LEU:HB2	1:A:153:PHE:CE1	2.40	0.57
1:A:71:GLY:O	1:A:75:LYS:HG3	2.05	0.57
2:B:101:ILE:HD13	2:B:101:ILE:N	2.06	0.57
2:B:107:GLU:O	2:B:108:ALA:HB3	2.04	0.56
1:A:94:LYS:HB2	1:A:106:ILE:HD11	1.87	0.56
1:A:151:LEU:HD22	1:A:152:THR:N	2.16	0.56
2:B:95:GLU:HB2	2:B:123:TYR:N	2.20	0.56
2:B:36:GLU:O	2:B:50:VAL:HG21	2.06	0.56
2:B:94:ARG:HG2	2:B:94:ARG:HH11	1.70	0.56
2:B:101:ILE:CD1	2:B:101:ILE:N	2.66	0.55
1:A:164:LYS:HE3	1:A:173:PRO:CB	2.36	0.55
2:B:133:ARG:NH1	2:B:133:ARG:HG3	2.18	0.55
1:A:27:ASP:O	2:B:149:ARG:NH2	2.40	0.55
1:A:121:TRP:HA	1:A:162:ASP:O	2.07	0.55
1:A:105:LEU:HD21	1:A:178:TRP:CE3	2.42	0.55
2:B:104:SER:O	2:B:106:THR:N	2.40	0.55
1:A:165:VAL:HB	1:A:174:VAL:HB	1.88	0.54
1:A:22:TYR:OH	1:A:24:HIS:HE1	1.89	0.54
2:B:163:MET:C	2:B:165:PRO:HD3	2.27	0.54
2:B:152:ASP:O	2:B:153:TRP:HB2	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:76:ARG:HG2	2:B:53:LEU:HD23	1.88	0.54
2:B:94:ARG:HB3	2:B:123:TYR:CE2	2.43	0.54
2:B:172:THR:HG23	2:B:185:THR:OG1	2.08	0.54
1:A:129:THR:OG1	1:A:129:THR:O	2.23	0.53
1:A:114:PRO:O	1:A:116:VAL:N	2.35	0.53
1:A:91:VAL:HA	1:A:106:ILE:O	2.08	0.53
2:B:94(A):LEU:HB3	2:B:179:SER:HB2	1.89	0.53
2:B:66:GLU:HG2	2:B:67:ILE:N	2.24	0.53
1:A:115:PRO:HA	1:A:137:PHE:CE1	2.44	0.53
1:A:151:LEU:CD1	1:A:153:PHE:HB3	2.39	0.52
1:A:170:LEU:HD12	1:A:171:GLU:H	1.73	0.52
1:A:139:VAL:HG22	2:B:12:LYS:HZ1	1.74	0.52
1:A:32:PHE:C	1:A:32:PHE:CD1	2.82	0.52
2:B:164:THR:N	2:B:165:PRO:HD3	2.23	0.52
2:B:94:ARG:NH1	2:B:94:ARG:HG2	2.25	0.51
2:B:125:ALA:HB2	2:B:155:PHE:CE2	2.46	0.51
1:A:151:LEU:HD13	1:A:152:THR:N	2.25	0.51
2:B:75:VAL:O	2:B:79:CYS:HB2	2.10	0.51
1:A:19:ILE:HD13	1:A:20:GLY:N	2.25	0.51
1:A:122:LEU:HD22	1:A:125:SER:C	2.31	0.51
2:B:145:THR:HG23	2:B:158:LEU:O	2.10	0.51
1:A:154:ILE:HG12	1:A:154:ILE:O	2.11	0.50
2:B:95:GLU:HB2	2:B:123:TYR:H	1.76	0.50
1:A:85:GLU:HB3	1:A:111:ASN:HD21	1.76	0.50
1:A:22:TYR:CE2	1:A:59:GLY:HA2	2.46	0.50
2:B:52:GLU:O	2:B:55:ARG:HG3	2.12	0.50
2:B:66:GLU:HG2	2:B:67:ILE:H	1.77	0.50
1:A:15:SER:HB2	2:B:7:PHE:HB2	1.94	0.49
1:A:44:ARG:HH11	1:A:44:ARG:CG	2.24	0.49
1:A:7:PHE:CE1	2:B:14:GLU:HG2	2.47	0.49
2:B:94:ARG:HG2	2:B:123:TYR:CD2	2.47	0.49
1:A:103:ASN:HD22	1:A:104:THR:N	2.00	0.49
1:A:135:THR:O	1:A:147:LYS:HE2	2.11	0.49
2:B:105:ARG:O	2:B:106:THR:CB	2.59	0.49
2:B:97:PRO:HB2	2:B:119:VAL:HG12	1.95	0.49
1:A:112:ILE:CD1	1:A:117:ILE:HD12	2.42	0.48
2:B:177:HIS:CG	2:B:178:PRO:HD2	2.47	0.48
1:A:110:ASP:OD1	1:A:111:ASN:N	2.45	0.48
2:B:12:LYS:O	2:B:28:THR:HA	2.13	0.48
1:A:14:GLN:HG2	2:B:8:VAL:HG22	1.96	0.48
1:A:123:ARG:HG3	1:A:158:ASP:CB	2.44	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:109:VAL:HG21	1:A:119:ILE:CG2	2.40	0.48
1:A:133:TYR:CD1	1:A:134:GLU:N	2.81	0.47
1:A:122:LEU:HD12	1:A:162:ASP:HB3	1.95	0.47
2:B:108:ALA:CB	2:B:113:ASN:OD1	2.62	0.47
1:A:140:ASN:HB2	1:A:144:SER:O	2.15	0.47
2:B:55:ARG:N	2:B:56:PRO:CD	2.78	0.47
1:A:123:ARG:CA	1:A:160:ILE:O	2.56	0.47
1:A:84:ASN:HB3	1:A:169:GLY:HA3	1.96	0.47
1:A:170:LEU:HD12	1:A:171:GLU:N	2.30	0.47
2:B:157:VAL:O	2:B:158:LEU:HD13	2.15	0.47
1:A:167:HIS:O	1:A:170:LEU:CB	2.62	0.47
2:B:163:MET:O	2:B:165:PRO:HD3	2.14	0.47
1:A:14:GLN:HA	2:B:7:PHE:O	2.15	0.46
2:B:110:ASN:O	2:B:111:HIS:CB	2.61	0.46
2:B:150:ASN:HB2	2:B:154:THR:O	2.15	0.46
1:A:175:LEU:H	1:A:175:LEU:HG	1.48	0.46
1:A:165:VAL:O	1:A:170:LEU:HD21	2.16	0.46
1:A:174:VAL:HG13	1:A:176:LYS:NZ	2.31	0.45
2:B:108:ALA:HA	2:B:113:ASN:HA	1.97	0.45
2:B:128:LYS:HE2	2:B:130:ARG:NH1	2.30	0.45
2:B:76:ASP:OD2	2:B:80:ARG:HD2	2.16	0.45
2:B:92:LEU:HA	2:B:92:LEU:HD12	1.82	0.45
2:B:88:THR:O	2:B:93:ARG:HG3	2.16	0.45
1:A:113:PHE:CD1	1:A:114:PRO:HA	2.51	0.45
1:A:44:ARG:HH11	1:A:44:ARG:HG2	1.82	0.45
2:B:160:MET:SD	2:B:160:MET:N	2.90	0.45
2:B:325(P):GLN:O	2:B:82:ASN:ND2	2.46	0.45
2:B:34:ARG:HG2	2:B:34:ARG:HH11	1.82	0.45
1:A:21:GLN:HE22	1:A:137:PHE:HB2	1.83	0.45
1:A:14:GLN:HB2	1:A:19:ILE:CG2	2.46	0.45
1:A:29:ASP:HA	4:A:1032:HOH:O	2.16	0.45
1:A:157:ASP:O	1:A:159:ASP:CA	2.64	0.44
2:B:128:LYS:HB3	2:B:176:GLU:HB2	1.99	0.44
2:B:114:THR:OG1	2:B:162:GLU:HG2	2.17	0.44
2:B:21:THR:HG22	2:B:24:ILE:CG1	2.45	0.44
2:B:37:TYR:CA	2:B:50:VAL:HG22	2.48	0.44
2:B:37:TYR:O	2:B:54:GLY:HA3	2.17	0.44
1:A:123:ARG:HD2	1:A:124:ASN:OD1	2.17	0.44
1:A:144:SER:HB3	2:B:34:ARG:HH12	1.82	0.44
2:B:17:TYR:CE1	2:B:83:TYR:HB2	2.52	0.44
2:B:94:ARG:NH1	2:B:153:TRP:HB3	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:166:HIS:CG	2:B:166:HIS:O	2.66	0.44
2:B:133:ARG:HG2	2:B:169:GLU:HG3	1.99	0.44
1:A:114:PRO:HB2	1:A:116:VAL:HG23	1.99	0.43
1:A:172:GLU:O	1:A:173:PRO:O	2.30	0.43
2:B:112:HIS:ND1	2:B:164:THR:HG23	2.33	0.43
1:A:127:SER:OG	1:A:128:VAL:N	2.51	0.43
1:A:120:THR:N	1:A:164:LYS:O	2.46	0.43
1:A:124:ASN:HB2	1:A:125:SER:H	1.56	0.43
1:A:164:LYS:HG3	1:A:173:PRO:CB	2.48	0.43
1:A:98:LEU:HA	1:A:98:LEU:HD12	1.80	0.43
2:B:74:GLU:HA	2:B:77:THR:OG1	2.18	0.43
1:A:176:LYS:HD3	1:A:176:LYS:HA	1.63	0.43
2:B:36:GLU:C	2:B:50:VAL:HG21	2.39	0.42
2:B:25:ARG:NH2	2:B:41:ASP:OD2	2.45	0.42
1:A:151:LEU:C	1:A:151:LEU:HD13	2.39	0.42
2:B:34:ARG:HG2	2:B:34:ARG:NH1	2.33	0.42
2:B:97:PRO:HB3	2:B:122:PHE:HB3	2.01	0.42
1:A:44:ARG:CG	1:A:44:ARG:NH1	2.81	0.42
2:B:111:HIS:O	2:B:112:HIS:HB2	2.18	0.42
2:B:101:ILE:CD1	2:B:186:VAL:HG11	2.45	0.42
2:B:37:TYR:CD2	2:B:38:VAL:CG2	3.02	0.42
2:B:167:GLN:C	2:B:169:GLU:H	2.22	0.42
1:A:85:GLU:HB3	1:A:111:ASN:ND2	2.35	0.41
2:B:94(A):LEU:HD22	2:B:179:SER:HA	2.01	0.41
2:B:107:GLU:O	2:B:108:ALA:C	2.54	0.41
1:A:88:GLN:HB3	1:A:88:GLN:HE21	1.64	0.41
1:A:33:TYR:CE1	1:A:42:VAL:HB	2.55	0.41
1:A:33:TYR:CE1	1:A:42:VAL:CG1	3.04	0.41
1:A:13:TYR:CZ	1:A:67:LYS:HG3	2.56	0.41
1:A:104:THR:CA	1:A:151:LEU:O	2.67	0.41
2:B:132:PHE:CD1	2:B:137:GLU:HA	2.55	0.41
2:B:101:ILE:CG1	2:B:188:TRP:CE3	2.97	0.41
2:B:103:LEU:O	2:B:104:SER:C	2.58	0.41
1:A:165:VAL:HG23	1:A:174:VAL:O	2.20	0.41
1:A:119:ILE:HA	1:A:164:LYS:O	2.21	0.40
1:A:72:ILE:HG22	1:A:76:ARG:HH21	1.86	0.40
2:B:68:LEU:HD12	2:B:68:LEU:O	2.21	0.40
2:B:18:THR:HB	2:B:23:ARG:HB3	2.02	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	176/194 (91%)	162 (92%)	8 (4%)	6 (3%)	3	5
2	B	196/222 (88%)	175 (89%)	16 (8%)	5 (3%)	5	9
All	All	372/416 (89%)	337 (91%)	24 (6%)	11 (3%)	4	7

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	125	SER
1	A	158	ASP
1	A	159	ASP
2	B	105	ARG
2	B	167	GLN
2	B	33	ASN
1	A	124	ASN
1	A	155	PRO
2	B	106	THR
2	B	112	HIS
1	A	173	PRO

### 5.3.2 Protein sidechains

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	153/175 (87%)	123 (80%)	30 (20%)	1	2
2	B	170/194 (88%)	148 (87%)	22 (13%)	4	7

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	323/369 (88%)	271 (84%)	52 (16%)	<b>2</b> <b>4</b>

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	VAL
1	A	10	THR
1	A	15	SER
1	A	19	ILE
1	A	21	GLN
1	A	24	HIS
1	A	25	GLU
1	A	40	LYS
1	A	44	ARG
1	A	53	LEU
1	A	57	GLN
1	A	73	LEU
1	A	80	THR
1	A	88	GLN
1	A	95	SER
1	A	103	ASN
1	A	117	ILE
1	A	119	ILE
1	A	120	THR
1	A	122	LEU
1	A	123	ARG
1	A	124	ASN
1	A	128	VAL
1	A	129	THR
1	A	136	SER
1	A	139	VAL
1	A	154	ILE
1	A	157	ASP
1	A	175	LEU
1	A	176	LYS
2	B	324(P)	SER
2	B	325(P)	GLN
2	B	15	CYS
2	B	21	THR
2	B	26	LEU
2	B	38	VAL
2	B	76	ASP

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Mol	Chain	Res	Type
2	B	77	THR
2	B	89	SER
2	B	90	THR
2	B	92	LEU
2	B	94	ARG
2	B	101	ILE
2	B	112	HIS
2	B	113	ASN
2	B	133	ARG
2	B	152	ASP
2	B	158	LEU
2	B	160	MET
2	B	164	THR
2	B	169	GLU
2	B	2(T)	SER

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	24	HIS
1	A	88	GLN
1	A	103	ASN
1	A	111	ASN
1	A	167	HIS
2	B	331(P)	HIS
2	B	64	GLN
2	B	166	HIS

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.



## 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$
3	NAG	B	495	2	14,14,15	0.61	0	17,19,21	0.72	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	NAG	B	495	2	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	495	NAG	O5-C5-C6-O6
3	B	495	NAG	C4-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	495	NAG	1	0

## 5.7 Other polymers

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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.