



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 10, 2020 – 07:42 AM BST

PDB ID : 1IEB  
Title : HISTOCOMPATIBILITY ANTIGEN  
Authors : Fremont, D.H.; Hendrickson, W.A.; Marrack, P.; Kappler, J.  
Deposited on : 1996-04-05  
Resolution : 2.70 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

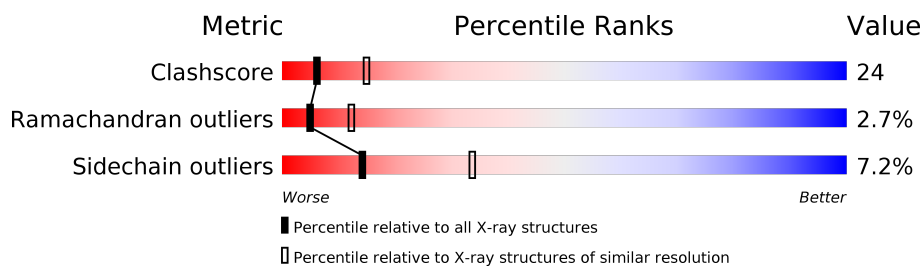
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)

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	192	
1	C	192	
2	B	227	
2	D	227	

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
3	NAG	A	194	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	C	194	X	-	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6672 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.

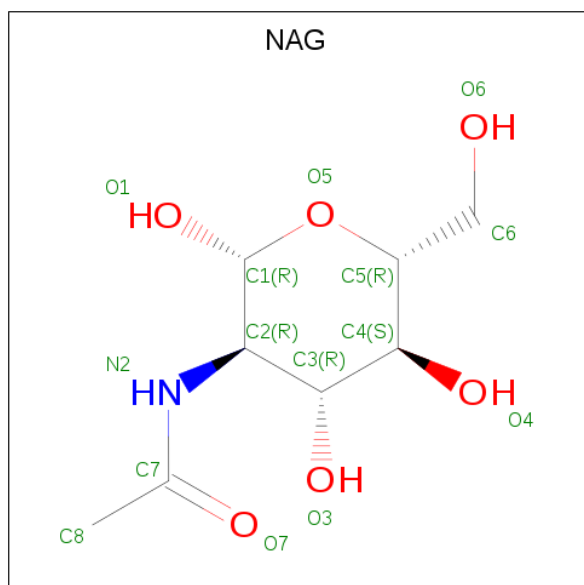
- Molecule 1 is a protein called MHC CLASS II I-EK.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	182	Total	C	N	O	S	0	0	0
			1488	959	243	282	4			
1	C	182	Total	C	N	O	S	0	0	0
			1488	959	243	282	4			

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

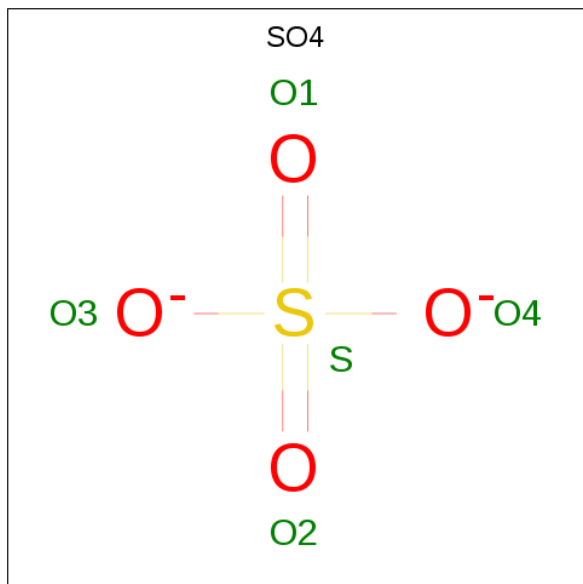
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1724	1092	302	323	7			
2	D	214	Total	C	N	O	S	0	0	0
			1724	1092	302	323	7			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula: C<sub>8</sub>H<sub>15</sub>NO<sub>6</sub>).



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

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula: O<sub>4</sub>S).



Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	1	Total	O S	0	0
			5	4 1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	39	Total	O	0	0
			39	39		
5	B	48	Total	O	0	0
			48	48		
5	C	27	Total	O	0	0
			27	27		

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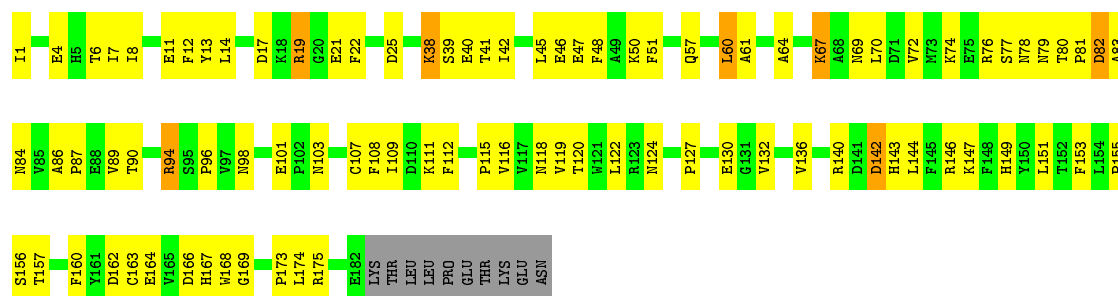
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	45	Total	O	0	0
			45	45		

### 3 Residue-property plots

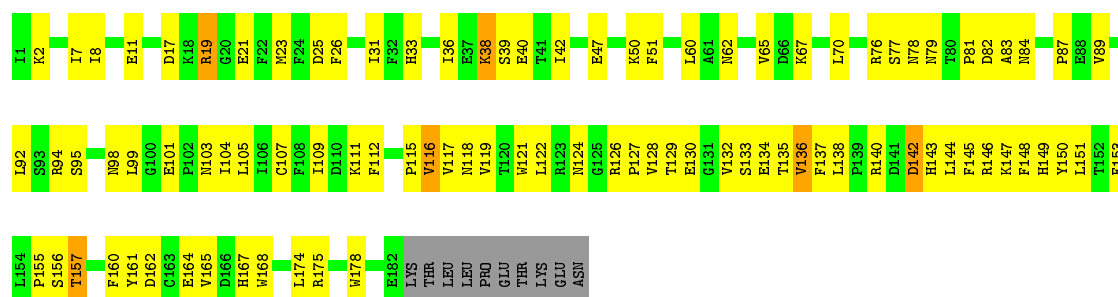
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded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

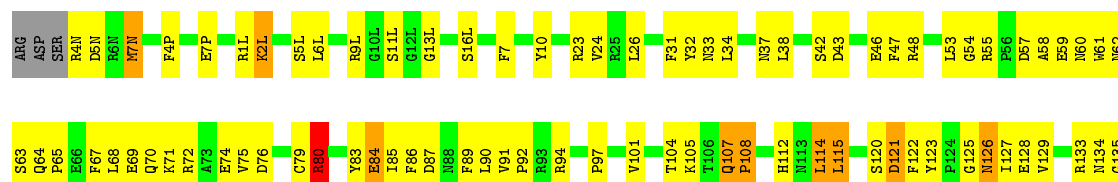
- Molecule 1: MHC CLASS II I-EK



- Molecule 1: MHC CLASS II I-EK

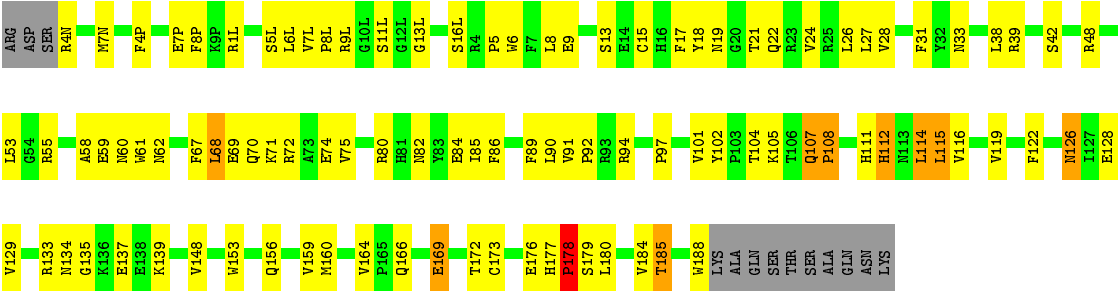


- Molecule 2: MHC CLASS II I-EK





● Molecule 2: MHC CLASS II I-EK





## 4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	77.53 Å 77.53 Å 319.48 Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	6.00 – 2.70	Depositor
% Data completeness (in resolution range)	83.6 (6.00-2.70)	Depositor
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
Refinement program	X-PLOR	Depositor
R, $R_{free}$	0.222 , 0.321	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6672	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	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, SO4

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	0.60	0/1530	0.80	0/2081
1	C	0.60	0/1530	0.79	0/2081
2	B	0.54	0/1769	0.81	2/2404 (0.1%)
2	D	0.56	0/1769	0.82	1/2404 (0.0%)
All	All	0.57	0/6598	0.81	3/8970 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1
2	B	0	3
All	All	0	4

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	108	PRO	N-CA-CB	5.81	110.28	103.30
2	D	108	PRO	N-CA-CB	5.56	109.97	103.30
2	B	80	ARG	NE-CZ-NH2	-5.11	117.75	120.30

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	B	10	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	B	123	TYR	Sidechain
2	B	32	TYR	Sidechain
1	C	150	TYR	Sidechain

## 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	1488	0	1412	90	0
1	C	1488	0	1412	84	0
2	B	1724	0	1622	89	0
2	D	1724	0	1622	79	0
3	A	28	0	26	1	0
3	B	14	0	13	1	0
3	C	28	0	26	3	0
3	D	14	0	13	0	0
4	D	5	0	0	0	0
5	A	39	0	0	6	0
5	B	48	0	0	3	0
5	C	27	0	0	3	0
5	D	45	0	0	2	0
All	All	6672	0	6146	310	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 24.

All (310) 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:147:LYS:HE3	1:A:149:HIS:HE1	1.12	1.11
1:C:147:LYS:HE3	1:C:149:HIS:HE1	1.12	1.10
1:C:147:LYS:HE3	1:C:149:HIS:CE1	2.03	0.93
1:A:147:LYS:HE3	1:A:149:HIS:CE1	2.03	0.93
1:A:87:PRO:HB3	1:A:112:PHE:HB3	1.53	0.89
2:B:134:ASN:HD21	2:B:169:GLU:HA	1.41	0.86
2:B:97:PRO:HB3	2:B:122:PHE:HB3	1.58	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:98:ASN:HB2	1:A:101:GLU:HG2	1.57	0.85
1:C:122:LEU:HD11	5:C:200:HOH:O	1.78	0.83
2:B:1(L):ARG:HD2	2:B:60:ASN:OD1	1.77	0.83
2:D:134:ASN:HD21	2:D:169:GLU:HA	1.45	0.82
2:D:91:VAL:HG11	5:D:235:HOH:O	1.81	0.80
1:A:77:SER:HB3	2:B:53:LEU:HD11	1.64	0.79
1:A:72:VAL:HG13	2:B:2(L):LYS:HA	1.64	0.79
2:B:43:ASP:HB3	5:B:231:HOH:O	1.80	0.79
2:B:7(P):GLU:HG3	2:B:67:PHE:CZ	2.19	0.78
2:D:116:VAL:HG22	2:D:160:MET:HG2	1.67	0.76
2:D:4(P):PHE:CE2	2:D:26:LEU:HD11	2.20	0.76
2:D:67:PHE:CE1	2:D:71:LYS:HD3	2.20	0.76
1:A:103:ASN:HB3	1:A:153:PHE:CE1	2.21	0.74
2:D:148:VAL:HB	2:D:156:GLN:HG3	1.71	0.73
2:D:69:GLU:OE2	2:D:72:ARG:HD2	1.88	0.72
2:B:23:ARG:HH11	2:B:23:ARG:HG2	1.54	0.72
2:B:140:THR:HG21	5:B:230:HOH:O	1.90	0.71
1:A:74:LYS:HD2	2:B:7:PHE:CD2	2.25	0.71
1:C:40:GLU:HG3	1:C:42:ILE:HD11	1.71	0.71
2:D:126:ASN:HD22	2:D:126:ASN:H	1.39	0.70
1:C:135:THR:HG21	1:C:148:PHE:HB2	1.74	0.69
1:C:128:VAL:HG11	1:C:151:LEU:HD11	1.75	0.69
1:A:87:PRO:HD3	1:A:167:HIS:CD2	2.27	0.69
1:C:98:ASN:HB2	1:C:101:GLU:HG2	1.73	0.69
1:C:135:THR:CG2	1:C:148:PHE:HB2	2.22	0.69
1:A:47:GLU:HG3	5:A:222:HOH:O	1.93	0.68
1:C:26:PHE:HB2	1:C:31:ILE:HD11	1.74	0.68
2:D:13(L):GLY:HA2	2:D:16(L):SER:HB2	1.74	0.68
1:C:84:ASN:OD1	2:D:16(L):SER:HB3	1.95	0.67
1:C:7:ILE:HD13	2:D:86:PHE:HD2	1.59	0.67
1:A:87:PRO:HB3	1:A:112:PHE:CB	2.25	0.67
2:B:75:VAL:O	2:B:79:CYS:HB2	1.97	0.65
1:A:96:PRO:HB2	5:A:214:HOH:O	1.96	0.65
2:D:94:ARG:HD2	2:D:178:PRO:O	1.96	0.65
2:D:115:LEU:HD21	2:D:188:TRP:CZ3	2.32	0.65
2:B:92:PRO:O	2:B:94:ARG:HG2	1.98	0.64
2:D:7(P):GLU:HG3	2:D:67:PHE:CZ	2.31	0.64
1:C:122:LEU:HD23	1:C:127:PRO:HA	1.79	0.64
2:D:58:ALA:O	2:D:62:ASN:HB2	1.97	0.64
2:D:4(P):PHE:HE2	2:D:26:LEU:HD11	1.62	0.64
2:B:127:ILE:HG12	2:B:128:GLU:N	2.13	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:87:PRO:CB	1:A:112:PHE:HB3	2.26	0.63
2:B:26:LEU:H	2:B:42:SER:HB2	1.63	0.63
2:B:55:ARG:O	2:B:59:GLU:HG3	1.99	0.63
2:D:70:GLN:O	2:D:74:GLU:HG3	1.98	0.63
1:A:101:GLU:HG3	1:A:101:GLU:O	1.98	0.62
1:A:89:VAL:HG23	1:A:174:LEU:HD23	1.80	0.62
1:C:36:ILE:O	1:C:60:LEU:HD21	1.99	0.62
1:A:82:ASP:H	2:B:33:ASN:HD22	1.48	0.61
1:A:122:LEU:HD23	1:A:127:PRO:HA	1.81	0.61
2:D:90:LEU:HD22	2:D:153:TRP:CH2	2.36	0.61
1:C:39:SER:HB2	1:C:60:LEU:HD11	1.83	0.61
1:A:74:LYS:HD2	2:B:7:PHE:CG	2.34	0.61
1:A:98:ASN:HB2	1:A:101:GLU:CG	2.29	0.60
2:B:90:LEU:HD22	2:B:153:TRP:CH2	2.35	0.60
1:C:134:GLU:HB2	1:C:149:HIS:CE1	2.36	0.60
2:B:76:ASP:HA	2:B:80:ARG:HG3	1.82	0.60
1:A:84:ASN:OD1	2:B:16(L):SER:HB3	2.02	0.60
1:A:79:ASN:O	1:A:81:PRO:HD3	2.01	0.60
2:B:101:VAL:HG11	2:B:188:TRP:HB2	1.82	0.60
2:B:23:ARG:NH1	2:B:23:ARG:HG2	2.17	0.60
1:A:143:HIS:H	1:A:143:HIS:CD2	2.20	0.59
2:D:97:PRO:HB3	2:D:122:PHE:HB3	1.85	0.59
1:C:115:PRO:HD3	1:C:145:PHE:CE2	2.38	0.59
2:D:97:PRO:HB2	2:D:119:VAL:CG1	2.33	0.59
2:B:13(L):GLY:HA2	2:B:16(L):SER:HB2	1.85	0.58
1:C:143:HIS:H	1:C:143:HIS:CD2	2.19	0.58
1:A:51:PHE:HA	2:B:4(N):ARG:HA	1.85	0.58
2:D:180:LEU:HD13	2:D:184:VAL:HG23	1.84	0.58
1:A:14:LEU:HD22	1:A:115:PRO:HG2	1.85	0.58
1:A:81:PRO:O	2:B:11(L):SER:HB2	2.04	0.57
1:A:1:ILE:O	3:B:199:NAG:H82	2.05	0.57
2:B:69:GLU:OE2	2:B:72:ARG:HD2	2.03	0.57
2:D:92:PRO:O	2:D:94:ARG:HG2	2.03	0.57
2:B:126:ASN:H	2:B:126:ASN:HD22	1.53	0.56
2:B:127:ILE:HB	2:B:177:HIS:HD2	1.70	0.56
1:C:99:LEU:HD21	1:C:157:THR:HG23	1.88	0.56
2:D:1(L):ARG:NH1	2:D:60:ASN:OD1	2.39	0.56
1:A:119:VAL:HB	1:A:149:HIS:CD2	2.41	0.56
2:B:37:ASN:O	2:B:54:GLY:HA3	2.06	0.56
1:A:107:CYS:HB3	1:A:149:HIS:HB2	1.88	0.55
1:C:7:ILE:HD13	2:D:86:PHE:CD2	2.41	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:19:ARG:NH1	1:C:115:PRO:O	2.39	0.55
2:B:164:VAL:O	2:B:166:GLN:HG3	2.05	0.55
1:C:81:PRO:O	2:D:11(L):SER:HB2	2.07	0.55
1:A:82:ASP:HB2	2:B:33:ASN:HD22	1.73	0.54
1:A:19:ARG:HB3	5:A:227:HOH:O	2.07	0.54
2:B:67:PHE:CE1	2:B:71:LYS:HD3	2.42	0.54
1:C:79:ASN:O	1:C:81:PRO:HD3	2.08	0.54
1:A:101:GLU:HG3	5:A:211:HOH:O	2.07	0.54
1:C:124:ASN:HA	1:C:160:PHE:CE1	2.43	0.54
1:C:119:VAL:HA	1:C:164:GLU:O	2.08	0.53
2:D:17:PHE:CD1	2:D:24:VAL:HG22	2.44	0.53
2:D:166:GLN:HB2	2:D:169:GLU:OE2	2.08	0.53
1:A:86:ALA:HB2	1:A:169:GLY:O	2.09	0.53
2:B:133:ARG:HH12	2:B:169:GLU:HB2	1.74	0.53
1:C:47:GLU:O	1:C:50:LYS:HG2	2.08	0.53
1:A:111:LYS:HE3	5:A:221:HOH:O	2.08	0.52
2:D:69:GLU:OE1	2:D:72:ARG:NH1	2.42	0.52
1:C:109:ILE:HD12	1:C:109:ILE:H	1.74	0.52
1:C:119:VAL:HB	1:C:149:HIS:CD2	2.44	0.52
2:B:5(N):ASP:HB2	2:B:85:ILE:HG23	1.91	0.52
1:C:117:VAL:HG12	1:C:167:HIS:HB2	1.90	0.52
1:C:89:VAL:HG21	1:C:165:VAL:HG21	1.90	0.52
1:C:2:LYS:HA	2:D:19:ASN:OD1	2.10	0.52
2:B:129:VAL:HB	2:B:159:VAL:HG21	1.90	0.52
1:A:115:PRO:O	1:A:116:VAL:HG13	2.10	0.51
1:A:83:ALA:O	2:B:34:LEU:HD11	2.11	0.51
2:D:8(P):PHE:HD1	5:D:208:HOH:O	1.93	0.51
1:C:135:THR:O	1:C:147:LYS:NZ	2.44	0.51
1:A:119:VAL:HA	1:A:164:GLU:O	2.10	0.51
1:A:118:ASN:HB2	1:A:166:ASP:HB3	1.93	0.51
1:C:87:PRO:HB3	1:C:112:PHE:HB3	1.93	0.51
1:C:11:GLU:OE1	1:C:62:ASN:HB3	2.11	0.51
2:D:126:ASN:HD22	2:D:126:ASN:N	2.05	0.51
2:D:5(L):SER:O	2:D:6(L):LEU:HD23	2.10	0.51
2:B:24:VAL:HG21	2:B:80:ARG:HD3	1.93	0.50
1:A:143:HIS:HB3	2:B:31:PHE:HE2	1.76	0.50
1:C:111:LYS:HG2	1:C:140:ARG:NH1	2.27	0.50
1:C:94:ARG:NH1	5:C:213:HOH:O	2.44	0.50
1:C:83:ALA:O	2:D:6:TRP:HZ2	1.94	0.50
1:C:87:PRO:HD3	1:C:167:HIS:CD2	2.47	0.50
2:D:90:LEU:HD22	2:D:153:TRP:CZ3	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:38:LYS:HD3	1:A:38:LYS:N	2.26	0.50
2:B:38:LEU:HD21	2:B:61:TRP:CZ3	2.47	0.50
1:A:41:THR:C	1:A:42:ILE:HD13	2.33	0.49
2:D:173:CYS:O	2:D:185:THR:HA	2.12	0.49
2:B:127:ILE:HG12	2:B:128:GLU:H	1.76	0.49
2:B:75:VAL:O	2:B:80:ARG:HG2	2.13	0.49
1:C:109:ILE:N	1:C:109:ILE:HD12	2.27	0.49
1:A:7:ILE:HA	1:A:25:ASP:O	2.13	0.49
1:C:103:ASN:HB3	1:C:153:PHE:CE1	2.48	0.49
2:D:1(L):ARG:HD2	2:D:60:ASN:OD1	2.12	0.49
1:C:135:THR:HG23	1:C:148:PHE:HB2	1.95	0.49
2:D:6:TRP:CZ3	2:D:33:ASN:HA	2.48	0.49
1:A:120:THR:HB	1:A:164:GLU:HB3	1.95	0.49
1:C:101:GLU:HG3	1:C:101:GLU:O	2.13	0.49
2:D:97:PRO:HB2	2:D:119:VAL:HG12	1.94	0.49
2:B:133:ARG:HB2	2:B:138:GLU:HB2	1.95	0.49
1:A:142:ASP:HB2	1:A:143:HIS:HD2	1.78	0.48
1:A:82:ASP:H	2:B:33:ASN:ND2	2.11	0.48
1:C:142:ASP:HB2	1:C:143:HIS:HD2	1.78	0.48
1:C:79:ASN:OD1	3:C:193:NAG:H62	2.13	0.48
2:D:75:VAL:O	2:D:80:ARG:HG3	2.13	0.48
1:C:132:VAL:HG12	1:C:151:LEU:HD13	1.95	0.48
1:A:143:HIS:HB3	2:B:31:PHE:CE2	2.49	0.48
1:A:47:GLU:O	1:A:50:LYS:HG2	2.13	0.48
1:C:134:GLU:OE1	1:C:149:HIS:NE2	2.46	0.48
1:C:38:LYS:HD3	1:C:38:LYS:N	2.28	0.48
2:B:105:LYS:HD3	2:B:105:LYS:C	2.34	0.48
2:B:83:TYR:O	2:B:84:GLU:C	2.51	0.48
2:D:104:THR:OG1	2:D:114:LEU:HD23	2.13	0.48
1:A:67:LYS:NZ	1:A:67:LYS:O	2.46	0.48
1:C:122:LEU:HA	1:C:126:ARG:O	2.13	0.48
2:D:115:LEU:HD21	2:D:188:TRP:CE3	2.50	0.47
2:B:37:ASN:HB3	5:B:211:HOH:O	2.13	0.47
2:B:97:PRO:CB	2:B:122:PHE:HB3	2.39	0.47
2:B:47:PHE:CE2	2:B:61:TRP:CE3	3.02	0.47
1:C:76:ARG:HG3	5:C:218:HOH:O	2.13	0.47
1:A:98:ASN:CB	1:A:101:GLU:HG2	2.39	0.47
1:A:132:VAL:HG12	1:A:151:LEU:HD13	1.96	0.47
2:B:115:LEU:HD21	2:B:188:TRP:CZ3	2.49	0.47
2:B:6(L):LEU:HD23	2:B:6(L):LEU:N	2.29	0.47
1:C:122:LEU:O	1:C:161:TYR:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:134:ASN:HD21	2:D:169:GLU:CA	2.22	0.47
1:A:14:LEU:HD13	1:A:115:PRO:HD2	1.96	0.47
1:C:174:LEU:HD12	1:C:175:ARG:N	2.29	0.47
1:C:99:LEU:CD2	1:C:157:THR:HG23	2.45	0.47
1:A:94:ARG:NH1	2:B:121:ASP:OD1	2.47	0.47
2:D:105:LYS:HD3	2:D:105:LYS:C	2.34	0.47
1:C:140:ARG:HD3	1:C:144:LEU:HB2	1.96	0.47
1:A:4:GLU:CD	2:D:48:ARG:HH21	2.19	0.47
1:A:167:HIS:O	1:A:169:GLY:N	2.48	0.46
1:A:70:LEU:O	1:A:74:LYS:HB2	2.15	0.46
1:A:11:GLU:HA	1:A:21:GLU:O	2.16	0.46
2:B:173:CYS:O	2:B:185:THR:HA	2.15	0.46
2:B:60:ASN:O	2:B:64:GLN:HG3	2.15	0.46
2:D:67:PHE:HE1	2:D:71:LYS:HD3	1.74	0.46
1:A:40:GLU:HG3	1:A:42:ILE:HD11	1.97	0.46
1:C:107:CYS:HB2	1:C:121:TRP:CZ2	2.49	0.46
2:D:7(L):VAL:HA	2:D:8(L):PRO:HD2	1.78	0.46
1:A:76:ARG:O	1:A:76:ARG:HG2	2.14	0.46
1:C:39:SER:CB	1:C:60:LEU:HD11	2.45	0.46
2:D:129:VAL:HB	2:D:159:VAL:HG21	1.98	0.46
2:D:55:ARG:O	2:D:59:GLU:HG3	2.15	0.46
2:B:126:ASN:N	2:B:126:ASN:HD22	2.13	0.46
2:B:38:LEU:HD22	2:B:57:ASP:HB2	1.98	0.46
2:D:105:LYS:NZ	2:D:107:GLN:HA	2.31	0.46
1:A:78:ASN:OD1	3:A:193:NAG:N2	2.49	0.46
1:A:74:LYS:O	1:A:79:ASN:ND2	2.50	0.45
1:C:92:LEU:HD23	1:C:92:LEU:N	2.31	0.45
1:C:11:GLU:HA	1:C:21:GLU:O	2.16	0.45
1:A:48:PHE:CE1	2:B:90:LEU:HD21	2.52	0.45
1:A:12:PHE:C	1:A:12:PHE:CD1	2.90	0.45
2:B:5(L):SER:C	2:B:6(L):LEU:HD23	2.37	0.45
2:D:101:VAL:HA	2:D:116:VAL:O	2.16	0.45
1:A:94:ARG:HH11	1:A:94:ARG:HG2	1.82	0.45
1:A:13:TYR:CE2	1:A:67:LYS:HG2	2.52	0.45
2:D:13:SER:HA	2:D:28:VAL:HA	1.99	0.45
1:A:78:ASN:O	1:A:78:ASN:CG	2.55	0.45
2:B:105:LYS:NZ	2:B:107:GLN:HA	2.32	0.45
1:A:167:HIS:C	1:A:169:GLY:H	2.20	0.44
1:C:134:GLU:OE1	1:C:149:HIS:CE1	2.70	0.44
1:A:50:LYS:HE2	1:A:51:PHE:HE2	1.83	0.44
1:C:21:GLU:OE1	1:C:137:PHE:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:160:PHE:CD1	1:C:160:PHE:C	2.91	0.44
1:C:51:PHE:HA	2:D:4(N):ARG:HA	1.99	0.44
2:B:38:LEU:HD13	2:B:58:ALA:HB2	1.99	0.44
2:B:63:SER:O	2:B:65:PRO:HD3	2.17	0.44
1:C:98:ASN:HB2	1:C:101:GLU:CG	2.44	0.44
1:A:87:PRO:HB2	1:A:109:ILE:CG2	2.47	0.44
1:A:50:LYS:HE2	1:A:51:PHE:CE2	2.53	0.44
2:B:114:LEU:HG	2:B:160:MET:HB3	1.99	0.44
1:C:78:ASN:CG	1:C:78:ASN:O	2.56	0.44
1:A:80:THR:HG22	2:B:11(L):SER:HB3	1.98	0.44
2:B:166:GLN:O	2:B:169:GLU:HG3	2.16	0.44
1:C:65:VAL:HG13	2:D:8(P):PHE:CD2	2.53	0.44
2:B:38:LEU:HD11	2:B:47:PHE:HB3	2.00	0.44
1:C:105:LEU:HA	1:C:105:LEU:HD23	1.78	0.44
1:C:89:VAL:CG2	1:C:165:VAL:HG21	2.48	0.43
1:A:87:PRO:CA	1:A:112:PHE:HB3	2.48	0.43
2:D:128:GLU:HB2	2:D:176:GLU:HB2	2.00	0.43
2:B:137:GLU:O	2:B:139:LYS:N	2.51	0.43
3:C:193:NAG:C1	3:C:193:NAG:O7	2.66	0.43
1:C:82:ASP:H	2:D:33:ASN:HD22	1.66	0.43
2:D:9(L):ARG:HD2	2:D:9(L):ARG:H	1.83	0.43
1:A:61:ALA:O	1:A:64:ALA:HB3	2.18	0.43
2:B:83:TYR:O	2:B:86:PHE:N	2.51	0.43
2:B:70:GLN:O	2:B:74:GLU:HG3	2.19	0.43
2:D:4(P):PHE:CZ	2:D:26:LEU:HD11	2.53	0.43
1:A:41:THR:O	1:A:42:ILE:HD13	2.18	0.43
2:B:58:ALA:O	2:B:62:ASN:HB2	2.19	0.43
2:B:87:ASP:HA	2:B:91:VAL:CG2	2.49	0.43
2:D:133:ARG:HH12	2:D:169:GLU:HB2	1.83	0.43
1:A:8:ILE:HB	1:A:25:ASP:HB3	2.00	0.43
2:B:134:ASN:ND2	2:B:169:GLU:HA	2.20	0.43
5:A:232:HOH:O	2:B:2(L):LYS:HG3	2.19	0.43
1:C:115:PRO:O	1:C:116:VAL:HG13	2.18	0.43
1:A:39:SER:OG	1:A:57:GLN:NE2	2.52	0.43
2:D:82:ASN:O	2:D:85:ILE:HB	2.19	0.43
1:A:22:PHE:CD1	1:A:22:PHE:C	2.92	0.42
1:C:138:LEU:HB2	1:C:146:ARG:HG3	2.01	0.42
2:D:26:LEU:H	2:D:42:SER:CB	2.33	0.42
1:C:23:MET:HA	1:C:33:HIS:HA	2.01	0.42
2:B:177:HIS:HB3	2:B:180:LEU:HG	2.00	0.42
1:C:118:ASN:OD1	3:C:194:NAG:O5	2.37	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:68:LEU:O	2:D:72:ARG:HB2	2.19	0.42
2:B:122:PHE:HE1	2:B:125:GLY:O	2.03	0.42
2:B:90:LEU:HA	2:B:90:LEU:HD23	1.82	0.42
2:D:177:HIS:C	2:D:179:SER:H	2.22	0.42
1:A:140:ARG:HB2	1:A:144:LEU:O	2.18	0.42
2:B:180:LEU:HD13	2:B:184:VAL:HG23	2.01	0.42
2:B:23:ARG:CG	2:B:23:ARG:NH1	2.80	0.42
2:B:46:GLU:HB2	2:B:48:ARG:NH1	2.34	0.42
1:C:140:ARG:HB2	1:C:144:LEU:O	2.20	0.42
1:C:2:LYS:NZ	2:D:18:TYR:O	2.45	0.42
1:A:163:CYS:O	1:A:175:ARG:HA	2.20	0.42
1:C:8:ILE:HB	1:C:25:ASP:HB3	2.00	0.42
2:B:4(P):PHE:HD2	2:B:74:GLU:OE1	2.03	0.42
1:C:174:LEU:HD12	1:C:175:ARG:H	1.85	0.42
1:C:70:LEU:HD13	2:D:9:GLU:N	2.34	0.42
2:D:164:VAL:O	2:D:164:VAL:HG23	2.19	0.42
1:A:103:ASN:HB3	1:A:153:PHE:CZ	2.55	0.42
1:A:109:ILE:H	1:A:109:ILE:HD12	1.85	0.42
1:C:132:VAL:HG12	1:C:151:LEU:CD1	2.50	0.42
1:A:116:VAL:HG23	1:A:116:VAL:O	2.20	0.42
2:B:9(L):ARG:H	2:B:9(L):ARG:HD2	1.85	0.42
2:D:5(L):SER:C	2:D:6(L):LEU:HD23	2.40	0.41
1:A:69:ASN:O	1:A:72:VAL:HB	2.21	0.41
2:D:38:LEU:HD21	2:D:61:TRP:CZ3	2.55	0.41
1:A:143:HIS:CD2	1:A:143:HIS:N	2.86	0.41
2:B:104:THR:OG1	2:B:114:LEU:HD23	2.20	0.41
2:B:133:ARG:HH12	2:B:169:GLU:CD	2.23	0.41
1:C:83:ALA:O	2:D:6:TRP:CZ2	2.74	0.41
1:C:81:PRO:HB2	2:D:5:PRO:HA	2.03	0.41
1:A:108:PHE:CE1	1:A:146:ARG:HB2	2.55	0.41
2:D:101:VAL:O	2:D:102:TYR:HB3	2.20	0.41
2:D:90:LEU:HA	2:D:90:LEU:HD23	1.59	0.41
2:B:166:GLN:HB2	2:B:169:GLU:OE2	2.20	0.41
2:B:176:GLU:HG3	2:B:183:PRO:HB3	2.03	0.41
1:A:82:ASP:HB2	2:B:33:ASN:HB3	2.03	0.41
2:B:68:LEU:HD12	2:B:68:LEU:HA	1.81	0.41
2:B:46:GLU:HB3	2:B:62:ASN:ND2	2.36	0.41
1:A:122:LEU:HB2	1:A:162:ASP:HB2	2.02	0.41
1:C:105:LEU:HD11	1:C:178:TRP:CE3	2.55	0.41
1:A:39:SER:OG	1:A:60:LEU:HD11	2.21	0.41
1:C:122:LEU:HB2	1:C:162:ASP:HB2	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:27:LEU:HD11	2:D:39:ARG:HD3	2.03	0.41
2:D:111:HIS:O	2:D:112:HIS:CB	2.68	0.40
2:D:4(P):PHE:HZ	2:D:15:CYS:SG	2.44	0.40
2:B:7(N):MET:HG2	2:B:7(N):MET:H	1.72	0.40
2:D:97:PRO:HB3	2:D:122:PHE:CB	2.50	0.40
1:A:124:ASN:HA	1:A:160:PHE:CE1	2.57	0.40
1:A:89:VAL:HG12	1:A:90:THR:N	2.37	0.40
2:B:7(P):GLU:HG3	2:B:67:PHE:CE1	2.55	0.40
1:C:121:TRP:O	1:C:127:PRO:HA	2.21	0.40
1:A:166:ASP:OD1	1:A:173:PRO:HG3	2.21	0.40
1:C:143:HIS:HB3	2:D:31:PHE:CE2	2.57	0.40
2:D:137:GLU:OE2	2:D:139:LYS:NZ	2.54	0.40
1:A:45:LEU:HD12	1:A:48:PHE:CZ	2.57	0.40
1:C:124:ASN:HA	1:C:160:PHE:CZ	2.55	0.40
2:D:133:ARG:HH12	2:D:169:GLU:CD	2.25	0.40
1:C:77:SER:HB3	2:D:53:LEU:HD11	2.02	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	A	180/192 (94%)	162 (90%)	14 (8%)	4 (2%)	6	17
1	C	180/192 (94%)	164 (91%)	12 (7%)	4 (2%)	6	17
2	B	212/227 (93%)	178 (84%)	27 (13%)	7 (3%)	4	8
2	D	212/227 (93%)	182 (86%)	24 (11%)	6 (3%)	5	11
All	All	784/838 (94%)	686 (88%)	77 (10%)	21 (3%)	5	12

All (21) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	107	GLN
2	B	108	PRO
2	D	107	GLN
2	D	108	PRO
1	A	17	ASP
1	A	142	ASP
1	A	168	TRP
2	B	2(L)	LYS
2	B	135	GLY
2	B	138	GLU
1	C	136	VAL
1	C	155	PRO
1	C	168	TRP
2	D	112	HIS
1	A	155	PRO
2	B	112	HIS
2	D	22	GLN
2	D	178	PRO
1	C	142	ASP
2	D	135	GLY
2	B	178	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	163/175 (93%)	151 (93%)	12 (7%)	13	32
1	C	163/175 (93%)	150 (92%)	13 (8%)	12	27
2	B	186/205 (91%)	174 (94%)	12 (6%)	17	38
2	D	186/205 (91%)	173 (93%)	13 (7%)	15	35
All	All	698/760 (92%)	648 (93%)	50 (7%)	14	34

All (50) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	THR

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Mol	Chain	Res	Type
1	A	19	ARG
1	A	38	LYS
1	A	46	GLU
1	A	60	LEU
1	A	67	LYS
1	A	82	ASP
1	A	94	ARG
1	A	130	GLU
1	A	136	VAL
1	A	156	SER
1	A	157	THR
2	B	7(N)	MET
2	B	80	ARG
2	B	84	GLU
2	B	89	PHE
2	B	114	LEU
2	B	115	LEU
2	B	120	SER
2	B	121	ASP
2	B	126	ASN
2	B	163	THR
2	B	169	GLU
2	B	172	THR
1	C	17	ASP
1	C	19	ARG
1	C	38	LYS
1	C	67	LYS
1	C	95	SER
1	C	104	ILE
1	C	116	VAL
1	C	129	THR
1	C	130	GLU
1	C	133	SER
1	C	136	VAL
1	C	156	SER
1	C	157	THR
2	D	7(N)	MET
2	D	8	LEU
2	D	21	THR
2	D	68	LEU
2	D	84	GLU
2	D	89	PHE

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Mol	Chain	Res	Type
2	D	114	LEU
2	D	115	LEU
2	D	126	ASN
2	D	169	GLU
2	D	172	THR
2	D	178	PRO
2	D	185	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	57	GLN
1	A	143	HIS
1	A	149	HIS
1	A	167	HIS
2	B	126	ASN
2	B	174	GLN
1	C	143	HIS
1	C	149	HIS
2	D	64	GLN
2	D	126	ASN
2	D	134	ASN
2	D	174	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 ⓘ

There are no monosaccharides in this entry.

## 5.6 Ligand geometry ⓘ

7 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	NAG	C	194	1	14,14,15	0.67	0	17,19,21	0.93	1 (5%)
3	NAG	A	193	1	14,14,15	0.55	0	17,19,21	0.56	0
3	NAG	C	193	1	14,14,15	0.55	0	17,19,21	0.90	0
3	NAG	D	199	2	14,14,15	0.48	0	17,19,21	0.98	2 (11%)
3	NAG	B	199	2	14,14,15	0.68	0	17,19,21	0.52	0
4	SO4	D	200	-	4,4,4	0.57	0	6,6,6	0.32	0
3	NAG	A	194	1	14,14,15	0.72	0	17,19,21	1.13	2 (11%)

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	C	194	1	1/1/5/7	1/6/23/26	0/1/1/1
3	NAG	A	193	1	-	3/6/23/26	0/1/1/1
3	NAG	C	193	1	-	3/6/23/26	0/1/1/1
3	NAG	D	199	2	-	2/6/23/26	0/1/1/1
3	NAG	B	199	2	-	0/6/23/26	0/1/1/1
3	NAG	A	194	1	1/1/5/7	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	194	NAG	O5-C1-C2	-2.66	107.09	111.29
3	D	199	NAG	C1-O5-C5	2.44	115.49	112.19
3	A	194	NAG	C1-C2-N2	-2.43	106.34	110.49
3	C	194	NAG	O5-C1-C2	-2.24	107.75	111.29
3	D	199	NAG	C4-C3-C2	-2.15	107.87	111.02

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	C	194	NAG	C1
3	A	194	NAG	C1

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	193	NAG	C1-C2-N2-C7
3	C	193	NAG	O5-C5-C6-O6
3	A	193	NAG	O5-C5-C6-O6
3	A	193	NAG	C4-C5-C6-O6
3	C	193	NAG	C4-C5-C6-O6
3	A	193	NAG	C1-C2-N2-C7
3	D	199	NAG	O5-C5-C6-O6
3	C	194	NAG	O5-C5-C6-O6
3	D	199	NAG	C4-C5-C6-O6

There are no ring outliers.

4 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	194	NAG	1	0
3	A	193	NAG	1	0
3	C	193	NAG	2	0
3	B	199	NAG	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 ⓘ

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.