



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 01:28 AM BST

PDB ID : 1IEA
Title : HISTOCOMPATIBILITY ANTIGEN
Authors : Fremont, D.H.; Hendrickson, W.A.; Marrack, P.; Kappler, J.
Deposited on : 1996-04-05
Resolution : 2.30 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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

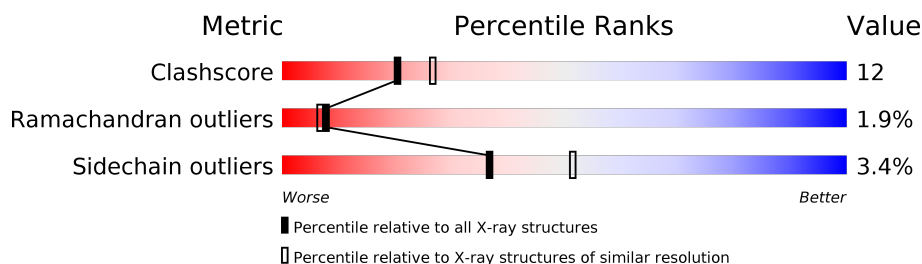
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)

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 ≥ 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	228	
2	D	228	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 6769 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
			1680	1063	290	321	6			
2	D	214	Total	C	N	O	S	0	0	0
			1680	1063	290	321	6			

- 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	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 water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	95	Total	O	0	0
			95	95		
4	B	79	Total	O	0	0
			79	79		
4	C	84	Total	O	0	0
			84	84		
4	D	91	Total	O	0	0
			91	91		

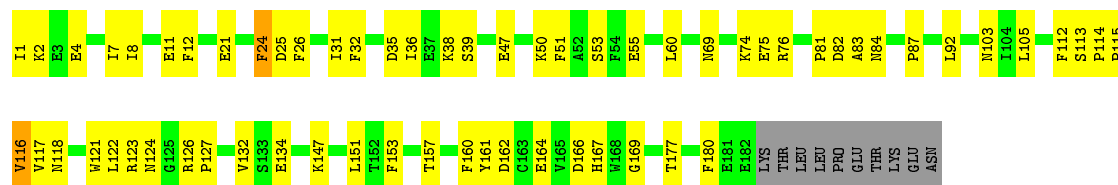
3 Residue-property plots

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.

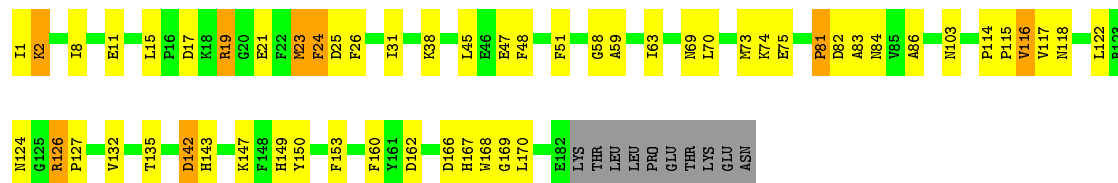
• Molecule 1: MHC CLASS II I-EK

Chain A: 



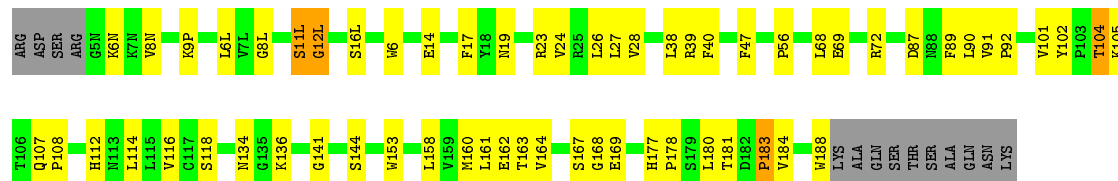
• Molecule 1: MHC CLASS II I-EK

Chain C: 



• Molecule 2: MHC CLASS II I-EK

Chain B: 



• Molecule 2: MHC CLASS II I-EK

Chain D: 





4 Data and refinement statistics

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

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	147.02Å 57.09Å 117.01Å 90.00° 91.52° 90.00°	Depositor
Resolution (Å)	6.00 – 2.30	Depositor
% Data completeness (in resolution range)	88.7 (6.00-2.30)	Depositor
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
Refinement program	X-PLOR	Depositor
R, R_{free}	0.202 , 0.274	Depositor
Estimated twinning fraction	No twinning to report.	Xtriage
Total number of atoms	6769	wwPDB-VP
Average B, all atoms (Å ²)	32.0	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

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	0.55	0/1530	0.75	0/2081
1	C	0.55	0/1530	0.76	0/2081
2	B	0.51	0/1722	0.77	1/2342 (0.0%)
2	D	0.53	0/1722	0.77	1/2342 (0.0%)
All	All	0.54	0/6504	0.76	2/8846 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	108	PRO	N-CA-CB	5.77	110.22	103.30
2	D	108	PRO	N-CA-CB	5.75	110.21	103.30

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	A	1488	0	1413	45	0
1	C	1488	0	1412	46	0
2	B	1680	0	1567	44	0
2	D	1680	0	1567	43	0
3	A	28	0	26	1	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	14	0	13	0	0
3	C	28	0	26	2	0
3	D	14	0	13	0	0
4	A	95	0	0	3	0
4	B	79	0	0	0	0
4	C	84	0	0	8	0
4	D	91	0	0	2	0
All	All	6769	0	6037	154	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 12.

All (154) 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:C:83:ALA:HB2	2:D:12(L):GLY:HA3	1.45	0.95
1:C:82:ASP:HA	2:D:11(L):SER:HA	1.68	0.76
2:B:23:ARG:HH11	2:B:23:ARG:HG2	1.52	0.74
2:B:114:LEU:HD22	2:B:160:MET:HB3	1.69	0.74
1:A:1:ILE:HG22	1:A:2:LYS:H	1.55	0.72
2:D:136:LYS:NZ	2:D:136:LYS:HB2	2.03	0.71
2:D:23:ARG:HH11	2:D:23:ARG:HG2	1.55	0.71
1:A:83:ALA:HB2	2:B:12(L):GLY:HA3	1.74	0.70
1:A:82:ASP:HA	2:B:11(L):SER:HA	1.72	0.69
1:A:122:LEU:HB2	1:A:162:ASP:HB2	1.74	0.69
1:C:122:LEU:HB2	1:C:162:ASP:HB2	1.72	0.69
1:A:51:PHE:O	2:B:6(N):LYS:HA	1.93	0.69
1:C:23:MET:SD	4:C:242:HOH:O	2.53	0.65
1:A:84:ASN:ND2	2:B:16(L):SER:HB3	2.13	0.63
1:A:2:LYS:HA	2:B:19:ASN:OD1	2.00	0.62
1:A:103:ASN:HB3	1:A:153:PHE:CE1	2.34	0.62
1:C:84:ASN:ND2	2:D:16(L):SER:HB3	2.13	0.62
2:D:65:PRO:O	2:D:69:GLU:HG2	2.00	0.60
1:C:143:HIS:H	1:C:143:HIS:CD2	2.20	0.60
1:A:124:ASN:HA	1:A:160:PHE:CZ	2.37	0.59
1:C:149:HIS:HD2	4:C:219:HOH:O	1.85	0.59
2:B:136:LYS:HB2	2:B:136:LYS:NZ	2.18	0.58
2:D:27:LEU:HD11	2:D:39:ARG:HD3	1.84	0.58
1:C:26:PHE:HB2	1:C:31:ILE:HD11	1.86	0.58
1:A:36:ILE:HG23	1:A:60:LEU:HD22	1.85	0.57
2:D:4(P):PHE:HZ	2:D:15:CYS:SG	2.27	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:PRO:HB3	2:B:6:TRP:CE3	2.40	0.57
1:C:19:ARG:NH1	1:C:115:PRO:O	2.39	0.56
1:C:168:TRP:CD2	3:C:194:NAG:H82	2.40	0.56
1:A:115:PRO:O	1:A:116:VAL:HG13	2.05	0.56
1:C:103:ASN:HB3	1:C:153:PHE:CE1	2.40	0.56
1:A:53:SER:OG	2:B:8(N):VAL:HG22	2.05	0.56
1:A:81:PRO:HB2	4:A:270:HOH:O	2.05	0.55
1:A:1:ILE:HG22	1:A:2:LYS:N	2.22	0.54
1:A:87:PRO:HB3	1:A:112:PHE:HB3	1.89	0.54
1:A:157:THR:HG22	1:A:180:PHE:HD2	1.72	0.54
1:C:82:ASP:HA	2:D:11(L):SER:CA	2.38	0.53
1:A:38:LYS:HB3	4:A:288:HOH:O	2.07	0.53
1:C:168:TRP:CE2	3:C:194:NAG:H82	2.44	0.53
1:C:11:GLU:HA	1:C:21:GLU:O	2.08	0.53
2:D:113:ASN:O	2:D:162:GLU:HA	2.09	0.53
2:D:66:GLU:HG2	4:D:256:HOH:O	2.09	0.53
1:A:76:ARG:HD3	2:B:56:PRO:HG2	1.92	0.52
2:D:136:LYS:HZ3	2:D:136:LYS:HB2	1.74	0.51
1:C:118:ASN:HB2	1:C:166:ASP:HB3	1.91	0.51
1:A:167:HIS:CD2	1:A:169:GLY:H	2.28	0.51
1:C:51:PHE:O	2:D:6(N):LYS:HA	2.11	0.51
1:A:26:PHE:HB2	1:A:31:ILE:HD11	1.91	0.51
2:B:141:GLY:O	2:B:162:GLU:HG3	2.11	0.50
2:D:55:ARG:O	2:D:59:GLU:HG3	2.11	0.50
2:D:5(P):ASN:ND2	2:D:67:PHE:HE1	2.10	0.50
1:C:124:ASN:HA	1:C:160:PHE:CZ	2.47	0.50
1:C:147:LYS:HD3	1:C:149:HIS:HE1	1.75	0.50
2:D:5(P):ASN:HD22	2:D:67:PHE:HE1	1.60	0.50
2:B:134:ASN:HD21	2:B:169:GLU:HG3	1.77	0.50
1:A:157:THR:HG22	1:A:180:PHE:CD2	2.47	0.49
1:C:69:ASN:O	1:C:73:MET:HG2	2.13	0.49
1:C:167:HIS:CD2	1:C:169:GLY:H	2.30	0.49
1:C:114:PRO:HB3	2:D:6:TRP:CE3	2.47	0.49
2:B:112:HIS:HA	2:B:164:VAL:HG22	1.94	0.49
1:C:167:HIS:HA	4:C:204:HOH:O	2.13	0.48
2:B:118:SER:HA	2:B:158:LEU:HD23	1.94	0.48
1:C:142:ASP:HB2	1:C:143:HIS:HD2	1.78	0.48
1:C:149:HIS:CD2	4:C:219:HOH:O	2.65	0.48
2:D:23:ARG:HH11	2:D:23:ARG:CG	2.26	0.48
1:C:19:ARG:HD3	1:C:116:VAL:CG1	2.44	0.47
1:A:123:ARG:HG3	1:A:161:TYR:CE2	2.49	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:101:VAL:HA	2:B:116:VAL:O	2.14	0.47
1:C:17:ASP:HB2	1:C:19:ARG:HG2	1.97	0.47
2:B:101:VAL:HG12	2:B:102:TYR:N	2.30	0.47
2:B:14:GLU:O	2:B:26:LEU:HD12	2.14	0.47
2:B:177:HIS:CD2	2:B:178:PRO:HD2	2.50	0.47
1:C:81:PRO:O	2:D:11(L):SER:HB2	2.15	0.47
2:D:11(L):SER:O	2:D:13(L):GLY:N	2.48	0.47
2:D:74:GLU:HA	2:D:77:THR:OG1	2.15	0.47
2:D:101:VAL:O	2:D:102:TYR:HB3	2.15	0.46
1:A:132:VAL:HG12	1:A:151:LEU:HD13	1.96	0.46
1:A:84:ASN:HD22	2:B:16(L):SER:HB3	1.80	0.46
2:B:68:LEU:HD13	2:B:72:ARG:NH2	2.31	0.46
2:D:172:THR:HG23	2:D:187:GLU:HG2	1.98	0.46
1:A:124:ASN:HA	1:A:160:PHE:CE1	2.50	0.46
2:D:120:SER:HB2	4:D:213:HOH:O	2.15	0.46
1:C:114:PRO:HD3	2:D:6:TRP:CE2	2.50	0.46
1:A:164:GLU:HG2	4:A:266:HOH:O	2.16	0.46
1:C:23:MET:HE3	1:C:24:PHE:C	2.36	0.45
1:C:135:THR:O	1:C:147:LYS:NZ	2.49	0.45
1:A:92:LEU:HD23	1:A:92:LEU:N	2.32	0.45
1:C:59:ALA:O	1:C:63:ILE:HG12	2.17	0.45
1:A:134:GLU:OE2	1:A:147:LYS:NZ	2.50	0.45
1:C:1:ILE:HG22	1:C:2:LYS:N	2.32	0.45
1:C:8:ILE:HB	1:C:25:ASP:HB3	1.99	0.45
1:C:45:LEU:HD12	1:C:48:PHE:CZ	2.51	0.45
1:C:132:VAL:HA	1:C:150:TYR:O	2.17	0.45
2:D:128:GLU:CD	2:D:130:ARG:HH22	2.19	0.45
2:B:23:ARG:HH21	2:D:43:ASP:CG	2.20	0.45
1:A:113:SER:OG	1:A:114:PRO:HA	2.17	0.45
3:A:194:NAG:O7	3:A:194:NAG:C1	2.65	0.45
2:D:161:LEU:HG	2:D:163:THR:HG23	1.98	0.44
1:A:69:ASN:HB3	2:B:9(P):LYS:HD2	1.98	0.44
1:A:11:GLU:HA	1:A:21:GLU:O	2.17	0.44
2:B:91:VAL:N	2:B:92:PRO:HD2	2.32	0.44
1:A:105:LEU:HD23	1:A:105:LEU:HA	1.90	0.44
1:C:143:HIS:HE1	4:C:227:HOH:O	2.01	0.44
2:D:97:PRO:HB3	2:D:122:PHE:HB3	1.99	0.43
2:D:133:ARG:NH1	2:D:163:THR:HG22	2.33	0.43
1:C:8:ILE:HG12	2:D:14:GLU:HG2	2.00	0.43
2:D:101:VAL:HA	2:D:116:VAL:O	2.18	0.43
2:B:161:LEU:HG	2:B:163:THR:HG23	1.99	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:38:LEU:HD11	2:B:47:PHE:HB3	2.00	0.43
1:C:147:LYS:HD3	1:C:149:HIS:CE1	2.53	0.43
1:C:19:ARG:NH2	4:C:214:HOH:O	2.52	0.43
1:A:12:PHE:CD1	1:A:12:PHE:C	2.92	0.43
2:D:32:TYR:CD2	2:D:53:LEU:HD21	2.52	0.43
2:D:68:LEU:HD13	2:D:72:ARG:NH2	2.33	0.43
1:C:126:ARG:HA	1:C:127:PRO:HD3	1.94	0.43
1:A:84:ASN:HD22	2:B:16(L):SER:CB	2.31	0.43
2:D:93:ARG:O	2:D:94:ARG:NH1	2.48	0.43
2:B:104:THR:OG1	2:B:114:LEU:HB3	2.19	0.43
2:B:90:LEU:HD22	2:B:153:TRP:CH2	2.54	0.43
2:B:27:LEU:HD11	2:B:39:ARG:HD3	2.00	0.42
1:A:8:ILE:HB	1:A:25:ASP:HB3	2.00	0.42
1:C:84:ASN:ND2	2:D:16(L):SER:CB	2.82	0.42
2:B:28:VAL:HB	2:B:40:PHE:HB3	2.01	0.42
1:C:15:LEU:HD23	1:C:15:LEU:HA	1.74	0.42
1:A:126:ARG:HA	1:A:127:PRO:HD3	1.87	0.42
2:B:87:ASP:O	2:B:92:PRO:HD3	2.20	0.42
1:C:58:GLY:HA3	4:C:245:HOH:O	2.20	0.42
2:D:46:GLU:HB2	2:D:48:ARG:NH1	2.35	0.42
1:A:118:ASN:HB2	1:A:166:ASP:HB3	2.02	0.42
2:B:101:VAL:O	2:B:102:TYR:HB3	2.20	0.42
2:B:116:VAL:HG12	2:B:158:LEU:HD22	2.00	0.42
1:A:4:GLU:HA	2:B:17:PHE:O	2.20	0.42
2:B:114:LEU:HD13	2:B:160:MET:SD	2.60	0.42
2:B:23:ARG:HG2	2:B:23:ARG:NH1	2.26	0.42
2:D:4(P):PHE:CD2	2:D:13:SER:HB2	2.54	0.42
1:A:24:PHE:HB2	1:A:32:PHE:CE1	2.55	0.41
2:B:69:GLU:OE1	2:B:72:ARG:NH1	2.53	0.41
2:B:144:SER:O	2:D:6(L):LEU:HA	2.20	0.41
1:C:70:LEU:O	1:C:74:LYS:HG3	2.20	0.41
1:A:47:GLU:O	1:A:50:LYS:HG2	2.20	0.41
2:B:17:PHE:CD1	2:B:24:VAL:HG22	2.56	0.41
1:C:86:ALA:HB1	1:C:170:LEU:CD2	2.51	0.41
2:D:132:PHE:CE2	2:D:137:GLU:HB2	2.56	0.41
2:B:6(L):LEU:HA	2:D:144:SER:O	2.21	0.41
1:C:47:GLU:HG2	4:C:237:HOH:O	2.21	0.41
1:A:7:ILE:HA	1:A:25:ASP:O	2.21	0.40
2:B:180:LEU:HD13	2:B:184:VAL:HG23	2.03	0.40
2:D:75:VAL:O	2:D:79:CYS:HB2	2.20	0.40
1:A:121:TRP:O	1:A:127:PRO:HA	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:74:LYS:HB3	1:A:74:LYS:HE2	1.89	0.40
1:A:35:ASP:O	1:A:39:SER:N	2.54	0.40
2:B:188:TRP:CE3	2:B:188:TRP:C	2.95	0.40
2:D:20:GLY:HA2	2:D:83:TYR:CZ	2.57	0.40
2:B:114:LEU:HD23	2:B:114:LEU:HA	1.90	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%)	175 (97%)	5 (3%)	0	100	100
1	C	180/192 (94%)	172 (96%)	6 (3%)	2 (1%)	14	15
2	B	212/228 (93%)	194 (92%)	10 (5%)	8 (4%)	3	1
2	D	212/228 (93%)	194 (92%)	13 (6%)	5 (2%)	6	4
All	All	784/840 (93%)	735 (94%)	34 (4%)	15 (2%)	8	7

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	107	GLN
2	D	107	GLN
2	B	8(L)	GLY
2	D	8(L)	GLY
2	D	12(L)	GLY
2	B	11(L)	SER
2	B	105	LYS
2	B	12(L)	GLY
1	C	142	ASP
2	D	105	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	167	SER
2	B	183	PRO
1	C	81	PRO
2	D	15(L)	GLY
2	B	168	GLY

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%)	157 (96%)	6 (4%)	34	48
1	C	163/175 (93%)	154 (94%)	9 (6%)	21	30
2	B	178/200 (89%)	174 (98%)	4 (2%)	52	69
2	D	178/200 (89%)	174 (98%)	4 (2%)	52	69
All	All	682/750 (91%)	659 (97%)	23 (3%)	37	51

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	PHE
1	A	55	GLU
1	A	75	GLU
1	A	116	VAL
1	A	117	VAL
1	A	177	THR
2	B	89	PHE
2	B	104	THR
2	B	181	THR
2	B	183	PRO
1	C	2	LYS
1	C	19	ARG
1	C	23	MET
1	C	24	PHE
1	C	38	LYS
1	C	75	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	C	116	VAL
1	C	117	VAL
1	C	126	ARG
2	D	23	ARG
2	D	89	PHE
2	D	104	THR
2	D	181	THR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (11) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	143	HIS
1	A	149	HIS
1	A	167	HIS
2	B	5(P)	ASN
2	B	70	GLN
1	C	57	GLN
1	C	143	HIS
1	C	149	HIS
1	C	167	HIS
2	D	5(P)	ASN
2	D	166	GLN

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 [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NAG	C	194	1	14,14,15	0.60	0	17,19,21	1.70	3 (17%)
3	NAG	D	199	2	14,14,15	0.81	0	17,19,21	1.19	2 (11%)
3	NAG	B	199	2	14,14,15	0.75	0	17,19,21	0.95	1 (5%)
3	NAG	A	193	1	14,14,15	0.53	0	17,19,21	0.72	0
3	NAG	C	193	1	14,14,15	0.47	0	17,19,21	0.58	0
3	NAG	A	194	1	14,14,15	0.54	0	17,19,21	1.18	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	-	2/6/23/26	0/1/1/1
3	NAG	D	199	2	-	4/6/23/26	0/1/1/1
3	NAG	B	199	2	-	3/6/23/26	0/1/1/1
3	NAG	A	193	1	-	2/6/23/26	0/1/1/1
3	NAG	C	193	1	-	0/6/23/26	0/1/1/1
3	NAG	A	194	1	-	2/6/23/26	0/1/1/1

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	194	NAG	C4-C3-C2	-3.56	105.80	111.02
3	C	194	NAG	C1-O5-C5	3.30	116.66	112.19
3	C	194	NAG	C1-C2-N2	2.95	115.53	110.49
3	D	199	NAG	C1-O5-C5	2.90	116.13	112.19
3	D	199	NAG	C8-C7-N2	-2.29	112.22	116.10
3	A	194	NAG	C4-C3-C2	-2.27	107.69	111.02
3	B	199	NAG	C1-O5-C5	2.26	115.25	112.19
3	A	194	NAG	C2-N2-C7	2.17	125.99	122.90

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	194	NAG	C1-C2-N2-C7
3	C	194	NAG	C1-C2-N2-C7
3	D	199	NAG	O5-C5-C6-O6
3	B	199	NAG	C1-C2-N2-C7
3	B	199	NAG	O5-C5-C6-O6
3	D	199	NAG	C1-C2-N2-C7
3	D	199	NAG	C3-C2-N2-C7
3	C	194	NAG	O5-C5-C6-O6
3	D	199	NAG	C4-C5-C6-O6
3	A	193	NAG	C4-C5-C6-O6
3	B	199	NAG	C3-C2-N2-C7
3	A	193	NAG	O5-C5-C6-O6
3	A	194	NAG	C4-C5-C6-O6

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	194	NAG	2	0
3	A	194	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.