



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 01:14 AM GMT

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 validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

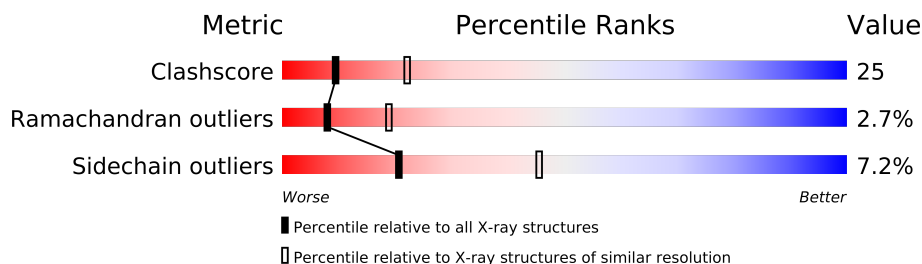
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : **NOT EXECUTED**
EDS : **NOT EXECUTED**
Percentile statistics : 21963
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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	79885	1939 (2.70-2.70)
Ramachandran outliers	78287	1905 (2.70-2.70)
Sidechain outliers	78261	1905 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Note EDS was not executed.

Mol	Chain	Length	Quality of chain
1	A	192	
1	C	192	
2	B	227	
2	D	227	

2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 6672 atoms, of which 0 are hydrogen and 0 are deuterium.

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.

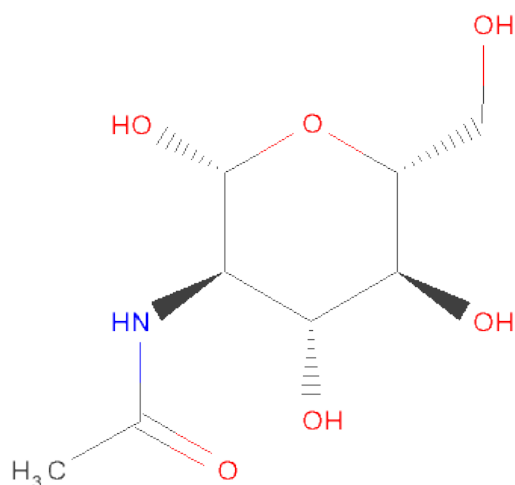
- Molecule 1 is a protein called MHC CLASS II I-EK.

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.

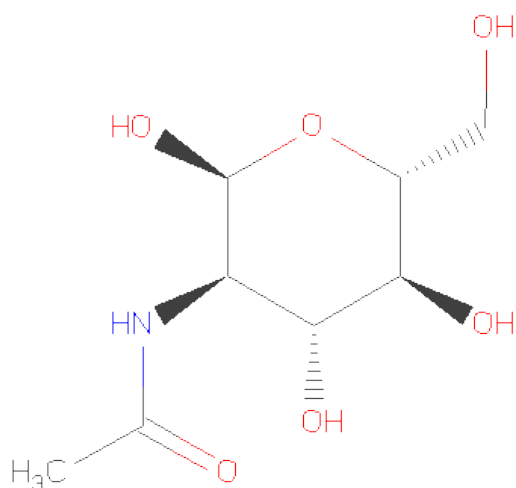
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	214	Total	C	N	O	S	0	0	0
			1724	1092	302	323	7			
2	D	214	Total	C	N	O	S	0	0	0
			1724	1092	302	323	7			

- Molecule 3 is SUGAR (N-ACETYL-D-GLUCOSAMINE) (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	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	D	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 4 is SUGAR (2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE) (three-letter code: NDG) (formula: C₈H₁₅NO₆).



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

- Molecule 5 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



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

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	39	Total	O	0	0
			39	39		
6	B	48	Total	O	0	0
			48	48		
6	C	27	Total	O	0	0
			27	27		
6	D	45	Total	O	0	0
			45	45		

Chain D: 

ARG	ASP	SER	R4N		M7N		F4P		E7P	F8P	K9P	R1L		S5L	L6L	V7L	P8L	R9L	G10L	S11L	G12L	G13L		S16L	R4	P5	W6	F7	L8	E9		S13	E14	C15	H16	F17	Y18	N19	G20	T21	Q22	R23	V24	R25	L26	L27	V28		F31	Y32	N33		L38	R39		S42		R48	
L53	G54	R55		A58	E59	N60	W61	N62		F67	L68	E69	Q70	K71	R72	A73	E74	V75		R80	H81	N82	Y83	E84	I85	F86		F89	L90	V91	P92	R93	R94		P97		V101	Y102	P103	T104	K105	T106	Q107	P108		H111	H112	N113	L114	L115	V116		V119		F122		N126	T127	E128
V129		R133	N134	G135	K136	E137	E138	K139		V148		W153		Q156		V159	M160		V164	P165	Q166		E169		T172	C173		E176	H177	H178	S179	L180		V184	T185		W188	LYS	ALA	GLN	SER	THR	SER	ALA	GLN	ASN	LYS												

4 Data and refinement statistics

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

Property	Value	Source
Space group	P 31 2 1	Depositor
Cell constants a, b, c, α , β , γ	77.53Å 77.53Å 319.48Å 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 ²)	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, NDG, 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 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1488	0	1412	91	0
1	C	1488	0	1412	84	0
2	B	1724	0	1622	89	0
2	D	1724	0	1622	79	0
3	A	14	0	13	1	0
3	B	14	0	13	1	0
3	C	14	0	13	2	0
3	D	14	0	13	0	0
4	A	14	0	13	1	0
4	C	14	0	13	1	0
5	D	5	0	0	0	0
6	A	39	0	0	6	0
6	B	48	0	0	3	0
6	C	27	0	0	3	0
6	D	45	0	0	2	0
All	All	6672	0	6146	311	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 25.

All (311) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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
1:A:98:ASN:HB2	1:A:101:GLU:HG2	1.57	0.85
1:C:122:LEU:HD11	6: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	6:D:235:HOH:O	1.81	0.80
1:A:77:SER:HB3	2:B:53:LEU:HD11	1.64	0.79
2:B:43:ASP:HB3	6:B:231:HOH:O	1.80	0.79
1:A:72:VAL:HG13	2:B:2(L):LYS:HA	1.64	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	6: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	6: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	6: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:D:7(P):GLU:HG3	2:D:67:PHE:CZ	2.31	0.64
2:B:92:PRO:O	2:B:94:ARG:HG2	1.98	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:127:ILE:HG12	2:B:128:GLU:N	2.13	0.64
1:A:87:PRO:CB	1:A:112:PHE:HB3	2.26	0.63
2:B:55:ARG:O	2:B:59:GLU:HG3	1.99	0.63
2:B:26:LEU:H	2:B:42:SER:HB2	1.63	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
2:B:23:ARG:NH1	2:B:23:ARG:HG2	2.17	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
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:D:92:PRO:O	2:D:94:ARG:HG2	2.03	0.57
2:B:69:GLU:OE2	2:B:72:ARG:HD2	2.03	0.57
2:B:126:ASN:H	2:B:126:ASN:HD22	1.53	0.56
1:A:168:TRP:CD1	4:A:194:NDG:H8C2	2.39	0.56
2:B:127:ILE:HB	2:B:177:HIS:HD2	1.70	0.56
2:D:1(L):ARG:NH1	2:D:60:ASN:OD1	2.39	0.56
1:C:99:LEU:HD21	1:C:157:THR:HG23	1.88	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:7:ILE:HD13	2:D:86:PHE:CD2	2.41	0.55
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
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:19:ARG:HB3	6:A:227:HOH:O	2.07	0.54
1:A:101:GLU:HG3	6: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
2:D:69:GLU:OE1	2:D:72:ARG:NH1	2.42	0.52
1:A:111:LYS:HE3	6:A:221:HOH:O	2.08	0.52
1:C:119:VAL:HB	1:C:149:HIS:CD2	2.44	0.52
1:C:109:ILE:HD12	1:C:109:ILE:H	1.74	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	6: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
2:D:126:ASN:HD22	2:D:126:ASN:N	2.05	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:5(L):SER:O	2:D:6(L):LEU:HD23	2.10	0.51
1:A:118:ASN:HB2	1:A:166:ASP:HB3	1.93	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:94:ARG:NH1	6:C:213:HOH:O	2.44	0.50
1:C:111:LYS:HG2	1:C:140:ARG:NH1	2.27	0.50
1:C:83:ALA:O	2:D:6:TRP:HZ2	1.94	0.50
2:D:90:LEU:HD22	2:D:153:TRP:CZ3	2.46	0.50
1:C:87:PRO:HD3	1:C:167:HIS:CD2	2.47	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(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:75:VAL:O	2:B:80:ARG:HG2	2.13	0.49
2:B:127:ILE:HG12	2:B:128:GLU:H	1.76	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
2:D:1(L):ARG:HD2	2:D:60:ASN:OD1	2.12	0.49
1:C:103:ASN:HB3	1:C:153:PHE:CE1	2.48	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:82:ASP:H	2:B:33:ASN:ND2	2.11	0.48
1:A:142:ASP:HB2	1:A:143:HIS:HD2	1.78	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:C:134:GLU:OE1	1:C:149:HIS:NE2	2.46	0.48
1:A:47:GLU:O	1:A:50:LYS:HG2	2.13	0.48
1:A:143:HIS:HB3	2:B:31:PHE:CE2	2.49	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:C:122:LEU:HA	1:C:126:ARG:O	2.13	0.48
1:A:67:LYS:NZ	1:A:67:LYS:O	2.46	0.48
2:D:115:LEU:HD21	2:D:188:TRP:CE3	2.50	0.47
2:B:37:ASN:HB3	6: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	6:C:218:HOH:O	2.13	0.47
1:A:98:ASN:CB	1:A:101:GLU:HG2	2.39	0.47
1:C:122:LEU:O	1:C:161:TYR:HA	2.15	0.47
2:D:134:ASN:HD21	2:D:169:GLU:CA	2.22	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:A:132:VAL:HG12	1:A:151:LEU:HD13	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:14:LEU:HD13	1:A:115:PRO:HD2	1.96	0.47
1:C:99:LEU:CD2	1:C:157:THR:HG23	2.45	0.47
1:C:174:LEU:HD12	1:C:175:ARG:N	2.29	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: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
2:B:173:CYS:O	2:B:185:THR:HA	2.15	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:C:39:SER:CB	1:C:60:LEU:HD11	2.45	0.46
1:A:76:ARG:O	1:A:76:ARG:HG2	2.14	0.46
2:D:55:ARG:O	2:D:59:GLU:HG3	2.15	0.46
2:D:129:VAL:HB	2:D:159:VAL:HG21	1.98	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
2:B:5(L):SER:C	2:B:6(L):LEU:HD23	2.37	0.45
1:A:12:PHE:C	1:A:12:PHE:CD1	2.90	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
2:B:105:LYS:NZ	2:B:107:GLN:HA	2.32	0.45
1:A:78:ASN:O	1:A:78:ASN:CG	2.55	0.45
1:C:134:GLU:OE1	1:C:149:HIS:CE1	2.70	0.44
1:A:167:HIS:C	1:A:169:GLY:H	2.20	0.44
1:A:50:LYS:HE2	1:A:51:PHE:HE2	1.83	0.44
1:C:160:PHE:CD1	1:C:160:PHE:C	2.91	0.44
1:C:21:GLU:OE1	1:C:137:PHE:HB2	2.17	0.44
1:C:51:PHE:HA	2:D:4(N):ARG:HA	1.99	0.44

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:98:ASN:HB2	1:C:101:GLU:CG	2.44	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: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
1:C:78:ASN:CG	1:C:78:ASN:O	2.56	0.44
2:B:114:LEU:HG	2:B:160:MET:HB3	1.99	0.44
2:B:166:GLN:O	2:B:169:GLU:HG3	2.16	0.44
1:A:80:THR:HG22	2:B:11(L):SER:HB3	1.98	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
3:C:193:NAG:O7	3:C:193:NAG:C1	2.66	0.43
1:C:82:ASP:H	2:D:33:ASN:HD22	1.66	0.43
2:B:137:GLU:O	2:B:139:LYS:N	2.51	0.43
2:D:9(L):ARG:HD2	2:D:9(L):ARG:H	1.83	0.43
2:B:83:TYR:O	2:B:86:PHE:N	2.51	0.43
1:A:61:ALA:O	1:A:64:ALA:HB3	2.18	0.43
2:D:4(P):PHE:CZ	2:D:26:LEU:HD11	2.53	0.43
2:B:70:GLN:O	2:B:74:GLU:HG3	2.19	0.43
2:D:133:ARG:HH12	2:D:169:GLU:HB2	1.83	0.43
2:B:58:ALA:O	2:B:62:ASN:HB2	2.19	0.43
1:A:41:THR:O	1:A:42:ILE:HD13	2.18	0.43
2:B:87:ASP:HA	2:B:91:VAL:CG2	2.49	0.43
2:B:134:ASN:ND2	2:B:169:GLU:HA	2.20	0.43
6: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:8:ILE:HB	1:A:25:ASP:HB3	2.00	0.43
2:D:82:ASN:O	2:D:85:ILE:HB	2.19	0.43
1:A:39:SER:OG	1:A:57:GLN:NE2	2.52	0.43
2:D:26:LEU:H	2:D:42:SER:CB	2.33	0.42
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
1:C:23:MET:HA	1:C:33:HIS:HA	2.01	0.42
2:D:68:LEU:O	2:D:72:ARG:HB2	2.19	0.42
2:B:177:HIS:HB3	2:B:180:LEU:HG	2.00	0.42
1:C:118:ASN:OD1	4:C:194:NDG:O	2.37	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:D:177:HIS:C	2:D:179:SER:H	2.22	0.42
2:B:23:ARG:CG	2:B:23:ARG:NH1	2.80	0.42
2:B:180:LEU:HD13	2:B:184:VAL:HG23	2.01	0.42
1:C:2:LYS:NZ	2:D:18:TYR:O	2.45	0.42
1:C:140:ARG:HB2	1:C:144:LEU:O	2.20	0.42
2:B:46:GLU:HB2	2:B:48:ARG:NH1	2.34	0.42
1:A:140:ARG:HB2	1:A:144:LEU:O	2.18	0.42
1:C:8:ILE:HB	1:C:25:ASP:HB3	2.00	0.42
1:A:163:CYS:O	1:A:175:ARG:HA	2.20	0.42
1:C:174:LEU:HD12	1:C:175:ARG:H	1.85	0.42
2:B:4(P):PHE:HD2	2:B:74:GLU:OE1	2.03	0.42
2:D:164:VAL:O	2:D:164:VAL:HG23	2.19	0.42
1:C:70:LEU:HD13	2:D:9:GLU:N	2.34	0.42
1:A:103:ASN:HB3	1:A:153:PHE:CZ	2.55	0.42
1:A:109:ILE:HD12	1:A:109:ILE:H	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
2:B:133:ARG:HH12	2:B:169:GLU:CD	2.23	0.41
1:A:143:HIS:CD2	1:A:143:HIS:N	2.86	0.41
1:C:81:PRO:HB2	2:D:5:PRO:HA	2.03	0.41
1:C:83:ALA:O	2:D:6:TRP:CZ2	2.74	0.41
2:B:104:THR:OG1	2:B:114:LEU:HD23	2.20	0.41
2:D:101:VAL:O	2:D:102:TYR:HB3	2.20	0.41
1:A:108:PHE:CE1	1:A:146:ARG:HB2	2.55	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
1:A:122:LEU:HB2	1:A:162:ASP:HB2	2.02	0.41
2:B:46:GLU:HB3	2:B:62:ASN:ND2	2.36	0.41
1:C:105:LEU:HD11	1:C:178:TRP:CE3	2.55	0.41
1:C:122:LEU:HB2	1:C:162:ASP:HB2	2.03	0.41
1:A:39:SER:OG	1:A:60:LEU:HD11	2.21	0.41
2:D:27:LEU:HD11	2:D:39:ARG:HD3	2.03	0.41
2:D:4(P):PHE:HZ	2:D:15:CYS:SG	2.44	0.40
2:D:111:HIS:O	2:D:112:HIS:CB	2.68	0.40
2:D:97:PRO:HB3	2:D:122:PHE:CB	2.50	0.40

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
2:B:7(N):MET:HG2	2:B:7(N):MET:H	1.72	0.40
1:C:121:TRP:O	1:C:127:PRO:HA	2.21	0.40
2:B:7(P):GLU:HG3	2:B:67:PHE:CE1	2.55	0.40
1:A:89:VAL:HG12	1:A:90:THR:N	2.37	0.40
1:A:124:ASN:HA	1:A:160:PHE:CE1	2.57	0.40
1:C:143:HIS:HB3	2:D:31:PHE:CE2	2.57	0.40
1:A:166:ASP:OD1	1:A:173:PRO:HG3	2.21	0.40
2:D:137:GLU:OE2	2:D:139:LYS:NZ	2.54	0.40
2:D:133:ARG:HH12	2:D:169:GLU:CD	2.25	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
1:C:77:SER:HB3	2:D:53:LEU:HD11	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	180/192 (94%)	162 (90%)	14 (8%)	4 (2%)	10	25
1	C	180/192 (94%)	164 (91%)	12 (7%)	4 (2%)	10	25
2	B	212/227 (93%)	178 (84%)	27 (13%)	7 (3%)	6	13
2	D	212/227 (93%)	182 (86%)	24 (11%)	6 (3%)	8	18
All	All	784/838 (94%)	686 (88%)	77 (10%)	21 (3%)	8	19

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

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Mol	Chain	Res	Type
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%)	20	43
1	C	163/175 (93%)	150 (92%)	13 (8%)	17	37
2	B	186/205 (91%)	174 (94%)	12 (6%)	24	51
2	D	186/205 (91%)	173 (93%)	13 (7%)	21	47
All	All	698/760 (92%)	648 (93%)	50 (7%)	21	45

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

Mol	Chain	Res	Type
1	A	6	THR
1	A	19	ARG
1	A	38	LYS
1	A	46	GLU
1	A	60	LEU
1	A	67	LYS
1	A	82	ASP

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

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Mol	Chain	Res	Type
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 chains 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 carbohydrates 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	A	193	1	12,14,15	0.50	0	15,19,21	0.50	0
4	NDG	A	194	1	12,14,15	0.71	0	15,19,21	0.77	0
3	NAG	B	199	2	12,14,15	0.70	0	15,19,21	0.49	0
3	NAG	C	193	1	12,14,15	0.42	0	15,19,21	0.76	0
4	NDG	C	194	1	12,14,15	0.50	0	15,19,21	0.73	0
3	NAG	D	199	2	12,14,15	0.34	0	15,19,21	0.61	0
5	SO4	D	200	-	4,4,4	0.92	0	6,6,6	0.39	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	A	193	1	-	0/6/23/26	0/1/1/1
4	NDG	A	194	1	-	0/6/23/26	0/1/1/1
3	NAG	B	199	2	-	0/6/23/26	1/1/1/1
3	NAG	C	193	1	-	0/6/23/26	0/1/1/1
4	NDG	C	194	1	-	0/6/23/26	0/1/1/1
3	NAG	D	199	2	-	0/6/23/26	1/1/1/1
5	SO4	D	200	-	-	0/0/0/0	0/0/0/0

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

All (2) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	D	199	NAG	C1-C2-C3-C4-C5-O5
3	B	199	NAG	C1-C2-C3-C4-C5-O5

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 will therefore be empty.

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

EDS was not executed - this section will therefore be empty.

6.3 Carbohydrates ⓘ

EDS was not executed - this section will therefore be empty.

6.4 Ligands ⓘ

EDS was not executed - this section will therefore be empty.

6.5 Other polymers ⓘ

EDS was not executed - this section will therefore be empty.