



# Full wwPDB X-ray Structure Validation Report ⓘ

Oct 14, 2017 – 04:14 PM EDT

PDB ID : 2BC4  
Title : Crystal structure of HLA-DM  
Authors : Nicholson, M.J.; Moradi, B.; Seth, N.P.; Xing, X.; Cuny, G.D.; Stein, R.L.;  
Wucherpfennig, K.W.  
Deposited on : unknown  
Resolution : 2.27 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

<http://wwpdb.org/validation/2016/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 : 1.7.2 (RC1), CSD as538be (2017)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20030345  
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20030345

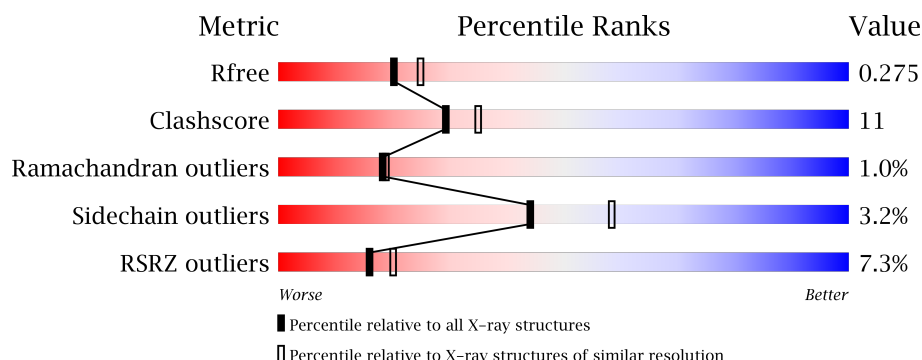
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.27 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))
$R_{free}$	100719	5609 (2.30-2.26)
Clashscore	112137	6364 (2.30-2.26)
Ramachandran outliers	110173	6281 (2.30-2.26)
Sidechain outliers	110143	6281 (2.30-2.26)
RSRZ outliers	101464	5639 (2.30-2.26)

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. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	211	<div> <div>4%</div> <div> <div></div> <div>74%</div> <div>13%</div> <div>•</div> <div>11%</div> </div> </div>
1	C	211	<div> <div>5%</div> <div> <div></div> <div>67%</div> <div>24%</div> <div>•</div> <div>8%</div> </div> </div>
2	B	211	<div> <div>6%</div> <div> <div></div> <div>65%</div> <div>24%</div> <div>•</div> <div>9%</div> </div> </div>
2	D	211	<div> <div>12%</div> <div> <div></div> <div>67%</div> <div>25%</div> <div>•</div> <div>7%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	BMA	C	215	-	-	-	X

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6667 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 HLA class II histocompatibility antigen, DM alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	188	Total	C	N	O	S	0	0	0
			1508	984	239	279	6			
1	C	195	Total	C	N	O	S	0	0	0
			1570	1024	247	293	6			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	204	ASP	-	FLAG tag	GB 18765715
A	205	TYR	-	FLAG tag	GB 18765715
A	206	LYS	-	FLAG tag	GB 18765715
A	207	ASP	-	FLAG tag	GB 18765715
A	208	ASP	-	FLAG tag	GB 18765715
A	209	ASP	-	FLAG tag	GB 18765715
A	210	ASP	-	FLAG tag	GB 18765715
A	211	LYS	-	FLAG tag	GB 18765715
C	204	ASP	-	FLAG tag	GB 18765715
C	205	TYR	-	FLAG tag	GB 18765715
C	206	LYS	-	FLAG tag	GB 18765715
C	207	ASP	-	FLAG tag	GB 18765715
C	208	ASP	-	FLAG tag	GB 18765715
C	209	ASP	-	FLAG tag	GB 18765715
C	210	ASP	-	FLAG tag	GB 18765715
C	211	LYS	-	FLAG tag	GB 18765715

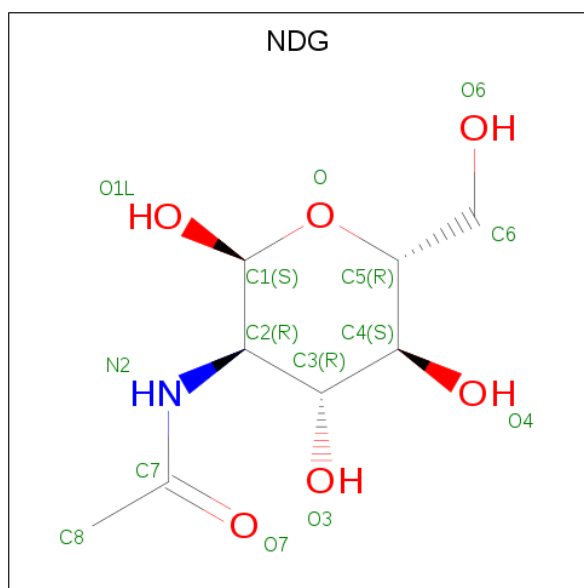
- Molecule 2 is a protein called HLA class II histocompatibility antigen, DM beta chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	191	Total	C	N	O	S	0	0	0
			1510	959	259	281	11			
2	D	197	Total	C	N	O	S	0	0	0
			1555	987	266	290	12			

There are 22 discrepancies between the modelled and reference sequences:

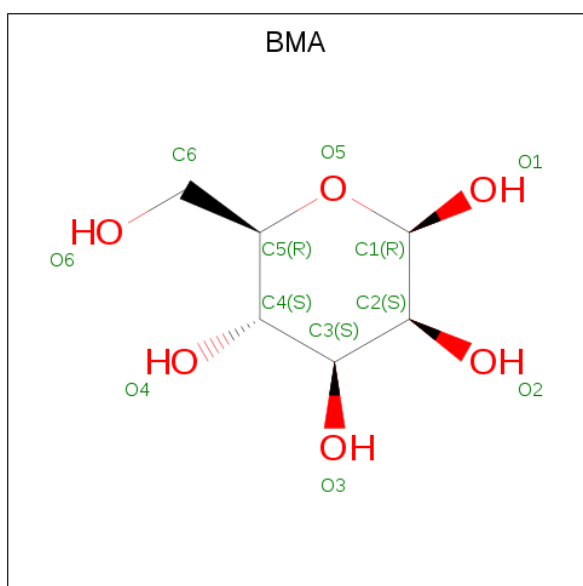
Chain	Residue	Modelled	Actual	Comment	Reference
B	201	LYS	-	KT3 tag	GB 4504399
B	202	PRO	-	KT3 tag	GB 4504399
B	203	PRO	-	KT3 tag	GB 4504399
B	204	THR	-	KT3 tag	GB 4504399
B	205	PRO	-	KT3 tag	GB 4504399
B	206	PRO	-	KT3 tag	GB 4504399
B	207	PRO	-	KT3 tag	GB 4504399
B	208	GLU	-	KT3 tag	GB 4504399
B	209	PRO	-	KT3 tag	GB 4504399
B	210	GLU	-	KT3 tag	GB 4504399
B	211	THR	-	KT3 tag	GB 4504399
D	201	LYS	-	KT3 tag	GB 4504399
D	202	PRO	-	KT3 tag	GB 4504399
D	203	PRO	-	KT3 tag	GB 4504399
D	204	THR	-	KT3 tag	GB 4504399
D	205	PRO	-	KT3 tag	GB 4504399
D	206	PRO	-	KT3 tag	GB 4504399
D	207	PRO	-	KT3 tag	GB 4504399
D	208	GLU	-	KT3 tag	GB 4504399
D	209	PRO	-	KT3 tag	GB 4504399
D	210	GLU	-	KT3 tag	GB 4504399
D	211	THR	-	KT3 tag	GB 4504399

- Molecule 3 is 2-(ACETYLAMINO)-2-DEOXY-A-D-GLUCOPYRANOSE (three-letter code: NDG) (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	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		

- Molecule 4 is BETA-D-MANNOSE (three-letter code: BMA) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			11	6	5		
4	A	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		
4	C	1	Total	C	O	0	0
			11	6	5		

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		
5	A	1	Total	Cl	0	0
			1	1		

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	1	Total	Cl	0	0
			1	1		
5	C	1	Total	Cl	0	0
			1	1		

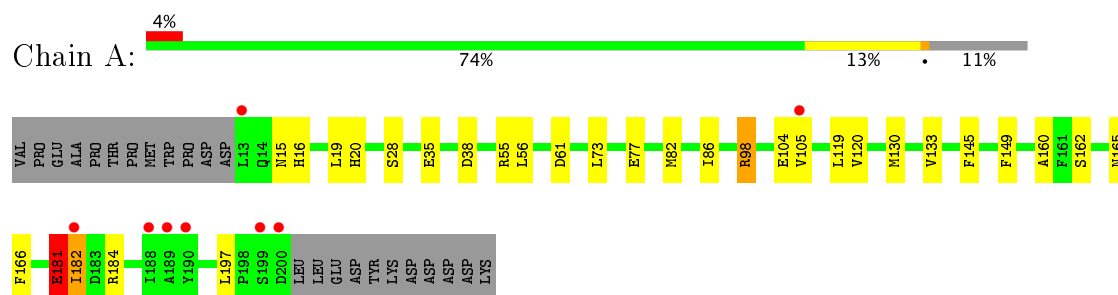
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	135	Total	O	0	0
			135	135		
6	B	96	Total	O	0	0
			96	96		
6	C	121	Total	O	0	0
			121	121		
6	D	68	Total	O	0	0
			68	68		

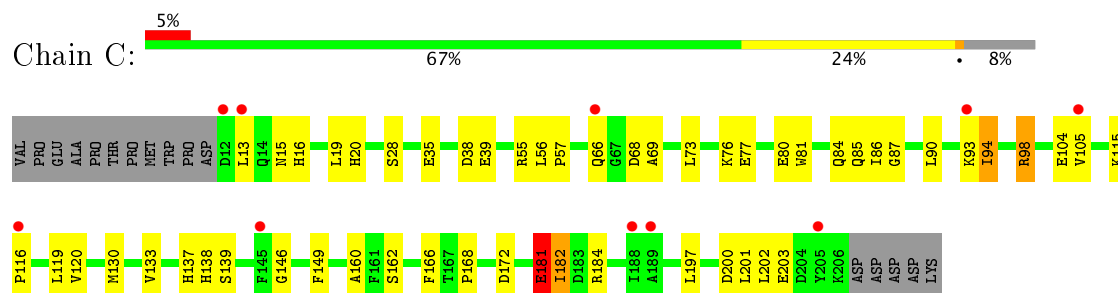
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

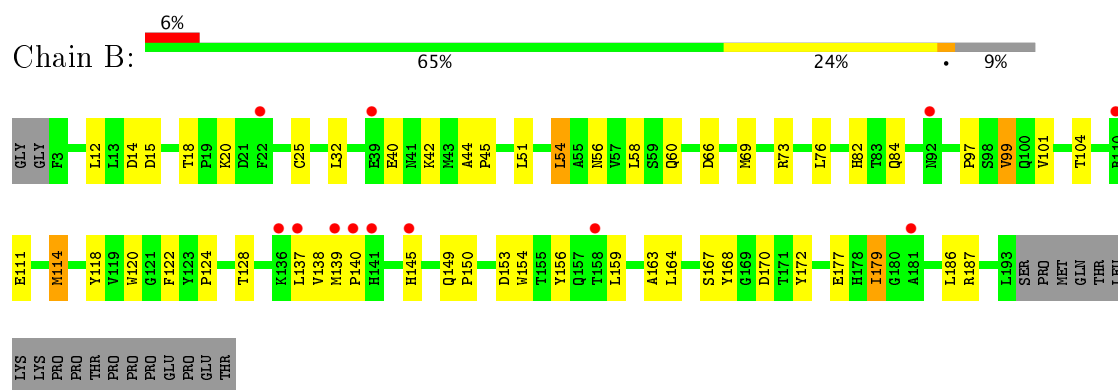
- Molecule 1: HLA class II histocompatibility antigen, DM alpha chain



- Molecule 1: HLA class II histocompatibility antigen, DM alpha chain



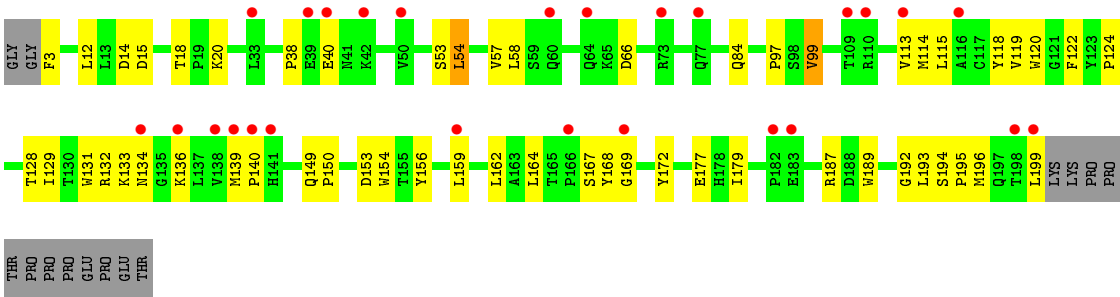
- Molecule 2: HLA class II histocompatibility antigen, DM beta chain



- Molecule 2: HLA class II histocompatibility antigen, DM beta chain







## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.07Å 108.42Å 110.21Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 2.27 29.40 – 2.20	Depositor EDS
% Data completeness (in resolution range)	99.7 (30.00-2.27) 99.1 (29.40-2.20)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.68 (at 2.20Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.229 , 0.268 0.234 , 0.275	Depositor DCC
$R_{free}$ test set	1477 reflections (2.69%)	DCC
Wilson B-factor (Å <sup>2</sup> )	35.5	Xtriage
Anisotropy	0.190	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 46.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.001 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	6667	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	39.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 30.98 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 1.1935e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup> Intensities estimated from amplitudes.

<sup>2</sup> Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality ⓘ

### 5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: BMA, NDG, CL

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	0.40	0/1561	0.80	3/2135 (0.1%)
1	C	0.40	0/1624	0.81	4/2220 (0.2%)
2	B	0.34	0/1556	0.61	0/2131
2	D	0.33	0/1602	0.63	1/2194 (0.0%)
All	All	0.37	0/6343	0.72	8/8680 (0.1%)

There are no bond length outliers.

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	98	ARG	NE-CZ-NH1	-14.63	112.98	120.30
1	C	98	ARG	NE-CZ-NH1	14.50	127.55	120.30
1	C	98	ARG	NE-CZ-NH2	-14.39	113.10	120.30
1	A	98	ARG	NE-CZ-NH2	14.16	127.38	120.30
1	C	98	ARG	CD-NE-CZ	7.57	134.20	123.60
1	A	98	ARG	CD-NE-CZ	7.48	134.07	123.60
2	D	194	SER	N-CA-C	5.60	126.13	111.00
1	C	68	ASP	N-CA-C	5.29	125.29	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	1508	0	1417	27	0
1	C	1570	0	1475	43	0
2	B	1510	0	1452	35	0
2	D	1555	0	1499	37	0
3	A	28	0	24	1	0
3	C	28	0	24	2	0
4	A	22	0	19	0	0
4	C	22	0	19	0	0
5	A	1	0	0	0	0
5	B	1	0	0	0	0
5	C	1	0	0	0	0
5	D	1	0	0	0	0
6	A	135	0	0	5	0
6	B	96	0	0	1	0
6	C	121	0	0	7	0
6	D	68	0	0	1	0
All	All	6667	0	5929	132	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 11.

All (132) 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:124:PRO:HD2	2:B:179:ILE:HD11	1.39	1.04
1:A:15:ASN:HB3	2:B:12:LEU:HD22	1.69	0.75
1:C:15:ASN:HB3	2:D:12:LEU:HD22	1.70	0.74
1:C:20:HIS:HD2	1:C:35:GLU:OE2	1.75	0.69
1:A:20:HIS:HD2	1:A:35:GLU:OE2	1.76	0.67
2:B:139:MET:N	2:B:140:PRO:HD3	2.11	0.66
1:A:133:VAL:HG21	1:A:162:SER:OG	2.00	0.61
3:C:212:NDG:H6C2	6:C:510:HOH:O	2.01	0.60
1:C:39:GLU:HA	6:C:618:HOH:O	2.01	0.60
1:C:130:MET:HE1	1:C:184:ARG:HH21	1.66	0.60
2:B:167:SER:HB2	2:B:170:ASP:OD2	2.02	0.60
1:C:133:VAL:HG21	1:C:162:SER:OG	2.01	0.59
2:D:167:SER:O	2:D:169:GLY:N	2.33	0.59
1:C:81:TRP:NE1	1:C:85:GLN:HG3	2.18	0.58
6:A:600:HOH:O	2:B:82:HIS:HE1	1.88	0.56
1:C:90:LEU:HB3	1:C:94:ILE:CD1	2.35	0.56
1:C:73:LEU:O	1:C:77:GLU:HG3	2.05	0.56
1:C:130:MET:CE	1:C:184:ARG:HH21	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:16:HIS:HE1	2:D:15:ASP:OD1	1.89	0.55
1:A:16:HIS:HE1	2:B:15:ASP:OD1	1.90	0.55
1:C:94:ILE:HD13	1:C:94:ILE:H	1.72	0.55
2:D:139:MET:N	2:D:140:PRO:HD3	2.22	0.54
1:A:130:MET:CE	1:A:184:ARG:HH21	2.20	0.54
2:B:114:MET:HE3	2:B:163:ALA:HB2	1.89	0.54
1:A:82:MET:O	1:A:86:ILE:O	2.24	0.54
1:C:55:ARG:HG3	1:C:56:LEU:HD13	1.91	0.53
1:A:182:ILE:HG22	1:A:182:ILE:O	2.09	0.53
1:A:19:LEU:O	1:A:35:GLU:HA	2.09	0.53
1:C:201:LEU:HD13	1:C:201:LEU:O	2.09	0.53
2:B:54:LEU:HD22	2:B:58:LEU:HG	1.91	0.53
2:D:54:LEU:HD22	2:D:58:LEU:HG	1.92	0.52
1:C:19:LEU:O	1:C:35:GLU:HA	2.09	0.52
2:D:97:PRO:HB3	2:D:122:PHE:HB3	1.91	0.52
1:A:55:ARG:HG3	1:A:56:LEU:HD13	1.92	0.51
2:B:97:PRO:HB3	2:B:122:PHE:HB3	1.93	0.51
1:A:73:LEU:O	1:A:77:GLU:HG3	2.09	0.51
2:B:51:LEU:HA	6:B:559:HOH:O	2.11	0.51
1:A:20:HIS:HE1	6:A:527:HOH:O	1.93	0.51
2:D:179:ILE:HG23	6:D:546:HOH:O	2.10	0.51
1:A:181:GLU:HA	1:A:181:GLU:OE1	2.11	0.50
2:B:101:VAL:HG23	2:B:187:ARG:HB3	1.94	0.50
1:C:181:GLU:OE1	1:C:181:GLU:HA	2.11	0.50
1:C:182:ILE:HG22	1:C:182:ILE:O	2.11	0.50
1:C:20:HIS:HE1	6:C:528:HOH:O	1.94	0.50
2:D:113:VAL:HB	2:D:164:LEU:HD12	1.94	0.50
2:B:128:THR:OG1	2:B:177:GLU:HB2	2.12	0.49
2:D:167:SER:C	2:D:169:GLY:H	2.15	0.49
2:B:164:LEU:HD22	2:B:172:TYR:CZ	2.47	0.49
2:D:119:VAL:HG21	2:D:129:ILE:HD11	1.94	0.49
1:C:149:PHE:O	1:C:160:ALA:HA	2.13	0.49
2:D:153:ASP:O	2:D:154:TRP:HB2	2.12	0.49
2:D:113:VAL:HG12	2:D:114:MET:N	2.28	0.48
2:D:128:THR:OG1	2:D:177:GLU:HB2	2.13	0.48
2:B:150:PRO:HB3	2:B:156:TYR:CE2	2.49	0.47
2:B:14:ASP:OD2	2:B:18:THR:HB	2.14	0.47
2:B:186:LEU:O	2:B:187:ARG:HD2	2.13	0.47
2:D:14:ASP:OD2	2:D:18:THR:HB	2.14	0.47
2:B:111:GLU:HB2	2:B:163:ALA:HB1	1.97	0.47
1:C:146:GLY:HA3	6:C:592:HOH:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:28:SER:O	1:C:130:MET:HG2	2.14	0.47
2:D:192:GLY:O	2:D:195:PRO:HD2	2.15	0.46
2:B:104:THR:CG2	2:B:114:MET:HG2	2.45	0.46
2:B:153:ASP:O	2:B:154:TRP:HB2	2.15	0.46
1:C:16:HIS:HD2	1:C:38:ASP:OD2	1.98	0.46
2:D:150:PRO:HB3	2:D:156:TYR:CE2	2.50	0.46
2:B:137:LEU:HD12	2:B:138:VAL:H	1.81	0.46
1:A:16:HIS:HD2	1:A:38:ASP:OD2	1.98	0.46
2:D:131:TRP:CD2	2:D:162:LEU:HD22	2.51	0.46
2:D:164:LEU:HD22	2:D:172:TYR:CZ	2.51	0.46
1:A:130:MET:HB3	1:A:181:GLU:HB2	1.98	0.46
2:D:14:ASP:OD2	2:D:20:LYS:HE2	2.16	0.46
1:A:149:PHE:O	1:A:160:ALA:HA	2.15	0.45
2:D:99:VAL:HA	2:D:118:TYR:O	2.17	0.45
2:B:139:MET:N	2:B:140:PRO:CD	2.80	0.45
3:A:212:NDG:H6C2	6:A:509:HOH:O	2.16	0.45
1:A:28:SER:O	1:A:130:MET:HG2	2.15	0.45
1:A:105:VAL:HA	1:A:120:VAL:O	2.17	0.45
2:B:56:ASN:O	2:B:60:GLN:HG3	2.17	0.45
2:D:54:LEU:CD2	2:D:58:LEU:HG	2.47	0.44
1:C:200:ASP:HB3	1:C:203:GLU:HB3	2.00	0.44
1:C:66:GLN:HG3	1:C:66:GLN:O	2.17	0.44
1:A:130:MET:HE3	1:A:184:ARG:HH21	1.81	0.44
1:A:61:ASP:HB2	6:A:551:HOH:O	2.16	0.44
2:D:133:LYS:O	2:D:134:ASN:HB2	2.16	0.44
2:D:124:PRO:HD2	2:D:179:ILE:HD11	2.00	0.44
2:D:124:PRO:CD	2:D:179:ILE:HD11	2.48	0.44
1:A:197:LEU:HD11	2:B:118:TYR:CE1	2.53	0.43
1:C:90:LEU:HB3	1:C:94:ILE:HD12	2.00	0.43
2:B:45:PRO:HG2	2:B:56:ASN:OD1	2.17	0.43
1:C:90:LEU:O	1:C:93:LYS:HB2	2.18	0.43
1:C:104:GLU:OE2	2:D:149:GLN:NE2	2.52	0.43
1:C:119:LEU:HD13	1:C:166:PHE:CE2	2.54	0.43
1:A:104:GLU:OE2	2:B:149:GLN:NE2	2.52	0.43
1:C:130:MET:HB3	1:C:181:GLU:HB2	2.00	0.43
2:D:53:SER:O	2:D:57:VAL:HG23	2.18	0.43
1:C:137:HIS:HE1	1:C:172:ASP:OD1	2.02	0.43
1:A:119:LEU:HD13	1:A:166:PHE:CE2	2.54	0.43
6:C:519:HOH:O	2:D:120:TRP:HB2	2.18	0.43
2:B:14:ASP:OD2	2:B:20:LYS:HE2	2.18	0.43
2:B:99:VAL:HA	2:B:118:TYR:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:HIS:O	1:C:139:SER:HB2	2.19	0.43
1:C:57:PRO:HD2	6:C:540:HOH:O	2.18	0.42
1:C:202:LEU:HD11	2:D:196:MET:CE	2.49	0.42
1:C:86:ILE:HG22	1:C:90:LEU:HD23	2.01	0.42
2:B:44:ALA:HA	2:B:45:PRO:HD3	1.92	0.42
1:C:105:VAL:HA	1:C:120:VAL:O	2.19	0.42
1:A:130:MET:HE1	1:A:184:ARG:HH21	1.83	0.42
6:C:600:HOH:O	2:D:199:LEU:HB3	2.19	0.42
1:C:119:LEU:HD13	1:C:166:PHE:CZ	2.55	0.42
1:C:16:HIS:CE1	2:D:15:ASP:OD1	2.71	0.42
1:C:87:GLY:H	1:C:90:LEU:HD23	1.85	0.41
3:C:212:NDG:H6C1	2:D:12:LEU:HD13	2.01	0.41
1:C:115:LYS:HA	1:C:116:PRO:HD3	1.98	0.41
1:C:76:LYS:O	1:C:80:GLU:HG3	2.19	0.41
1:A:16:HIS:CE1	2:B:15:ASP:OD1	2.72	0.41
1:C:197:LEU:HD12	1:C:197:LEU:N	2.35	0.41
6:A:518:HOH:O	2:B:120:TRP:HB2	2.19	0.41
1:C:94:ILE:HD11	2:D:3:PHE:CZ	2.55	0.41
2:D:115:LEU:HD21	2:D:189:TRP:CE2	2.55	0.41
2:D:132:ARG:HA	2:D:136:LYS:O	2.21	0.41
1:A:119:LEU:HD13	1:A:166:PHE:CZ	2.56	0.41
2:D:119:VAL:HG21	2:D:129:ILE:CD1	2.50	0.41
2:D:164:LEU:HD12	2:D:164:LEU:C	2.41	0.41
1:A:15:ASN:OD1	2:B:20:LYS:HG3	2.21	0.41
2:B:69:MET:O	2:B:73:ARG:HG3	2.21	0.41
2:B:40:GLU:CG	2:B:42:LYS:HE2	2.51	0.41
2:D:38:PRO:C	2:D:40:GLU:H	2.24	0.41
1:C:90:LEU:HB3	1:C:94:ILE:HD11	2.03	0.40
2:B:25:CYS:HB3	2:B:32:LEU:HD11	2.03	0.40
2:B:164:LEU:HD12	2:B:164:LEU:C	2.41	0.40
1:A:145:PHE:CD1	1:A:165:ASN:ND2	2.89	0.40
1:C:115:LYS:O	1:C:168:PRO:HD2	2.21	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	186/211 (88%)	179 (96%)	5 (3%)	2 (1%)	17	16
1	C	193/211 (92%)	182 (94%)	7 (4%)	4 (2%)	8	6
2	B	189/211 (90%)	182 (96%)	6 (3%)	1 (0%)	32	38
2	D	195/211 (92%)	182 (93%)	12 (6%)	1 (0%)	32	38
All	All	763/844 (90%)	725 (95%)	30 (4%)	8 (1%)	18	19

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	D	168	TYR
1	A	182	ILE
1	C	182	ILE
1	C	13	LEU
1	C	181	GLU
1	A	181	GLU
2	B	168	TYR
1	C	69	ALA

### 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	167/189 (88%)	165 (99%)	2 (1%)	75	86
1	C	174/189 (92%)	170 (98%)	4 (2%)	56	71
2	B	169/187 (90%)	160 (95%)	9 (5%)	26	34
2	D	175/187 (94%)	168 (96%)	7 (4%)	36	48
All	All	685/752 (91%)	663 (97%)	22 (3%)	44	58

All (22) residues with a non-rotameric sidechain are listed below:



Mol	Chain	Res	Type
1	A	98	ARG
1	A	181	GLU
2	B	54	LEU
2	B	66	ASP
2	B	76	LEU
2	B	84	GLN
2	B	99	VAL
2	B	114	MET
2	B	145	HIS
2	B	159	LEU
2	B	179	ILE
1	C	84	GLN
1	C	94	ILE
1	C	98	ARG
1	C	181	GLU
2	D	54	LEU
2	D	66	ASP
2	D	84	GLN
2	D	99	VAL
2	D	159	LEU
2	D	187	ARG
2	D	193	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	16	HIS
1	A	20	HIS
1	A	50	ASN
1	A	125	ASN
1	A	137	HIS
2	B	78	ASN
2	B	82	HIS
2	B	108	ASN
2	B	157	GLN
1	C	16	HIS
1	C	20	HIS
1	C	125	ASN
1	C	137	HIS
2	D	70	GLN
2	D	78	ASN
2	D	108	ASN
2	D	157	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 12 ligands modelled in this entry, 4 are monoatomic - leaving 8 for Mogul analysis.

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	NDG	A	212	1,3	14,14,15	0.76	0	15,19,21	0.77	1 (6%)
3	NDG	A	213	3,4	14,14,15	0.71	0	15,19,21	0.80	1 (6%)
4	BMA	A	214	3,4	11,11,12	0.73	0	13,15,17	0.41	0
4	BMA	A	215	4	11,11,12	0.53	0	13,15,17	0.65	0
3	NDG	C	212	1,3	14,14,15	0.69	0	15,19,21	0.79	1 (6%)
3	NDG	C	213	3,4	14,14,15	0.70	0	15,19,21	0.77	0
4	BMA	C	214	3,4	11,11,12	0.75	0	13,15,17	0.42	0
4	BMA	C	215	4	11,11,12	0.50	0	13,15,17	0.65	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	NDG	A	212	1,3	-	0/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NDG	A	213	3,4	-	2/6/23/26	0/1/1/1
4	BMA	A	214	3,4	-	0/2/19/22	0/1/1/1
4	BMA	A	215	4	-	0/2/19/22	0/1/1/1
3	NDG	C	212	1,3	-	0/6/23/26	0/1/1/1
3	NDG	C	213	3,4	-	2/6/23/26	0/1/1/1
4	BMA	C	214	3,4	-	0/2/19/22	0/1/1/1
4	BMA	C	215	4	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	212	NDG	C2-N2-C7	-2.12	119.85	122.94
3	C	212	NDG	C2-N2-C7	-2.08	119.91	122.94
3	A	213	NDG	C2-N2-C7	-2.01	120.00	122.94

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	213	NDG	O7-C7-N2-C2
3	A	213	NDG	O7-C7-N2-C2
3	C	213	NDG	C8-C7-N2-C2
3	A	213	NDG	C8-C7-N2-C2

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	212	NDG	1	0
3	C	212	NDG	2	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 ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	188/211 (89%)	0.15	8 (4%) 36 41	20, 31, 52, 67	0
1	C	195/211 (92%)	0.14	10 (5%) 29 35	20, 34, 60, 70	0
2	B	191/211 (90%)	0.23	12 (6%) 21 26	22, 38, 58, 72	0
2	D	197/211 (93%)	0.77	26 (13%) 4 5	22, 46, 68, 74	0
All	All	771/844 (91%)	0.33	56 (7%) 16 20	20, 37, 63, 74	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	141	HIS	6.2
2	B	141	HIS	5.7
2	D	136	LYS	5.3
2	B	139	MET	4.4
2	D	198	THR	4.1
2	D	110	ARG	4.0
2	D	60	GLN	3.9
2	D	140	PRO	3.9
2	D	139	MET	3.8
1	C	12	ASP	3.6
2	D	40	GLU	3.6
2	D	169	GLY	3.3
2	B	140	PRO	3.2
1	A	105	VAL	3.0
2	B	39	GLU	3.0
2	B	92	ASN	2.9
1	A	189	ALA	2.9
1	A	182	ILE	2.9
2	D	134	ASN	2.9
2	D	64	GLN	2.8
2	B	110	ARG	2.8

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Mol	Chain	Res	Type	RSRZ
2	D	183	GLU	2.8
2	D	138	VAL	2.7
2	D	73	ARG	2.6
2	D	39	GLU	2.6
2	D	77	GLN	2.6
1	C	93	LYS	2.6
1	A	13	LEU	2.6
1	C	188	ILE	2.6
1	C	13	LEU	2.6
2	B	145	HIS	2.5
1	C	205	TYR	2.5
1	C	189	ALA	2.5
2	D	50	VAL	2.5
1	C	105	VAL	2.4
1	C	145	PHE	2.4
1	A	188	ILE	2.4
2	D	116	ALA	2.4
2	D	182	PRO	2.3
1	C	66	GLN	2.3
2	B	158	THR	2.3
2	B	22	PHE	2.2
2	D	166	PRO	2.2
2	D	42	LYS	2.2
2	B	181	ALA	2.2
1	A	190	TYR	2.1
1	A	200	ASP	2.1
1	C	116	PRO	2.1
2	B	137	LEU	2.1
2	D	159	LEU	2.1
2	B	136	LYS	2.1
2	D	113	VAL	2.1
2	D	199	LEU	2.0
2	D	109	THR	2.0
1	A	199	SER	2.0
2	D	33	LEU	2.0

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

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	BMA	C	215	11/12	0.61	0.35	2.72	77,79,81,81	0
3	NDG	A	213	14/15	0.75	0.21	0.73	56,59,62,67	0
3	NDG	C	213	14/15	0.84	0.19	0.20	55,59,61,63	0
3	NDG	A	212	14/15	0.85	0.16	-0.59	40,43,46,52	0
3	NDG	C	212	14/15	0.91	0.14	-0.91	39,42,45,50	0
4	BMA	C	214	11/12	0.81	0.15	-	67,69,72,75	0
4	BMA	A	215	11/12	0.71	0.40	-	78,79,81,81	0
5	CL	D	502	1/1	0.96	0.29	-	51,51,51,51	0
5	CL	C	504	1/1	0.82	0.44	-	71,71,71,71	0
5	CL	B	501	1/1	0.90	0.22	-	57,57,57,57	0
4	BMA	A	214	11/12	0.54	0.31	-	70,71,73,76	0
5	CL	A	503	1/1	0.88	0.51	-	68,68,68,68	0

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

There are no such residues in this entry.