



# Full wwPDB X-ray Structure Validation Report ⓘ

Sep 27, 2018 – 03:53 PM EDT

PDB ID : 1D5M  
Title : X-RAY CRYSTAL STRUCTURE OF HLA-DR4 COMPLEXED WITH PEP-TIDE AND SEB  
Authors : Swain, A.L.; Crowther, R.; Kammlott, U.  
Deposited on : 1999-10-07  
Resolution : 2.00 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 : 1.7.3 (157068), CSD as539be (2018)  
Xtriage (Phenix) : 1.13  
EDS : rb-20031172  
Percentile statistics : 20171227.v01 (using entries in the PDB archive December 27th 2017)  
Refmac : 5.8.0158  
CCP4 : 7.0 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : rb-20031172

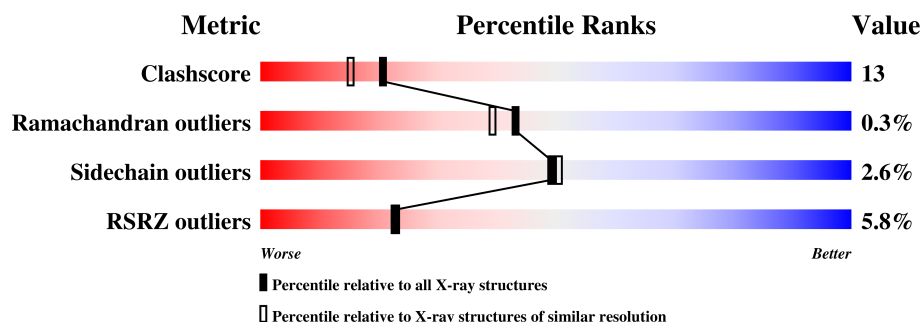
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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	122126	8267 (2.00-2.00)
Ramachandran outliers	120053	8166 (2.00-2.00)
Sidechain outliers	120020	8165 (2.00-2.00)
RSRZ outliers	108989	7011 (2.00-2.00)

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	181	<div> <div>3%</div> <div>78%</div> <div>19%</div> <div>• •</div> </div>
2	B	192	<div> <div>5%</div> <div>67%</div> <div>25%</div> <div>• 6%</div> </div>
3	C	239	<div> <div>8%</div> <div>71%</div> <div>22%</div> <div>• 5%</div> </div>
4	D	9	<div> <div>67%</div> <div>33%</div> </div>

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5076 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.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	178	Total	C	N	O	S	0	0	0
			1464	949	238	272	5			

- Molecule 2 is a protein called HLA CLASS II HISTOCOMPATIBILITY ANTIGEN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	181	Total	C	N	O	S	0	0	0
			1499	948	263	283	5			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	180	VAL	LEU	CONFLICT	UNP P13760

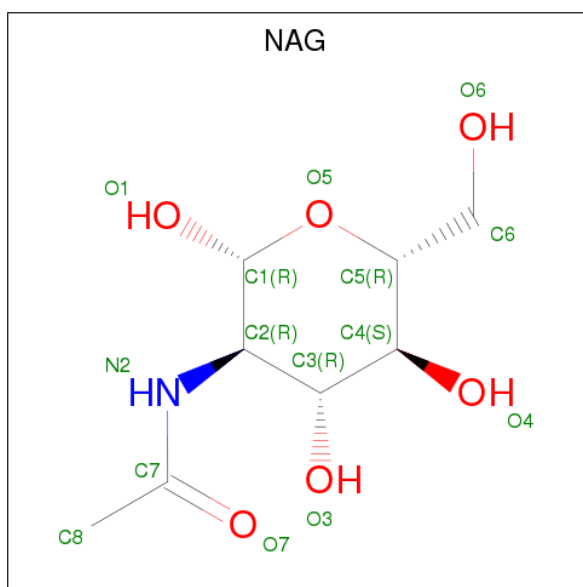
- Molecule 3 is a protein called ENTEROTOXIN TYPE B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	226	Total	C	N	O	S	0	0	0
			1884	1208	304	362	10			

- Molecule 4 is a protein called INHIBITOR.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	D	9	Total	C	N	O	S	0	1	1
			70	43	13	11	3			

- Molecule 5 is N-ACETYL-D-GLUCOSAMINE (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

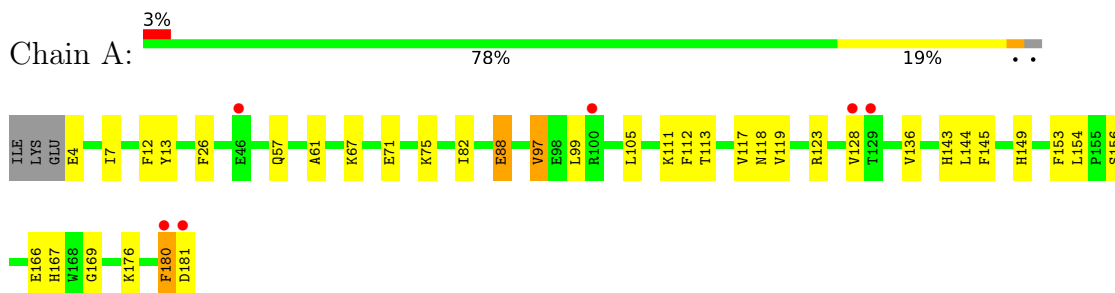
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	52	Total	O	0	0
			52	52		
6	B	38	Total	O	0	0
			38	38		
6	C	51	Total	O	0	0
			51	51		
6	D	4	Total	O	0	0
			4	4		

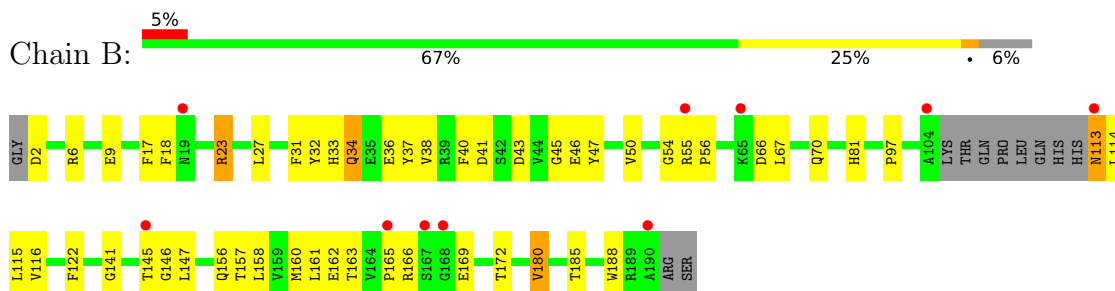
### 3 Residue-property plots [i](#)

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.

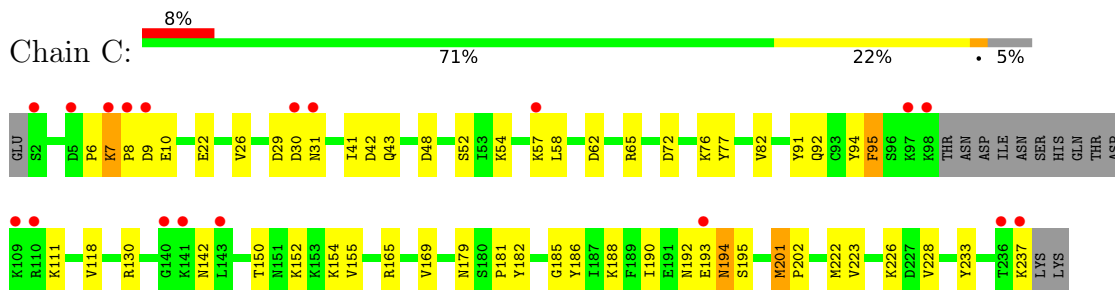
- Molecule 1: HLA CLASS II HISTOCOMPATIBILITY ANTIGEN



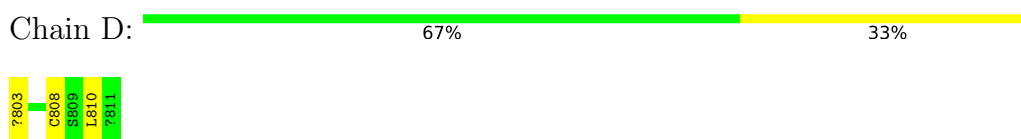
- Molecule 2: HLA CLASS II HISTOCOMPATIBILITY ANTIGEN



- Molecule 3: ENTEROTOXIN TYPE B



- Molecule 4: INHIBITOR



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	82.38Å 93.34Å 99.68Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.90 – 2.00 19.89 – 1.99	Depositor EDS
% Data completeness (in resolution range)	92.9 (19.90-2.00) 92.2 (19.89-1.99)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.22 (at 1.99Å)	Xtriage
Refinement program	CNS 0.9	Depositor
R, $R_{free}$	0.236 , 0.260 0.234 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	19.7	Xtriage
Anisotropy	0.245	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 51.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	5076	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	23.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.97% of the height of the origin peak. No significant pseudotranslation is detected.*

<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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CY1, NH2, NAG, ACE, ALC

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	0.44	1/1509 (0.1%)	0.68	1/2058 (0.0%)
2	B	0.35	0/1539	0.64	0/2091
3	C	0.35	0/1927	0.59	0/2592
4	D	0.57	0/36	1.19	0/44
All	All	0.38	1/5011 (0.0%)	0.64	1/6785 (0.0%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	97	VAL	CB-CG1	-6.57	1.39	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	88	GLU	N-CA-C	-5.16	97.07	111.00

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	1464	0	1400	45	0
2	B	1499	0	1407	52	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	1884	0	1821	41	0
4	D	70	0	76	5	0
5	A	14	0	13	0	0
6	A	52	0	0	0	0
6	B	38	0	0	1	0
6	C	51	0	0	0	0
6	D	4	0	0	1	0
All	All	5076	0	4717	127	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 13.

All (127) 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:97:VAL:CG1	1:A:180:PHE:HE2	1.51	1.23
3:C:194:ASN:HD22	3:C:194:ASN:C	1.58	1.05
1:A:97:VAL:CG1	1:A:180:PHE:CE2	2.41	1.02
1:A:97:VAL:HG12	1:A:180:PHE:HE2	1.22	1.02
1:A:97:VAL:HG12	1:A:180:PHE:CE2	1.97	0.99
1:A:97:VAL:HG11	1:A:180:PHE:HE2	1.25	0.98
3:C:152:LYS:HB2	3:C:155:VAL:HG22	1.49	0.94
3:C:223:VAL:HB	3:C:228:VAL:HG11	1.50	0.91
1:A:61:ALA:HB1	4:D:808[B]:CY1:HM2	1.55	0.89
3:C:194:ASN:C	3:C:194:ASN:ND2	2.27	0.87
1:A:97:VAL:HG11	1:A:180:PHE:CE2	2.06	0.84
2:B:147:LEU:HA	2:B:157:THR:HG22	1.62	0.80
3:C:29:ASP:OD1	3:C:169:VAL:HG11	1.85	0.76
2:B:161:LEU:HG	2:B:163:THR:HG23	1.71	0.72
1:A:57:GLN:HB2	3:C:92:GLN:OE1	1.89	0.71
3:C:223:VAL:HB	3:C:228:VAL:CG1	2.20	0.70
1:A:143:HIS:CE1	2:B:31:PHE:CE2	2.80	0.69
1:A:143:HIS:CE1	2:B:31:PHE:CZ	2.81	0.69
3:C:7:LYS:NZ	3:C:10:GLU:OE1	2.26	0.68
3:C:91:TYR:CE2	3:C:92:GLN:NE2	2.61	0.68
2:B:116:VAL:HG22	2:B:160:MET:HG2	1.74	0.68
2:B:97:PRO:HB3	2:B:122:PHE:HB3	1.75	0.68
2:B:37:TYR:HD1	2:B:38:VAL:HG23	1.59	0.66
3:C:194:ASN:O	3:C:194:ASN:ND2	2.28	0.66
2:B:161:LEU:HG	2:B:163:THR:CG2	2.26	0.66
1:A:167:HIS:CD2	1:A:169:GLY:H	2.14	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:223:VAL:CB	3:C:228:VAL:HG11	2.26	0.64
3:C:194:ASN:HD22	3:C:195:SER:N	1.95	0.64
2:B:145:THR:HG22	2:B:158:LEU:H	1.61	0.64
2:B:113:ASN:HD22	2:B:114:LEU:N	1.95	0.64
1:A:144:LEU:HD21	2:B:34:GLN:OE1	1.98	0.64
3:C:76:LYS:HE3	3:C:77:TYR:CE1	2.35	0.62
2:B:172:THR:CG2	2:B:185:THR:HG23	2.30	0.61
1:A:82:ILE:HB	2:B:33:HIS:ND1	2.18	0.59
1:A:88:GLU:OE1	1:A:111:LYS:HE2	2.01	0.59
2:B:147:LEU:HA	2:B:157:THR:CG2	2.31	0.59
2:B:81:HIS:HE1	4:D:803:ACE:O	1.84	0.59
3:C:150:THR:HG21	3:C:155:VAL:HG21	1.84	0.58
2:B:38:VAL:CG2	2:B:54:GLY:HA3	2.33	0.58
3:C:94:TYR:O	3:C:95:PHE:HB3	2.02	0.58
2:B:37:TYR:CD1	2:B:38:VAL:HG23	2.40	0.57
2:B:163:THR:C	2:B:165:PRO:HD3	2.25	0.57
2:B:141:GLY:O	2:B:162:GLU:HG3	2.06	0.56
1:A:144:LEU:CD2	2:B:34:GLN:OE1	2.54	0.56
1:A:112:PHE:O	1:A:113:THR:HG23	2.05	0.55
3:C:8:PRO:O	3:C:9:ASP:HB2	2.07	0.54
1:A:112:PHE:O	1:A:113:THR:CG2	2.56	0.53
1:A:105:LEU:HG	1:A:153:PHE:CE2	2.42	0.53
3:C:57:LYS:HD2	3:C:58:LEU:HG	1.90	0.53
3:C:130:ARG:NH1	3:C:226:LYS:HB2	2.24	0.53
1:A:99:LEU:CD1	1:A:156:SER:HA	2.40	0.52
2:B:115:LEU:HD11	2:B:188:TRP:CE3	2.45	0.52
1:A:97:VAL:HG12	1:A:180:PHE:CZ	2.44	0.52
3:C:165:ARG:O	3:C:169:VAL:HG23	2.10	0.52
3:C:154:LYS:HB3	3:C:222:MET:CE	2.41	0.52
2:B:67:LEU:HD11	4:D:810:LEU:HD21	1.92	0.51
3:C:7:LYS:HB2	3:C:7:LYS:HZ3	1.76	0.51
2:B:180:VAL:HG23	6:B:1352:HOH:O	2.11	0.51
2:B:38:VAL:HG23	2:B:54:GLY:HA3	1.93	0.51
2:B:32:TYR:O	2:B:33:HIS:HB2	2.11	0.50
3:C:181:PRO:HG2	3:C:182:TYR:CD1	2.47	0.50
1:A:71:GLU:O	1:A:75:LYS:HG3	2.12	0.50
2:B:36:GLU:HG2	2:B:50:VAL:HG21	1.94	0.49
1:A:117:VAL:HG12	1:A:118:ASN:N	2.27	0.49
1:A:99:LEU:HD11	1:A:156:SER:HA	1.95	0.48
3:C:30:ASP:OD2	3:C:31:ASN:N	2.46	0.48
3:C:188:LYS:HE3	3:C:190:ILE:HD11	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:118:ASN:HB2	1:A:166:GLU:HB2	1.97	0.47
1:A:113:THR:HG22	1:A:145:PHE:HD1	1.79	0.47
1:A:12:PHE:HA	2:B:9:GLU:O	2.15	0.47
2:B:172:THR:HG23	2:B:185:THR:HG23	1.96	0.47
1:A:4:GLU:OE2	2:B:18:PHE:CD2	2.69	0.46
3:C:54:LYS:NZ	3:C:62:ASP:HB3	2.31	0.46
1:A:112:PHE:C	1:A:113:THR:HG23	2.35	0.46
1:A:12:PHE:CD1	1:A:12:PHE:C	2.88	0.46
1:A:67:LYS:O	1:A:71:GLU:HG3	2.15	0.46
2:B:147:LEU:HD12	2:B:157:THR:CG2	2.46	0.46
2:B:45:GLY:O	2:B:46:GLU:HG3	2.15	0.46
2:B:32:TYR:CE2	2:B:33:HIS:CD2	3.04	0.46
1:A:119:VAL:HB	1:A:149:HIS:CE1	2.51	0.46
1:A:82:ILE:HB	2:B:33:HIS:CE1	2.51	0.46
2:B:23:ARG:NH2	2:B:43:ASP:OD1	2.49	0.46
4:D:808[B]:CY1:HM3	6:D:1445:HOH:O	2.17	0.45
3:C:154:LYS:HB3	3:C:222:MET:HE2	1.98	0.45
1:A:176:LYS:HA	1:A:176:LYS:HD2	1.73	0.45
3:C:65:ARG:HB2	3:C:95:PHE:CD2	2.51	0.45
1:A:4:GLU:HA	2:B:17:PHE:O	2.17	0.45
2:B:55:ARG:HB3	2:B:56:PRO:HD3	1.99	0.45
1:A:113:THR:CG2	1:A:144:LEU:HA	2.47	0.44
2:B:156:GLN:O	2:B:157:THR:CG2	2.66	0.44
3:C:22:GLU:O	3:C:26:VAL:HG13	2.18	0.44
3:C:223:VAL:CG2	3:C:228:VAL:HG11	2.48	0.44
2:B:40:PHE:HB2	2:B:47:TYR:CE2	2.52	0.44
1:A:167:HIS:HD2	1:A:169:GLY:H	1.60	0.44
2:B:113:ASN:HD22	2:B:114:LEU:H	1.63	0.44
1:A:143:HIS:NE2	2:B:31:PHE:CE2	2.87	0.43
2:B:31:PHE:CE2	2:B:36:GLU:HB2	2.53	0.43
3:C:201:MET:HG3	3:C:202:PRO:HD2	2.01	0.43
3:C:41:ILE:HD13	3:C:52:SER:HB2	2.00	0.43
2:B:166:ARG:HG2	2:B:169:GLU:CD	2.39	0.43
1:A:123:ARG:HB2	1:A:128:VAL:HG21	2.01	0.43
3:C:82:VAL:HG21	3:C:118:VAL:HG13	2.01	0.43
1:A:113:THR:HG22	1:A:145:PHE:CD1	2.54	0.43
2:B:2:ASP:OD1	2:B:6:ARG:NH1	2.37	0.43
2:B:115:LEU:HD23	2:B:115:LEU:HA	1.91	0.43
3:C:6:PRO:HG2	3:C:186:TYR:CD1	2.54	0.42
3:C:185:GLY:HA2	3:C:233:TYR:O	2.20	0.42
3:C:192:ASN:O	3:C:193:GLU:HB2	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:95:PHE:CZ	3:C:111:LYS:HB2	2.55	0.42
1:A:113:THR:HG23	1:A:144:LEU:HD22	2.00	0.42
1:A:82:ILE:CB	2:B:33:HIS:ND1	2.82	0.42
3:C:179:ASN:OD1	3:C:237:LYS:NZ	2.52	0.42
3:C:41:ILE:O	3:C:42:ASP:HB2	2.20	0.42
1:A:13:TYR:CE2	1:A:67:LYS:HG3	2.54	0.42
2:B:145:THR:CG2	2:B:158:LEU:H	2.29	0.42
2:B:156:GLN:O	2:B:157:THR:HG23	2.19	0.42
3:C:181:PRO:HG2	3:C:182:TYR:CE1	2.55	0.42
1:A:7:ILE:HG12	1:A:26:PHE:HD1	1.85	0.41
2:B:55:ARG:N	2:B:56:PRO:CD	2.83	0.41
1:A:99:LEU:CD1	1:A:180:PHE:CE1	3.04	0.41
1:A:82:ILE:N	2:B:33:HIS:CE1	2.88	0.41
2:B:27:LEU:HD23	2:B:41:ASP:HA	2.03	0.41
2:B:38:VAL:CG2	2:B:54:GLY:CA	2.98	0.41
3:C:43:GLN:HG2	3:C:48:ASP:O	2.21	0.41
2:B:145:THR:HG23	2:B:146:GLY:O	2.20	0.41
3:C:7:LYS:HB2	3:C:7:LYS:NZ	2.36	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	176/181 (97%)	173 (98%)	2 (1%)	1 (1%)	27	21
2	B	177/192 (92%)	171 (97%)	6 (3%)	0	100	100
3	C	222/239 (93%)	211 (95%)	10 (4%)	1 (0%)	31	25
4	D	5/9 (56%)	5 (100%)	0	0	100	100
All	All	580/621 (93%)	560 (97%)	18 (3%)	2 (0%)	43	39

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	95	PHE
1	A	136	VAL

### 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	163/166 (98%)	160 (98%)	3 (2%)	62	66
2	B	163/173 (94%)	157 (96%)	6 (4%)	37	35
3	C	210/225 (93%)	205 (98%)	5 (2%)	52	54
4	D	4/4 (100%)	4 (100%)	0	100	100
All	All	540/568 (95%)	526 (97%)	14 (3%)	49	50

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	154	LEU
1	A	180	PHE
1	A	181	ASP
2	B	23	ARG
2	B	34	GLN
2	B	66	ASP
2	B	70	GLN
2	B	113	ASN
2	B	180	VAL
3	C	7	LYS
3	C	72	ASP
3	C	142	ASN
3	C	194	ASN
3	C	201	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	167	HIS

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Mol	Chain	Res	Type
1	A	177	HIS
2	B	19	ASN
2	B	81	HIS
2	B	113	ASN
2	B	120	ASN
3	C	23	ASN
3	C	171	ASN
3	C	194	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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	$\# Z  > 2$
4	ALC	D	804	4	10,11,12	1.13	1 (10%)	11,13,15	1.02	1 (9%)
4	CY1	D	808[A]	-	10,10,11	1.73	3 (30%)	6,11,13	1.40	1 (16%)
4	CY1	D	808[B]	-	10,10,11	1.98	2 (20%)	6,11,13	1.96	1 (16%)

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
4	ALC	D	804	4	-	0/4/14/16	0/1/1/1
4	CY1	D	808[A]	-	-	0/5/9/11	0/0/0/0
4	CY1	D	808[B]	-	-	0/5/9/11	0/0/0/0

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	808[B]	CY1	CD-SG	-2.76	1.77	1.82
4	D	808[A]	CY1	CD-SG	-2.35	1.78	1.82
4	D	808[A]	CY1	CD-NE	2.50	1.47	1.44
4	D	804	ALC	CA-C	2.86	1.54	1.50
4	D	808[A]	CY1	CB-SG	3.28	1.89	1.81
4	D	808[B]	CY1	CB-SG	4.82	1.93	1.81

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	808[A]	CY1	CA-CB-SG	-2.34	107.20	113.08
4	D	804	ALC	CG-CB-CA	2.40	117.56	114.39
4	D	808[B]	CY1	CB-SG-CD	3.97	108.56	102.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	808[A]	CY1	1	0
4	D	808[B]	CY1	2	0

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
5	NAG	A	1201	1	14,14,15	0.49	0	17,19,21	0.95	1 (5%)

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
5	NAG	A	1201	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1201	NAG	C4-C3-C2	-2.44	107.44	111.02

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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

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	178/181 (98%)	0.13	6 (3%) 45 44	11, 19, 35, 46	0
2	B	181/192 (94%)	0.42	10 (5%) 25 25	12, 23, 44, 53	0
3	C	226/239 (94%)	0.51	18 (7%) 12 12	13, 23, 47, 64	0
4	D	5/9 (55%)	0.13	0 100 100	8, 8, 16, 18	0
All	All	590/621 (95%)	0.36	34 (5%) 23 23	8, 22, 43, 64	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
3	C	8	PRO	5.8
3	C	110	ARG	5.4
2	B	65	LYS	5.1
2	B	190	ALA	4.7
2	B	104	ALA	4.6
3	C	9	ASP	4.4
3	C	7	LYS	4.3
3	C	98	LYS	4.1
1	A	180	PHE	4.1
3	C	5	ASP	4.1
3	C	2	SER	4.0
2	B	55	ARG	3.9
3	C	30	ASP	3.8
2	B	113	ASN	3.8
3	C	109	LYS	3.7
3	C	193	GLU	3.6
3	C	97	LYS	3.5
3	C	57	LYS	3.3
1	A	100	ARG	3.1
1	A	129	THR	3.0
2	B	145	THR	2.9

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Mol	Chain	Res	Type	RSRZ
3	C	31	ASN	2.7
2	B	19	ASN	2.5
3	C	143	LEU	2.4
2	B	168	GLY	2.4
3	C	237	LYS	2.4
1	A	181	ASP	2.3
2	B	165	PRO	2.2
2	B	167	SER	2.1
3	C	140	GLY	2.1
3	C	141	LYS	2.1
1	A	128	VAL	2.0
1	A	46	GLU	2.0
3	C	236	THR	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
4	ALC	D	804	11/12	0.88	0.16	6,8,11,13	0
4	CY1	D	808[A]	11/12	0.91	0.22	7,14,15,16	6
4	CY1	D	808[B]	11/12	0.91	0.22	7,14,20,22	6

## 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. 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	B-factors(Å <sup>2</sup> )	Q<0.9
5	NAG	A	1201	14/15	0.74	0.21	34,37,39,43	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.