



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:51 PM GMT

PDB ID : 1HHU  
Title : Balhimycin in complex with D-Ala-D-Ala  
Authors : Lehmann, C.; Bunkoczi, G.; Sheldrick, G.M.; Vertessy, L.  
Deposited on : 2000-12-28  
Resolution : 0.89 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.

---

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

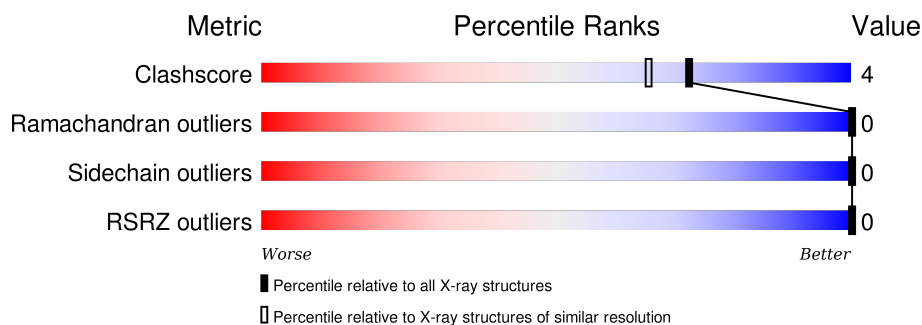
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 0.89 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	102246	1082 (1.08-0.72)
Ramachandran outliers	100387	1008 (1.08-0.72)
Sidechain outliers	100360	1010 (1.08-0.72)
RSRZ outliers	91569	1002 (1.08-0.72)

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	7	<div><div></div><div>100%</div></div>
1	B	7	<div><div></div><div>100%</div></div>
1	C	7	<div><div></div><div>100%</div></div>
1	D	7	<div><div></div><div>100%</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	MPD	B	1016	X	-	-	-

## 2 Entry composition [i](#)

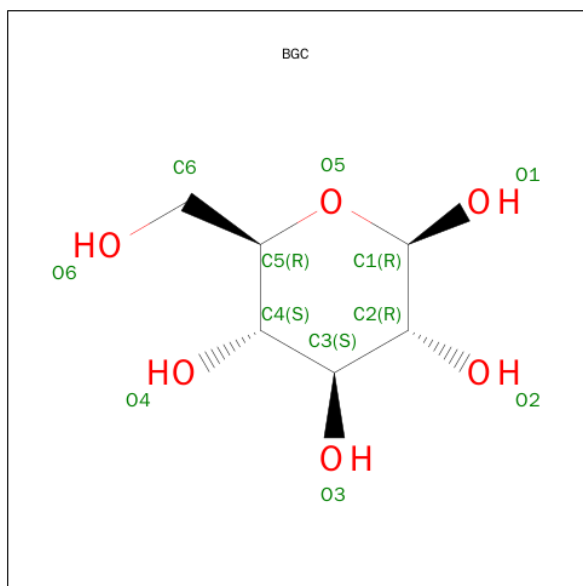
There are 7 unique types of molecules in this entry. The entry contains 1062 atoms, of which 366 are hydrogens and 0 are deuteriums.

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 BALHIMYCIN.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	7	Total	C	Cl	H	N	O	0	0	0
			129	53	2	49	8	17			
1	B	7	Total	C	Cl	H	N	O	0	0	0
			129	53	2	49	8	17			
1	C	7	Total	C	Cl	H	N	O	0	0	0
			129	53	2	49	8	17			
1	D	7	Total	C	Cl	H	N	O	0	0	0
			129	53	2	49	8	17			

- Molecule 2 is SUGAR (BETA-D-GLUCOSE) (three-letter code: BGC) (formula: C<sub>6</sub>H<sub>12</sub>O<sub>6</sub>).



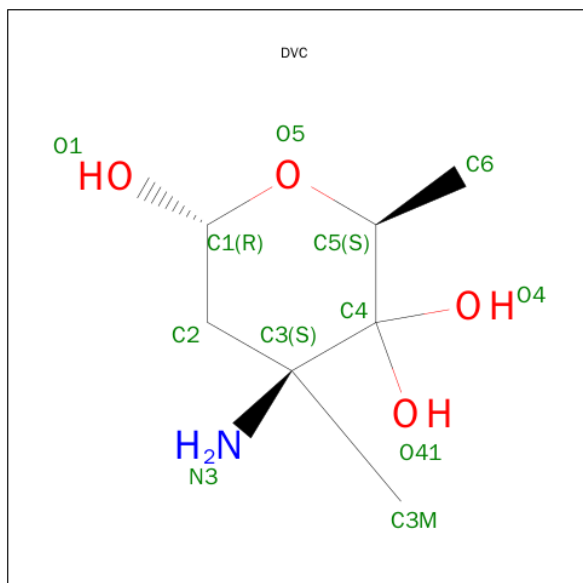
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			22	6	11	5		
2	B	1	Total	C	H	O	0	0
			22	6	11	5		

*Continued on next page...*

Continued from previous page...

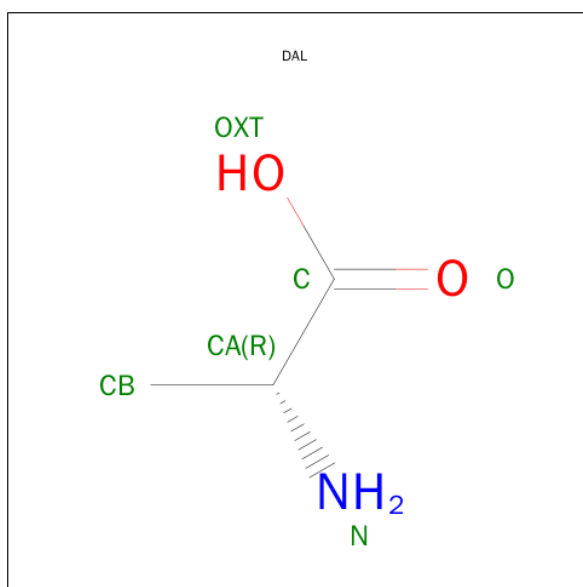
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	H	O	0	0
			22	6	11	5		
2	D	1	Total	C	H	O	0	0
			22	6	11	5		

- Molecule 3 is SUGAR ((2R,4S,6S)-4-AZANYL-4,6-DIMETHYL-OXANE-2,5,5-TRIOL) (three-letter code: DVC) (formula: C<sub>7</sub>H<sub>15</sub>NO<sub>4</sub>).



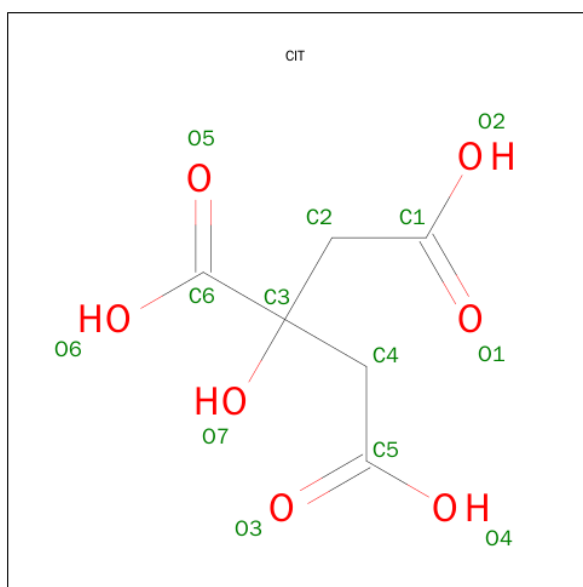
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	H	N	O	0	0
			23	7	12	1	3		
3	B	1	Total	C	H	N	O	0	0
			23	7	12	1	3		
3	C	1	Total	C	H	N	O	0	0
			23	7	12	1	3		
3	D	1	Total	C	H	N	O	0	0
			23	7	12	1	3		

- Molecule 4 is D-ALANINE (three-letter code: DAL) (formula: C<sub>3</sub>H<sub>7</sub>NO<sub>2</sub>).



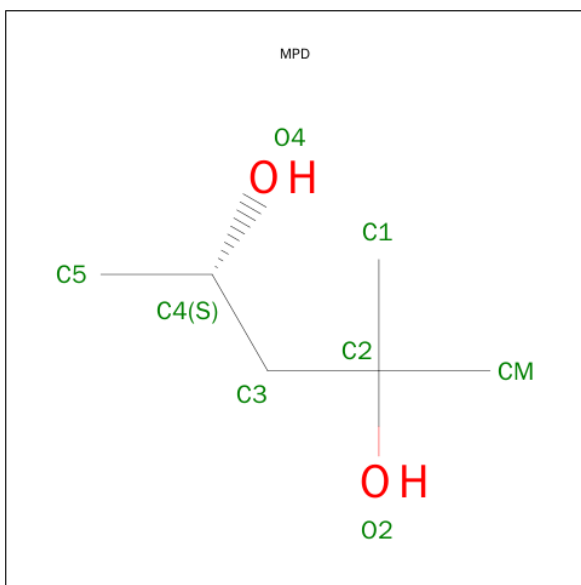
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	H	N	O	0	0
			9	3	4	1	1		
4	A	1	Total	C	H	N	O	0	0
			11	3	5	1	2		
4	B	1	Total	C	H	N	O	0	0
			9	3	4	1	1		
4	B	1	Total	C	H	N	O	0	0
			11	3	5	1	2		
4	C	1	Total	C	H	N	O	0	0
			9	3	4	1	1		
4	C	1	Total	C	H	N	O	0	0
			11	3	5	1	2		
4	D	1	Total	C	H	N	O	0	0
			9	3	4	1	1		
4	D	1	Total	C	H	N	O	0	0
			11	3	5	1	2		

- Molecule 5 is CITRIC ACID (three-letter code: CIT) (formula: C<sub>6</sub>H<sub>8</sub>O<sub>7</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	1
			36	12	10	14		
5	A	1	Total	C	H	O	0	1
			36	12	10	14		
5	A	1	Total	C	H	O	0	1
			23	8	7	8		
5	A	1	Total	C	H	O	0	1
			35	12	10	13		
5	B	1	Total	C	H	O	0	0
			18	6	5	7		

- Molecule 6 is (4S)-2-METHYL-2,4-PENTANEDIOL (three-letter code: MPD) (formula:  $C_6H_{14}O_2$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			8	6	2		
6	A	1	Total	C	O	0	0
			5	4	1		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	48	Total	O	0	0
			48	48		
7	B	34	Total	O	0	0
			34	34		
7	C	22	Total	O	0	0
			22	22		
7	D	21	Total	O	0	0
			21	21		



### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: BALHIMYCIN

Chain A:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: BALHIMYCIN

Chain B:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: BALHIMYCIN

Chain C:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: BALHIMYCIN

Chain D:  100%

There are no outlier residues recorded for this chain.

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	22.70Å 27.99Å 44.49Å 90.00° 93.18° 90.00°	Depositor
Resolution (Å)	27.99 – 0.89 23.68 – 0.89	Depositor EDS
% Data completeness (in resolution range)	99.4 (27.99-0.89) 99.0 (23.68-0.89)	Depositor EDS
$R_{merge}$	0.02	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	6.57 (at 0.89Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.084 , 0.100 0.092 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	3.9	Xtriage
Anisotropy	0.147	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.44 , 105.2	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 42290 reflections	Xtriage
$F_o, F_c$ correlation	0.99	EDS
Total number of atoms	1062	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	7.0	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 58.43 % 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 2.0476e-05. 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, 0.375 respectively for untwinned datasets, and 0.333, 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: MPD, BGC, GHP, DAL, CIT, DVC, OMZ, MLU, 3FG, OMY

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	0.43	0/7	0.76	0/8
1	B	0.49	0/7	0.84	0/8
1	C	0.36	0/7	0.72	0/8
1	D	0.59	0/7	0.78	0/8
All	All	0.47	0/28	0.78	0/32

There are no bond length outliers.

There are no bond angle outliers.

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	80	49	45	0	0
1	B	80	49	43	0	0
1	C	80	49	45	0	0
1	D	80	49	45	0	0
2	A	11	11	10	0	0
2	B	11	11	10	0	0
2	C	11	11	10	0	0
2	D	11	11	10	0	0
3	A	11	12	13	0	0

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	11	12	13	0	0
3	C	11	12	13	0	0
3	D	11	12	13	0	0
4	A	11	9	11	0	0
4	B	11	9	11	0	0
4	C	11	9	11	0	0
4	D	11	9	11	0	0
5	A	93	37	33	3	0
5	B	13	5	5	1	0
6	A	5	0	7	0	0
6	B	8	0	10	0	0
7	A	48	0	0	0	0
7	B	34	0	0	0	0
7	C	22	0	0	0	0
7	D	21	0	0	0	0
All	All	696	366	369	4	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 4.

All (4) 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)
5:A:1015[B]:CIT:O2	5:A:1017[B]:CIT:O4	1.65	1.12
5:A:1015[B]:CIT:C1	5:A:1017[B]:CIT:O4	2.50	0.56
5:A:1015[B]:CIT:H22	5:A:1015[B]:CIT:O3	2.18	0.43
5:B:1015:CIT:O2	5:B:1015:CIT:C6	2.67	0.42

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	1/7 (14%)	0	1 (100%)	0	100	100
1	B	1/7 (14%)	1 (100%)	0	0	100	100
1	C	1/7 (14%)	0	1 (100%)	0	100	100
1	D	1/7 (14%)	1 (100%)	0	0	100	100
All	All	4/28 (14%)	2 (50%)	2 (50%)	0	100	100

There are no Ramachandran outliers to report.

### 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	1/1 (100%)	1 (100%)	0	100	100
1	B	1/1 (100%)	1 (100%)	0	100	100
1	C	1/1 (100%)	1 (100%)	0	100	100
1	D	1/1 (100%)	1 (100%)	0	100	100
All	All	4/4 (100%)	4 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

24 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$
1	MLU	A	1	1	7,8,9	1.00	0	4,9,11	1.42	1 (25%)
1	OMZ	A	2	1	13,14,15	0.82	0	17,19,21	1.19	2 (11%)
1	GHP	A	4	1,2	10,11,12	0.88	0	12,14,16	0.86	0
1	GHP	A	5	1	10,11,12	0.91	0	12,14,16	0.99	0
1	OMY	A	6	1,3	13,14,15	0.72	0	17,19,21	1.14	1 (5%)
1	3FG	A	7	1	9,13,13	0.72	0	14,18,18	0.74	0
1	MLU	B	1	1	7,8,9	1.31	1 (14%)	4,9,11	3.08	3 (75%)
1	OMZ	B	2	1	13,14,15	0.90	0	17,19,21	1.24	3 (17%)
1	GHP	B	4	1,2	10,11,12	0.70	0	12,14,16	0.97	0
1	GHP	B	5	1	10,11,12	0.82	0	12,14,16	1.06	0
1	OMY	B	6	1,3	13,14,15	0.97	1 (7%)	17,19,21	1.36	2 (11%)
1	3FG	B	7	1	9,13,13	1.05	1 (11%)	14,18,18	1.03	1 (7%)
1	MLU	C	1	1	7,8,9	0.74	0	4,9,11	1.34	1 (25%)
1	OMZ	C	2	1	13,14,15	1.11	2 (15%)	17,19,21	1.30	4 (23%)
1	GHP	C	4	1,2	10,11,12	0.95	0	12,14,16	1.03	0
1	GHP	C	5	1	10,11,12	0.86	0	12,14,16	1.00	1 (8%)
1	OMY	C	6	1,3	13,14,15	0.86	1 (7%)	17,19,21	1.45	3 (17%)
1	3FG	C	7	1	9,13,13	0.92	0	14,18,18	0.94	0
1	MLU	D	1	1	7,8,9	0.73	0	4,9,11	1.93	2 (50%)
1	OMZ	D	2	1	13,14,15	1.00	2 (15%)	17,19,21	1.41	3 (17%)
1	GHP	D	4	1,2	10,11,12	0.62	0	12,14,16	0.93	0
1	GHP	D	5	1	10,11,12	0.75	0	12,14,16	0.99	0
1	OMY	D	6	1,3	13,14,15	0.77	0	17,19,21	1.16	1 (5%)
1	3FG	D	7	1	9,13,13	1.02	0	14,18,18	0.98	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
1	MLU	A	1	1	-	0/4/8/10	0/0/0/0
1	OMZ	A	2	1	-	0/8/10/12	0/1/1/1
1	GHP	A	4	1,2	-	0/4/6/8	0/1/1/1
1	GHP	A	5	1	-	0/4/6/8	0/1/1/1

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	OMY	A	6	1,3	-	0/8/10/12	0/1/1/1
1	3FG	A	7	1	-	0/4/8/8	0/1/1/1
1	MLU	B	1	1	-	0/4/8/10	0/0/0/0
1	OMZ	B	2	1	-	0/8/10/12	0/1/1/1
1	GHP	B	4	1,2	-	0/4/6/8	0/1/1/1
1	GHP	B	5	1	-	0/4/6/8	0/1/1/1
1	OMY	B	6	1,3	-	0/8/10/12	0/1/1/1
1	3FG	B	7	1	-	0/4/8/8	0/1/1/1
1	MLU	C	1	1	-	0/4/8/10	0/0/0/0
1	OMZ	C	2	1	-	0/8/10/12	0/1/1/1
1	GHP	C	4	1,2	-	0/4/6/8	0/1/1/1
1	GHP	C	5	1	-	0/4/6/8	0/1/1/1
1	OMY	C	6	1,3	-	0/8/10/12	0/1/1/1
1	3FG	C	7	1	-	0/4/8/8	0/1/1/1
1	MLU	D	1	1	-	0/4/8/10	0/0/0/0
1	OMZ	D	2	1	-	0/8/10/12	0/1/1/1
1	GHP	D	4	1,2	-	0/4/6/8	0/1/1/1
1	GHP	D	5	1	-	0/4/6/8	0/1/1/1
1	OMY	D	6	1,3	-	0/8/10/12	0/1/1/1
1	3FG	D	7	1	-	0/4/8/8	0/1/1/1

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	1	MLU	CD1-CG	-2.62	1.35	1.51
1	C	2	OMZ	CZ-CE1	-2.18	1.37	1.39
1	B	7	3FG	CG1-CB	2.05	1.42	1.39
1	D	2	OMZ	CA-CB	2.06	1.58	1.54
1	C	2	OMZ	OH-CZ	2.12	1.40	1.36
1	D	2	OMZ	OH-CZ	2.27	1.41	1.36
1	C	6	OMY	OCZ-CZ	2.38	1.41	1.36
1	B	6	OMY	OCZ-CZ	2.51	1.41	1.36

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1	MLU	CD2-CG-CD1	-4.04	90.23	110.55
1	C	6	OMY	CG-CB-CA	-3.44	107.15	111.96
1	A	6	OMY	CG-CB-CA	-3.34	107.28	111.96
1	C	6	OMY	CD1-CE1-CZ	-3.25	119.41	121.22
1	B	6	OMY	CG-CB-CA	-3.13	107.59	111.96
1	D	1	MLU	O-C-CA	-3.11	117.23	125.44

*Continued on next page...*

*Continued from previous page...*

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2	OMZ	O-C-CA	-3.02	117.46	125.44
1	A	2	OMZ	O-C-CA	-3.00	117.50	125.44
1	B	2	OMZ	O-C-CA	-3.00	117.51	125.44
1	D	6	OMY	CG-CB-CA	-2.91	107.90	111.96
1	D	2	OMZ	CD1-CE1-CZ	-2.88	119.62	121.22
1	C	2	OMZ	O-C-CA	-2.83	117.95	125.44
1	A	1	MLU	O-C-CA	-2.72	118.26	125.44
1	B	1	MLU	O-C-CA	-2.55	118.71	125.44
1	B	6	OMY	CD1-CE1-CZ	-2.45	119.86	121.22
1	B	7	3FG	CD1-CG1-CB	-2.41	117.95	120.14
1	C	1	MLU	O-C-CA	-2.33	119.29	125.44
1	C	2	OMZ	CD2-CE2-CZ	-2.21	118.22	120.49
1	C	5	GHP	C6-C5-C4	-2.04	117.52	119.87
1	B	2	OMZ	CE2-CZ-CE1	2.03	120.64	118.57
1	C	2	OMZ	CE2-CZ-CE1	2.06	120.67	118.57
1	C	2	OMZ	C-CA-N	2.10	114.22	109.83
1	C	6	OMY	CE2-CZ-CE1	2.16	120.76	118.57
1	D	1	MLU	CD1-CG-CB	2.16	119.14	111.11
1	B	2	OMZ	C-CA-N	2.33	114.71	109.83
1	D	2	OMZ	CE2-CZ-CE1	2.36	120.97	118.57
1	A	2	OMZ	C-CA-N	2.45	114.95	109.83
1	B	1	MLU	CD1-CG-CB	3.86	125.44	111.11

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

27 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
5	CIT	A	1015[A]	-	3,12,12	0.81	0	3,17,17	3.08	2 (66%)
5	CIT	A	1015[B]	-	3,12,12	0.62	0	3,17,17	4.09	2 (66%)
5	CIT	A	1016[A]	-	3,12,12	1.34	1 (33%)	3,17,17	3.60	2 (66%)
5	CIT	A	1016[B]	-	3,12,12	1.25	1 (33%)	3,17,17	0.64	0
5	CIT	A	1017[A]	-	3,11,12	0.50	0	3,15,17	5.39	3 (100%)
5	CIT	A	1017[B]	-	3,12,12	1.14	0	3,17,17	2.06	2 (66%)
5	CIT	A	1018[A]	-	3,12,12	1.45	1 (33%)	3,17,17	3.01	2 (66%)
5	CIT	A	1018[B]	-	3,11,12	3.24	1 (33%)	3,15,17	5.64	3 (100%)
6	MPD	A	1019	-	4,4,7	1.01	0	6,6,10	3.66	3 (50%)
4	DAL	A	11	4	3,4,5	0.95	0	0,4,6	0.00	-
4	DAL	A	12	4	2,5,5	0.18	0	0,6,6	0.00	-
2	BGC	A	8	1	11,11,12	0.57	0	14,15,17	0.64	0
3	DVC	A	9	1	5,11,12	0.72	0	7,18,20	1.24	1 (14%)
5	CIT	B	1015	-	3,12,12	0.59	0	3,17,17	2.39	2 (66%)
6	MPD	B	1016	-	6,7,7	1.24	1 (16%)	7,10,10	1.26	1 (14%)
4	DAL	B	11	4	3,4,5	0.79	0	0,4,6	0.00	-
4	DAL	B	12	4	2,5,5	0.44	0	0,6,6	0.00	-
2	BGC	B	8	1	11,11,12	0.94	1 (9%)	14,15,17	0.92	0
3	DVC	B	9	1	5,11,12	0.62	0	7,18,20	1.15	0
4	DAL	C	11	4	3,4,5	0.93	0	0,4,6	0.00	-
4	DAL	C	12	4	2,5,5	0.36	0	0,6,6	0.00	-
2	BGC	C	8	1	11,11,12	0.58	0	14,15,17	0.64	0
3	DVC	C	9	1	5,11,12	0.81	0	7,18,20	1.24	0
4	DAL	D	11	4	3,4,5	0.60	0	0,4,6	0.00	-
4	DAL	D	12	4	2,5,5	0.13	0	0,6,6	0.00	-
2	BGC	D	8	1	11,11,12	0.93	1 (9%)	14,15,17	0.99	0
3	DVC	D	9	1	5,11,12	0.51	0	7,18,20	1.31	1 (14%)

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	CIT	A	1015[A]	-	-	0/6/16/16	0/0/0/0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	CIT	A	1015[B]	-	-	0/6/16/16	0/0/0/0
5	CIT	A	1016[A]	-	-	0/6/16/16	0/0/0/0
5	CIT	A	1016[B]	-	-	0/6/16/16	0/0/0/0
5	CIT	A	1017[A]	-	-	0/7/15/16	0/0/0/0
5	CIT	A	1017[B]	-	-	0/6/16/16	0/0/0/0
5	CIT	A	1018[A]	-	-	0/6/16/16	0/0/0/0
5	CIT	A	1018[B]	-	-	0/7/15/16	0/0/0/0
6	MPD	A	1019	-	-	0/0/0/5	0/0/0/0
4	DAL	A	11	4	-	0/0/2/4	0/0/0/0
4	DAL	A	12	4	-	0/0/4/4	0/0/0/0
2	BGC	A	8	1	-	0/2/19/22	0/1/1/1
3	DVC	A	9	1	-	0/0/22/24	0/0/1/1
5	CIT	B	1015	-	-	0/6/16/16	0/0/0/0
6	MPD	B	1016	-	1/1/2/2	0/5/5/5	0/0/0/0
4	DAL	B	11	4	-	0/0/2/4	0/0/0/0
4	DAL	B	12	4	-	0/0/4/4	0/0/0/0
2	BGC	B	8	1	-	0/2/19/22	0/1/1/1
3	DVC	B	9	1	-	0/0/22/24	0/0/1/1
4	DAL	C	11	4	-	0/0/2/4	0/0/0/0
4	DAL	C	12	4	-	0/0/4/4	0/0/0/0
2	BGC	C	8	1	-	0/2/19/22	0/1/1/1
3	DVC	C	9	1	-	0/0/22/24	0/0/1/1
4	DAL	D	11	4	-	0/0/2/4	0/0/0/0
4	DAL	D	12	4	-	0/0/4/4	0/0/0/0
2	BGC	D	8	1	-	0/2/19/22	0/1/1/1
3	DVC	D	9	1	-	0/0/22/24	0/0/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	8	BGC	O5-C1	-2.61	1.39	1.43
6	B	1016	MPD	O4-C4	-2.53	1.30	1.43
2	B	8	BGC	O5-C1	-2.19	1.40	1.43
5	A	1016[A]	CIT	O7-C3	-2.16	1.39	1.43
5	A	1018[A]	CIT	O7-C3	2.10	1.46	1.43
5	A	1016[B]	CIT	C2-C3	2.12	1.57	1.54
5	A	1018[B]	CIT	C4-C3	5.30	1.62	1.54

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1018[B]	CIT	C3-C4-C5	-8.85	100.81	114.96

*Continued on next page...*

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	1015[B]	CIT	C3-C4-C5	-6.52	104.53	114.96
5	A	1016[A]	CIT	C3-C2-C1	-5.82	105.66	114.96
5	A	1015[A]	CIT	C3-C4-C5	-4.75	107.37	114.96
5	A	1017[A]	CIT	C4-C3-C2	-4.25	99.49	109.81
6	A	1019	MPD	C3-C2-CM	-3.94	100.62	111.05
5	B	1015	CIT	C3-C4-C5	-3.36	109.58	114.96
5	A	1018[B]	CIT	C2-C3-C4	-3.33	101.71	109.81
5	A	1017[A]	CIT	C3-C2-C1	-2.71	110.63	114.96
5	A	1017[B]	CIT	C3-C2-C1	-2.71	110.63	114.96
5	A	1015[B]	CIT	C3-C2-C1	-2.56	110.86	114.96
5	B	1015	CIT	C4-C3-C2	-2.39	104.09	109.81
5	A	1015[A]	CIT	C3-C2-C1	-2.35	111.21	114.96
5	A	1018[A]	CIT	C3-C2-C1	-2.29	111.30	114.96
6	A	1019	MPD	CM-C2-C1	-2.22	105.16	111.05
5	A	1016[A]	CIT	C4-C3-C2	-2.08	104.84	109.81
3	A	9	DVC	C2-C3-C4	2.11	109.28	107.10
6	B	1016	MPD	C2-C3-C4	2.13	126.71	116.66
3	D	9	DVC	C3M-C3-C2	2.20	114.06	110.74
5	A	1017[B]	CIT	C4-C3-C2	2.28	115.26	109.81
5	A	1018[B]	CIT	O7-C3-C2	2.45	114.19	109.22
5	A	1018[A]	CIT	C3-C4-C5	4.58	122.28	114.96
6	A	1019	MPD	O2-C2-C3	7.63	125.99	107.78
5	A	1017[A]	CIT	O7-C3-C4	7.86	125.19	109.22

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
6	B	1016	MPD	C4

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	1015[B]	CIT	3	0
5	A	1017[B]	CIT	2	0
5	B	1015	CIT	1	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	1/7 (14%)	-0.51	0 100 100	4, 4, 4, 4	0
1	B	1/7 (14%)	-0.92	0 100 100	5, 5, 5, 5	0
1	C	1/7 (14%)	-0.85	0 100 100	4, 4, 4, 4	0
1	D	1/7 (14%)	-0.76	0 100 100	4, 4, 4, 4	0
All	All	4/28 (14%)	-0.76	0 100 100	4, 4, 4, 5	0

There are no RSRZ outliers to report.

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

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
1	GHP	A	5	11/12	1.00	0.04	-	2,2,3,4	0
1	MLU	C	1	9/10	0.99	0.05	-	5,10,27,27	0
1	3FG	B	7	13/13	1.00	0.04	-	2,3,5,8	0
1	OMY	A	6	14/15	1.00	0.04	-	2,2,3,4	0
1	OMY	B	6	14/15	0.99	0.05	-	2,2,3,5	0
1	OMZ	B	2	14/15	1.00	0.04	-	3,3,4,7	0
1	GHP	C	5	11/12	1.00	0.05	-	2,2,3,4	0
1	3FG	A	7	13/13	1.00	0.04	-	2,3,4,7	0
1	GHP	D	4	11/12	1.00	0.05	-	2,2,3,3	0
1	MLU	A	1	9/10	0.97	0.09	-	4,12,28,28	0
1	MLU	B	1	9/10	0.96	0.11	-	5,21,62,62	0
1	OMZ	D	2	14/15	1.00	0.04	-	3,3,4,7	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	GHP	C	4	11/12	1.00	0.04	-	2,2,3,3	0
1	GHP	B	4	11/12	1.00	0.04	-	2,2,3,3	0
1	GHP	A	4	11/12	1.00	0.04	-	2,2,3,3	0
1	3FG	D	7	13/13	0.99	0.04	-	2,3,10,15	0
1	OMY	C	6	14/15	1.00	0.04	-	2,2,3,4	0
1	3FG	C	7	13/13	1.00	0.04	-	2,4,9,13	0
1	MLU	D	1	9/10	0.99	0.05	-	5,9,19,19	0
1	OMZ	C	2	14/15	1.00	0.04	-	2,3,4,6	0
1	GHP	B	5	11/12	1.00	0.04	-	2,2,3,4	0
1	GHP	D	5	11/12	1.00	0.04	-	2,2,3,4	0
1	OMZ	A	2	14/15	1.00	0.04	-	2,3,4,5	0
1	OMY	D	6	14/15	0.99	0.05	-	2,2,3,5	0

### 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

### 6.4 Ligands ⓘ

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( $\text{\AA}^2$ )	Q<0.9
4	DAL	C	11	5/6	0.99	0.05	-	4,4,7,7	0
4	DAL	A	11	5/6	1.00	0.03	-	3,5,8,8	0
3	DVC	C	9	11/12	0.99	0.04	-	3,4,9,9	0
3	DVC	D	9	11/12	0.99	0.04	-	2,4,7,7	0
5	CIT	A	1018[B]	12/13	0.97	0.16	-	7,12,21,32	17
5	CIT	A	1018[A]	13/13	0.97	0.16	-	4,6,12,13	18
5	CIT	A	1016[A]	13/13	0.99	0.09	-	3,5,8,11	18
4	DAL	D	11	5/6	0.99	0.05	-	3,4,6,6	0
5	CIT	A	1016[B]	13/13	0.99	0.09	-	4,7,12,17	18
4	DAL	D	12	6/6	1.00	0.04	-	3,3,7,7	0
6	MPD	A	1019	5/8	0.93	0.31	-	5,5,8,12	5
3	DVC	B	9	11/12	0.99	0.04	-	2,4,7,7	0
2	BGC	A	8	11/12	1.00	0.04	-	2,4,6,7	0
4	DAL	B	11	5/6	1.00	0.04	-	4,5,9,9	0

*Continued on next page...*

*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BGC	C	8	11/12	1.00	0.04	-	3,4,6,7	0
2	BGC	D	8	11/12	0.99	0.04	-	3,6,9,12	0
4	DAL	B	12	6/6	1.00	0.04	-	3,4,6,6	0
4	DAL	A	12	6/6	1.00	0.04	-	3,3,6,6	0
5	CIT	A	1017[A]	12/13	0.98	0.12	-	5,7,11,14	5
3	DVC	A	9	11/12	0.99	0.04	-	3,4,9,9	0
5	CIT	A	1015[B]	13/13	0.99	0.06	-	3,4,8,10	18
6	MPD	B	1016	8/8	0.85	0.28	-	3,5,11,13	7
5	CIT	A	1017[B]	13/13	0.98	0.12	-	4,6,11,14	6
5	CIT	B	1015	13/13	0.93	0.15	-	3,6,17,17	18
5	CIT	A	1015[A]	13/13	0.99	0.06	-	2,4,7,9	18
4	DAL	C	12	6/6	1.00	0.04	-	3,4,8,8	0
2	BGC	B	8	11/12	0.99	0.04	-	3,6,9,11	0

## 6.5 Other polymers

There are no such residues in this entry.