



# Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 07:30 PM GMT

PDB ID : 1HHC  
Title : Decaplanin second P21-Form  
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Deposited on : 2000-12-22  
Resolution : 1.13 Å(reported)

This is a full wwPDB 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/ValidationPDFNotes.html>

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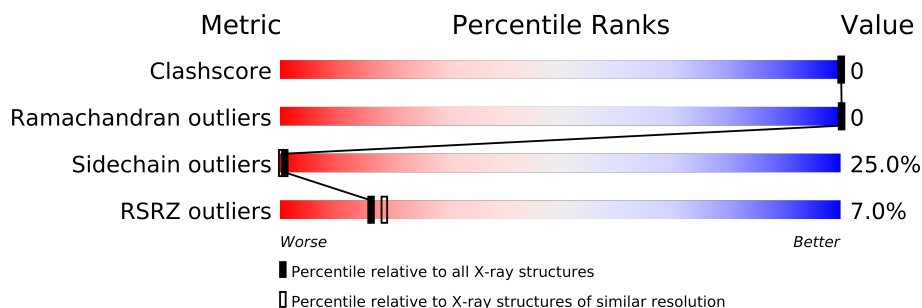
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.15 2013  
Xtriage (Phenix) : dev-1323  
EDS : stable22639  
Percentile statistics : 21963  
Refmac : 5.8.0049  
CCP4 : 6.3.0 (Settle)  
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 1.13 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	1354 (1.20-1.04)
Ramachandran outliers	78287	1287 (1.20-1.04)
Sidechain outliers	78261	1285 (1.20-1.04)
RSRZ outliers	66119	1225 (1.20-1.04)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	7	
1	B	7	
1	C	7	
1	D	7	

## 2 Entry composition i

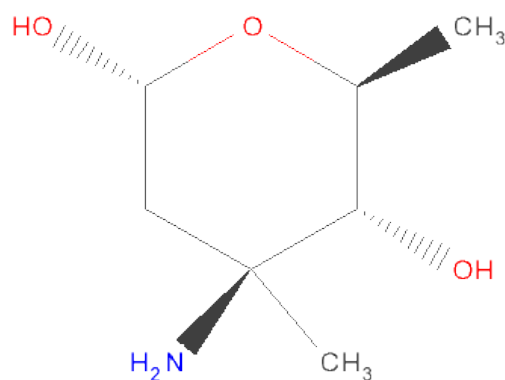
There are 5 unique types of molecules in this entry. The entry contains 629 atoms, of which 0 are hydrogen and 0 are deuterium.

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 DECAPLANIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	7	Total	C	Cl	N	O	0	0	0
			79	53	1	8	17			
1	B	7	Total	C	Cl	N	O	0	0	0
			76	50	1	8	17			
1	C	7	Total	C	Cl	N	O	0	0	0
			79	53	1	8	17			
1	D	7	Total	C	Cl	N	O	0	0	0
			79	53	1	8	17			

- Molecule 2 is SUGAR ((1R,3S,4R,5S)-3-AMINO-2,3,6-TRIDEOXY-3-METHYL-ALPHA-L-ARABINO-HEXOPYRANOSE) (three-letter code: ERE) (formula: C<sub>7</sub>H<sub>15</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			10	7	1	2		
2	B	1	Total	C	N	O	0	0
			10	7	1	2		

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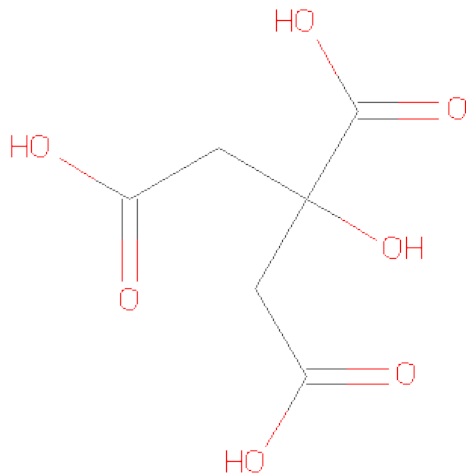
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			10	7	1	2		
2	D	1	Total	C	N	O	0	0
			10	7	1	2		

- Molecule 3 is a polymer of unknown type called SUGAR (2-MER).

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	2	Total	C	O	0	0
			21	12	9		
3	B	2	Total	C	O	0	0
			21	12	9		
3	C	2	Total	C	O	0	0
			21	12	9		
3	D	2	Total	C	O	0	0
			21	12	9		

- Molecule 4 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
4	D	1	Total	C	O	0	0
			13	6	7		
4	A	1	Total	C	O	0	0
			13	6	7		
4	C	1	Total	C	O	0	0
			3	1	2		

- Molecule 5 is water.

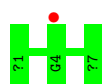
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	41	Total 41	O 41	0	0
5	B	42	Total 42	O 42	0	0
5	C	38	Total 38	O 38	0	0
5	D	42	Total 42	O 42	0	0

### 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.

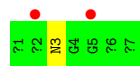
- Molecule 1: DECAPLANIN

Chain A: 



- Molecule 1: DECAPLANIN

Chain B: 



- Molecule 1: DECAPLANIN

Chain C: 

There are no outlier residues recorded for this chain.

- Molecule 1: DECAPLANIN

Chain D: 

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, $\alpha$ , $\beta$ , $\gamma$	28.95Å 31.91Å 34.73Å 90.00° 109.87° 90.00°	Depositor
Resolution (Å)	18.08 – 1.13 18.10 – 1.13	Depositor EDS
% Data completeness (in resolution range)	96.8 (18.08-1.13) 89.8 (18.10-1.13)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.23 (at 1.13Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, $R_{free}$	0.224 , 0.264 0.206 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	5.3	Xtriage
Anisotropy	0.258	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.42 , 84.7	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 21506 reflections	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	629	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	8.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.88% of the height of the origin peak. No significant pseudotranslation is detected.*

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, GHP, RAM, OMZ, ERE, CIT, MLU, 3FG, OMX

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	0.70	0/7	1.21	0/8
1	B	0.98	0/7	2.41	0/8
1	C	0.70	0/7	0.87	0/8
1	D	0.39	0/7	1.16	0/8
All	All	0.72	0/28	1.53	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 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	79	0	0	0	0
1	B	76	0	0	0	0
1	C	79	0	0	0	0
1	D	79	0	0	0	0
2	A	10	0	0	0	0
2	B	10	0	0	0	0
2	C	10	0	0	0	0
2	D	10	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	21	0	0	0	0
3	B	21	0	0	0	0
3	C	21	0	0	0	0
3	D	21	0	0	0	0
4	A	13	0	0	0	0
4	C	3	0	0	0	0
4	D	13	0	0	0	0
5	A	41	0	0	0	0
5	B	42	0	0	0	0
5	C	38	0	0	0	0
5	D	42	0	0	0	0
All	All	629	0	0	0	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 0.

There are no clashes within the asymmetric unit.

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	1/7 (14%)	1 (100%)	0	0	100	100
1	B	1/7 (14%)	0	1 (100%)	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%)	0	1 (100%)	0	0
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%)	3 (75%)	1 (25%)	1	0

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	3	ASN

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 chains 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	8,8,9	5.47	3 (37%)	6,9,11	1.21	1 (16%)
1	OMZ	A	2	1	14,14,15	5.70	2 (14%)	17,19,21	2.58	2 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
1	GHP	A	4	1,3	11,11,12	6.34	2 (18%)	12,14,16	11.87	5 (41%)
1	GHP	A	5	1	11,11,12	6.43	2 (18%)	12,14,16	6.90	3 (25%)
1	OMX	A	6	1,2	13,13,14	4.51	2 (15%)	15,17,19	1.76	4 (26%)
1	3FG	A	7	1	13,13,13	1.14	0	18,18,18	1.62	5 (27%)
1	MLU	B	1	1	4,5,9	8.54	3 (75%)	1,5,11	5.17	1 (100%)
1	OMZ	B	2	1	14,14,15	5.84	2 (14%)	17,19,21	1.27	3 (17%)
1	GHP	B	4	1,3	11,11,12	5.90	3 (27%)	12,14,16	10.03	4 (33%)
1	GHP	B	5	1	11,11,12	5.53	3 (27%)	12,14,16	13.55	3 (25%)
1	OMX	B	6	1,2	13,13,14	3.64	1 (7%)	15,17,19	2.40	7 (46%)
1	3FG	B	7	1	13,13,13	1.03	0	18,18,18	1.27	2 (11%)
1	MLU	C	1	1	8,8,9	6.81	3 (37%)	6,9,11	0.80	0
1	OMZ	C	2	1	14,14,15	6.06	3 (21%)	17,19,21	1.68	5 (29%)
1	GHP	C	4	1,3	11,11,12	5.23	2 (18%)	12,14,16	10.81	1 (8%)
1	GHP	C	5	1	11,11,12	6.64	2 (18%)	12,14,16	11.21	5 (41%)
1	OMX	C	6	1,2	13,13,14	3.77	2 (15%)	15,17,19	1.37	3 (20%)
1	3FG	C	7	1	13,13,13	0.87	0	18,18,18	1.75	3 (16%)
1	MLU	D	1	1	8,8,9	6.56	3 (37%)	6,9,11	1.57	2 (33%)
1	OMZ	D	2	1	14,14,15	5.99	3 (21%)	17,19,21	1.52	3 (17%)
1	GHP	D	4	1,3	11,11,12	5.59	3 (27%)	12,14,16	10.04	4 (33%)
1	GHP	D	5	1	11,11,12	6.02	2 (18%)	12,14,16	8.66	4 (33%)
1	OMX	D	6	1,2	13,13,14	4.28	1 (7%)	15,17,19	2.55	7 (46%)
1	3FG	D	7	1	13,13,13	1.07	0	18,18,18	1.69	4 (22%)

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	-	0/6/8/10	0/0/0/0
1	OMZ	A	2	1	-	0/8/10/12	0/1/1/1
1	GHP	A	4	1,3	-	0/4/6/8	0/1/1/1
1	GHP	A	5	1	-	0/4/6/8	0/1/1/1
1	OMX	A	6	1,2	-	0/8/10/12	0/1/1/1
1	3FG	A	7	1	-	0/8/8/8	0/1/1/1
1	MLU	B	1	1	-	0/2/4/10	0/0/0/0
1	OMZ	B	2	1	-	0/8/10/12	0/1/1/1

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

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	2	OMZ	O-C	22.20	1.26	1.11
1	D	2	OMZ	O-C	21.89	1.26	1.11
1	B	2	OMZ	O-C	21.55	1.26	1.11
1	A	5	GHP	O-C	21.15	1.26	1.11
1	C	5	GHP	O-C	20.96	1.25	1.11
1	A	2	OMZ	O-C	20.95	1.25	1.11
1	A	4	GHP	O-C	20.26	1.25	1.11
1	D	5	GHP	O-C	19.34	1.24	1.11
1	B	4	GHP	O-C	18.83	1.24	1.11
1	C	1	MLU	O-C	18.72	1.24	1.11
1	D	1	MLU	O-C	17.88	1.23	1.11
1	D	4	GHP	O-C	17.85	1.23	1.11
1	B	5	GHP	O-C	17.62	1.23	1.11
1	C	4	GHP	O-C	16.64	1.22	1.11
1	B	1	MLU	O-C	15.85	1.22	1.11
1	A	6	OMX	O-C	15.83	1.22	1.11
1	D	6	OMX	O-C	14.99	1.21	1.11
1	A	1	MLU	O-C	14.80	1.21	1.11
1	C	6	OMX	O-C	13.08	1.20	1.11
1	B	6	OMX	O-C	12.71	1.20	1.11
1	C	5	GHP	CA-C	6.56	1.55	1.48
1	B	1	MLU	CA-N	5.82	1.51	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	4	GHP	CA-C	4.81	1.53	1.48
1	D	5	GHP	CA-C	4.53	1.53	1.48
1	B	4	GHP	CA-C	4.03	1.52	1.48
1	D	1	MLU	CA-N	3.91	1.51	1.46
1	C	4	GHP	CA-C	3.87	1.52	1.48
1	C	1	MLU	CA-C	3.76	1.55	1.48
1	B	5	GHP	CA-C	3.64	1.52	1.48
1	D	4	GHP	CA-C	3.53	1.52	1.48
1	A	1	MLU	CA-N	3.44	1.51	1.46
1	B	4	GHP	C6-C1	-3.27	1.33	1.39
1	D	1	MLU	CA-C	3.06	1.54	1.48
1	D	2	OMZ	CG-CB	-2.90	1.47	1.51
1	D	4	GHP	C6-C1	-2.86	1.34	1.39
1	B	2	OMZ	CA-CB	2.74	1.59	1.54
1	C	2	OMZ	CZ-CE1	-2.70	1.36	1.39
1	C	2	OMZ	CA-C	2.64	1.53	1.48
1	B	5	GHP	C1-CA	2.47	1.56	1.52
1	B	1	MLU	CA-C	2.29	1.52	1.48
1	A	1	MLU	CA-C	2.27	1.52	1.48
1	A	6	OMX	CD2-CG	2.24	1.42	1.39
1	A	2	OMZ	CA-C	2.24	1.52	1.48
1	A	5	GHP	CA-C	2.23	1.50	1.48
1	D	2	OMZ	OH-CZ	2.21	1.41	1.36
1	C	1	MLU	CA-N	2.15	1.49	1.46
1	C	6	OMX	CE2-CD2	-2.13	1.34	1.38

All (81) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	5	GHP	C-CA-N	-46.68	107.98	113.27
1	A	4	GHP	C-CA-N	-40.66	108.66	113.27
1	C	5	GHP	C-CA-N	-38.10	108.95	113.27
1	C	4	GHP	C-CA-N	-37.34	109.04	113.27
1	D	4	GHP	C-CA-N	-34.31	109.38	113.27
1	B	4	GHP	C-CA-N	-34.29	109.38	113.27
1	D	5	GHP	C-CA-N	-29.22	109.96	113.27
1	A	5	GHP	C-CA-N	-23.31	110.63	113.27
1	A	2	OMZ	CD1-CE1-CZ	-9.14	116.38	121.13
1	D	6	OMX	CE1-CD1-CG	5.76	127.30	121.20
1	B	6	OMX	CD1-CE1-CZ	-5.25	113.54	119.87
1	B	1	MLU	CN-N-CA	-5.17	106.50	113.92
1	D	5	GHP	C3-C2-C1	4.84	126.33	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	6	OMX	CE1-CD1-CG	4.71	126.19	121.20
1	C	5	GHP	C5-C6-C1	-4.24	116.71	121.20
1	D	6	OMX	CD1-CE1-CZ	-4.08	114.95	119.87
1	D	4	GHP	C3-C2-C1	-3.95	117.02	121.20
1	A	4	GHP	C5-C6-C1	3.81	125.23	121.20
1	A	6	OMX	CG-CB-CA	-3.69	106.28	111.75
1	A	2	OMZ	CD1-CE1-CL	3.65	124.29	118.55
1	B	5	GHP	C2-C3-C4	-3.64	115.48	119.87
1	D	2	OMZ	CB-CA-N	3.64	114.75	109.14
1	D	6	OMX	OC-CB-CA	-3.60	100.37	109.21
1	C	5	GHP	C3-C2-C1	3.60	125.01	121.20
1	D	6	OMX	CD1-CG-CB	3.56	125.83	120.75
1	C	7	3FG	CD2-CZ-CD1	3.55	124.32	119.21
1	C	7	3FG	CG2-CD2-CZ	-3.45	115.38	120.43
1	D	2	OMZ	CG-CB-CA	3.44	116.85	111.75
1	C	5	GHP	C2-C3-C4	-3.38	115.79	119.87
1	D	7	3FG	CD2-CZ-CD1	3.38	124.09	119.21
1	C	2	OMZ	CD2-CE2-CZ	-3.28	116.93	120.50
1	D	7	3FG	CD1-CG1-CB	-3.25	117.24	120.05
1	A	6	OMX	OC-CB-CA	-3.23	101.28	109.21
1	D	7	3FG	CG2-CD2-CZ	-3.06	115.94	120.43
1	C	6	OMX	OC-CB-CA	-3.03	101.77	109.21
1	C	2	OMZ	CB-CA-N	2.92	113.64	109.14
1	A	5	GHP	C6-C5-C4	2.86	123.31	119.87
1	C	5	GHP	C6-C5-C4	2.85	123.30	119.87
1	A	7	3FG	CD2-CG2-CB	2.82	122.48	120.05
1	D	5	GHP	C2-C3-C4	-2.81	116.48	119.87
1	D	1	MLU	CG-CB-CA	2.81	123.54	115.45
1	B	4	GHP	C3-C2-C1	2.80	124.17	121.20
1	B	4	GHP	C6-C1-C2	-2.77	114.66	118.33
1	A	5	GHP	C3-C2-C1	2.77	124.13	121.20
1	B	6	OMX	OC-CB-CG	2.75	117.15	111.09
1	C	2	OMZ	CD1-CE1-CZ	2.74	122.55	121.13
1	C	6	OMX	CD2-CG-CB	-2.66	116.96	120.75
1	B	7	3FG	CD1-CG1-CB	-2.65	117.76	120.05
1	C	2	OMZ	C-CA-N	2.63	116.20	111.94
1	A	6	OMX	CD1-CG-CB	2.60	124.47	120.75
1	A	6	OMX	OC-CB-CG	2.52	116.65	111.09
1	A	7	3FG	OXT-C-O	2.50	129.72	124.07
1	A	4	GHP	C6-C1-C2	-2.49	115.03	118.33
1	A	1	MLU	CB-CA-N	-2.46	104.69	110.54
1	D	1	MLU	CB-CA-N	-2.46	104.69	110.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	4	GHP	C5-C6-C1	2.45	123.79	121.20
1	A	7	3FG	OD2-CD2-CG2	2.44	126.21	119.78
1	A	4	GHP	C6-C1-CA	2.43	123.96	120.60
1	B	4	GHP	C5-C6-C1	2.41	123.75	121.20
1	B	6	OMX	CD2-CG-CB	-2.36	117.39	120.75
1	B	7	3FG	OXT-C-O	2.35	129.39	124.07
1	A	7	3FG	O-C-CA	-2.35	113.75	121.27
1	C	2	OMZ	CE2-CZ-CE1	2.33	120.82	118.80
1	A	4	GHP	C2-C3-C4	2.31	122.65	119.87
1	D	2	OMZ	CE2-CZ-CE1	2.30	120.79	118.80
1	D	6	OMX	CD2-CG-CB	-2.27	117.51	120.75
1	D	7	3FG	C-CA-N	2.24	114.11	108.21
1	D	5	GHP	C2-C1-CA	2.24	123.69	120.60
1	B	2	OMZ	C-CA-N	2.22	115.55	111.94
1	B	5	GHP	C3-C2-C1	2.20	123.53	121.20
1	A	7	3FG	OD2-CD2-CZ	-2.18	114.04	119.78
1	C	7	3FG	CD2-CG2-CB	2.18	121.94	120.05
1	D	4	GHP	C2-C3-C4	2.18	122.49	119.87
1	B	2	OMZ	CD1-CE1-CZ	-2.17	120.00	121.13
1	D	6	OMX	CG-CB-CA	-2.13	108.59	111.75
1	B	2	OMZ	CD2-CG-CB	2.07	123.70	120.75
1	B	6	OMX	OC-CB-CA	-2.06	104.15	109.21
1	B	6	OMX	CE2-CD2-CG	-2.03	119.05	121.20
1	D	6	OMX	OC-CB-CG	2.03	115.56	111.09
1	C	6	OMX	CB-CA-N	2.01	112.24	109.14
1	B	6	OMX	CD1-CG-CB	2.01	123.62	120.75

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 5.5 Carbohydrates ⓘ

8 carbohydrates 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	RAM	A	10	3	9,10,11	1.95	3 (33%)	10,14,16	2.72	5 (50%)
3	BGC	A	9	1,3	10,11,12	1.80	2 (20%)	11,15,17	1.86	4 (36%)
3	RAM	B	10	3	9,10,11	2.67	3 (33%)	10,14,16	1.89	1 (10%)
3	BGC	B	9	1,3	10,11,12	1.35	2 (20%)	11,15,17	2.53	3 (27%)
3	RAM	C	10	3	9,10,11	2.15	2 (22%)	10,14,16	0.87	0
3	BGC	C	9	1,3	10,11,12	1.24	1 (10%)	11,15,17	1.74	1 (9%)
3	RAM	D	10	3	9,10,11	2.06	1 (11%)	10,14,16	2.33	6 (60%)
3	BGC	D	9	1,3	10,11,12	1.27	1 (10%)	11,15,17	1.24	1 (9%)

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	RAM	A	10	3	-	0/0/17/20	0/1/1/1
3	BGC	A	9	1,3	-	0/2/19/22	0/1/1/1
3	RAM	B	10	3	-	0/0/17/20	0/1/1/1
3	BGC	B	9	1,3	-	0/2/19/22	0/1/1/1
3	RAM	C	10	3	-	0/0/17/20	0/1/1/1
3	BGC	C	9	1,3	-	0/2/19/22	0/1/1/1
3	RAM	D	10	3	-	0/0/17/20	0/1/1/1
3	BGC	D	9	1,3	-	0/2/19/22	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	10	RAM	C3-C2	-6.07	1.39	1.52
3	C	10	RAM	C3-C2	-5.49	1.40	1.52
3	D	10	RAM	C3-C2	-5.17	1.41	1.52
3	B	10	RAM	O5-C5	-4.43	1.37	1.45
3	A	10	RAM	C3-C2	-3.98	1.44	1.52
3	A	9	BGC	O4-C4	3.56	1.51	1.43
3	A	9	BGC	O3-C3	3.26	1.50	1.43
3	A	10	RAM	O5-C5	-2.89	1.40	1.45
3	D	9	BGC	O4-C4	2.85	1.49	1.43
3	B	9	BGC	O4-C4	2.61	1.49	1.43
3	A	10	RAM	C4-C3	2.37	1.58	1.52
3	B	9	BGC	O5-C5	2.17	1.49	1.45
3	C	10	RAM	O5-C5	-2.10	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	9	BGC	O4-C4	2.07	1.48	1.43
3	B	10	RAM	O2-C2	2.01	1.47	1.43

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	9	BGC	O5-C5-C4	-6.36	102.58	110.65
3	B	10	RAM	C4-C3-C2	5.14	117.40	110.50
3	A	10	RAM	O5-C5-C6	-4.95	100.07	108.03
3	C	9	BGC	O5-C5-C4	-4.83	104.53	110.65
3	A	10	RAM	O3-C3-C2	-4.11	102.42	109.94
3	B	9	BGC	C4-C3-C2	-3.77	105.45	110.50
3	A	10	RAM	O5-C5-C4	3.67	115.77	110.22
3	D	10	RAM	O3-C3-C2	3.56	116.45	109.94
3	A	10	RAM	C3-C4-C5	-3.33	104.30	109.84
3	D	10	RAM	O5-C5-C6	-3.28	102.77	108.03
3	A	9	BGC	O5-C5-C4	-3.22	106.57	110.65
3	A	9	BGC	O5-C5-C6	-3.01	103.82	106.98
3	B	9	BGC	O2-C2-C3	-2.96	103.78	110.18
3	D	10	RAM	C6-C5-C4	-2.68	108.71	113.06
3	A	9	BGC	O3-C3-C4	-2.57	104.59	110.35
3	D	10	RAM	O5-C5-C4	-2.53	106.40	110.22
3	D	9	BGC	C6-C5-C4	2.45	118.91	113.00
3	D	10	RAM	O4-C4-C3	2.42	115.77	110.35
3	A	9	BGC	C6-C5-C4	2.34	118.64	113.00
3	A	10	RAM	C4-C3-C2	-2.33	107.38	110.50
3	D	10	RAM	C4-C3-C2	2.06	113.27	110.50

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	$\# Z  > 2$
4	CIT	A	1002	-	12,12,12	1.40	2 (16%)	17,17,17	1.79	5 (29%)
2	ERE	A	8	1	9,10,11	1.02	0	12,15,17	1.14	1 (8%)
2	ERE	B	8	1	9,10,11	0.66	0	12,15,17	1.39	2 (16%)
4	CIT	C	1003	-	2,2,12	0.55	0	1,1,17	0.56	0
2	ERE	C	8	1	9,10,11	0.66	0	12,15,17	1.37	1 (8%)
4	CIT	D	1001	-	12,12,12	1.22	2 (16%)	17,17,17	1.85	4 (23%)
2	ERE	D	8	1	9,10,11	1.34	2 (22%)	12,15,17	1.36	1 (8%)

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	CIT	A	1002	-	-	0/16/16/16	0/0/0/0
2	ERE	A	8	1	-	0/0/17/19	0/1/1/1
2	ERE	B	8	1	-	0/0/17/19	0/1/1/1
4	CIT	C	1003	-	-	0/0/0/16	0/0/0/0
2	ERE	C	8	1	-	0/0/17/19	0/1/1/1
4	CIT	D	1001	-	-	0/16/16/16	0/0/0/0
2	ERE	D	8	1	-	0/0/17/19	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	8	ERE	C2-C3	-2.92	1.49	1.53
4	A	1002	CIT	O4-C5	-2.52	1.21	1.30
4	D	1001	CIT	C2-C3	2.41	1.56	1.53
4	D	1001	CIT	O4-C5	-2.24	1.22	1.30
4	A	1002	CIT	C3-C6	-2.17	1.50	1.53
2	D	8	ERE	O4-C4	2.10	1.47	1.42

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	1001	CIT	O6-C6-C3	4.79	119.86	112.89
2	C	8	ERE	O5-C5-C5A	-3.57	102.29	108.03
2	B	8	ERE	C2-C3-C4	-3.06	104.30	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	1002	CIT	O4-C5-C4	2.97	125.08	114.63
4	A	1002	CIT	O4-C5-O3	-2.96	115.76	123.30
2	A	8	ERE	C5A-C5-C4	-2.95	107.30	112.59
2	D	8	ERE	O5-C5-C5A	-2.94	103.31	108.03
4	D	1001	CIT	C2-C3-C6	-2.74	103.77	110.12
2	B	8	ERE	C3A-C3-C2	2.71	118.47	112.14
4	A	1002	CIT	O5-C6-C3	-2.70	118.48	122.20
4	A	1002	CIT	C2-C3-C6	-2.45	104.45	110.12
4	D	1001	CIT	O4-C5-C4	2.44	123.24	114.63
4	D	1001	CIT	O3-C5-C4	-2.41	115.09	122.74
4	A	1002	CIT	C4-C3-C6	2.14	115.08	110.12

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

## 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	7/7 (100%)	1.29	1 (14%) 3 5	4, 5, 8, 9	0
1	B	7/7 (100%)	1.76	2 (28%) 1 1	3, 4, 7, 11	0
1	C	7/7 (100%)	0.83	0 100 100	3, 4, 5, 6	0
1	D	7/7 (100%)	1.23	0 100 100	3, 4, 6, 7	0
All	All	28/28 (100%)	1.28	3 (10%) 16 8	3, 5, 8, 11	0

All (3) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	5	GHP	2.6
1	B	2	OMZ	2.5
1	A	4	GHP	2.2

### 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
1	GHP	B	5	11/12	0.11	2.50	2,3,4,4	0
1	GHP	C	5	11/12	0.10	1.29	2,3,4,6	0
1	MLU	D	1	9/10	0.11	1.00	6,7,8,9	0
1	GHP	D	5	11/12	0.10	0.81	2,3,3,6	0
1	GHP	A	5	11/12	0.08	-6.50	4,5,6,7	0
1	OMX	C	6	13/14	0.07	-	2,3,3,4	0
1	OMX	D	6	13/14	0.07	-	2,3,3,4	0

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Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
1	MLU	B	1	6/10	0.15	-	9,10,11,12	0
1	GHP	D	4	11/12	0.10	-	3,3,4,4	0
1	3FG	B	7	13/13	0.10	-	2,2,3,4	0
1	OMZ	B	2	14/15	0.11	-	5,6,8,8	0
1	3FG	A	7	13/13	0.09	-	7,8,10,11	0
1	MLU	C	1	9/10	0.11	-	4,5,7,8	0
1	OMZ	C	2	14/15	0.07	-	3,4,5,6	0
1	3FG	D	7	13/13	0.09	-	3,3,6,6	0
1	3FG	C	7	13/13	0.08	-	4,5,7,8	0
1	GHP	A	4	11/12	0.11	-	3,4,4,4	0
1	GHP	B	4	11/12	0.09	-	3,4,4,5	0
1	OMX	A	6	13/14	0.10	-	5,5,6,6	0
1	OMX	B	6	13/14	0.09	-	2,3,4,4	0
1	MLU	A	1	9/10	0.12	-	6,7,9,11	0
1	OMZ	D	2	14/15	0.10	-	4,5,6,7	0
1	OMZ	A	2	14/15	0.08	-	4,5,5,6	0
1	GHP	C	4	11/12	0.09	-	2,2,3,3	0

### 6.3 Carbohydrates ⓘ

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	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
3	BGC	D	9	11/12	0.11	-	5,5,7,7	0
3	BGC	B	9	11/12	0.12	-	5,7,8,9	0
3	RAM	B	10	10/11	0.13	-	6,7,9,10	0
3	BGC	A	9	11/12	0.10	-	4,5,6,6	0
3	RAM	D	10	10/11	0.11	-	6,7,9,9	0
3	BGC	C	9	11/12	0.10	-	3,4,4,6	0
3	RAM	C	10	10/11	0.10	-	5,6,9,9	0
3	RAM	A	10	10/11	0.15	-	7,9,12,13	0

### 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	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
4	CIT	D	1001	13/13	0.08	-5.44	4,4,5,5	0
2	ERE	D	8	10/11	0.10	-	3,4,5,7	0
2	ERE	A	8	10/11	0.09	-	6,7,9,10	0
2	ERE	C	8	10/11	0.10	-	4,5,5,7	0
2	ERE	B	8	10/11	0.07	-	3,4,5,6	0
4	CIT	A	1002	13/13	0.23	-	2,5,7,7	13
4	CIT	C	1003	3/13	0.08	-	8,8,8,8	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.