



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 07:50 PM GMT

PDB ID : 1HHA
Title : Decaplanin first P6122-Form
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Deposited on : 2000-12-22
Resolution : 1.90 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
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

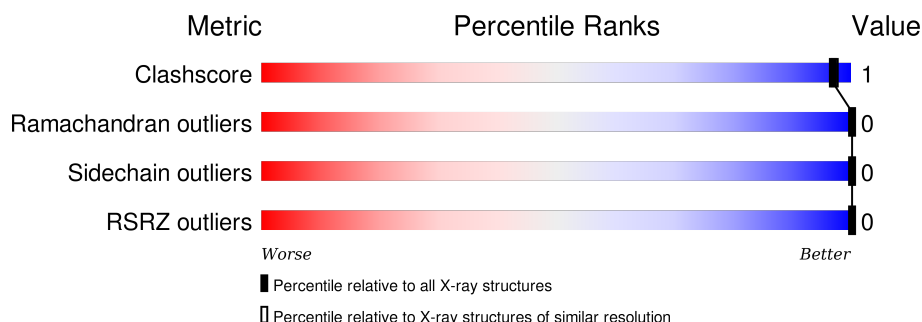
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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	5398 (1.90-1.90)
Ramachandran outliers	100387	5338 (1.90-1.90)
Sidechain outliers	100360	5339 (1.90-1.90)
RSRZ outliers	91569	4766 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. 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	100%
1	B	7	100%
1	C	7	100%
1	D	7	100%

2 Entry composition [i](#)

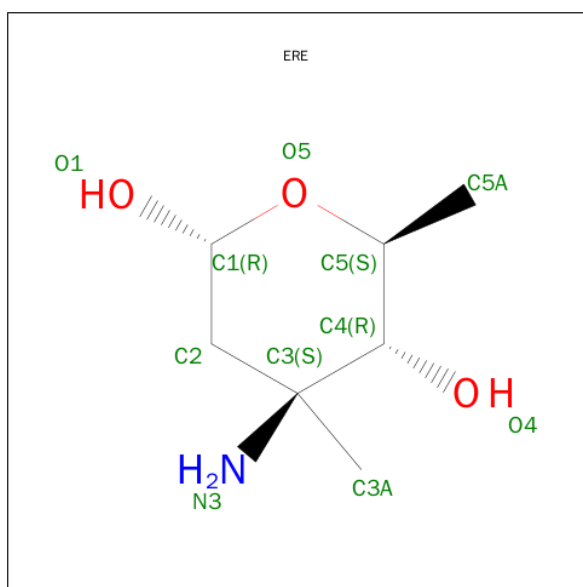
There are 5 unique types of molecules in this entry. The entry contains 532 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 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
			79	53	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: C₇H₁₅NO₃).



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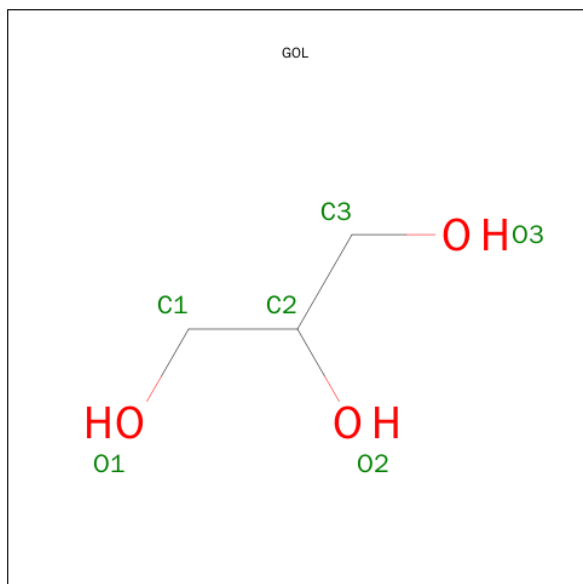
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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			10	7	1	2		
2	D	1	Total	C	N	O	0	0
			10	7	1	2		

- 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 GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total	C	O	0	1
			12	6	6		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	16	Total 16	O 16	0	0
5	B	28	Total 28	O 28	0	0
5	C	18	Total 18	O 18	0	0
5	D	11	Total 12	O 12	0	1

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:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: DECAPLANIN

Chain B:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: DECAPLANIN

Chain C:  100%

There are no outlier residues recorded for this chain.

- Molecule 1: DECAPLANIN

Chain D:  100%

There are no outlier residues recorded for this chain.

4 Data and refinement statistics

Property	Value	Source
Space group	P 61 2 2	Depositor
Cell constants a, b, c, α , β , γ	64.36Å 64.36Å 84.13Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	23.23 – 1.90 23.23 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (23.23-1.90) 97.7 (23.23-1.90)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.49 (at 1.90Å)	Xtriage
Refinement program	SHELXL-97	Depositor
R, R_{free}	0.220 , 0.265 0.272 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	15.8	Xtriage
Anisotropy	0.373	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 118.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 8592 reflections	Xtriage
F_o, F_c correlation	0.89	EDS
Total number of atoms	532	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 8.53% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: GOL, BGC, GHP, RAM, OMZ, ERE, 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	0.77	0/7	1.88	0/8
1	B	0.92	0/7	2.60	0/8
1	C	0.88	0/7	1.94	0/8
1	D	0.81	0/7	1.67	0/8
All	All	0.85	0/28	2.05	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	79	0	43	0	0
1	B	79	0	44	0	0
1	C	79	0	43	0	0
1	D	79	0	43	0	0
2	A	10	0	13	0	0
2	B	10	0	13	0	0
2	C	10	0	13	0	0
2	D	10	0	13	0	0
3	A	21	0	18	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	21	0	18	0	0
3	C	21	0	18	0	0
3	D	21	0	18	0	0
4	B	12	0	16	0	0
4	D	6	0	8	1	0
5	A	16	0	0	0	0
5	B	28	0	0	0	0
5	C	18	0	0	0	0
5	D	12	0	0	1	0
All	All	532	0	321	1	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 1.

All (1) 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)
4:D:1001:GOL:O1	5:D:2007[B]:HOH:O	2.14	0.64

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%)	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%)	1 (25%)	3 (75%)	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	0.73	0	4,9,11	1.60	1 (25%)
1	OMZ	A	2	1	13,14,15	1.11	1 (7%)	17,19,21	2.21	8 (47%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
1	GHP	A	4	1,3	10,11,12	1.50	2 (20%)	12,14,16	2.11	5 (41%)
1	GHP	A	5	1	10,11,12	1.05	0	12,14,16	3.14	6 (50%)
1	OMX	A	6	1,2	12,13,14	1.20	1 (8%)	15,17,19	2.49	8 (53%)
1	3FG	A	7	1	9,13,13	1.23	2 (22%)	14,18,18	1.93	5 (35%)
1	MLU	B	1	1	7,8,9	0.73	0	4,9,11	1.65	1 (25%)
1	OMZ	B	2	1	13,14,15	1.13	1 (7%)	17,19,21	2.58	8 (47%)
1	GHP	B	4	1,3	10,11,12	1.57	2 (20%)	12,14,16	2.43	6 (50%)
1	GHP	B	5	1	10,11,12	1.07	1 (10%)	12,14,16	2.92	6 (50%)
1	OMX	B	6	1,2	12,13,14	1.15	1 (8%)	15,17,19	2.71	8 (53%)
1	3FG	B	7	1	9,13,13	1.33	2 (22%)	14,18,18	1.85	4 (28%)
1	MLU	C	1	1	7,8,9	0.75	0	4,9,11	1.88	1 (25%)
1	OMZ	C	2	1	13,14,15	1.24	2 (15%)	17,19,21	2.43	7 (41%)
1	GHP	C	4	1,3	10,11,12	1.67	2 (20%)	12,14,16	2.35	4 (33%)
1	GHP	C	5	1	10,11,12	1.08	1 (10%)	12,14,16	2.83	6 (50%)
1	OMX	C	6	1,2	12,13,14	1.12	1 (8%)	15,17,19	2.53	7 (46%)
1	3FG	C	7	1	9,13,13	1.25	1 (11%)	14,18,18	1.99	4 (28%)
1	MLU	D	1	1	7,8,9	0.74	0	4,9,11	2.10	1 (25%)
1	OMZ	D	2	1	13,14,15	1.16	1 (7%)	17,19,21	2.35	7 (41%)
1	GHP	D	4	1,3	10,11,12	1.55	2 (20%)	12,14,16	1.87	4 (33%)
1	GHP	D	5	1	10,11,12	1.13	1 (10%)	12,14,16	2.74	5 (41%)
1	OMX	D	6	1,2	12,13,14	1.13	1 (8%)	15,17,19	2.43	7 (46%)
1	3FG	D	7	1	9,13,13	1.15	0	14,18,18	1.92	4 (28%)

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	1,3	-	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	-	0/4/8/8	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

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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	-	0/4/8/8	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	1,3	-	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	-	0/4/8/8	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	1,3	-	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	-	0/4/8/8	0/1/1/1

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	7	3FG	CB-CA	2.02	1.54	1.52
1	A	7	3FG	CG1-CB	2.03	1.42	1.39
1	B	2	OMZ	OH-CZ	2.03	1.40	1.36
1	C	7	3FG	CB-CA	2.04	1.54	1.52
1	B	7	3FG	CG1-CB	2.05	1.42	1.39
1	D	4	GHP	O4-C4	2.09	1.42	1.37
1	A	4	GHP	O4-C4	2.09	1.42	1.37
1	C	2	OMZ	CA-CB	2.09	1.58	1.54
1	B	4	GHP	O4-C4	2.11	1.42	1.37
1	C	5	GHP	C1-CA	2.11	1.54	1.52
1	B	5	GHP	C1-CA	2.13	1.54	1.52
1	A	2	OMZ	OH-CZ	2.14	1.40	1.36
1	D	2	OMZ	OH-CZ	2.20	1.41	1.36
1	B	6	OMX	OH-CZ	2.20	1.42	1.37
1	C	6	OMX	OH-CZ	2.23	1.42	1.37
1	D	5	GHP	C1-CA	2.28	1.54	1.52
1	C	4	GHP	O4-C4	2.30	1.42	1.37
1	C	2	OMZ	OH-CZ	2.30	1.41	1.36
1	B	7	3FG	CB-CA	2.32	1.54	1.52
1	A	6	OMX	OH-CZ	2.34	1.42	1.37
1	D	6	OMX	OH-CZ	2.35	1.42	1.37
1	A	4	GHP	C1-CA	2.91	1.55	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	4	GHP	C1-CA	3.08	1.55	1.52
1	D	4	GHP	C1-CA	3.10	1.55	1.52
1	C	4	GHP	C1-CA	3.30	1.55	1.52

All (123) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	6	OMX	CD2-CG-CD1	-5.34	111.50	118.31
1	C	6	OMX	CD2-CG-CD1	-5.00	111.94	118.31
1	A	6	OMX	CD2-CG-CD1	-4.82	112.16	118.31
1	D	6	OMX	CD2-CG-CD1	-4.43	112.67	118.31
1	A	5	GHP	C6-C1-C2	-4.33	112.78	118.31
1	B	6	OMX	CE2-CZ-CE1	-4.31	113.64	119.79
1	B	2	OMZ	CE2-CZ-CE1	-4.25	114.26	118.57
1	B	4	GHP	C6-C1-C2	-4.24	112.90	118.31
1	D	1	MLU	O-C-CA	-4.12	114.55	125.44
1	C	4	GHP	C6-C1-C2	-4.11	113.06	118.31
1	C	6	OMX	CE2-CZ-CE1	-3.98	114.12	119.79
1	B	5	GHP	C2-C3-C4	-3.91	115.35	119.87
1	D	2	OMZ	CD2-CG-CD1	-3.87	114.14	118.79
1	B	2	OMZ	CD2-CG-CD1	-3.85	114.17	118.79
1	A	7	3FG	CD1-CG1-CB	-3.84	116.65	120.14
1	C	5	GHP	C6-C1-C2	-3.81	113.45	118.31
1	D	5	GHP	C6-C1-C2	-3.79	113.48	118.31
1	A	5	GHP	C2-C3-C4	-3.77	115.51	119.87
1	C	2	OMZ	CD2-CG-CD1	-3.72	114.32	118.79
1	C	2	OMZ	O-C-CA	-3.69	115.70	125.44
1	C	1	MLU	O-C-CA	-3.68	115.71	125.44
1	B	5	GHP	C6-C1-C2	-3.63	113.68	118.31
1	A	4	GHP	C6-C1-C2	-3.59	113.73	118.31
1	A	2	OMZ	CD2-CG-CD1	-3.52	114.56	118.79
1	B	7	3FG	CD1-CG1-CB	-3.49	116.97	120.14
1	B	2	OMZ	O-C-CA	-3.46	116.30	125.44
1	C	2	OMZ	CE2-CZ-CE1	-3.45	115.08	118.57
1	C	5	GHP	C2-C3-C4	-3.43	115.90	119.87
1	A	2	OMZ	O-C-CA	-3.40	116.45	125.44
1	D	6	OMX	CE2-CZ-CE1	-3.39	114.97	119.79
1	D	2	OMZ	CE2-CZ-CE1	-3.36	115.16	118.57
1	A	6	OMX	CE2-CZ-CE1	-3.32	115.06	119.79
1	D	5	GHP	C2-C3-C4	-3.32	116.03	119.87
1	C	7	3FG	CD1-CG1-CB	-3.30	117.14	120.14
1	D	7	3FG	CD1-CG1-CB	-3.30	117.14	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	2	OMZ	O-C-CA	-3.27	116.81	125.44
1	D	7	3FG	CG2-CB-CA	-3.26	115.17	119.35
1	B	1	MLU	O-C-CA	-3.25	116.85	125.44
1	D	4	GHP	C6-C1-C2	-3.19	114.24	118.31
1	A	1	MLU	O-C-CA	-3.16	117.08	125.44
1	C	7	3FG	CG2-CB-CA	-3.14	115.32	119.35
1	A	2	OMZ	CE2-CZ-CE1	-3.00	115.53	118.57
1	C	4	GHP	C5-C4-C3	-2.99	115.53	119.79
1	A	4	GHP	C5-C4-C3	-2.56	116.14	119.79
1	D	4	GHP	C5-C4-C3	-2.42	116.34	119.79
1	B	4	GHP	C5-C4-C3	-2.37	116.42	119.79
1	B	6	OMX	O-C-CA	-2.28	119.41	125.44
1	A	7	3FG	CG2-CB-CA	-2.22	116.51	119.35
1	B	7	3FG	CG2-CB-CA	-2.11	116.64	119.35
1	A	6	OMX	O-C-CA	-2.06	119.99	125.44
1	A	4	GHP	C1-CA-N	2.02	117.29	112.54
1	D	6	OMX	CE2-CD2-CG	2.02	123.28	121.20
1	C	5	GHP	C6-C5-C4	2.04	122.22	119.87
1	A	7	3FG	CZ-CD1-CG1	2.04	123.40	120.39
1	B	4	GHP	C6-C1-CA	2.08	124.29	120.70
1	D	7	3FG	CD2-CG2-CB	2.12	122.08	120.14
1	D	5	GHP	C2-C1-CA	2.16	124.43	120.70
1	C	7	3FG	CD2-CG2-CB	2.22	122.16	120.14
1	A	2	OMZ	CE1-CD1-CG	2.24	123.94	120.32
1	B	5	GHP	C6-C5-C4	2.24	122.46	119.87
1	B	4	GHP	C1-CA-N	2.30	117.96	112.54
1	B	7	3FG	CD2-CG2-CB	2.35	122.28	120.14
1	B	6	OMX	CE2-CD2-CG	2.38	123.65	121.20
1	A	2	OMZ	CD2-CG-CB	2.44	124.30	120.72
1	C	6	OMX	CE2-CD2-CG	2.46	123.73	121.20
1	D	2	OMZ	CE1-CD1-CG	2.49	124.35	120.32
1	A	5	GHP	C6-C5-C4	2.50	122.75	119.87
1	B	2	OMZ	CD2-CG-CB	2.50	124.39	120.72
1	A	5	GHP	C2-C1-CA	2.52	125.06	120.70
1	B	2	OMZ	CE1-CD1-CG	2.54	124.42	120.32
1	A	6	OMX	CE2-CD2-CG	2.54	123.81	121.20
1	A	6	OMX	CD2-CE2-CZ	2.57	122.84	119.87
1	A	7	3FG	CG1-CB-CA	2.57	122.65	119.35
1	B	5	GHP	C2-C1-CA	2.68	125.32	120.70
1	C	2	OMZ	CE1-CD1-CG	2.68	124.64	120.32
1	D	6	OMX	CD2-CE2-CZ	2.68	122.96	119.87
1	C	5	GHP	C2-C1-CA	2.74	125.44	120.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	6	OMX	CD2-CE2-CZ	2.75	123.05	119.87
1	C	6	OMX	CD2-CE2-CZ	2.77	123.07	119.87
1	C	6	OMX	CD1-CG-CB	2.83	124.86	120.72
1	A	7	3FG	CD2-CG2-CB	2.84	122.72	120.14
1	A	4	GHP	C5-C6-C1	2.88	124.16	121.20
1	D	4	GHP	C3-C2-C1	2.90	124.18	121.20
1	A	2	OMZ	CD2-CE2-CZ	2.94	123.51	120.49
1	C	2	OMZ	C-CA-N	3.10	116.30	109.83
1	B	7	3FG	CG1-CB-CA	3.12	123.36	119.35
1	D	4	GHP	C5-C6-C1	3.13	124.42	121.20
1	D	6	OMX	CE1-CD1-CG	3.15	124.44	121.20
1	C	6	OMX	OC-CB-CG	3.18	118.19	111.16
1	B	2	OMZ	C-CA-N	3.24	116.59	109.83
1	D	2	OMZ	CD2-CE2-CZ	3.25	123.83	120.49
1	B	6	OMX	OC-CB-CG	3.27	118.39	111.16
1	A	6	OMX	OC-CB-CG	3.36	118.60	111.16
1	D	6	OMX	CD1-CG-CB	3.37	125.66	120.72
1	C	6	OMX	CE1-CD1-CG	3.42	124.72	121.20
1	A	6	OMX	CD1-CG-CB	3.45	125.77	120.72
1	D	5	GHP	C1-CA-N	3.48	120.74	112.54
1	A	2	OMZ	C-CA-N	3.49	117.13	109.83
1	C	5	GHP	C1-CA-N	3.51	120.82	112.54
1	D	2	OMZ	CG-CB-CA	3.51	116.87	111.96
1	A	6	OMX	CE1-CD1-CG	3.55	124.86	121.20
1	B	5	GHP	C1-CA-N	3.56	120.94	112.54
1	B	6	OMX	CD1-CG-CB	3.56	125.94	120.72
1	C	4	GHP	C3-C2-C1	3.64	124.94	121.20
1	C	2	OMZ	CG-CB-CA	3.72	117.16	111.96
1	A	4	GHP	C3-C2-C1	3.73	125.04	121.20
1	D	7	3FG	CG1-CB-CA	3.76	124.18	119.35
1	C	4	GHP	C5-C6-C1	3.77	125.08	121.20
1	A	2	OMZ	CG-CB-CA	3.82	117.30	111.96
1	D	6	OMX	OC-CB-CG	3.83	119.62	111.16
1	B	4	GHP	C5-C6-C1	3.91	125.22	121.20
1	C	2	OMZ	CD2-CE2-CZ	3.94	124.54	120.49
1	B	6	OMX	CE1-CD1-CG	3.95	125.26	121.20
1	A	5	GHP	C1-CA-N	3.99	121.94	112.54
1	B	2	OMZ	CD2-CE2-CZ	4.07	124.67	120.49
1	C	7	3FG	CG1-CB-CA	4.10	124.61	119.35
1	B	4	GHP	C3-C2-C1	4.11	125.43	121.20
1	D	2	OMZ	C-CA-N	4.37	118.96	109.83
1	B	2	OMZ	CG-CB-CA	4.80	118.67	111.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	5	GHP	C3-C2-C1	6.33	127.71	121.20
1	C	5	GHP	C3-C2-C1	6.40	127.78	121.20
1	B	5	GHP	C3-C2-C1	6.84	128.24	121.20
1	A	5	GHP	C3-C2-C1	7.27	128.68	121.20

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

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	10,10,11	3.09	1 (10%)	14,14,16	1.22	1 (7%)
3	BGC	A	9	1,3	11,11,12	1.81	2 (18%)	14,15,17	1.47	3 (21%)
3	RAM	B	10	3	10,10,11	3.00	2 (20%)	14,14,16	1.29	2 (14%)
3	BGC	B	9	1,3	11,11,12	1.84	3 (27%)	14,15,17	1.41	3 (21%)
3	RAM	C	10	3	10,10,11	3.00	2 (20%)	14,14,16	1.19	1 (7%)
3	BGC	C	9	1,3	11,11,12	1.85	3 (27%)	14,15,17	1.56	3 (21%)
3	RAM	D	10	3	10,10,11	3.02	1 (10%)	14,14,16	1.44	2 (14%)
3	BGC	D	9	1,3	11,11,12	1.82	3 (27%)	14,15,17	1.37	1 (7%)

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 (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	10	RAM	C2-C3	-8.94	1.40	1.52
3	D	10	RAM	C2-C3	-8.78	1.40	1.52
3	B	10	RAM	C2-C3	-8.64	1.40	1.52
3	C	10	RAM	C2-C3	-8.54	1.40	1.52
3	A	9	BGC	O6-C6	-2.54	1.31	1.42
3	B	9	BGC	O6-C6	-2.49	1.31	1.42
3	D	9	BGC	O6-C6	-2.43	1.31	1.42
3	C	9	BGC	O6-C6	-2.31	1.32	1.42
3	C	9	BGC	O3-C3	2.01	1.47	1.43
3	B	10	RAM	O2-C2	2.01	1.47	1.43
3	D	9	BGC	O3-C3	2.15	1.48	1.43
3	C	10	RAM	O2-C2	2.20	1.48	1.43
3	B	9	BGC	O3-C3	2.23	1.48	1.43
3	A	9	BGC	O4-C4	4.24	1.53	1.43
3	D	9	BGC	O4-C4	4.42	1.53	1.43
3	B	9	BGC	O4-C4	4.47	1.53	1.43
3	C	9	BGC	O4-C4	4.70	1.54	1.43

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	10	RAM	C3-C4-C5	-2.34	105.77	109.72
3	B	10	RAM	C3-C4-C5	-2.16	106.07	109.72
3	A	9	BGC	C1-C2-C3	2.09	112.01	109.54
3	A	9	BGC	O5-C5-C6	2.24	112.19	107.35
3	B	9	BGC	O3-C3-C2	2.24	114.04	110.00
3	C	9	BGC	O5-C5-C6	2.50	112.76	107.35
3	B	9	BGC	O2-C2-C1	2.51	114.24	109.21
3	C	9	BGC	O3-C3-C2	2.55	114.61	110.00
3	A	9	BGC	O3-C3-C2	2.69	114.85	110.00
3	C	9	BGC	O2-C2-C1	2.82	114.86	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	9	BGC	O5-C5-C6	2.85	113.51	107.35
3	C	10	RAM	C1-C2-C3	3.15	113.27	109.54
3	B	10	RAM	C1-C2-C3	3.33	113.48	109.54
3	A	10	RAM	C1-C2-C3	3.43	113.60	109.54
3	D	9	BGC	O2-C2-C1	3.46	116.14	109.21
3	D	10	RAM	C1-C2-C3	3.79	114.03	109.54

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.6 Ligand geometry [i](#)

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
2	ERE	A	8	1	8,10,11	1.19	1 (12%)	7,15,17	1.60	1 (14%)
4	GOL	B	1002[A]	-	5,5,5	0.19	0	5,5,5	0.46	0
4	GOL	B	1002[B]	-	5,5,5	0.17	0	5,5,5	0.40	0
2	ERE	B	8	1	8,10,11	1.17	1 (12%)	7,15,17	1.50	1 (14%)
2	ERE	C	8	1	8,10,11	1.23	1 (12%)	7,15,17	1.47	1 (14%)
4	GOL	D	1001	-	5,5,5	0.22	0	5,5,5	0.47	0
2	ERE	D	8	1	8,10,11	1.05	0	7,15,17	1.34	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
2	ERE	A	8	1	-	0/0/17/19	0/1/1/1
4	GOL	B	1002[A]	-	-	0/4/4/4	0/0/0/0
4	GOL	B	1002[B]	-	-	0/4/4/4	0/0/0/0
2	ERE	B	8	1	-	0/0/17/19	0/1/1/1
2	ERE	C	8	1	-	0/0/17/19	0/1/1/1
4	GOL	D	1001	-	-	0/4/4/4	0/0/0/0
2	ERE	D	8	1	-	0/0/17/19	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	8	ERE	C2-C3	-2.54	1.50	1.53
2	B	8	ERE	C2-C3	-2.32	1.51	1.53
2	A	8	ERE	C2-C3	-2.29	1.51	1.53

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	8	ERE	C1-C2-C3	3.11	116.43	111.46
2	C	8	ERE	C1-C2-C3	3.37	116.85	111.46
2	B	8	ERE	C1-C2-C3	3.39	116.88	111.46
2	A	8	ERE	C1-C2-C3	3.66	117.31	111.46

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	D	1001	GOL	1	0

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, 95th 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 ²)	Q<0.9
1	A	1/7 (14%)	1.05	0 100 100	43, 43, 43, 43	0
1	B	1/7 (14%)	0.51	0 100 100	38, 38, 38, 38	0
1	C	1/7 (14%)	1.30	0 100 100	38, 38, 38, 38	0
1	D	1/7 (14%)	1.06	0 100 100	35, 35, 35, 35	0
All	All	4/28 (14%)	0.98	0 100 100	35, 38, 38, 43	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, 95th 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 ²)	Q<0.9
1	OMX	A	6	13/14	0.83	0.14	-	30,32,34,34	0
1	MLU	D	1	9/10	0.85	0.19	-	33,43,52,53	0
1	GHP	C	4	11/12	0.85	0.16	-	27,29,31,32	0
1	GHP	D	4	11/12	0.87	0.14	-	29,31,35,36	0
1	OMZ	D	2	14/15	0.78	0.19	-	33,36,37,49	0
1	GHP	C	5	11/12	0.83	0.14	-	29,31,37,38	0
1	MLU	B	1	9/10	0.84	0.17	-	29,32,35,35	0
1	OMX	B	6	13/14	0.82	0.16	-	30,33,36,37	0
1	GHP	D	5	11/12	0.82	0.16	-	29,32,36,41	0
1	MLU	A	1	9/10	0.70	0.28	-	50,57,65,68	0
1	3FG	C	7	13/13	0.77	0.19	-	30,35,46,49	0
1	3FG	D	7	13/13	0.81	0.14	-	37,42,53,58	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(\AA^2)	Q<0.9
1	MLU	C	1	9/10	0.81	0.23	-	33,38,47,50	0
1	GHP	B	4	11/12	0.90	0.12	-	26,30,32,32	0
1	3FG	B	7	13/13	0.81	0.16	-	31,33,37,41	0
1	GHP	B	5	11/12	0.79	0.17	-	28,32,37,43	0
1	OMZ	A	2	14/15	0.87	0.17	-	32,37,45,50	0
1	OMZ	C	2	14/15	0.87	0.14	-	26,31,32,37	0
1	GHP	A	5	11/12	0.84	0.14	-	29,31,34,35	0
1	3FG	A	7	13/13	0.82	0.17	-	31,36,40,43	0
1	GHP	A	4	11/12	0.83	0.15	-	30,33,35,35	0
1	OMX	D	6	13/14	0.84	0.15	-	29,31,32,37	0
1	OMZ	B	2	14/15	0.79	0.16	-	30,33,36,47	0
1	OMX	C	6	13/14	0.81	0.16	-	30,33,36,38	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, 95th 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(\AA^2)	Q<0.9
3	BGC	C	9	11/12	0.89	0.11	-	29,31,36,36	0
3	BGC	A	9	11/12	0.77	0.15	-	37,40,45,49	0
3	RAM	A	10	10/11	0.76	0.25	-	42,46,54,64	0
3	RAM	B	10	10/11	0.89	0.12	-	31,36,39,41	0
3	RAM	C	10	10/11	0.74	0.19	-	27,31,35,39	0
3	RAM	D	10	10/11	0.87	0.14	-	31,39,44,51	0
3	BGC	D	9	11/12	0.82	0.17	-	33,38,45,53	0
3	BGC	B	9	11/12	0.86	0.14	-	29,32,37,38	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, 95th 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(\AA^2)	Q<0.9
2	ERE	C	8	10/11	0.78	0.17	-	31,35,39,41	0
2	ERE	D	8	10/11	0.83	0.14	-	30,34,37,40	0
2	ERE	A	8	10/11	0.83	0.13	-	29,33,37,38	0
2	ERE	B	8	10/11	0.81	0.17	-	33,37,42,42	0
4	GOL	B	1002[B]	6/6	0.71	0.45	-	40,45,47,50	6
4	GOL	B	1002[A]	6/6	0.71	0.45	-	42,45,45,48	6
4	GOL	D	1001	6/6	0.68	0.35	-	29,44,49,58	5

6.5 Other polymers [i](#)

There are no such residues in this entry.