



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:22 PM UTC

PDB ID : 6EBP / pdb_00006ebp
Title : Crystal Structure of the Class Ie Ribonucleotide Reductase Beta Subunit from *Aerococcus urinae* in Activated Form
Authors : Palowitch, G.M.; Boal, A.K.
Deposited on : 2018-08-06
Resolution : 1.59 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

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

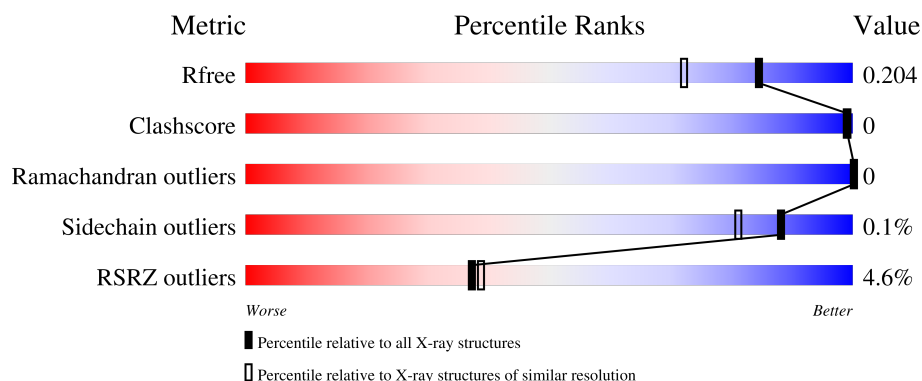
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.59 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4673 (1.60-1.60)
Clashscore	190562	4931 (1.60-1.60)
Ramachandran outliers	187476	4831 (1.60-1.60)
Sidechain outliers	187428	4830 (1.60-1.60)
RSRZ outliers	180081	4672 (1.60-1.60)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. 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	355	2% 85% • 15%
1	B	355	5% 86% • 12%
1	C	355	3% 85% 14%
1	D	355	6% 86% • 12%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 10705 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 Ribonucleoside-diphosphate reductase, beta subunit.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	303	Total	C	N	O	S	0	0	0
			2468	1596	400	466	6			
1	B	311	Total	C	N	O	S	0	0	0
			2538	1637	414	481	6			
1	C	304	Total	C	N	O	S	0	0	0
			2479	1602	404	467	6			
1	D	311	Total	C	N	O	S	0	0	0
			2538	1637	414	481	6			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-17	MET	-	initiating methionine	UNP A0A178HFF8
A	-16	GLY	-	expression tag	UNP A0A178HFF8
A	-15	SER	-	expression tag	UNP A0A178HFF8
A	-14	SER	-	expression tag	UNP A0A178HFF8
A	-13	HIS	-	expression tag	UNP A0A178HFF8
A	-12	HIS	-	expression tag	UNP A0A178HFF8
A	-11	HIS	-	expression tag	UNP A0A178HFF8
A	-10	HIS	-	expression tag	UNP A0A178HFF8
A	-9	HIS	-	expression tag	UNP A0A178HFF8
A	-8	HIS	-	expression tag	UNP A0A178HFF8
A	-7	SER	-	expression tag	UNP A0A178HFF8
A	-6	SER	-	expression tag	UNP A0A178HFF8
A	-5	GLY	-	expression tag	UNP A0A178HFF8
A	-4	LEU	-	expression tag	UNP A0A178HFF8
A	-3	VAL	-	expression tag	UNP A0A178HFF8
A	-2	PRO	-	expression tag	UNP A0A178HFF8
A	-1	ARG	-	expression tag	UNP A0A178HFF8
A	0	GLY	-	expression tag	UNP A0A178HFF8
A	1	SER	-	expression tag	UNP A0A178HFF8
A	89	SER	ALA	conflict	UNP A0A178HFF8
A	226	ALA	VAL	conflict	UNP A0A178HFF8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	245	ASP	TYR	conflict	UNP A0A178HFF8
A	249	GLY	ASP	conflict	UNP A0A178HFF8
A	256	HIS	ARG	conflict	UNP A0A178HFF8
B	-17	MET	-	initiating methionine	UNP A0A178HFF8
B	-16	GLY	-	expression tag	UNP A0A178HFF8
B	-15	SER	-	expression tag	UNP A0A178HFF8
B	-14	SER	-	expression tag	UNP A0A178HFF8
B	-13	HIS	-	expression tag	UNP A0A178HFF8
B	-12	HIS	-	expression tag	UNP A0A178HFF8
B	-11	HIS	-	expression tag	UNP A0A178HFF8
B	-10	HIS	-	expression tag	UNP A0A178HFF8
B	-9	HIS	-	expression tag	UNP A0A178HFF8
B	-8	HIS	-	expression tag	UNP A0A178HFF8
B	-7	SER	-	expression tag	UNP A0A178HFF8
B	-6	SER	-	expression tag	UNP A0A178HFF8
B	-5	GLY	-	expression tag	UNP A0A178HFF8
B	-4	LEU	-	expression tag	UNP A0A178HFF8
B	-3	VAL	-	expression tag	UNP A0A178HFF8
B	-2	PRO	-	expression tag	UNP A0A178HFF8
B	-1	ARG	-	expression tag	UNP A0A178HFF8
B	0	GLY	-	expression tag	UNP A0A178HFF8
B	1	SER	-	expression tag	UNP A0A178HFF8
B	89	SER	ALA	conflict	UNP A0A178HFF8
B	226	ALA	VAL	conflict	UNP A0A178HFF8
B	245	ASP	TYR	conflict	UNP A0A178HFF8
B	249	GLY	ASP	conflict	UNP A0A178HFF8
B	256	HIS	ARG	conflict	UNP A0A178HFF8
C	-17	MET	-	initiating methionine	UNP A0A178HFF8
C	-16	GLY	-	expression tag	UNP A0A178HFF8
C	-15	SER	-	expression tag	UNP A0A178HFF8
C	-14	SER	-	expression tag	UNP A0A178HFF8
C	-13	HIS	-	expression tag	UNP A0A178HFF8
C	-12	HIS	-	expression tag	UNP A0A178HFF8
C	-11	HIS	-	expression tag	UNP A0A178HFF8
C	-10	HIS	-	expression tag	UNP A0A178HFF8
C	-9	HIS	-	expression tag	UNP A0A178HFF8
C	-8	HIS	-	expression tag	UNP A0A178HFF8
C	-7	SER	-	expression tag	UNP A0A178HFF8
C	-6	SER	-	expression tag	UNP A0A178HFF8
C	-5	GLY	-	expression tag	UNP A0A178HFF8
C	-4	LEU	-	expression tag	UNP A0A178HFF8
C	-3	VAL	-	expression tag	UNP A0A178HFF8

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	PRO	-	expression tag	UNP A0A178HFF8
C	-1	ARG	-	expression tag	UNP A0A178HFF8
C	0	GLY	-	expression tag	UNP A0A178HFF8
C	1	SER	-	expression tag	UNP A0A178HFF8
C	89	SER	ALA	conflict	UNP A0A178HFF8
C	226	ALA	VAL	conflict	UNP A0A178HFF8
C	245	ASP	TYR	conflict	UNP A0A178HFF8
C	249	GLY	ASP	conflict	UNP A0A178HFF8
C	256	HIS	ARG	conflict	UNP A0A178HFF8
D	-17	MET	-	initiating methionine	UNP A0A178HFF8
D	-16	GLY	-	expression tag	UNP A0A178HFF8
D	-15	SER	-	expression tag	UNP A0A178HFF8
D	-14	SER	-	expression tag	UNP A0A178HFF8
D	-13	HIS	-	expression tag	UNP A0A178HFF8
D	-12	HIS	-	expression tag	UNP A0A178HFF8
D	-11	HIS	-	expression tag	UNP A0A178HFF8
D	-10	HIS	-	expression tag	UNP A0A178HFF8
D	-9	HIS	-	expression tag	UNP A0A178HFF8
D	-8	HIS	-	expression tag	UNP A0A178HFF8
D	-7	SER	-	expression tag	UNP A0A178HFF8
D	-6	SER	-	expression tag	UNP A0A178HFF8
D	-5	GLY	-	expression tag	UNP A0A178HFF8
D	-4	LEU	-	expression tag	UNP A0A178HFF8
D	-3	VAL	-	expression tag	UNP A0A178HFF8
D	-2	PRO	-	expression tag	UNP A0A178HFF8
D	-1	ARG	-	expression tag	UNP A0A178HFF8
D	0	GLY	-	expression tag	UNP A0A178HFF8
D	1	SER	-	expression tag	UNP A0A178HFF8
D	89	SER	ALA	conflict	UNP A0A178HFF8
D	226	ALA	VAL	conflict	UNP A0A178HFF8
D	245	ASP	TYR	conflict	UNP A0A178HFF8
D	249	GLY	ASP	conflict	UNP A0A178HFF8
D	256	HIS	ARG	conflict	UNP A0A178HFF8

- Molecule 2 is CALCIUM ION (CCD ID: CA) (formula: Ca).

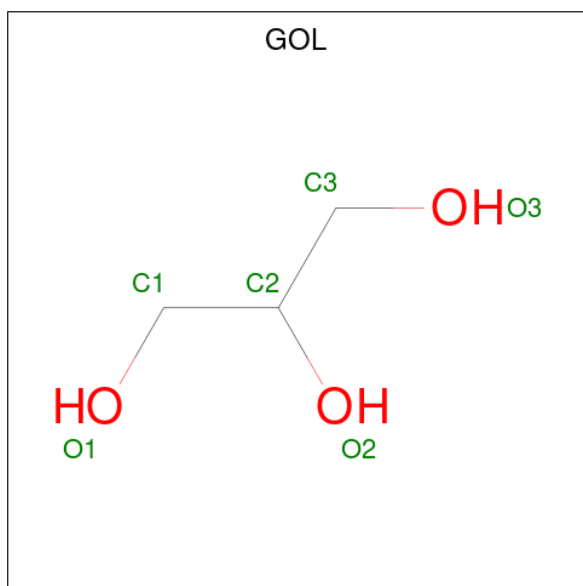
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	3	Total Ca 3 3	0	0
2	B	1	Total Ca 1 1	0	0
2	C	1	Total Ca 1 1	0	0

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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	D	1	Total	Ca	0	0
			1	1		

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			6	3	3		
3	A	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		
3	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	196	Total	O	0	0
			196	196		
4	B	166	Total	O	0	0
			166	166		
4	C	159	Total	O	0	0
			159	159		
4	D	131	Total	O	0	0
			131	131		

- Molecule 1: Ribonucleoside-diphosphate reductase, beta subunit



F314

PHE
SER
GLY
SER
GLY
SER
TYR
ILE
ILE
GLY
THR
SER
GLU
GLU
THR
LEU
ASP
GLU
ASP
TRP
ASP
PHE

4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	80.00Å 109.42Å 83.86Å 90.00° 90.06° 90.00°	Depositor
Resolution (Å)	35.18 – 1.59 35.18 – 1.59	Depositor EDS
% Data completeness (in resolution range)	94.9 (35.18-1.59) 96.2 (35.18-1.59)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.56 (at 1.58Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.163 , 0.179 0.188 , 0.204	Depositor DCC
R_{free} test set	9317 reflections (4.20%)	wwPDB-VP
Wilson B-factor (Å ²)	13.2	Xtriage
Anisotropy	0.055	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 31.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	0.000 for l,k,-h 0.146 for h,-k,-l 0.006 for l,-k,h	Xtriage
Reported twinning fraction	0.544 for H, K, L 0.456 for -h,-k,l	Depositor
Outliers	2 of 186690 reflections (0.001%)	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	10705	wwPDB-VP
Average B, all atoms (Å ²)	14.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.30% 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, 0.333 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: CA, DAH, GOL

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	0.53	0/2516	0.75	0/3416
1	B	0.53	0/2588	0.76	0/3513
1	C	0.53	0/2527	0.76	0/3430
1	D	0.55	0/2588	0.78	0/3513
All	All	0.54	0/10219	0.76	0/13872

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	2468	0	2403	0	0
1	B	2538	0	2457	2	0
1	C	2479	0	2416	1	0
1	D	2538	0	2457	2	0
2	A	3	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	12	0	14	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	12	0	12	0	0
4	A	196	0	0	0	0
4	B	166	0	0	0	0
4	C	159	0	0	0	0
4	D	131	0	0	0	0
All	All	10705	0	9759	5	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 0.

All (5) 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:C:85:ASP:OD2	1:C:123:DAH:OE2	2.27	0.52
1:B:85:ASP:OD2	1:B:123:DAH:OE2	2.33	0.46
1:D:85:ASP:OD2	1:D:123:DAH:OE2	2.35	0.45
1:D:221:TYR:CZ	1:D:225:VAL:HG11	2.52	0.44
1:B:221:TYR:CZ	1:B:225:VAL:HG11	2.55	0.42

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	300/355 (84%)	298 (99%)	2 (1%)	0	100	100
1	B	308/355 (87%)	305 (99%)	3 (1%)	0	100	100
1	C	301/355 (85%)	299 (99%)	2 (1%)	0	100	100
1	D	308/355 (87%)	306 (99%)	2 (1%)	0	100	100
All	All	1217/1420 (86%)	1208 (99%)	9 (1%)	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	265/310 (86%)	264 (100%)	1 (0%)	84	75
1	B	272/310 (88%)	272 (100%)	0	100	100
1	C	266/310 (86%)	266 (100%)	0	100	100
1	D	272/310 (88%)	272 (100%)	0	100	100
All	All	1075/1240 (87%)	1074 (100%)	1 (0%)	88	81

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

Mol	Chain	Res	Type
1	A	53	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	20	GLN
1	A	99	ASN
1	A	111	ASN
1	B	20	GLN
1	B	53	ASN
1	B	99	ASN
1	B	111	ASN
1	B	222	GLN
1	B	256	HIS
1	C	72	GLN
1	C	99	ASN
1	C	256	HIS
1	C	275	ASN
1	C	282	ASN
1	D	20	GLN
1	D	99	ASN

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Mol	Chain	Res	Type
1	D	111	ASN
1	D	256	HIS
1	D	312	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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	DAH	D	123	1	12,13,14	1.53	1 (8%)	12,17,19	0.80	0
1	DAH	B	123	1	12,13,14	1.66	1 (8%)	12,17,19	1.06	1 (8%)
1	DAH	C	123	1	12,13,14	1.71	1 (8%)	12,17,19	1.15	1 (8%)
1	DAH	A	123	1	12,13,14	1.58	1 (8%)	12,17,19	0.94	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
1	DAH	D	123	1	-	0/5/6/8	0/1/1/1
1	DAH	B	123	1	-	0/5/6/8	0/1/1/1
1	DAH	C	123	1	-	0/5/6/8	0/1/1/1
1	DAH	A	123	1	-	0/5/6/8	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	123	DAH	CZ-CE2	5.68	1.49	1.40
1	B	123	DAH	CZ-CE2	5.48	1.49	1.40
1	D	123	DAH	CZ-CE2	5.07	1.48	1.40
1	A	123	DAH	CZ-CE2	4.97	1.48	1.40

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	123	DAH	CD1-CG-CD2	2.19	121.58	118.55
1	B	123	DAH	CD1-CG-CD2	2.06	121.39	118.55
1	A	123	DAH	CB-CG-CD2	-2.02	116.96	120.43

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	D	123	DAH	1	0
1	B	123	DAH	1	0
1	C	123	DAH	1	0

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	GOL	A	405	2	5,5,5	0.29	0	5,5,5	0.24	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	GOL	C	402	2	5,5,5	0.26	0	5,5,5	0.23	0
3	GOL	A	404	2	5,5,5	0.29	0	5,5,5	0.20	0
3	GOL	C	403	2	5,5,5	0.27	0	5,5,5	0.26	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	A	405	2	-	0/4/4/4	-
3	GOL	C	402	2	-	0/4/4/4	-
3	GOL	A	404	2	-	1/4/4/4	-
3	GOL	C	403	2	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	404	GOL	O2-C2-C3-O3

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, 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	302/355 (85%)	0.18	7 (2%) 61 64	6, 11, 21, 26	0
1	B	310/355 (87%)	0.42	18 (5%) 29 29	6, 13, 23, 31	0
1	C	303/355 (85%)	0.32	9 (2%) 52 55	8, 12, 21, 34	0
1	D	310/355 (87%)	0.63	22 (7%) 22 22	8, 15, 26, 35	0
All	All	1225/1420 (86%)	0.39	56 (4%) 37 39	6, 13, 23, 35	0

All (56) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	306	ALA	4.7
1	A	305	SER	4.2
1	A	53	ASN	3.8
1	D	234	ALA	3.8
1	D	56	VAL	3.5
1	B	310	GLU	3.2
1	A	231	GLU	3.1
1	A	304	LEU	3.1
1	B	308	ALA	3.1
1	B	314	PHE	3.0
1	B	292	GLU	2.9
1	D	314	PHE	2.9
1	D	4	ASN	2.8
1	D	53	ASN	2.8
1	D	227	LYS	2.8
1	B	55	PRO	2.7
1	D	311	ASN	2.7
1	B	56	VAL	2.6
1	D	225	VAL	2.6
1	B	307	ARG	2.6
1	D	232	LYS	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	54	ILE	2.6
1	B	297	ALA	2.6
1	C	292	GLU	2.6
1	B	54	ILE	2.6
1	B	4	ASN	2.6
1	A	232	LYS	2.5
1	A	163	ASP	2.5
1	D	174	LEU	2.5
1	B	53	ASN	2.4
1	C	307	ARG	2.4
1	D	310	GLU	2.4
1	B	43	ARG	2.3
1	B	286	GLU	2.3
1	D	231	GLU	2.3
1	C	163	ASP	2.3
1	B	311	ASN	2.2
1	D	55	PRO	2.2
1	D	286	GLU	2.2
1	D	292	GLU	2.2
1	C	231	GLU	2.2
1	C	305	SER	2.1
1	C	7	ASP	2.1
1	B	299	GLU	2.1
1	B	300	VAL	2.1
1	C	306	ALA	2.1
1	D	226	ALA	2.1
1	D	312	HIS	2.0
1	D	32	ILE	2.0
1	D	163	ASP	2.0
1	B	301	PHE	2.0
1	C	18	PHE	2.0
1	B	304	LEU	2.0
1	D	228	LEU	2.0
1	D	283	LEU	2.0
1	C	53	ASN	2.0

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. 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	B-factors($\text{\AA}^2$)	Q<0.9
1	DAH	A	123	13/14	0.89	0.10	11,13,15,15	0
1	DAH	C	123	13/14	0.89	0.10	11,13,16,16	0
1	DAH	B	123	13/14	0.90	0.10	12,15,18,18	0
1	DAH	D	123	13/14	0.90	0.09	14,17,19,20	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides 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, 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	B-factors($\text{\AA}^2$)	Q<0.9
3	GOL	C	403	6/6	0.75	0.18	21,21,21,21	0
3	GOL	C	402	6/6	0.87	0.12	18,19,19,19	0
3	GOL	A	405	6/6	0.87	0.13	24,24,24,24	0
3	GOL	A	404	6/6	0.92	0.10	19,20,20,20	0
2	CA	A	403	1/1	0.98	0.07	20,20,20,20	0
2	CA	A	401	1/1	0.99	0.02	12,12,12,12	0
2	CA	D	401	1/1	0.99	0.02	13,13,13,13	0
2	CA	A	402	1/1	0.99	0.07	16,16,16,16	0
2	CA	C	401	1/1	1.00	0.02	11,11,11,11	0
2	CA	B	401	1/1	1.00	0.02	11,11,11,11	0

6.5 Other polymers [i](#)

There are no such residues in this entry.