



# Full wwPDB X-ray Structure Validation Report ⓘ

May 24, 2020 – 12:35 am BST

PDB ID : 2RCC  
Title : Crystal structure of putative class I ribonucleotide reductase (NP\_241368.1)  
from *Bacillus halodurans* at 1.90 Å resolution  
Authors : Joint Center for Structural Genomics (JCSG)  
Deposited on : 2007-09-19  
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](mailto:validation@mail.wwpdb.org)

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

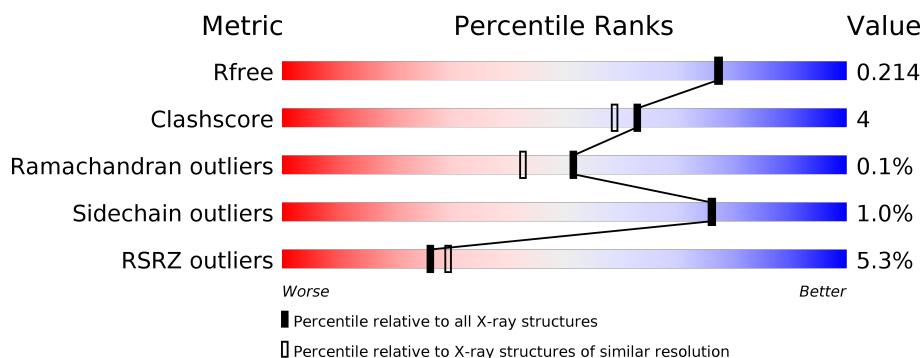
# 1 Overall quality at a glance

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))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (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  $\geq 3$ , 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	346	<div> <div>4%</div> <div> <div></div> <div>80%</div> <div>10%</div> <div>10%</div> </div> </div>
1	B	346	<div> <div>%</div> <div> <div></div> <div>78%</div> <div>19%</div> </div> </div>
1	C	346	<div> <div>8%</div> <div> <div></div> <div>80%</div> <div>9%</div> <div>10%</div> </div> </div>

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 7885 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.

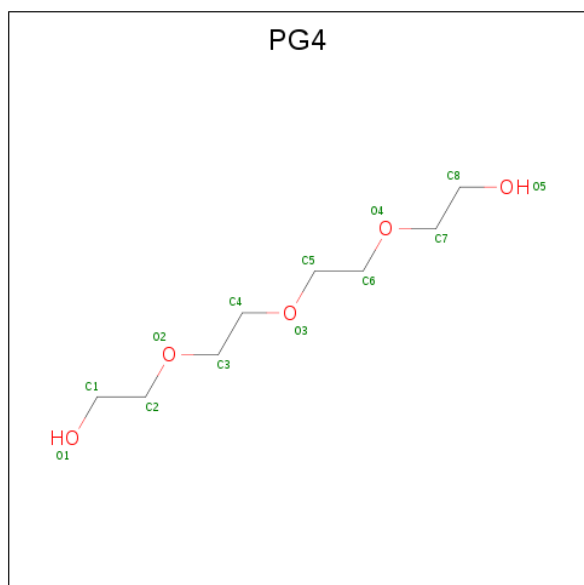
- Molecule 1 is a protein called Ribonucleoside-diphosphate reductase subunit beta.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	313	Total	C	N	O	Se	0	14	0
			2596	1698	399	487	12			
1	B	280	Total	C	N	O	Se	0	5	0
			2322	1526	350	434	12			
1	C	311	Total	C	N	O	Se	0	7	0
			2547	1656	397	484	10			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	LEADER SEQUENCE	UNP Q9KFH7
B	0	GLY	-	LEADER SEQUENCE	UNP Q9KFH7
C	0	GLY	-	LEADER SEQUENCE	UNP Q9KFH7

- Molecule 2 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: C<sub>8</sub>H<sub>18</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			13	8	5		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula:  $C_4H_{10}O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			6	4	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			5	3	2		
3	C	1	Total	C	O	0	0
			5	3	2		
3	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is ZINC ION (three-letter code: ZN) (formula: Zn).

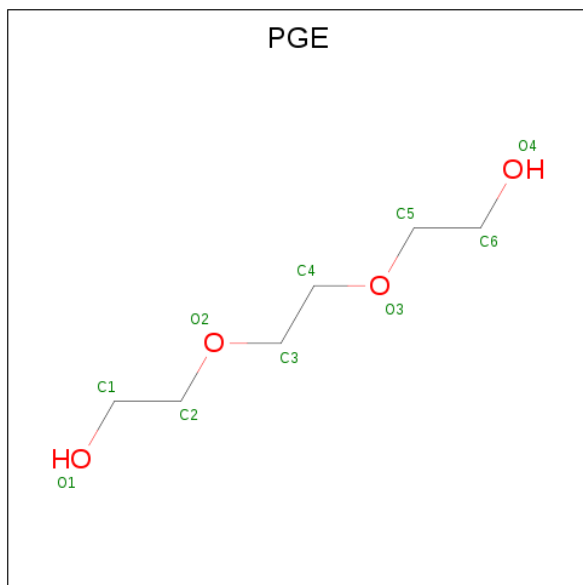
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	2	Total	Zn	0	0
			2	2		
4	C	2	Total	Zn	0	0
			2	2		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

- Molecule 6 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula:  $C_6H_{14}O_4$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	B	1	Total	C	O	0	0
			10	6	4		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



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

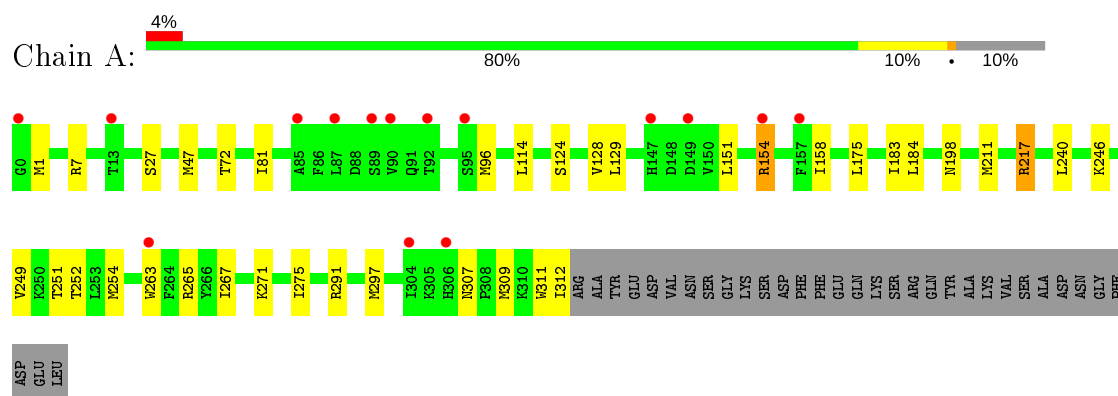
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	126	Total	O	0	0
			126	126		
8	B	104	Total	O	0	0
			104	104		
8	C	110	Total	O	0	0
			110	110		

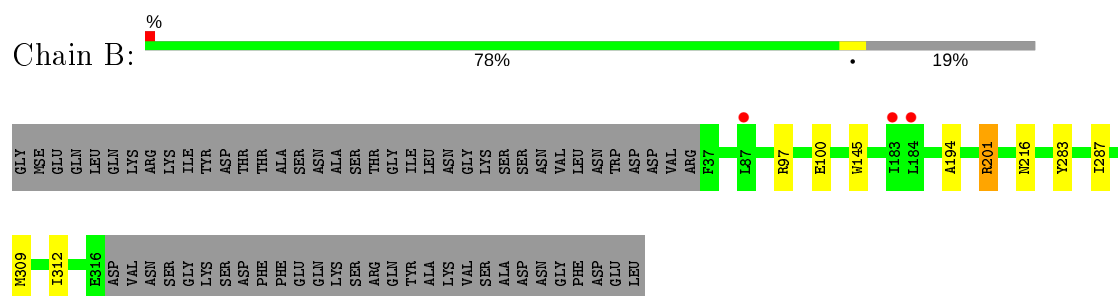
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

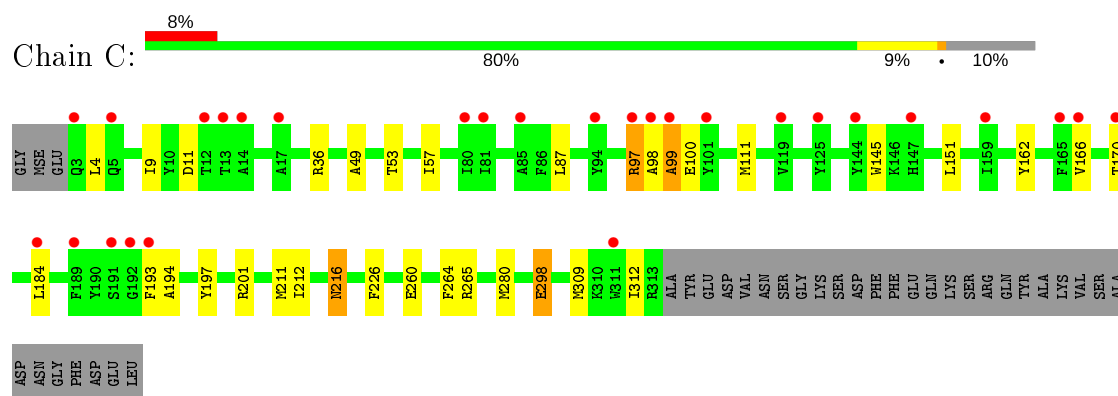
- Molecule 1: Ribonucleoside-diphosphate reductase subunit beta



- Molecule 1: Ribonucleoside-diphosphate reductase subunit beta



- Molecule 1: Ribonucleoside-diphosphate reductase subunit beta



## 4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	175.26Å 72.78Å 111.77Å 90.00° 124.90° 90.00°	Depositor
Resolution (Å)	28.50 – 1.90 28.50 – 1.90	Depositor EDS
% Data completeness (in resolution range)	99.5 (28.50-1.90) 99.5 (28.50-1.90)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.13 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.3.0040, PHENIX	Depositor
R, $R_{free}$	0.183 , 0.215 0.187 , 0.214	Depositor DCC
$R_{free}$ test set	4538 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	28.8	Xtriage
Anisotropy	0.123	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 56.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	7885	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.78% of the height of the origin peak. No significant pseudotranslation is detected.*

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

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.



## 5 Model quality [i](#)

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

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, ZN, PGE, EDO, PG4, PEG

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	0.71	0/2690	0.85	11/3638 (0.3%)
1	B	0.75	0/2391	0.77	3/3231 (0.1%)
1	C	0.86	3/2621 (0.1%)	0.89	9/3549 (0.3%)
All	All	0.78	3/7702 (0.0%)	0.84	23/10418 (0.2%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	298	GLU	CG-CD	6.00	1.60	1.51
1	C	298	GLU	CB-CG	5.99	1.63	1.52
1	C	260	GLU	CD-OE1	-5.28	1.19	1.25

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	217	ARG	NE-CZ-NH1	12.40	126.50	120.30
1	A	217	ARG	NE-CZ-NH2	-9.55	115.53	120.30
1	B	201	ARG	NE-CZ-NH1	9.26	124.93	120.30
1	C	97[A]	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	C	97[B]	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	A	154[A]	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	A	154[B]	ARG	NE-CZ-NH2	-6.94	116.83	120.30
1	B	97	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	A	217	ARG	CG-CD-NE	6.88	126.24	111.80
1	B	201	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	A	217	ARG	CD-NE-CZ	6.21	132.29	123.60
1	A	291	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	A	265	ARG	NE-CZ-NH1	5.99	123.29	120.30
1	C	97[A]	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	C	97[B]	ARG	NE-CZ-NH1	5.97	123.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	36	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	A	7	ARG	NE-CZ-NH1	5.91	123.25	120.30
1	C	36	ARG	NE-CZ-NH1	5.81	123.21	120.30
1	C	265	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	A	154[A]	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	A	154[B]	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	C	201	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	C	100	GLU	N-CA-CB	5.04	119.67	110.60

There are no chirality outliers.

There are no planarity outliers.

## 5.2 Too-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 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	2596	0	2505	36	0
1	B	2322	0	2234	5	0
1	C	2547	0	2428	23	0
2	A	13	0	18	0	0
3	A	7	0	10	0	0
3	B	10	0	12	3	0
3	C	14	0	15	1	0
4	B	2	0	0	0	0
4	C	2	0	0	0	0
5	B	4	0	6	0	0
6	B	10	0	14	0	0
7	B	12	0	16	0	0
7	C	6	0	8	1	0
8	A	126	0	0	1	0
8	B	104	0	0	0	0
8	C	110	0	0	0	0
All	All	7885	0	7266	63	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 (63) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:154[A]:ARG:HD2	1:A:263[A]:TRP:NE1	1.46	1.28
1:A:154[A]:ARG:HD2	1:A:263[A]:TRP:CE2	1.87	1.09
1:A:128:VAL:HG23	1:A:211:MSE:HE1	1.48	0.96
1:C:87:LEU:HB3	1:C:184:LEU:HD11	1.53	0.90
1:A:154[A]:ARG:CD	1:A:263[A]:TRP:NE1	2.36	0.87
1:A:47:MSE:HE1	1:A:114:LEU:HD12	1.61	0.82
1:C:11:ASP:OD2	3:C:403:PEG:C3	2.37	0.72
1:A:96:MSE:HE2	3:B:406:PEG:C4	2.19	0.72
1:C:98:ALA:O	1:C:99:ALA:HB3	1.90	0.72
1:C:98:ALA:O	1:C:99:ALA:CB	2.41	0.69
1:A:72[A]:THR:HG21	1:A:271:LYS:HB3	1.75	0.68
1:B:309:MSE:HE2	1:B:312:ILE:HD11	1.74	0.68
1:A:124[A]:SER:HB3	1:A:211:MSE:HE3	1.76	0.68
1:A:154[A]:ARG:HD2	1:A:263[A]:TRP:CD1	2.30	0.66
1:C:87:LEU:HD22	1:C:184:LEU:HD13	1.76	0.65
1:C:309:MSE:HE2	1:C:312:ILE:HD11	1.78	0.65
1:A:128:VAL:HG23	1:A:211:MSE:CE	2.26	0.65
1:A:128:VAL:CG2	1:A:211:MSE:HE1	2.26	0.63
1:A:309:MSE:HE2	1:A:312[A]:ILE:HG13	1.80	0.63
1:A:263[B]:TRP:CZ2	1:A:267:ILE:HD12	2.35	0.61
1:A:154[A]:ARG:HD2	1:A:263[A]:TRP:HE1	1.57	0.61
1:C:4:LEU:HG	1:C:170:THR:HA	1.82	0.60
1:C:309:MSE:CE	1:C:312:ILE:HD11	2.33	0.58
1:A:309:MSE:HE3	1:A:311:TRP:CZ2	2.39	0.57
1:A:251:THR:HA	1:A:254:MSE:HE2	1.87	0.56
1:C:49:ALA:HB2	7:C:402:GOL:H2	1.87	0.56
1:A:124[B]:SER:HB2	1:A:211:MSE:HE3	1.88	0.56
1:C:87:LEU:HD22	1:C:184:LEU:CD1	2.36	0.55
1:A:307:ASN:HD21	1:A:312[B]:ILE:CG2	2.20	0.55
1:B:194:ALA:HB1	1:B:309:MSE:HE1	1.88	0.55
1:A:263[B]:TRP:CE2	1:A:267:ILE:HD12	2.41	0.54
1:C:193:PHE:CD1	1:C:212:ILE:HG23	2.43	0.54
1:A:81:ILE:HG23	1:A:129:LEU:HD13	1.89	0.53
1:C:309:MSE:HE2	1:C:312:ILE:CD1	2.37	0.53
1:A:96:MSE:CE	3:B:406:PEG:C4	2.90	0.49
1:C:97[B]:ARG:HD3	1:C:166:VAL:HG22	1.93	0.49
1:A:158:ILE:HD12	1:A:184:LEU:HD21	1.95	0.48
1:B:283:TYR:CE2	1:B:287[B]:ILE:HD11	2.48	0.48
1:C:162:TYR:O	1:C:166:VAL:HG23	2.13	0.48
1:A:128:VAL:CG2	1:A:211:MSE:CE	2.90	0.48
1:A:249:VAL:HG11	1:A:297[B]:MSE:HG3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:145:TRP:HA	1:C:151:LEU:HD23	1.96	0.46
1:C:111:MSE:HE1	1:C:226:PHE:CE1	2.50	0.46
1:A:307:ASN:HD21	1:A:312[B]:ILE:HG21	1.81	0.45
1:C:57:ILE:HD12	1:C:211:MSE:HE2	1.99	0.45
1:A:198:ASN:HB2	1:A:275[A]:ILE:HD11	1.98	0.44
1:A:249:VAL:HG11	1:A:297[A]:MSE:HG3	2.01	0.43
1:C:264:PHE:CE1	1:C:280:MSE:HE3	2.54	0.43
1:A:175:LEU:HD22	1:A:240:LEU:HD13	2.01	0.42
1:C:97[B]:ARG:CD	1:C:166:VAL:HG13	2.49	0.42
1:A:47:MSE:HE3	8:A:352:HOH:O	2.18	0.42
1:A:154[A]:ARG:CD	1:A:263[A]:TRP:HE1	2.25	0.42
1:A:27:SER:HB2	1:B:145:TRP:CZ2	2.54	0.42
1:C:194:ALA:HB1	1:C:309:MSE:HE1	2.02	0.42
1:C:193:PHE:HB3	1:C:197:TYR:CE2	2.55	0.41
1:A:309:MSE:O	1:A:312[B]:ILE:HG22	2.21	0.41
1:B:100:GLU:HG2	3:B:406:PEG:C4	2.50	0.41
1:C:87:LEU:CB	1:C:184:LEU:HD11	2.37	0.41
1:A:246:LYS:HG2	1:A:297[A]:MSE:SE	2.70	0.41
1:A:151:LEU:HA	1:A:263[A]:TRP:CZ2	2.56	0.41
1:C:216:ASN:HD22	1:C:216:ASN:C	2.23	0.41
1:A:183:ILE:CD1	1:A:252:THR:HG22	2.51	0.40
1:A:309:MSE:HE2	1:A:312[A]:ILE:CG1	2.49	0.40

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	324/346 (94%)	318 (98%)	6 (2%)	0	100	100
1	B	283/346 (82%)	280 (99%)	3 (1%)	0	100	100
1	C	316/346 (91%)	306 (97%)	9 (3%)	1 (0%)	41	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	923/1038 (89%)	904 (98%)	18 (2%)	1 (0%)	51 43

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	99	ALA

### 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	280/302 (93%)	278 (99%)	2 (1%)	84 84
1	B	249/302 (82%)	247 (99%)	2 (1%)	81 82
1	C	272/302 (90%)	268 (98%)	4 (2%)	65 62
All	All	801/906 (88%)	793 (99%)	8 (1%)	76 76

All (8) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MSE
1	A	217	ARG
1	B	201	ARG
1	B	216	ASN
1	C	9	ILE
1	C	53	THR
1	C	216	ASN
1	C	298	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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	$\# Z  > 2$
7	GOL	B	405	-	5,5,5	0.51	0	5,5,5	0.39	0
5	EDO	B	402	-	3,3,3	0.39	0	2,2,2	1.09	0
7	GOL	B	404	-	5,5,5	0.54	0	5,5,5	0.53	0
6	PGE	B	403	-	9,9,9	0.43	0	8,8,8	0.46	0
7	GOL	C	402	-	5,5,5	0.79	0	5,5,5	1.17	0
3	PEG	C	403	-	4,4,6	0.17	0	3,3,5	0.58	0
3	PEG	C	404	-	4,4,6	0.43	0	3,3,5	0.24	0
3	PEG	A	347	-	6,6,6	0.54	0	5,5,5	0.38	0
2	PG4	A	346	-	12,12,12	0.47	0	11,11,11	0.45	0
3	PEG	B	407	-	3,3,6	0.31	0	2,2,5	0.51	0
3	PEG	C	405	-	3,3,6	0.33	0	2,2,5	0.40	0
3	PEG	B	406	-	5,5,6	0.63	0	4,4,5	0.42	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
7	GOL	B	405	-	-	0/4/4/4	-
5	EDO	B	402	-	-	0/1/1/1	-
7	GOL	B	404	-	-	2/4/4/4	-
6	PGE	B	403	-	-	2/7/7/7	-
7	GOL	C	402	-	-	2/4/4/4	-
3	PEG	C	403	-	-	0/2/2/4	-
3	PEG	C	404	-	-	1/2/2/4	-
3	PEG	A	347	-	-	2/4/4/4	-
2	PG4	A	346	-	-	1/10/10/10	-
3	PEG	B	407	-	-	1/1/1/4	-
3	PEG	C	405	-	-	1/1/1/4	-
3	PEG	B	406	-	-	2/3/3/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	B	404	GOL	O1-C1-C2-C3
7	C	402	GOL	O1-C1-C2-C3
2	A	346	PG4	O4-C7-C8-O5
6	B	403	PGE	O3-C5-C6-O4
3	C	404	PEG	O1-C1-C2-O2
3	A	347	PEG	O2-C3-C4-O4
7	B	404	GOL	O1-C1-C2-O2
7	C	402	GOL	O1-C1-C2-O2
3	B	406	PEG	O1-C1-C2-O2
3	B	407	PEG	O1-C1-C2-O2
6	B	403	PGE	O1-C1-C2-O2
3	C	405	PEG	O1-C1-C2-O2
3	A	347	PEG	C4-C3-O2-C2
3	B	406	PEG	C1-C2-O2-C3

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	402	GOL	1	0
3	C	403	PEG	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	406	PEG	3	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, 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	302/346 (87%)	-0.00	15 (4%) 28 32	11, 22, 41, 62	0
1	B	270/346 (78%)	-0.11	3 (1%) 80 82	13, 19, 32, 59	0
1	C	301/346 (86%)	0.37	28 (9%) 8 10	7, 24, 37, 53	0
All	All	873/1038 (84%)	0.09	46 (5%) 26 29	7, 22, 38, 62	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	0	GLY	9.8
1	A	90	VAL	9.6
1	C	99	ALA	6.0
1	C	166	VAL	5.2
1	A	306	HIS	4.8
1	C	159	ILE	3.9
1	C	13	THR	3.9
1	C	12	THR	3.6
1	C	170	THR	3.4
1	C	3	GLN	3.3
1	C	17	ALA	3.3
1	A	157	PHE	3.2
1	C	147	HIS	3.2
1	C	101	TYR	3.1
1	A	92	THR	3.0
1	A	87	LEU	3.0
1	A	85	ALA	2.9
1	C	5	GLN	2.9
1	C	311	TRP	2.9
1	B	184	LEU	2.9
1	C	165	PHE	2.8
1	C	144	TYR	2.8
1	A	304	ILE	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	184	LEU	2.7
1	A	13	THR	2.6
1	C	193	PHE	2.6
1	C	189	PHE	2.5
1	A	89	SER	2.5
1	C	192	GLY	2.5
1	B	87	LEU	2.5
1	C	94	TYR	2.5
1	A	263[A]	TRP	2.5
1	C	191	SER	2.4
1	C	85	ALA	2.4
1	C	98	ALA	2.3
1	C	97[A]	ARG	2.3
1	C	14	ALA	2.3
1	C	81	ILE	2.3
1	C	80	ILE	2.2
1	A	154[A]	ARG	2.1
1	C	119	VAL	2.1
1	A	95	SER	2.1
1	A	149	ASP	2.1
1	A	147	HIS	2.1
1	C	125	TYR	2.0
1	B	183	ILE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
3	PEG	A	347	7/7	0.73	0.13	47,58,63,68	0
3	PEG	C	404	5/7	0.77	0.21	52,52,59,60	5
6	PGE	B	403	10/10	0.83	0.32	43,70,77,79	0
7	GOL	B	405	6/6	0.88	0.34	35,51,52,55	0
3	PEG	C	403	5/7	0.89	0.21	47,54,57,59	0
7	GOL	B	404	6/6	0.90	0.12	52,64,66,71	0
2	PG4	A	346	13/13	0.91	0.14	39,47,59,60	0
7	GOL	C	402	6/6	0.93	0.41	30,44,48,60	0
5	EDO	B	402	4/4	0.94	0.11	26,32,35,40	0
3	PEG	B	407	4/7	0.94	0.14	45,45,55,55	0
3	PEG	B	406	6/7	0.94	0.23	20,29,51,56	0
3	PEG	C	405	4/7	0.95	0.10	54,54,55,62	0
4	ZN	C	400	1/1	0.97	0.04	52,52,52,52	1
4	ZN	B	400	1/1	0.99	0.05	38,38,38,38	1
4	ZN	C	401	1/1	0.99	0.02	40,40,40,40	1
4	ZN	B	401	1/1	1.00	0.07	27,27,27,27	1

## 6.5 Other polymers [i](#)

There are no such residues in this entry.