



# Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 05:03 AM GMT

PDB ID : 1C2T  
Title : NEW INSIGHTS INTO INHIBITOR DESIGN FROM THE CRYSTAL STRUCTURE AND NMR STUDIES OF E. COLI GAR TRANSFORMYLASE IN COMPLEX WITH BETA-GAR AND 10-FORMYL-5,8,10-TRIDE AZAFOLICACID.  
Authors : Greasley, S.E.; Yamashita, M.M.; Cai, H.; Benkovic, S.J.; Boger, D.L.; Wilson, I.A.  
Deposited on : 1999-07-26  
Resolution : 2.10 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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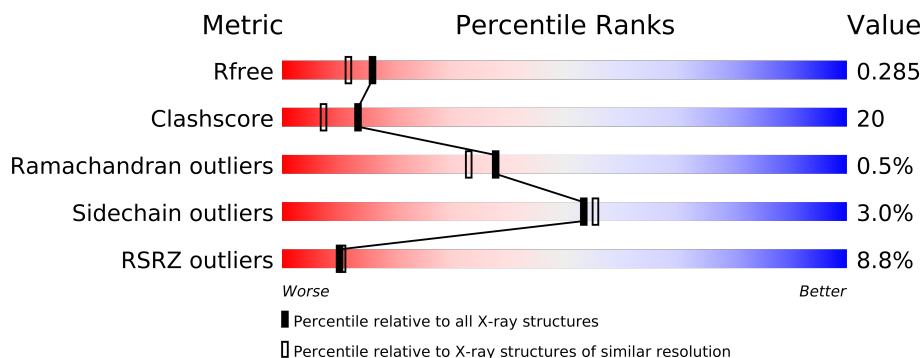
The following versions of software and data (see [references](#)) were used in the production of this report:

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 2.10 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))
$R_{free}$	66092	3012 (2.10-2.10)
Clashscore	79885	3649 (2.10-2.10)
Ramachandran outliers	78287	3610 (2.10-2.10)
Sidechain outliers	78261	3611 (2.10-2.10)
RSRZ outliers	66119	3013 (2.10-2.10)

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	212	
1	B	212	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
3	GAR	A	223	-	X
3	GAR	B	221	-	X

## 2 Entry composition

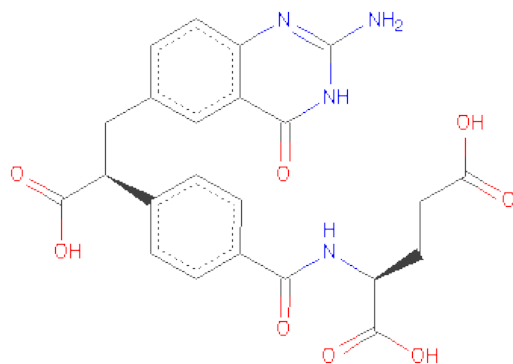
There are 4 unique types of molecules in this entry. The entry contains 3537 atoms, of which 0 are hydrogen and 0 are deuterium.

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 GLYCINAMIDE RIBONUCLEOTIDE TRANSFORMYLASE.

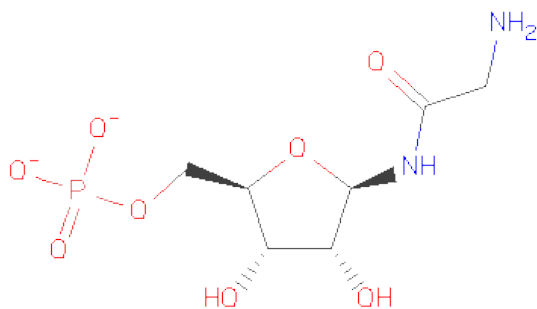
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	209	Total	C	N	O	S	0	0	0
			1617	1024	287	301	5			
1	B	209	Total	C	N	O	S	0	0	0
			1617	1024	287	301	5			

- Molecule 2 is 10-FORMYL-5,8,10-TRIDEAZAFOLICACID (three-letter code: NHS) (formula:  $C_{23}H_{22}N_4O_8$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			35	23	4	8		
2	A	1	Total	C	N	O	0	0
			35	23	4	8		

- Molecule 3 is GLYCINAMIDE RIBONUCLEOTIDE (three-letter code: GAR) (formula:  $C_7H_{13}N_2O_8P$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	B	1	Total	C	N	O	P	0	0
			18	7	2	8	1		
3	A	1	Total	C	N	O	P	0	0
			18	7	2	8	1		

- Molecule 4 is water.

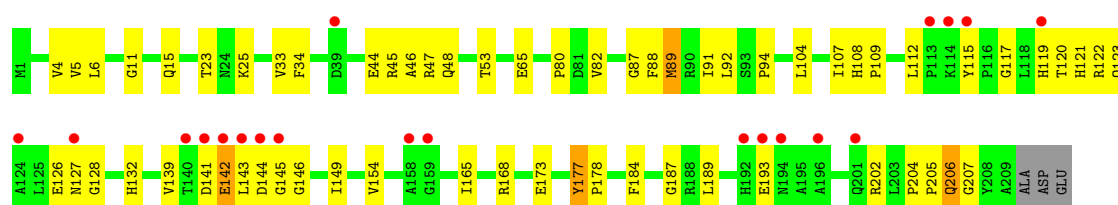
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	94	Total	O	0	0
			94	94		
4	B	103	Total	O	0	0
			103	103		

### 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.

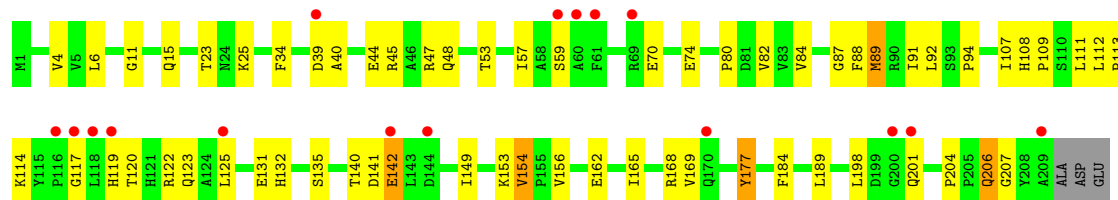
#### • Molecule 1: GLYCINAMIDE RIBONUCLEOTIDE TRANSFORMYLASE

Chain A: 



#### • Molecule 1: GLYCINAMIDE RIBONUCLEOTIDE TRANSFORMYLASE

Chain B: 



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	40.25Å 112.79Å 46.96Å 90.00° 101.50° 90.00°	Depositor
Resolution (Å)	20.00 – 2.10 17.46 – 2.10	Depositor EDS
% Data completeness (in resolution range)	78.9 (20.00-2.10) 92.1 (17.46-2.10)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.90 (at 2.11Å)	Xtriage
Refinement program	CNS 0.3	Depositor
R, $R_{free}$	0.227 , 0.265 0.242 , 0.285	Depositor DCC
$R_{free}$ test set	1085 reflections (5.18%)	DCC
Wilson B-factor (Å <sup>2</sup> )	23.3	Xtriage
Anisotropy	0.606	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 39.1	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 22019 reflections	Xtriage
$F_o, F_c$ correlation	0.92	EDS
Total number of atoms	3537	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.93% 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: GAR, NHS

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	0.50	0/1654	0.73	0/2248
1	B	0.45	0/1654	0.68	0/2248
All	All	0.48	0/3308	0.70	0/4496

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	1617	0	1592	74	0
1	B	1617	0	1592	56	0
2	A	35	0	20	5	0
2	B	35	0	21	5	0
3	A	18	0	13	8	0
3	B	18	0	13	7	0
4	A	94	0	0	5	0
4	B	103	0	0	3	0
All	All	3537	0	3251	134	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 20.

All (134) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:B:89:MET:HE3	3:B:221:GAR:H241	1.04	1.13
1:B:89:MET:CE	3:B:221:GAR:H241	1.64	1.09
1:A:91:ILE:HD12	1:A:143:LEU:HD11	1.42	1.02
1:B:89:MET:HE3	3:B:221:GAR:N24	1.76	1.00
1:A:202:ARG:NH2	1:B:113:PRO:HG3	1.76	0.99
1:A:202:ARG:CZ	1:B:113:PRO:HG3	1.95	0.96
1:B:140:THR:HG22	1:B:142:GLU:HG2	1.52	0.92
2:A:222:NHS:H10	3:A:223:GAR:N24	1.89	0.86
1:B:87:GLY:HA2	3:B:221:GAR:H19	1.41	0.84
1:A:112:LEU:HD21	1:A:144:ASP:HB3	1.59	0.83
1:A:89:MET:CE	3:A:223:GAR:H241	1.91	0.83
1:B:131:GLU:OE2	1:B:153:LYS:HD3	1.80	0.81
1:A:91:ILE:CD1	1:A:143:LEU:HD11	2.11	0.81
1:A:154:VAL:HG21	1:A:168:ARG:HG2	1.63	0.80
1:A:89:MET:CE	3:A:223:GAR:N24	2.47	0.78
1:A:23:THR:OG1	1:A:25:LYS:HG3	1.84	0.78
1:B:23:THR:OG1	1:B:25:LYS:HG3	1.83	0.77
1:B:132:HIS:HB3	1:B:165:ILE:HD11	1.67	0.77
1:A:11:GLY:HA2	4:A:227:HOH:O	1.86	0.76
1:A:109:PRO:HG2	1:A:120:THR:HG21	1.69	0.75
1:B:15:GLN:HE21	1:B:45:ARG:HH11	1.33	0.74
1:A:91:ILE:HD12	1:A:143:LEU:CD1	2.18	0.73
1:A:119:HIS:O	1:A:123:GLN:HG3	1.90	0.72
1:B:11:GLY:HA2	4:B:289:HOH:O	1.89	0.71
1:A:89:MET:HE1	3:A:223:GAR:H241	1.56	0.69
1:A:112:LEU:HD21	1:A:144:ASP:O	1.94	0.67
1:A:112:LEU:CD2	1:A:144:ASP:O	2.42	0.67
2:A:222:NHS:H10	3:A:223:GAR:C23	2.24	0.67
1:A:206:GLN:CA	1:A:206:GLN:HE21	2.07	0.67
1:A:115:TYR:CE2	1:A:123:GLN:HB3	2.28	0.67
1:A:15:GLN:HE21	1:A:45:ARG:HH11	1.41	0.66
1:B:206:GLN:HG3	1:B:206:GLN:O	1.94	0.66
1:A:132:HIS:O	1:A:154:VAL:HG12	1.97	0.65
1:B:156:VAL:HG22	1:B:165:ILE:HD12	1.79	0.65
2:A:222:NHS:H10	3:A:223:GAR:H231	1.80	0.64
1:B:23:THR:HG21	1:B:25:LYS:NZ	2.13	0.64
1:B:162:GLU:HG2	4:B:261:HOH:O	1.98	0.63
1:A:126:GLU:C	1:A:128:GLY:H	2.02	0.63
1:A:154:VAL:CG2	1:A:168:ARG:HG2	2.29	0.63

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:122:ARG:O	1:A:126:GLU:HG3	1.99	0.63
1:A:23:THR:HG21	1:A:25:LYS:NZ	2.14	0.62
1:A:94:PRO:HA	1:A:141:ASP:OD1	1.99	0.62
1:B:47:ARG:NH1	1:B:53:THR:OG1	2.33	0.61
1:B:119:HIS:O	1:B:123:GLN:HG3	2.00	0.61
1:B:132:HIS:CB	1:B:165:ILE:HD11	2.30	0.59
2:B:220:NHS:H10	3:B:221:GAR:H231	1.84	0.58
1:A:47:ARG:NH1	1:A:53:THR:OG1	2.36	0.58
1:A:132:HIS:HB3	1:A:165:ILE:HD11	1.85	0.57
1:B:140:THR:HG22	1:B:142:GLU:CG	2.32	0.57
1:B:4:VAL:HG23	1:B:80:PRO:HB3	1.85	0.57
1:B:6:LEU:HD22	1:B:34:PHE:HB2	1.86	0.56
1:A:108:HIS:HE1	1:A:117:GLY:O	1.89	0.55
1:A:132:HIS:CB	1:A:165:ILE:HD11	2.37	0.55
2:B:220:NHS:H10	3:B:221:GAR:C23	2.37	0.54
1:B:149:ILE:HD13	1:B:189:LEU:HD21	1.88	0.54
1:B:107:ILE:O	1:B:107:ILE:HG23	2.08	0.54
1:B:15:GLN:NE2	1:B:45:ARG:HH11	2.05	0.54
1:B:94:PRO:HA	1:B:141:ASP:OD1	2.08	0.53
1:B:141:ASP:HA	2:B:220:NHS:HN22	1.72	0.53
1:A:88:PHE:CE2	1:A:92:LEU:HD21	2.44	0.53
1:A:206:GLN:HB2	4:A:280:HOH:O	2.09	0.53
1:B:82:VAL:HB	1:B:184:PHE:CE2	2.43	0.53
1:A:88:PHE:HE2	1:A:92:LEU:HD21	1.73	0.53
1:A:107:ILE:O	1:A:107:ILE:HG23	2.07	0.53
1:A:206:GLN:HA	1:A:206:GLN:HE21	1.72	0.52
1:A:89:MET:HA	1:A:89:MET:HE2	1.91	0.52
1:A:115:TYR:CE2	1:A:123:GLN:CB	2.91	0.52
1:A:112:LEU:HD23	1:A:144:ASP:O	2.11	0.50
2:B:220:NHS:H10	3:B:221:GAR:N24	2.27	0.50
1:B:198:LEU:O	1:B:201:GLN:HG2	2.13	0.49
1:A:82:VAL:HB	1:A:184:PHE:CE2	2.48	0.49
1:A:15:GLN:NE2	1:A:45:ARG:HH11	2.10	0.48
1:B:88:PHE:HE2	1:B:92:LEU:HD21	1.78	0.48
1:A:187:GLY:HA2	4:A:278:HOH:O	2.13	0.48
1:A:204:PRO:HG2	1:A:207:GLY:O	2.12	0.48
1:A:126:GLU:C	1:A:128:GLY:N	2.67	0.48
1:A:126:GLU:O	1:A:128:GLY:N	2.46	0.48
1:B:109:PRO:HG2	1:B:120:THR:HG21	1.96	0.48
1:A:65:GLU:HA	4:A:249:HOH:O	2.13	0.48
1:B:88:PHE:CE2	1:B:92:LEU:HD21	2.49	0.47
1:A:142:GLU:HB2	1:A:145:GLY:HA3	1.96	0.47

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:149:ILE:HD13	1:A:189:LEU:HD21	1.96	0.47
1:A:132:HIS:O	1:A:154:VAL:N	2.48	0.47
1:A:23:THR:HG21	1:A:25:LYS:HZ1	1.78	0.47
1:B:156:VAL:HG22	1:B:165:ILE:CD1	2.44	0.47
1:B:154:VAL:HG13	1:B:168:ARG:HD2	1.96	0.47
1:B:112:LEU:HD12	1:B:135:SER:HB2	1.96	0.47
1:B:140:THR:CG2	1:B:142:GLU:HG2	2.34	0.46
1:B:132:HIS:O	1:B:154:VAL:N	2.48	0.46
1:B:57:ILE:HG22	1:B:59:SER:H	1.80	0.46
1:A:89:MET:CE	1:A:89:MET:HA	2.45	0.46
1:A:109:PRO:HG2	1:A:120:THR:CG2	2.44	0.45
1:A:132:HIS:C	1:A:154:VAL:HG12	2.36	0.45
1:A:120:THR:OG1	1:A:121:HIS:N	2.49	0.45
1:B:70:GLU:O	1:B:74:GLU:HG2	2.17	0.45
1:B:108:HIS:HE1	1:B:117:GLY:O	2.00	0.45
1:B:114:LYS:HG3	4:B:266:HOH:O	2.16	0.45
1:A:6:LEU:HD22	1:A:34:PHE:HB2	1.99	0.45
1:B:165:ILE:O	1:B:169:VAL:HG23	2.17	0.45
1:B:204:PRO:HG2	1:B:207:GLY:O	2.17	0.44
1:B:89:MET:HA	1:B:89:MET:CE	2.47	0.44
1:A:89:MET:HE3	3:A:223:GAR:N24	2.29	0.44
1:A:177:TYR:HB3	1:A:178:PRO:HD3	2.00	0.44
1:A:104:LEU:HG	1:A:139:VAL:HB	1.99	0.44
1:B:122:ARG:HH11	1:B:122:ARG:HG3	1.83	0.44
1:A:142:GLU:HG2	1:A:142:GLU:H	1.34	0.44
1:B:23:THR:HG21	1:B:25:LYS:HZ1	1.80	0.44
1:A:144:ASP:OD1	2:A:222:NHS:OA2	2.36	0.44
1:B:84:VAL:HG13	1:B:177:TYR:OH	2.18	0.43
1:A:5:VAL:C	1:A:6:LEU:HD23	2.39	0.43
1:B:91:ILE:HA	2:B:220:NHS:C8	2.49	0.43
1:B:39:ASP:O	1:B:40:ALA:C	2.56	0.43
1:B:4:VAL:CG2	1:B:80:PRO:HB3	2.48	0.43
1:B:142:GLU:H	1:B:142:GLU:HG2	1.24	0.42
1:B:122:ARG:HG3	1:B:122:ARG:NH1	2.33	0.42
1:B:125:LEU:HD22	1:B:162:GLU:CD	2.39	0.42
1:A:115:TYR:CD2	1:A:123:GLN:NE2	2.88	0.42
1:B:125:LEU:HB3	1:B:162:GLU:OE2	2.19	0.42
1:A:44:GLU:O	1:A:48:GLN:HG2	2.20	0.42
1:A:112:LEU:HD12	1:A:112:LEU:HA	1.83	0.42
1:A:87:GLY:HA2	3:A:223:GAR:H19	1.84	0.42
1:A:23:THR:CB	1:A:25:LYS:HZ2	2.31	0.41
1:A:115:TYR:HD2	1:A:123:GLN:NE2	2.18	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:141:ASP:HA	2:A:222:NHS:HN22	1.86	0.41
1:A:193:GLU:HB2	4:A:313:HOH:O	2.19	0.41
1:A:4:VAL:HG23	1:A:80:PRO:HB3	2.02	0.41
1:B:44:GLU:O	1:B:48:GLN:HG2	2.21	0.41
1:B:111:LEU:O	1:B:114:LYS:HB2	2.20	0.41
1:A:143:LEU:HD12	1:A:143:LEU:HA	1.57	0.41
1:A:108:HIS:CD2	1:A:112:LEU:HD13	2.56	0.40
1:A:107:ILE:HD11	1:A:173:GLU:HG2	2.03	0.40
1:A:33:VAL:HG21	1:A:46:ALA:HB2	2.02	0.40
1:A:154:VAL:HG22	1:A:168:ARG:CD	2.51	0.40
1:A:142:GLU:O	1:A:145:GLY:N	2.36	0.40

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	207/212 (98%)	194 (94%)	11 (5%)	2 (1%)	22	14
1	B	207/212 (98%)	200 (97%)	7 (3%)	0	100	100
All	All	414/424 (98%)	394 (95%)	18 (4%)	2 (0%)	38	33

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	127	ASN
1	A	146	GLY

### 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	169/171 (99%)	164 (97%)	5 (3%)	53	55
1	B	169/171 (99%)	164 (97%)	5 (3%)	53	55
All	All	338/342 (99%)	328 (97%)	10 (3%)	53	55

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	89	MET
1	A	142	GLU
1	A	177	TYR
1	A	205	PRO
1	A	206	GLN
1	B	89	MET
1	B	142	GLU
1	B	154	VAL
1	B	177	TYR
1	B	206	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	99	HIS
1	A	123	GLN
1	A	127	ASN
1	A	206	GLN
1	B	15	GLN
1	B	123	GLN

### 5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

4 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	NHS	A	222	-	37,37,37	2.39	13 (35%)	50,52,52	1.85	11 (22%)
3	GAR	A	223	-	18,18,18	2.18	4 (22%)	26,26,26	1.80	5 (19%)
2	NHS	B	220	-	37,37,37	2.44	17 (45%)	50,52,52	1.82	10 (20%)
3	GAR	B	221	-	18,18,18	2.39	5 (27%)	26,26,26	1.54	5 (19%)

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	NHS	A	222	-	-	0/29/29/29	0/1/3/3
3	GAR	A	223	-	-	0/12/28/28	0/1/1/1
2	NHS	B	220	-	-	0/29/29/29	0/1/3/3
3	GAR	B	221	-	-	0/12/28/28	0/1/1/1

All (39) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	222	NHS	C14-C10	6.33	1.62	1.52
2	A	222	NHS	C2-N3	6.15	1.46	1.36
2	B	220	NHS	C8A-N1	6.03	1.48	1.37
2	B	220	NHS	C2-N3	5.74	1.46	1.36
3	B	221	GAR	P15-O18	-5.67	1.42	1.51
3	A	223	GAR	P15-O17	5.66	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	221	GAR	P15-O17	5.43	1.61	1.51
3	A	223	GAR	P15-O18	-5.24	1.43	1.51
2	A	222	NHS	C8A-N1	4.78	1.45	1.37
2	B	220	NHS	C14-C10	4.50	1.59	1.52
3	B	221	GAR	C3-N19	4.41	1.48	1.43
2	A	222	NHS	C4-C4A	3.71	1.53	1.39
2	B	220	NHS	C13-C14	3.57	1.45	1.39
3	B	221	GAR	P15-O16	3.51	1.58	1.51
2	B	220	NHS	C4-C4A	3.40	1.52	1.39
3	A	223	GAR	P15-O16	3.33	1.58	1.51
2	A	222	NHS	C15-C14	3.30	1.44	1.39
2	B	220	NHS	C12-C11	3.14	1.44	1.39
2	B	220	NHS	C13-C12	3.03	1.44	1.38
2	A	222	NHS	C2-N1	-2.99	1.29	1.33
2	B	220	NHS	C8-C7	2.92	1.42	1.36
2	B	220	NHS	C2-NA2	2.92	1.36	1.32
2	B	220	NHS	C-N	2.88	1.40	1.34
3	A	223	GAR	P15-O12	-2.83	1.53	1.61
2	B	220	NHS	CA-N	2.60	1.51	1.45
2	A	222	NHS	C13-C14	2.51	1.43	1.39
2	A	222	NHS	C8-C7	2.45	1.41	1.36
2	A	222	NHS	O2-CT	2.39	1.38	1.30
2	A	222	NHS	CA-CT	2.38	1.59	1.52
2	B	220	NHS	C2-N1	-2.38	1.30	1.33
3	B	221	GAR	P15-O12	-2.30	1.55	1.61
2	A	222	NHS	C12-C11	2.29	1.43	1.39
2	A	222	NHS	C16-C11	2.19	1.43	1.39
2	B	220	NHS	O2-CT	2.16	1.37	1.30
2	B	220	NHS	C15-C14	2.15	1.42	1.39
2	B	220	NHS	C5-C6	2.14	1.42	1.37
2	A	222	NHS	C2-NA2	2.07	1.35	1.32
2	B	220	NHS	C11-C	2.06	1.54	1.50
2	B	220	NHS	CA-CT	2.05	1.58	1.52

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	222	NHS	C6-C9-C10	6.61	123.24	112.63
2	B	220	NHS	C6-C9-C10	5.78	121.91	112.63
3	A	223	GAR	O4-C3-N19	-5.37	104.67	109.91
2	A	222	NHS	OA1-CA1-OA2	-5.22	112.27	124.07
2	B	220	NHS	OA1-CA1-OA2	-4.90	112.99	124.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	220	NHS	CA-N-C	4.56	131.98	121.80
3	B	221	GAR	C21-C23-N24	4.20	121.39	112.55
2	B	220	NHS	C9-C10-CA1	4.14	118.01	111.22
2	A	222	NHS	C9-C10-CA1	4.03	117.81	111.22
3	A	223	GAR	C21-C23-N24	3.24	119.36	112.55
3	A	223	GAR	C3-N19-C21	3.20	127.96	122.57
2	A	222	NHS	C9-C10-C14	3.16	117.84	112.03
3	A	223	GAR	O12-P15-O16	-3.09	97.40	105.86
2	B	220	NHS	CT-CA-N	3.00	118.27	110.53
2	A	222	NHS	CA-N-C	2.98	128.46	121.80
2	A	222	NHS	CG-CB-CA	2.98	118.83	112.99
2	B	220	NHS	C4A-C8A-N1	-2.94	120.15	122.86
2	B	220	NHS	CG-CB-CA	2.93	118.74	112.99
3	B	221	GAR	C3-N19-C21	2.92	127.49	122.57
2	B	220	NHS	C4A-C4-N3	2.86	117.80	115.40
2	A	222	NHS	C4A-C8A-N1	-2.75	120.32	122.86
2	A	222	NHS	CT-CA-N	2.65	117.35	110.53
2	A	222	NHS	C4A-C4-N3	2.63	117.61	115.40
3	B	221	GAR	O12-P15-O16	-2.49	99.06	105.86
2	B	220	NHS	C14-C10-CA1	2.48	113.46	109.56
3	B	221	GAR	C1-C2-C3	2.46	106.23	101.35
2	A	222	NHS	C14-C10-CA1	2.46	113.42	109.56
3	B	221	GAR	O18-P15-O12	2.45	113.26	105.93
2	A	222	NHS	C4-C4A-C8A	-2.40	116.39	119.40
3	A	223	GAR	O18-P15-O12	2.26	112.69	105.93
2	B	220	NHS	C4-C4A-C8A	-2.11	116.75	119.40

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	209/212 (98%)	0.62	20 (9%) 8 9	14, 26, 49, 52	0
1	B	209/212 (98%)	0.72	16 (7%) 13 15	16, 31, 49, 56	0
All	All	418/424 (98%)	0.67	36 (8%) 10 11	14, 30, 49, 56	0

All (36) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	200	GLY	7.1
1	B	39	ASP	5.4
1	B	201	GLN	3.8
1	A	141	ASP	3.6
1	A	144	ASP	3.5
1	B	209	ALA	3.4
1	A	143	LEU	3.3
1	B	59	SER	3.3
1	A	115	TYR	3.2
1	A	39	ASP	3.2
1	A	158	ALA	3.2
1	B	118	LEU	3.1
1	B	69	ARG	3.0
1	A	145	GLY	3.0
1	A	142	GLU	2.9
1	B	170	GLN	2.9
1	A	201	GLN	2.8
1	A	159	GLY	2.7
1	A	127	ASN	2.6
1	B	60	ALA	2.6
1	A	194	ASN	2.6
1	B	142	GLU	2.5
1	B	116	PRO	2.5
1	A	196	ALA	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	117	GLY	2.3
1	A	124	ALA	2.3
1	A	119	HIS	2.2
1	B	61	PHE	2.2
1	A	192	HIS	2.2
1	A	193	GLU	2.2
1	A	113	PRO	2.1
1	B	144	ASP	2.1
1	A	140	THR	2.1
1	B	125	LEU	2.0
1	A	114	LYS	2.0
1	B	119	HIS	2.0

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

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

## 6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	GAR	B	221	18/18	0.46	5.54	58,61,62,62	0
3	GAR	A	223	18/18	0.38	4.83	50,56,61,61	0
2	NHS	B	220	35/35	0.23	0.78	41,47,52,53	0
2	NHS	A	222	35/35	0.21	0.08	32,43,53,53	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.