



Full wwPDB X-ray Structure Validation Report ⓘ

May 17, 2020 – 10:11 am BST

PDB ID : 3R5G
Title : Crystal structure of the adenylyl cyclase CyaB from *P. aeruginosa*
Authors : Topal, H.; Steegborn, C.
Deposited on : 2011-03-18
Resolution : 1.50 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 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

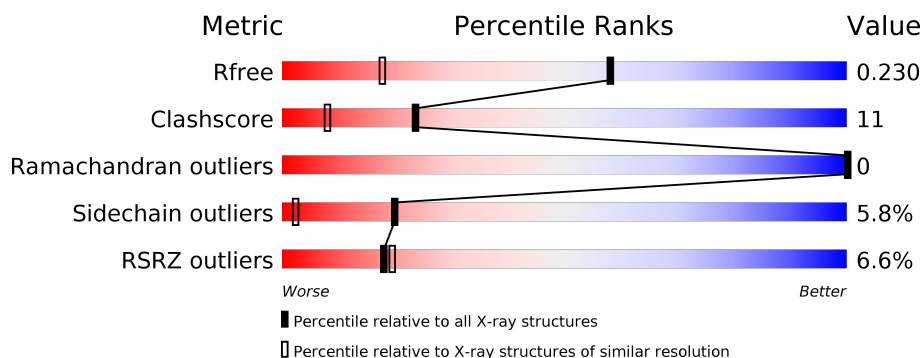
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.50 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	2936 (1.50-1.50)
Clashscore	141614	3144 (1.50-1.50)
Ramachandran outliers	138981	3066 (1.50-1.50)
Sidechain outliers	138945	3064 (1.50-1.50)
RSRZ outliers	127900	2884 (1.50-1.50)

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 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	198	<div> <div>7%</div> <div> <div></div> <div>80%</div> <div>14%</div> <div>• • •</div> </div> </div>
1	B	198	<div> <div>7%</div> <div> <div></div> <div>78%</div> <div>17%</div> <div>• •</div> </div> </div>

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3377 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 CyaB.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	195	Total	C	N	O	S	0	0	0
			1523	956	266	290	11			
1	B	196	Total	C	N	O	S	0	0	0
			1531	962	267	291	11			

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	219	GLY	-	EXPRESSION TAG	UNP Q9HZ23
B	219	GLY	-	EXPRESSION TAG	UNP Q9HZ23

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C₃H₈O₃).



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

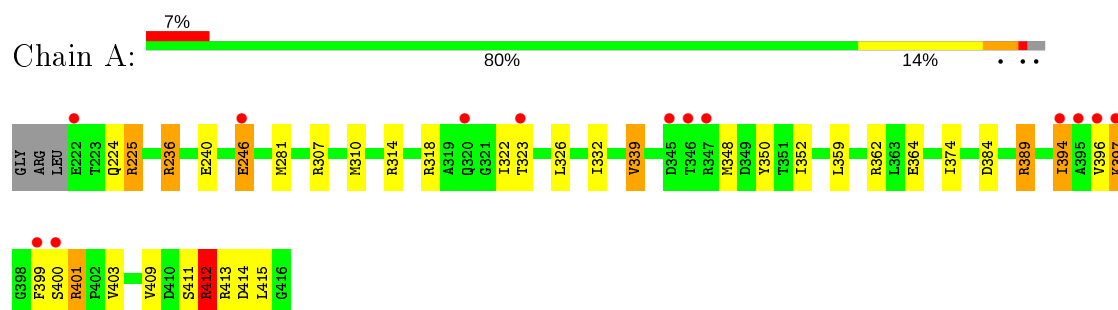
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	163	Total 163	O 163	0	0
3	B	154	Total 154	O 154	0	0

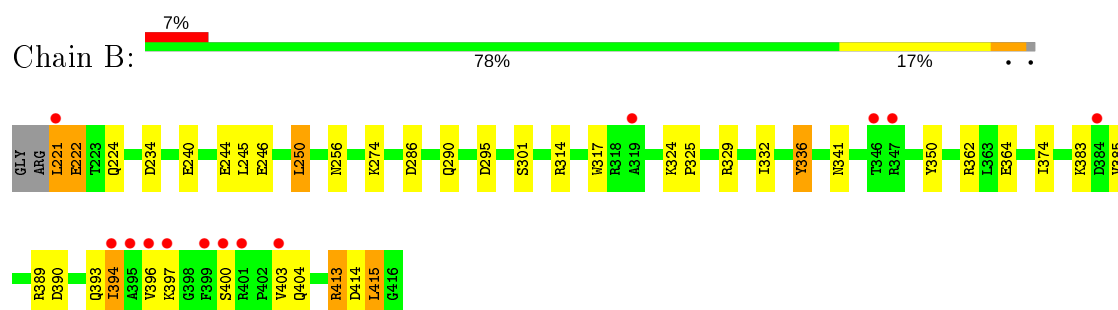
3 Residue-property plots [i](#)

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: CyaB



• Molecule 1: CyaB



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	51.36Å 36.31Å 94.76Å 90.00° 98.76° 90.00°	Depositor
Resolution (Å)	47.78 – 1.50 47.78 – 1.50	Depositor EDS
% Data completeness (in resolution range)	100.0 (47.78-1.50) 91.2 (47.78-1.50)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.91 (at 1.50Å)	Xtriage
Refinement program	REFMAC 5.5.0110	Depositor
R, R_{free}	0.186 , 0.230 0.183 , 0.230	Depositor DCC
R_{free} test set	2548 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	16.3	Xtriage
Anisotropy	0.062	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 43.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	3377	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 48.66 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 8.3307e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

² 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 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	1.30	2/1543 (0.1%)	1.28	14/2070 (0.7%)
1	B	1.31	2/1551 (0.1%)	1.33	12/2081 (0.6%)
All	All	1.30	4/3094 (0.1%)	1.30	26/4151 (0.6%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	240	GLU	CG-CD	5.62	1.60	1.51
1	A	350	TYR	CB-CG	-5.61	1.43	1.51
1	B	301	SER	CB-OG	5.09	1.48	1.42
1	B	404	GLN	N-CA	5.04	1.56	1.46

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	414	ASP	CB-CG-OD2	-14.47	105.28	118.30
1	B	390	ASP	CB-CG-OD1	8.59	126.03	118.30
1	B	390	ASP	CB-CG-OD2	-8.49	110.66	118.30
1	A	384	ASP	CB-CG-OD1	7.95	125.46	118.30
1	B	336	TYR	CB-CG-CD1	-7.67	116.40	121.00
1	B	414	ASP	CB-CG-OD1	6.73	124.36	118.30
1	A	310	MET	CG-SD-CE	6.59	110.75	100.20
1	B	234	ASP	CB-CG-OD1	6.51	124.16	118.30
1	A	412	ARG	NE-CZ-NH1	-6.50	117.05	120.30
1	A	414	ASP	CB-CG-OD2	-6.24	112.69	118.30
1	A	307	ARG	NE-CZ-NH1	-6.23	117.18	120.30
1	A	413	ARG	NE-CZ-NH1	6.23	123.42	120.30
1	B	314	ARG	NE-CZ-NH1	-6.02	117.29	120.30
1	B	329	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	B	389	ARG	NE-CZ-NH2	-5.80	117.40	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	415	LEU	CA-CB-CG	5.78	128.58	115.30
1	A	339	VAL	CB-CA-C	-5.69	100.59	111.40
1	A	389	ARG	NE-CZ-NH1	-5.68	117.46	120.30
1	A	348	MET	CG-SD-CE	-5.61	91.23	100.20
1	A	389	ARG	NE-CZ-NH2	5.59	123.09	120.30
1	A	389	ARG	CG-CD-NE	5.58	123.53	111.80
1	B	250	LEU	CB-CG-CD2	-5.41	101.81	111.00
1	B	295	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	A	236	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	384	ASP	CB-CG-OD2	-5.29	113.53	118.30
1	A	415	LEU	CB-CG-CD2	-5.25	102.08	111.00

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	1523	0	1542	43	0
1	B	1531	0	1553	27	1
2	B	6	0	8	0	0
3	A	163	0	0	7	0
3	B	154	0	0	7	1
All	All	3377	0	3103	69	2

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 11.

All (69) 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:281:MET:HG2	3:A:432:HOH:O	1.25	1.27
1:A:396:VAL:HG23	1:A:399:PHE:HB2	1.48	0.94
1:A:400:SER:H	1:A:401:ARG:HH12	0.97	0.92
1:A:396:VAL:CG2	1:A:399:PHE:HB2	1.99	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:394:ILE:HD13	1:B:396:VAL:HG23	1.51	0.92
1:A:400:SER:N	1:A:401:ARG:HH12	1.77	0.83
1:A:400:SER:H	1:A:401:ARG:NH1	1.76	0.82
1:A:394:ILE:HD13	1:A:396:VAL:CG1	2.10	0.82
1:B:240:GLU:HG3	3:B:60:HOH:O	1.81	0.81
1:B:290:GLN:NE2	3:B:463:HOH:O	2.16	0.79
1:A:400:SER:HB3	1:A:401:ARG:HH11	1.49	0.77
1:B:240:GLU:HB2	1:B:324:LYS:HE2	1.67	0.76
1:A:394:ILE:HD13	1:A:396:VAL:HG13	1.65	0.76
1:A:396:VAL:HG23	1:A:399:PHE:CD2	2.22	0.74
1:B:246:GLU:CD	1:B:246:GLU:H	1.93	0.72
1:A:225:ARG:HG2	1:A:225:ARG:HH11	1.53	0.71
1:A:225:ARG:HG2	1:A:225:ARG:NH1	2.09	0.67
1:B:222:GLU:OE2	3:B:461:HOH:O	2.13	0.65
1:A:396:VAL:HG23	1:A:399:PHE:CB	2.23	0.65
1:B:256:ASN:HD22	1:B:317:TRP:HE1	1.46	0.62
1:A:396:VAL:CG2	1:A:399:PHE:CB	2.75	0.62
1:A:412:ARG:H	1:A:412:ARG:CZ	2.13	0.61
1:A:396:VAL:HG22	1:A:399:PHE:HB2	1.82	0.61
1:A:339:VAL:HG13	1:A:352:ILE:HG22	1.83	0.59
1:B:246:GLU:HB2	3:B:436:HOH:O	2.05	0.57
1:A:400:SER:CB	1:A:401:ARG:NH1	2.70	0.55
1:A:396:VAL:CG2	1:A:399:PHE:CD2	2.89	0.55
1:A:400:SER:HB3	1:A:401:ARG:NH1	2.18	0.54
1:A:401:ARG:H	1:A:401:ARG:NH1	2.06	0.54
1:B:413:ARG:HG3	3:B:71:HOH:O	2.09	0.53
1:B:394:ILE:HD13	1:B:396:VAL:CG2	2.32	0.53
1:A:394:ILE:CD1	1:A:396:VAL:CG1	2.86	0.52
1:A:396:VAL:HG23	1:A:399:PHE:CG	2.44	0.51
1:A:400:SER:N	1:A:401:ARG:NH1	2.45	0.51
1:A:225:ARG:HD2	3:A:158:HOH:O	2.10	0.51
1:A:396:VAL:HG23	1:A:399:PHE:HD2	1.75	0.51
1:B:394:ILE:H	1:B:394:ILE:HD12	1.76	0.50
1:A:362:ARG:NH2	1:A:397:LYS:HB2	2.27	0.50
1:A:339:VAL:HG13	1:A:352:ILE:CG2	2.42	0.49
1:B:256:ASN:ND2	1:B:317:TRP:HE1	2.09	0.49
1:A:332:ILE:HB	1:A:374:ILE:HG22	1.95	0.48
1:B:240:GLU:O	1:B:244:GLU:HG3	2.14	0.47
1:A:281:MET:CG	3:A:432:HOH:O	2.09	0.47
1:A:318:ARG:HA	1:A:322:ILE:O	2.14	0.47
1:B:393:GLN:HA	1:B:403:VAL:O	2.14	0.47

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:ARG:HH21	1:A:397:LYS:HB2	1.81	0.46
1:B:332:ILE:HB	1:B:374:ILE:HG22	1.98	0.46
1:A:246:GLU:HB2	3:A:200:HOH:O	2.15	0.45
1:A:396:VAL:CG2	1:A:399:PHE:CG	2.99	0.45
1:A:359:LEU:HB2	1:A:399:PHE:CZ	2.51	0.45
1:A:412:ARG:HB2	1:A:412:ARG:HE	1.44	0.44
1:A:236:ARG:NE	1:A:236:ARG:HA	2.33	0.44
1:A:389:ARG:NH1	3:A:175:HOH:O	2.51	0.44
1:B:246:GLU:HG2	3:B:451:HOH:O	2.17	0.44
1:B:394:ILE:N	1:B:394:ILE:HD12	2.33	0.44
1:B:397:LYS:HE3	3:B:465:HOH:O	2.16	0.44
1:B:245:LEU:HD23	1:B:250:LEU:HA	2.00	0.43
1:B:221:LEU:HD23	1:B:341:ASN:HD22	1.83	0.43
1:A:409:VAL:HG11	1:B:415:LEU:HD11	2.01	0.42
1:B:286:ASP:OD2	1:B:350:TYR:OH	2.34	0.42
1:A:394:ILE:HD12	1:A:394:ILE:H	1.85	0.42
1:A:411:SER:HB2	1:A:412:ARG:NH1	2.34	0.42
1:B:394:ILE:CD1	1:B:403:VAL:HB	2.50	0.42
1:B:324:LYS:HG2	1:B:325:PRO:HD2	2.03	0.41
3:A:476:HOH:O	1:B:385:VAL:HG22	2.21	0.41
1:A:314:ARG:HD3	1:A:326:LEU:O	2.20	0.41
3:A:476:HOH:O	1:B:385:VAL:CG2	2.68	0.41
1:A:401:ARG:NH1	1:A:401:ARG:N	2.69	0.40
1:B:362:ARG:NH1	1:B:362:ARG:HG2	2.36	0.40

All (2) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:162:HOH:O	3:B:418:HOH:O[1_565]	2.02	0.18
1:B:336:TYR:OH	1:B:336:TYR:OH[2_656]	2.02	0.18

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	193/198 (98%)	191 (99%)	2 (1%)	0	100	100
1	B	194/198 (98%)	192 (99%)	2 (1%)	0	100	100
All	All	387/396 (98%)	383 (99%)	4 (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	164/166 (99%)	154 (94%)	10 (6%)	18	2
1	B	165/166 (99%)	156 (94%)	9 (6%)	21	3
All	All	329/332 (99%)	310 (94%)	19 (6%)	20	2

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	224	GLN
1	A	225	ARG
1	A	246	GLU
1	A	323	THR
1	A	364	GLU
1	A	394	ILE
1	A	397	LYS
1	A	401	ARG
1	A	403	VAL
1	A	412	ARG
1	B	221	LEU
1	B	222	GLU
1	B	224	GLN
1	B	274	LYS
1	B	364	GLU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	383	LYS
1	B	394	ILE
1	B	400	SER
1	B	413	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	256	ASN
1	B	256	ASN
1	B	290	GLN
1	B	341	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

1 ligand is 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	GOL	B	1	-	5,5,5	0.52	0	5,5,5	1.19	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
2	GOL	B	1	-	-	2/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1	GOL	O1-C1-C2-O2
2	B	1	GOL	O1-C1-C2-C3

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	195/198 (98%)	0.09	13 (6%) 17 19	8, 18, 42, 51	0
1	B	196/198 (98%)	0.09	13 (6%) 18 19	8, 18, 37, 46	0
All	All	391/396 (98%)	0.09	26 (6%) 18 19	8, 18, 41, 51	0

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	396	VAL	7.1
1	A	396	VAL	5.3
1	A	399	PHE	5.3
1	A	395	ALA	5.2
1	A	397	LYS	5.1
1	B	399	PHE	3.7
1	B	395	ALA	3.6
1	B	401	ARG	3.2
1	B	221	LEU	3.2
1	B	397	LYS	3.1
1	B	347	ARG	2.9
1	A	222	GLU	2.8
1	B	346	THR	2.8
1	A	320	GLN	2.6
1	A	323	THR	2.6
1	B	400	SER	2.6
1	A	394	ILE	2.5
1	B	319	ALA	2.4
1	A	346	THR	2.4
1	B	403	VAL	2.3
1	A	347	ARG	2.2
1	A	246	GLU	2.1
1	A	400	SER	2.1
1	A	345	ASP	2.1

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	394	ILE	2.0
1	B	384	ASP	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, 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(\AA^2)	Q<0.9
2	GOL	B	1	6/6	0.76	0.14	25,25,28,39	0

6.5 Other polymers [i](#)

There are no such residues in this entry.