



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 05:40 PM UTC

PDB ID : 1NSS / pdb_00001nss
Title : Crystal structure of galactose mutarotase from *Lactococcus lactis* mutant D243A complexed with glucose
Authors : Holden, H.M.; Thoden, J.B.
Deposited on : 2003-01-28
Resolution : 1.85 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

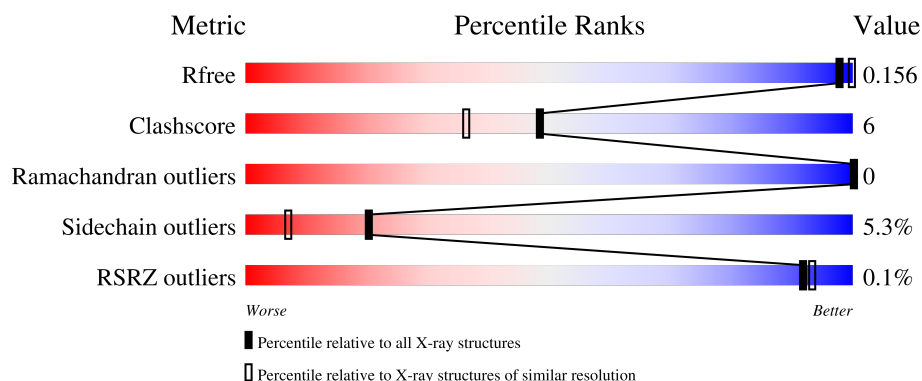
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	347	 80% 15% ..
1	B	347	 82% 15% ..

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5816 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.

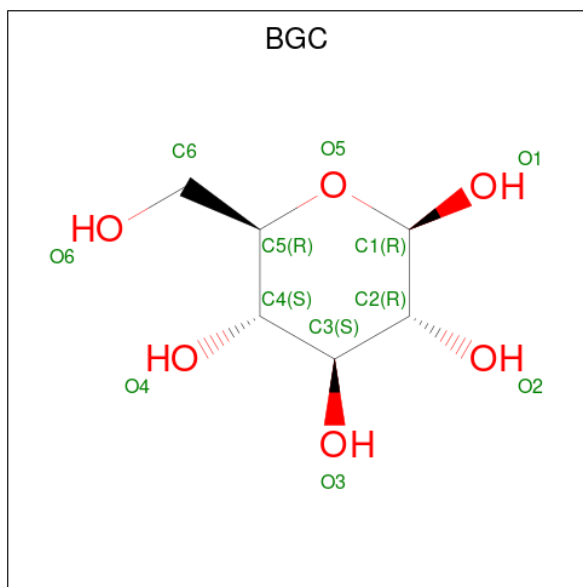
- Molecule 1 is a protein called GALACTOSE MUTAROTASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	339	Total	C	N	O	S	0	2	0
			2650	1674	447	526	3			
1	B	346	Total	C	N	O	S	0	2	0
			2723	1717	466	537	3			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	2	SER	GLU	cloning artifact	UNP Q9ZB17
A	243	ALA	ASP	engineered mutation	UNP Q9ZB17
A	340	LEU	-	expression tag	UNP Q9ZB17
A	341	GLU	-	expression tag	UNP Q9ZB17
A	342	HIS	-	expression tag	UNP Q9ZB17
A	343	HIS	-	expression tag	UNP Q9ZB17
A	344	HIS	-	expression tag	UNP Q9ZB17
A	345	HIS	-	expression tag	UNP Q9ZB17
A	346	HIS	-	expression tag	UNP Q9ZB17
A	347	HIS	-	expression tag	UNP Q9ZB17
B	2	SER	GLU	cloning artifact	UNP Q9ZB17
B	243	ALA	ASP	engineered mutation	UNP Q9ZB17
B	340	LEU	-	expression tag	UNP Q9ZB17
B	341	GLU	-	expression tag	UNP Q9ZB17
B	342	HIS	-	expression tag	UNP Q9ZB17
B	343	HIS	-	expression tag	UNP Q9ZB17
B	344	HIS	-	expression tag	UNP Q9ZB17
B	345	HIS	-	expression tag	UNP Q9ZB17
B	346	HIS	-	expression tag	UNP Q9ZB17
B	347	HIS	-	expression tag	UNP Q9ZB17

- Molecule 2 is beta-D-glucopyranose (CCD ID: BGC) (formula: C₆H₁₂O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			12	6	6		
2	B	1	Total	C	O	0	0
			12	6	6		

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Na	0	0
			1	1		

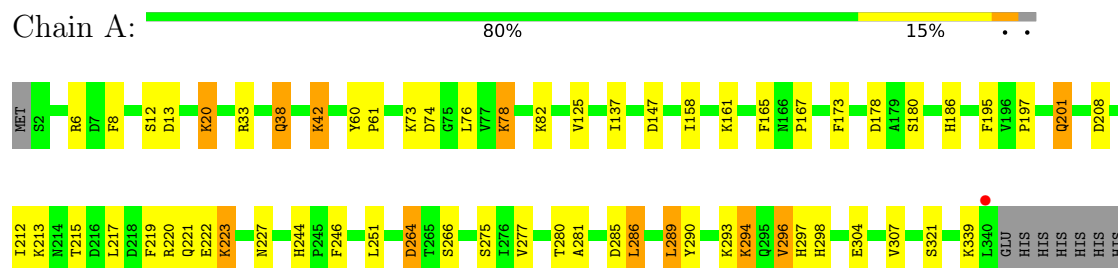
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	196	Total	O	0	0
			196	196		
4	B	222	Total	O	0	0
			222	222		

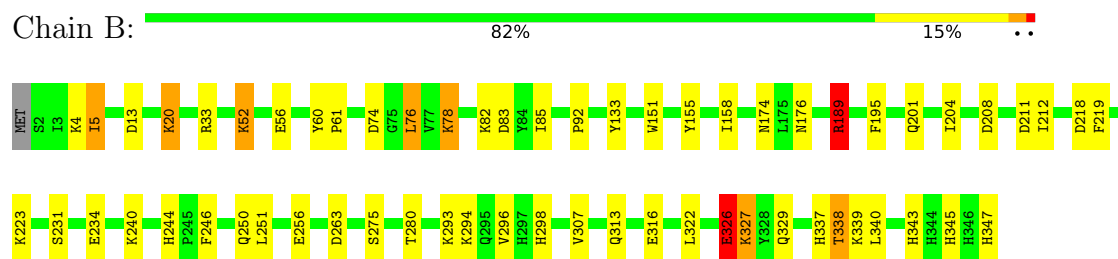
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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: GALACTOSE MUTAROTASE



• Molecule 1: GALACTOSE MUTAROTASE



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	44.90Å 76.20Å 210.90Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	30.00 – 1.85 30.00 – 1.85	Depositor EDS
% Data completeness (in resolution range)	96.8 (30.00-1.85) 96.7 (30.00-1.85)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.47 (at 1.81Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.161 , 0.212 0.158 , 0.156	Depositor DCC
R_{free} test set	6252 reflections (9.96%)	wwPDB-VP
Wilson B-factor (Å ²)	22.1	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 90.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5816	wwPDB-VP
Average B, all atoms (Å ²)	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.88% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: BGC, NA

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	1.09	0/2710	1.46	15/3668 (0.4%)
1	B	1.11	1/2789 (0.0%)	1.45	19/3774 (0.5%)
All	All	1.10	1/5499 (0.0%)	1.46	34/7442 (0.5%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	13	ASP	CG-OD1	-5.14	1.15	1.25

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	244	HIS	O-C-N	8.86	127.38	121.71
1	A	13	ASP	CA-CB-CG	-8.08	104.52	112.60
1	A	33	ARG	N-CA-CB	-7.23	98.71	111.08
1	B	33	ARG	N-CA-CB	-7.17	98.83	111.08
1	A	307	VAL	N-CA-C	-6.91	99.82	109.21
1	A	244	HIS	O-C-N	6.43	125.82	121.71
1	A	33	ARG	N-CA-C	6.17	119.59	109.72
1	B	296	VAL	CB-CA-C	-6.10	103.08	111.49
1	B	307	VAL	N-CA-C	-5.90	101.10	108.89
1	A	289	LEU	N-CA-C	5.85	118.27	108.96
1	B	33	ARG	N-CA-C	5.83	119.05	109.72
1	B	347	HIS	CA-CB-CG	-5.83	107.97	113.80
1	B	231	SER	N-CA-C	5.78	118.22	110.35
1	B	189	ARG	N-CA-CB	5.76	120.36	110.68
1	B	307	VAL	N-CA-CB	5.76	116.81	110.53
1	B	13	ASP	CA-CB-CG	-5.74	106.86	112.60
1	A	38	GLN	N-CA-C	5.73	118.11	109.23
1	A	76	LEU	N-CA-C	5.67	118.48	109.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	204	ILE	N-CA-C	-5.65	103.90	110.05
1	B	244	HIS	N-CA-C	5.53	117.17	108.55
1	A	290	TYR	CB-CA-C	-5.49	101.91	110.74
1	B	345	HIS	CA-CB-CG	-5.45	108.35	113.80
1	B	326	GLU	CB-CA-C	5.34	118.56	109.53
1	B	133	TYR	N-CA-C	5.34	116.37	109.65
1	A	246	PHE	CA-CB-CG	-5.33	108.47	113.80
1	B	211	ASP	CA-CB-CG	-5.33	107.27	112.60
1	B	337	HIS	CA-CB-CG	-5.32	108.48	113.80
1	A	244	HIS	N-CA-C	5.25	116.74	108.55
1	A	173	PHE	CA-CB-CG	-5.17	108.63	113.80
1	A	125	VAL	N-CA-CB	5.13	117.93	111.46
1	B	189	ARG	CB-CA-C	5.07	118.99	109.71
1	B	76	LEU	N-CA-C	5.03	116.71	108.52
1	A	217	LEU	CA-C-N	-5.00	115.77	122.42
1	A	217	LEU	C-N-CA	-5.00	115.77	122.42

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	2650	0	2595	32	0
1	B	2723	0	2644	27	0
2	A	12	0	12	0	0
2	B	12	0	12	0	0
3	A	1	0	0	0	0
4	A	196	0	0	1	0
4	B	222	0	0	1	0
All	All	5816	0	5263	59	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 6.

All (59) 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:264:ASP:HB3	1:A:339:LYS:HG2	1.68	0.75
1:A:20:LYS:HD2	1:A:147:ASP:OD2	1.86	0.75
1:B:263:ASP:H	1:B:343:HIS:HD1	1.37	0.73
1:A:180:SER:HA	1:A:296:VAL:HG13	1.72	0.70
1:A:161:LYS:HE3	4:A:1560:HOH:O	1.93	0.69
1:A:201:GLN:NE2	1:A:201:GLN:H	1.94	0.66
1:B:338:THR:HG22	1:B:339:LYS:HG3	1.78	0.65
1:A:294:LYS:NZ	1:A:294:LYS:HB2	2.15	0.62
1:A:201:GLN:H	1:A:201:GLN:CD	2.09	0.60
1:B:158[B]:ILE:HD11	1:B:327:LYS:HG3	1.83	0.60
1:B:338:THR:CG2	1:B:339:LYS:HG3	2.32	0.60
1:A:212:ILE:O	1:A:215:THR:HG23	2.04	0.57
1:B:52:LYS:HE2	1:B:56:GLU:OE2	2.04	0.57
1:A:289:LEU:HD23	1:A:294:LYS:HA	1.89	0.53
1:B:313:GLN:HG2	4:B:2552:HOH:O	2.09	0.52
1:A:213:LYS:HG2	1:A:220:ARG:CZ	2.40	0.52
1:A:73:LYS:NZ	1:A:74:ASP:OD2	2.37	0.51
1:B:52:LYS:O	1:B:56:GLU:HG3	2.11	0.50
1:A:251:LEU:HD23	1:A:251:LEU:N	2.26	0.50
1:B:78:LYS:HG3	1:B:83:ASP:OD1	2.12	0.49
1:B:189:ARG:NH2	1:B:256:GLU:O	2.45	0.49
1:A:219:PHE:CE2	1:A:223:LYS:HG2	2.48	0.48
1:B:4:LYS:C	1:B:5:ILE:HG12	2.38	0.47
1:A:20:LYS:HD2	1:A:147:ASP:CG	2.39	0.47
1:B:340:LEU:HD12	1:B:340:LEU:HA	1.68	0.47
1:A:197:PRO:HD2	1:A:208:ASP:O	2.15	0.46
1:A:285:ASP:O	1:A:286:LEU:C	2.58	0.46
1:A:221:GLN:O	1:A:222:GLU:C	2.57	0.45
1:B:60:TYR:N	1:B:61:PRO:CD	2.78	0.45
1:A:180:SER:O	1:A:296:VAL:HG11	2.17	0.45
1:B:82:LYS:HB3	1:B:82:LYS:HE3	1.76	0.44
1:B:218:ASP:O	1:B:223:LYS:HE2	2.19	0.43
1:B:322:LEU:HD12	1:B:326:GLU:HG2	2.00	0.43
1:A:280:THR:O	1:A:281:ALA:C	2.61	0.43
1:B:246:PHE:O	1:B:275:SER:HB2	2.19	0.43
1:B:155:TYR:O	1:B:329:GLN:HA	2.19	0.43
1:B:74:ASP:HA	1:B:92:PRO:O	2.17	0.43
1:B:174:ASN:OD1	1:B:176:ASN:HB2	2.18	0.43
1:A:60:TYR:N	1:A:61:PRO:CD	2.81	0.42
1:A:280:THR:O	1:A:298:HIS:HA	2.19	0.42
1:B:20:LYS:HB3	1:B:20:LYS:HE3	1.84	0.42
1:A:297:HIS:O	1:A:298:HIS:HB2	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:137:ILE:HD13	1:A:137:ILE:HG21	1.86	0.42
1:A:277:VAL:HB	1:A:304:GLU:HB2	2.02	0.42
1:A:294:LYS:NZ	1:A:294:LYS:CB	2.82	0.42
1:B:280:THR:O	1:B:298:HIS:HA	2.19	0.42
1:A:227:ASN:N	1:A:227:ASN:HD22	2.18	0.41
1:A:38:GLN:HB2	1:A:42:LYS:O	2.21	0.41
1:B:219:PHE:CE2	1:B:223:LYS:HG3	2.56	0.41
1:A:178:ASP:OD2	1:A:293:LYS:NZ	2.49	0.41
1:B:76:LEU:HD12	1:B:85:ILE:HG13	2.03	0.41
1:A:78:LYS:HA	1:A:82:LYS:O	2.20	0.41
1:A:165:PHE:CD2	1:A:167:PRO:HD3	2.57	0.40
1:B:208:ASP:OD2	1:B:208:ASP:N	2.52	0.40
1:B:151:TRP:CD1	1:B:151:TRP:C	3.00	0.40
1:A:8:PHE:HB3	1:A:12:SER:OG	2.21	0.40
1:B:251:LEU:N	1:B:251:LEU:HD23	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	339/347 (98%)	318 (94%)	21 (6%)	0	100	100
1	B	346/347 (100%)	330 (95%)	16 (5%)	0	100	100
All	All	685/694 (99%)	648 (95%)	37 (5%)	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	293/299 (98%)	278 (95%)	15 (5%)	21	7
1	B	300/299 (100%)	284 (95%)	16 (5%)	20	7
All	All	593/598 (99%)	562 (95%)	31 (5%)	20	7

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	ARG
1	A	20	LYS
1	A	42	LYS
1	A	78	LYS
1	A	186	HIS
1	A	195	PHE
1	A	201	GLN
1	A	223	LYS
1	A	264	ASP
1	A	266	SER
1	A	275	SER
1	A	286	LEU
1	A	294	LYS
1	A	296	VAL
1	A	321	SER
1	B	5	ILE
1	B	20	LYS
1	B	52	LYS
1	B	78	LYS
1	B	189	ARG
1	B	195	PHE
1	B	201	GLN
1	B	212	ILE
1	B	234	GLU
1	B	240	LYS
1	B	250	GLN
1	B	293	LYS
1	B	294	LYS
1	B	326	GLU
1	B	327	LYS
1	B	338	THR

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

Mol	Chain	Res	Type
1	A	201	GLN
1	A	227	ASN
1	B	43	HIS
1	B	201	GLN
1	B	224	GLN
1	B	227	ASN
1	B	306	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 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	$\# Z > 2$
2	BGC	B	2400	-	12,12,12	0.56	0	17,17,17	1.44	2 (11%)
2	BGC	A	1400	-	12,12,12	0.72	0	17,17,17	1.12	1 (5%)

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	BGC	B	2400	-	-	0/2/22/22	0/1/1/1
2	BGC	A	1400	-	-	0/2/22/22	0/1/1/1

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2400	BGC	O5-C1-C2	-3.73	103.75	110.30
2	B	2400	BGC	O6-C6-C5	-2.33	103.40	111.33
2	A	1400	BGC	C3-C4-C5	-2.29	106.07	110.23

There are no chirality outliers.

There are no torsion outliers.

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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	339/347 (97%)	-0.57	1 (0%) 90 92	18, 28, 59, 93	2 (0%)
1	B	346/347 (99%)	-0.76	0 100 100	16, 24, 52, 66	2 (0%)
All	All	685/694 (98%)	-0.67	1 (0%) 92 93	16, 26, 57, 93	4 (0%)

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	340	LEU	2.9

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 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(Å ²)	Q<0.9
3	NA	A	1401	1/1	0.91	0.10	51,51,51,51	0
2	BGC	A	1400	12/12	0.93	0.10	27,51,100,100	0
2	BGC	B	2400	12/12	0.94	0.10	28,45,100,100	0

6.5 Other polymers [i](#)

There are no such residues in this entry.