



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 02:19 PM UTC

PDB ID : 4WKT / pdb_00004wkt
Title : n-Alkylboronic Acid Inhibitors Reveal Determinants of Ligand Specificity in the Quorum-Quenching and Siderophore Biosynthetic Enzyme PvdQ
Authors : Wu, R.; Clevenger, K.D.; Fast, W.; Liu, D.
Deposited on : 2014-10-03
Resolution : 1.78 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

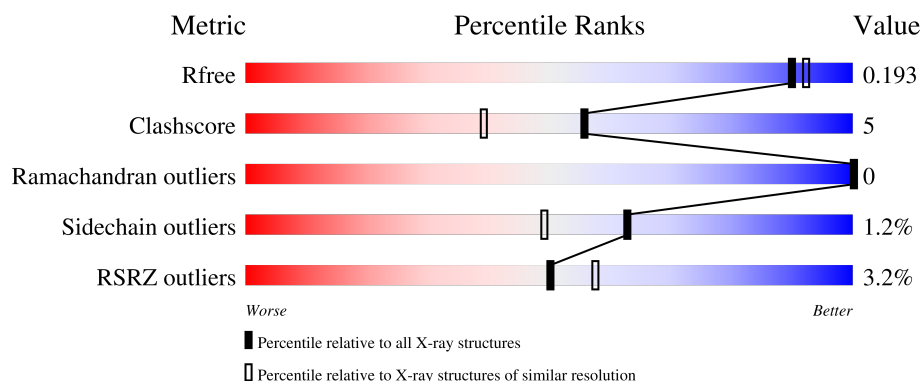
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.78 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	1365 (1.78-1.78)
Clashscore	190562	1395 (1.78-1.78)
Ramachandran outliers	187476	1382 (1.78-1.78)
Sidechain outliers	187428	1382 (1.78-1.78)
RSRZ outliers	180081	1365 (1.78-1.78)

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	C	548	3% 92% 7%
2	A	165	4% 93% 7%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	204	-	X	X	-
4	GOL	C	804	-	-	X	-

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6361 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 Acyl-homoserine lactone acylase PvdQ.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	548	Total	C	N	O	S	0	5	0
			4291	2700	783	797	11			

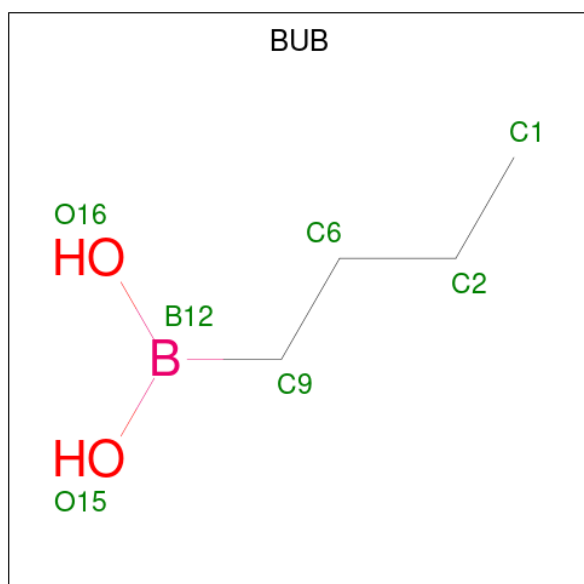
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	763	ALA	-	expression tag	UNP Q9I194
C	764	ALA	-	expression tag	UNP Q9I194

- Molecule 2 is a protein called Acyl-homoserine lactone acylase PvdQ.

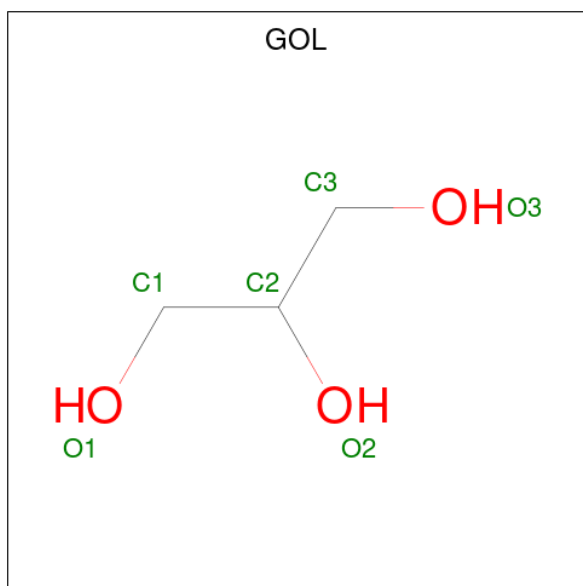
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	A	165	Total	C	N	O	S	0	5	0
			1300	825	234	239	2			

- Molecule 3 is 1-BUTANE BORONIC ACID (CCD ID: BUB) (formula: $C_4H_{11}BO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	C	1	Total	B	C	O	0	1
			12	2	8	2		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



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

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

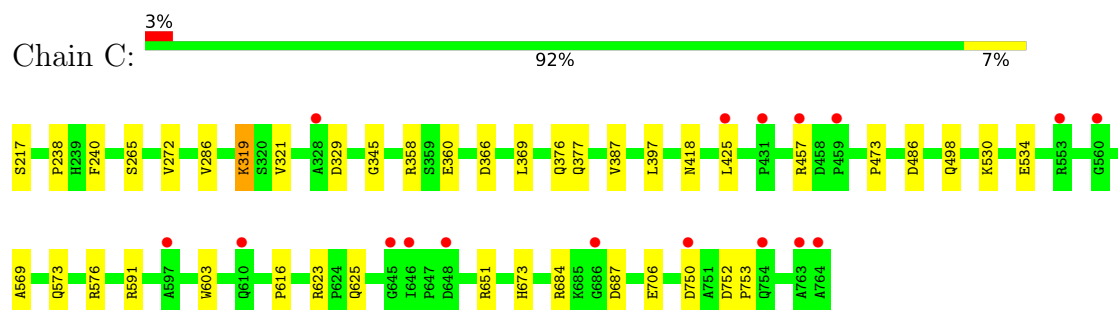
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	475	Total O 475 475	0	0
5	A	175	Total O 175 175	0	0

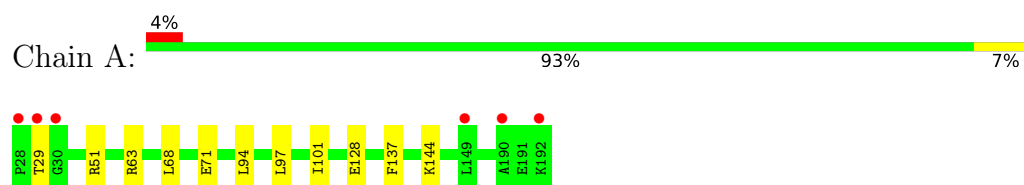
3 Residue-property plots [i](#)

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: Acyl-homoserine lactone acylase PvdQ



- Molecule 2: Acyl-homoserine lactone acylase PvdQ



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	121.29Å 167.51Å 95.03Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	47.51 – 1.78 47.51 – 1.78	Depositor EDS
% Data completeness (in resolution range)	99.8 (47.51-1.78) 91.4 (47.51-1.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.30 (at 1.78Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.9_1678)	Depositor
R, R_{free}	0.165 , 0.192 0.171 , 0.193	Depositor DCC
R_{free} test set	2000 reflections (2.17%)	wwPDB-VP
Wilson B-factor (Å ²)	22.4	Xtriage
Anisotropy	0.313	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 48.7	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	0.97	EDS
Total number of atoms	6361	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.18% 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: GOL, BUB

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	C	0.43	0/4405	0.74	0/5994
2	A	0.46	0/1344	0.69	0/1824
All	All	0.44	0/5749	0.72	0/7818

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

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	C	4291	0	4201	39	0
2	A	1300	0	1280	14	0
3	C	12	0	20	2	0
4	A	36	0	48	5	0
4	C	72	0	96	12	0
5	A	175	0	0	4	1
5	C	475	0	0	13	1
All	All	6361	0	5645	53	1

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 5.

All (53) 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)
2:A:144:LYS:HB3	4:A:204:GOL:H2	1.43	0.99
1:C:673:HIS:NE2	5:C:1289:HOH:O	2.10	0.83
2:A:137:PHE:HZ	4:A:204:GOL:H11	1.45	0.80
1:C:369:LEU:HD12	4:C:804:GOL:H11	1.63	0.78
1:C:457:ARG:NH1	5:C:1282:HOH:O	2.14	0.77
2:A:29:THR:OG1	5:A:456:HOH:O	2.05	0.75
2:A:71[B]:GLU:OE1	5:A:461:HOH:O	2.10	0.69
1:C:651:ARG:NE	5:C:1268:HOH:O	2.26	0.69
2:A:51[B]:ARG:NH2	2:A:128:GLU:OE1	2.22	0.69
2:A:71[B]:GLU:OE2	5:A:436:HOH:O	2.10	0.69
2:A:137:PHE:CZ	4:A:204:GOL:H11	2.27	0.68
1:C:360:GLU:OE1	5:C:902:HOH:O	2.12	0.67
2:A:128:GLU:OE2	5:A:405:HOH:O	2.13	0.65
1:C:217[A]:SER:HB3	1:C:238:PRO:HA	1.86	0.57
1:C:569:ALA:O	1:C:573:GLN:HG3	2.05	0.56
1:C:591:ARG:NH2	4:C:813:GOL:O2	2.39	0.56
1:C:366:ASP:H	4:C:804:GOL:C1	2.19	0.55
1:C:366:ASP:H	4:C:804:GOL:H12	1.71	0.55
1:C:376[A]:GLN:OE1	5:C:1094:HOH:O	2.18	0.53
1:C:603:TRP:CD2	1:C:616:PRO:HB2	2.44	0.52
1:C:603:TRP:CD1	4:C:807:GOL:H2	2.45	0.51
2:A:94:LEU:HA	4:A:202:GOL:H2	1.95	0.49
1:C:265:SER:OG	1:C:272:VAL:HA	2.13	0.49
1:C:369:LEU:HD12	4:C:804:GOL:C1	2.37	0.48
1:C:625:GLN:OE1	1:C:625:GLN:N	2.32	0.48
1:C:217[A]:SER:CB	1:C:238:PRO:HA	2.44	0.48
1:C:418:ASN:ND2	5:C:1042:HOH:O	2.47	0.46
1:C:750:ASP:OD2	5:C:903:HOH:O	2.21	0.46
1:C:750:ASP:CG	5:C:903:HOH:O	2.58	0.46
1:C:486:ASP:OD1	4:C:810:GOL:O1	2.26	0.46
1:C:345:GLY:HA3	4:C:804:GOL:H2	1.97	0.46
1:C:329:ASP:OD1	1:C:329:ASP:N	2.49	0.44
5:C:1090:HOH:O	2:A:68[B]:LEU:HD13	2.16	0.44
1:C:623:ARG:NE	5:C:1367:HOH:O	2.41	0.44
1:C:369:LEU:HD13	4:C:804:GOL:H31	2.00	0.43
1:C:358:ARG:NH1	5:C:1122:HOH:O	2.22	0.43
1:C:752:ASP:HA	1:C:753:PRO:HD3	1.90	0.43
1:C:286:VAL:H	3:C:801[A]:BUB:HO15	1.62	0.42
1:C:377:GLN:HA	1:C:397:LEU:HD23	2.00	0.42
1:C:369:LEU:CD1	4:C:804:GOL:H31	2.48	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:A:137:PHE:CZ	4:A:204:GOL:C1	3.01	0.42
1:C:217[A]:SER:HB2	3:C:801[A]:BUB:HO15	1.84	0.42
2:A:63[B]:ARG:HA	2:A:137:PHE:CZ	2.54	0.42
1:C:369:LEU:HA	1:C:369:LEU:HD23	1.76	0.42
4:C:812:GOL:C1	5:C:1324:HOH:O	2.68	0.42
1:C:319:LYS:HB2	1:C:319:LYS:HE2	1.73	0.42
1:C:576:ARG:NH1	5:C:1236:HOH:O	2.53	0.41
1:C:321:VAL:HG21	2:A:101:ILE:HG23	2.02	0.41
2:A:63[A]:ARG:HA	2:A:137:PHE:CZ	2.55	0.41
1:C:418:ASN:HB3	1:C:473:PRO:HD2	2.02	0.40
1:C:530:LYS:HE3	1:C:534:GLU:OE2	2.21	0.40
1:C:684:ARG:HD3	4:C:813:GOL:H31	2.03	0.40
1:C:687:ASP:OD1	1:C:687:ASP:N	2.50	0.40

All (1) 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)
5:C:963:HOH:O	5:A:335:HOH:O[8_455]	1.94	0.26

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	C	550/548 (100%)	534 (97%)	16 (3%)	0	100	100
2	A	168/165 (102%)	165 (98%)	3 (2%)	0	100	100
All	All	718/713 (101%)	699 (97%)	19 (3%)	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	C	446/447 (100%)	439 (98%)	7 (2%)	55	38
2	A	125/121 (103%)	124 (99%)	1 (1%)	73	63
All	All	571/568 (100%)	563 (99%)	8 (1%)	63	44

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

Mol	Chain	Res	Type
1	C	240[A]	PHE
1	C	240[B]	PHE
1	C	319	LYS
1	C	387	VAL
1	C	425	LEU
1	C	498	GLN
1	C	706	GLU
2	A	97	LEU

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

Mol	Chain	Res	Type
1	C	539	ASN
1	C	678	ASN
1	C	737	GLN
1	C	756	GLN

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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

20 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	$\# Z > 2$
3	BUB	C	801[B]	1	3,5,6	0.33	0	2,4,6	1.47	1 (50%)
4	GOL	C	807	-	5,5,5	0.41	0	5,5,5	0.16	0
4	GOL	A	204	-	5,5,5	0.58	0	5,5,5	1.81	2 (40%)
4	GOL	C	809	-	5,5,5	0.38	0	5,5,5	0.23	0
4	GOL	C	812	-	5,5,5	0.36	0	5,5,5	0.37	0
3	BUB	C	801[A]	1	3,5,6	0.32	0	2,4,6	2.19	1 (50%)
4	GOL	C	806	-	5,5,5	0.37	0	5,5,5	0.38	0
4	GOL	A	205	-	5,5,5	0.38	0	5,5,5	0.34	0
4	GOL	C	811	-	5,5,5	0.36	0	5,5,5	0.32	0
4	GOL	C	810	-	5,5,5	0.38	0	5,5,5	0.18	0
4	GOL	A	203	-	5,5,5	0.37	0	5,5,5	0.45	0
4	GOL	A	206	-	5,5,5	0.35	0	5,5,5	0.33	0
4	GOL	C	813	-	5,5,5	0.38	0	5,5,5	0.30	0
4	GOL	C	808	-	5,5,5	0.39	0	5,5,5	0.29	0
4	GOL	C	805	-	5,5,5	0.40	0	5,5,5	0.47	0
4	GOL	A	202	-	5,5,5	0.35	0	5,5,5	0.36	0
4	GOL	A	201	-	5,5,5	0.36	0	5,5,5	0.40	0
4	GOL	C	803	-	5,5,5	0.50	0	5,5,5	0.54	0
4	GOL	C	802	-	5,5,5	0.35	0	5,5,5	0.38	0
4	GOL	C	804	-	5,5,5	0.54	0	5,5,5	0.34	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	BUB	C	801[B]	1	-	1/2/3/4	-
4	GOL	C	807	-	-	2/4/4/4	-
4	GOL	A	204	-	-	4/4/4/4	-
4	GOL	C	809	-	-	2/4/4/4	-
4	GOL	C	812	-	-	2/4/4/4	-
3	BUB	C	801[A]	1	-	2/2/3/4	-
4	GOL	C	806	-	-	2/4/4/4	-
4	GOL	A	205	-	-	2/4/4/4	-
4	GOL	C	811	-	-	2/4/4/4	-
4	GOL	C	810	-	-	4/4/4/4	-
4	GOL	A	203	-	-	2/4/4/4	-
4	GOL	A	206	-	-	2/4/4/4	-
4	GOL	C	813	-	-	2/4/4/4	-
4	GOL	C	808	-	-	2/4/4/4	-
4	GOL	C	805	-	-	4/4/4/4	-
4	GOL	A	202	-	-	4/4/4/4	-
4	GOL	A	201	-	-	2/4/4/4	-
4	GOL	C	803	-	-	4/4/4/4	-
4	GOL	C	802	-	-	2/4/4/4	-
4	GOL	C	804	-	-	4/4/4/4	-

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	801[A]	BUB	B12-C9-C6	-3.09	107.50	115.19
4	A	204	GOL	O1-C1-C2	2.73	122.68	110.38
4	A	204	GOL	O3-C3-C2	-2.38	99.68	110.38
3	C	801[B]	BUB	B12-C9-C6	-2.07	110.05	115.19

There are no chirality outliers.

All (51) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	C	801[A]	BUB	C1-C2-C6-C9
3	C	801[B]	BUB	C2-C6-C9-B12
4	C	802	GOL	O1-C1-C2-C3
4	C	803	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	C	803	GOL	C1-C2-C3-O3
4	C	804	GOL	C1-C2-C3-O3
4	C	805	GOL	O1-C1-C2-C3
4	C	805	GOL	C1-C2-C3-O3
4	C	808	GOL	O1-C1-C2-C3
4	C	809	GOL	O1-C1-C2-C3
4	C	811	GOL	O1-C1-C2-O2
4	C	811	GOL	O1-C1-C2-C3
4	C	812	GOL	O1-C1-C2-C3
4	C	813	GOL	O1-C1-C2-O2
4	C	813	GOL	O1-C1-C2-C3
4	A	201	GOL	O1-C1-C2-C3
4	A	202	GOL	C1-C2-C3-O3
4	A	203	GOL	O1-C1-C2-C3
4	A	204	GOL	O1-C1-C2-C3
4	A	205	GOL	O1-C1-C2-C3
4	C	803	GOL	O2-C2-C3-O3
4	C	804	GOL	O1-C1-C2-O2
4	A	206	GOL	O1-C1-C2-O2
3	C	801[A]	BUB	C2-C6-C9-B12
4	C	804	GOL	O1-C1-C2-C3
4	C	806	GOL	O1-C1-C2-C3
4	C	807	GOL	O1-C1-C2-C3
4	C	810	GOL	O1-C1-C2-C3
4	C	810	GOL	C1-C2-C3-O3
4	A	202	GOL	O1-C1-C2-C3
4	A	204	GOL	C1-C2-C3-O3
4	A	206	GOL	O1-C1-C2-C3
4	C	802	GOL	O1-C1-C2-O2
4	C	803	GOL	O1-C1-C2-O2
4	C	804	GOL	O2-C2-C3-O3
4	C	807	GOL	O1-C1-C2-O2
4	C	808	GOL	O1-C1-C2-O2
4	C	809	GOL	O1-C1-C2-O2
4	C	810	GOL	O1-C1-C2-O2
4	A	201	GOL	O1-C1-C2-O2
4	A	202	GOL	O2-C2-C3-O3
4	A	203	GOL	O1-C1-C2-O2
4	A	204	GOL	O1-C1-C2-O2
4	C	805	GOL	O2-C2-C3-O3
4	C	812	GOL	O1-C1-C2-O2
4	A	205	GOL	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
4	C	805	GOL	O1-C1-C2-O2
4	A	204	GOL	O2-C2-C3-O3
4	A	202	GOL	O1-C1-C2-O2
4	C	810	GOL	O2-C2-C3-O3
4	C	806	GOL	O1-C1-C2-O2

There are no ring outliers.

8 monomers are involved in 19 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	807	GOL	1	0
4	A	204	GOL	4	0
4	C	812	GOL	1	0
3	C	801[A]	BUB	2	0
4	C	810	GOL	1	0
4	C	813	GOL	2	0
4	A	202	GOL	1	0
4	C	804	GOL	7	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 [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	C	548/548 (100%)	0.07	17 (3%)	51	59	9, 31, 61, 79	5 (0%)
2	A	165/165 (100%)	-0.24	6 (3%)	46	52	11, 23, 45, 113	5 (3%)
All	All	713/713 (100%)	-0.00	23 (3%)	50	57	9, 29, 60, 113	10 (1%)

All (23) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	A	28	PRO	5.4
1	C	764	ALA	5.0
1	C	553	ARG	4.9
1	C	328	ALA	4.4
2	A	29	THR	3.7
2	A	192	LYS	3.6
2	A	190	ALA	3.1
1	C	560	GLY	2.9
2	A	30	GLY	2.9
1	C	754	GLN	2.8
1	C	648	ASP	2.7
1	C	597	ALA	2.4
1	C	750	ASP	2.4
1	C	763	ALA	2.2
2	A	149	LEU	2.2
1	C	425	LEU	2.2
1	C	645	GLY	2.2
1	C	459	PRO	2.2
1	C	431	PRO	2.1
1	C	610	GLN	2.1
1	C	646	ILE	2.1
1	C	686	GLY	2.1
1	C	457	ARG	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 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
4	GOL	C	812	6/6	0.59	0.21	99,105,106,107	0
4	GOL	C	813	6/6	0.63	0.21	90,98,99,102	0
4	GOL	C	810	6/6	0.66	0.24	78,94,100,102	0
4	GOL	A	206	6/6	0.75	0.24	85,94,96,99	0
4	GOL	A	202	6/6	0.76	0.22	39,65,68,70	0
4	GOL	A	203	6/6	0.77	0.19	49,71,73,75	0
4	GOL	A	201	6/6	0.79	0.23	76,80,84,87	0
4	GOL	C	811	6/6	0.79	0.21	94,97,99,102	0
4	GOL	C	807	6/6	0.80	0.17	74,77,80,80	0
4	GOL	C	808	6/6	0.80	0.23	62,78,79,80	0
4	GOL	C	803	6/6	0.82	0.21	29,48,59,60	0
4	GOL	A	205	6/6	0.83	0.17	53,69,73,76	0
4	GOL	A	204	6/6	0.83	0.22	21,26,47,49	0
4	GOL	C	806	6/6	0.85	0.17	30,80,89,90	0
4	GOL	C	805	6/6	0.86	0.14	38,48,63,65	0
4	GOL	C	809	6/6	0.86	0.16	66,73,78,82	0
3	BUB	C	801[B]	6/7	0.87	0.21	19,38,49,51	6
3	BUB	C	801[A]	6/7	0.87	0.21	19,29,44,46	6
4	GOL	C	804	6/6	0.87	0.16	33,48,54,61	0
4	GOL	C	802	6/6	0.93	0.14	25,64,74,77	0

6.5 Other polymers [i](#)

There are no such residues in this entry.