wwPDB X-ray Structure Validation Summary Report (i)

Mar 6, 2026 – 05:40 AM UTC

PDB ID	:	5D4J / pdb_00005d4j
Title	:	Chloride-bound form of a copper nitrite reductase from Alcaligenes faecals
Authors	:	Fukuda, Y.; Tse, K.M.; Nakane, T.; Nakatsu, T.; Suzuki, M.; Sugahara, M.; Inoue, S.; Yumoto, F.; Matsugaki, N.; Nango, E.; Tono, K.; Joti, Y.; Kameshima, T.; Song, C.; Yabashi, M.; Nureki, O.; Murphy, M.E.P.; Inoue, T.; Iwata, S.; Mizohata, E.
Deposited on	:	2015-08-07
Resolution	:	2.00 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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 (i) 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 (i)) were used in the production of this report:

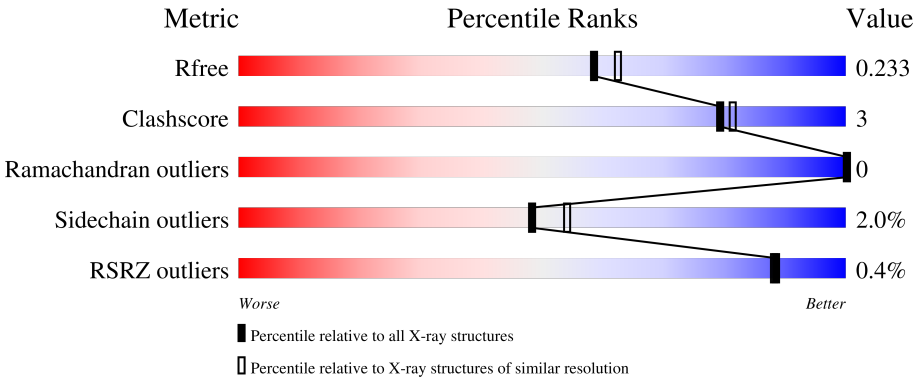
MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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 <=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	342	89% 9% .
1	B	342	% 87% 11% .
1	C	342	% 88% 10% .

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 8149 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 Copper-containing nitrite reductase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	335	Total	C	N	O	S	0	1	0
			2563	1640	431	481	11			
1	B	336	Total	C	N	O	S	0	0	0
			2560	1639	430	480	11			
1	C	336	Total	C	N	O	S	0	0	0
			2560	1639	430	480	11			

There are 15 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	3	MET	-	initiating methionine	UNP P38501
A	341	LEU	-	expression tag	UNP P38501
A	342	VAL	-	expression tag	UNP P38501
A	343	PRO	-	expression tag	UNP P38501
A	344	ARG	-	expression tag	UNP P38501
B	3	MET	-	initiating methionine	UNP P38501
B	341	LEU	-	expression tag	UNP P38501
B	342	VAL	-	expression tag	UNP P38501
B	343	PRO	-	expression tag	UNP P38501
B	344	ARG	-	expression tag	UNP P38501
C	3	MET	-	initiating methionine	UNP P38501
C	341	LEU	-	expression tag	UNP P38501
C	342	VAL	-	expression tag	UNP P38501
C	343	PRO	-	expression tag	UNP P38501
C	344	ARG	-	expression tag	UNP P38501

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Cu	0	0
			2	2		

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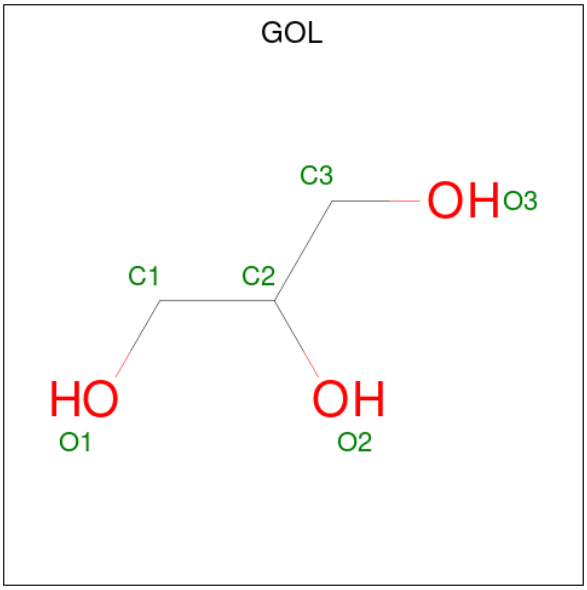
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	2	Total Cu 2 2	0	0
2	C	2	Total Cu 2 2	0	0

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Cl 1 1	0	0
3	B	1	Total Cl 1 1	0	0
3	C	1	Total Cl 1 1	0	0

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



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

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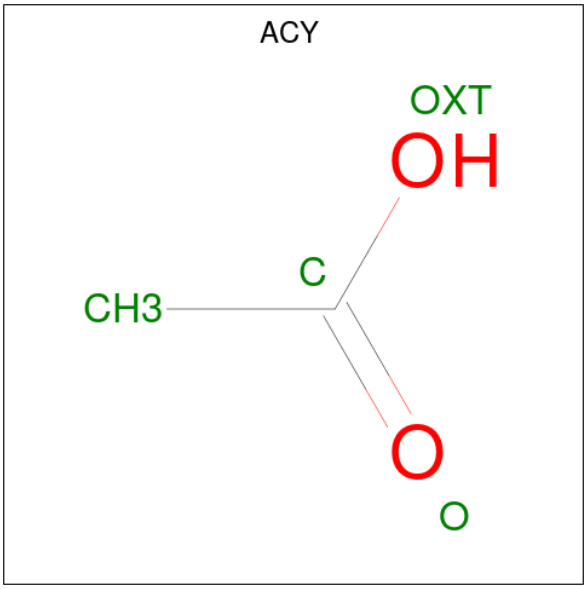
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0
4	C	1	Total C O 6 3 3	0	0

- Molecule 5 is ACETIC ACID (CCD ID: ACY) (formula: $C_2H_4O_2$).



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

- Molecule 6 is water.

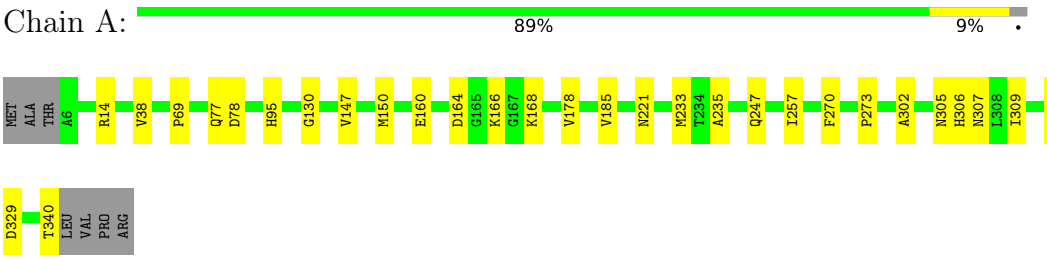
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	114	Total O 114 114	0	0
6	B	118	Total O 118 118	0	0
6	C	153	Total O 153 153	0	0

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.

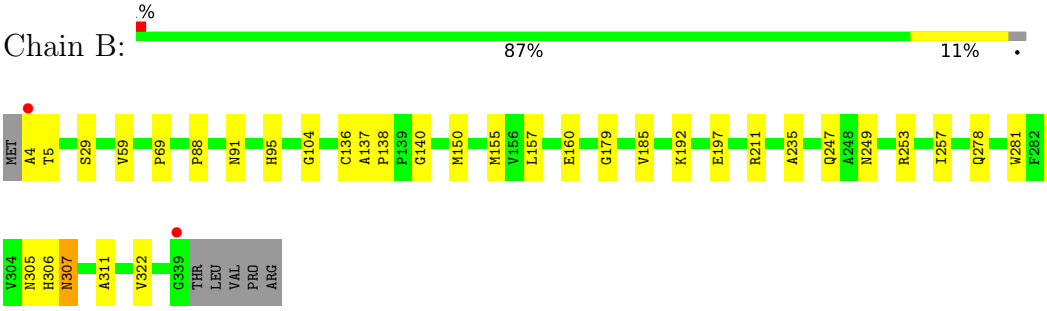
• Molecule 1: Copper-containing nitrite reductase

Chain A:



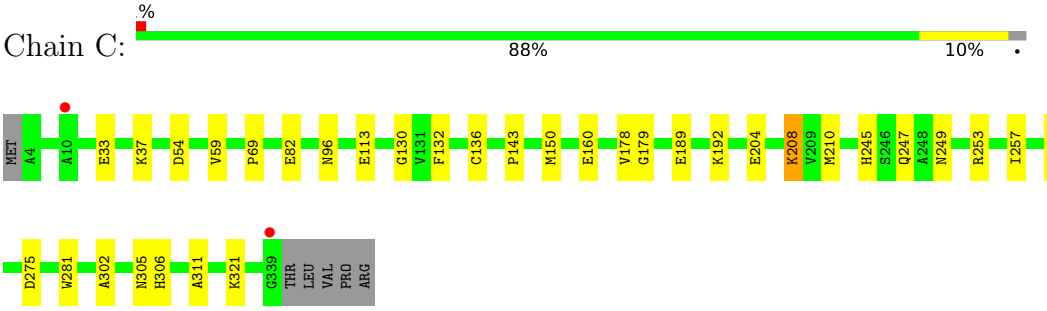
• Molecule 1: Copper-containing nitrite reductase

Chain B:



• Molecule 1: Copper-containing nitrite reductase

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	61.40Å 102.21Å 144.51Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.79 – 2.00 24.79 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.6 (24.79-2.00) 99.6 (24.79-2.00)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.13 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.182 , 0.232 0.183 , 0.233	Depositor DCC
R_{free} test set	2979 reflections (4.79%)	wwPDB-VP
Wilson B-factor (Å^2)	32.4	Xtriage
Anisotropy	0.088	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.39 , 40.4	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.97	EDS
Total number of atoms	8149	wwPDB-VP
Average B, all atoms (Å^2)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.71% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CU, CL, ACY, 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	1.13	4/2634 (0.2%)	1.10	4/3592 (0.1%)
1	B	1.12	0/2631	1.12	11/3588 (0.3%)
1	C	1.14	1/2631 (0.0%)	1.10	2/3588 (0.1%)
All	All	1.13	5/7896 (0.1%)	1.11	17/10768 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
1	C	0	1
All	All	0	3

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	273	PRO	CA-C	5.74	1.57	1.52
1	C	82	GLU	N-CA	-5.44	1.40	1.46
1	A	147	VAL	CA-CB	5.21	1.60	1.54
1	A	185	VAL	C-O	-5.20	1.17	1.24
1	A	178	VAL	CA-CB	5.08	1.60	1.53

The worst 5 of 17 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	303	TYR	N-CA-C	-6.34	97.94	108.34
1	B	211	ARG	NE-CZ-NH2	6.26	124.83	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	137	ALA	CA-C-N	-6.01	114.19	120.38
1	B	137	ALA	C-N-CA	-6.01	114.19	120.38
1	A	309	ILE	N-CA-C	-5.76	104.89	110.42

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	306	HIS	Peptide
1	B	306	HIS	Peptide
1	C	306	HIS	Peptide

5.2 Too-close contacts (i)

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	2563	0	2485	13	0
1	B	2560	0	2485	14	0
1	C	2560	0	2485	19	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	1	0
4	A	18	0	24	0	0
4	B	12	0	16	0	0
4	C	30	0	40	2	0
5	A	4	0	3	0	0
5	B	4	0	3	0	0
5	C	4	0	3	0	0
6	A	114	0	0	2	0
6	B	118	0	0	0	0
6	C	153	0	0	1	0
All	All	8149	0	7544	42	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 3.

The worst 5 of 42 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:C:257:ILE:HG12	3:C:601:CL:CL	2.16	0.83
1:C:59:VAL:HG13	4:C:608:GOL:H31	1.80	0.62
1:C:54:ASP:HA	4:C:607:GOL:H2	1.82	0.62
1:C:143:PRO:HB2	1:C:210:MET:CE	2.38	0.53
1:A:168:LYS:HG3	6:A:703:HOH:O	2.07	0.53

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	334/342 (98%)	327 (98%)	7 (2%)	0	100	100
1	B	334/342 (98%)	327 (98%)	7 (2%)	0	100	100
1	C	334/342 (98%)	330 (99%)	4 (1%)	0	100	100
All	All	1002/1026 (98%)	984 (98%)	18 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains (i)

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	265/270 (98%)	262 (99%)	3 (1%)	65	73
1	B	264/270 (98%)	257 (97%)	7 (3%)	39	42
1	C	264/270 (98%)	258 (98%)	6 (2%)	44	49
All	All	793/810 (98%)	777 (98%)	16 (2%)	48	54

5 of 16 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	208	LYS
1	C	192	LYS
1	B	197	GLU
1	C	160	GLU
1	B	192	LYS

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

Mol	Chain	Res	Type
1	A	15	GLN
1	A	115	ASN
1	C	163	HIS
1	C	296	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 22 ligands modelled in this entry, 9 are monoatomic - leaving 13 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	$\#\|Z\| > 2$
5	ACY	C	609	-	3,3,3	0.87	0	3,3,3	0.68	0
4	GOL	B	505	-	5,5,5	0.36	0	5,5,5	1.37	0
4	GOL	C	607	-	5,5,5	0.52	0	5,5,5	1.51	2 (40%)
4	GOL	A	505	-	5,5,5	0.35	0	5,5,5	1.37	1 (20%)
4	GOL	A	506	-	5,5,5	0.42	0	5,5,5	0.72	0
5	ACY	A	507	-	3,3,3	1.06	0	3,3,3	0.17	0
5	ACY	B	506	-	3,3,3	1.22	0	3,3,3	1.18	0
4	GOL	C	606	-	5,5,5	0.28	0	5,5,5	0.66	0
4	GOL	A	504	-	5,5,5	0.65	0	5,5,5	1.65	1 (20%)
4	GOL	B	504	-	5,5,5	0.48	0	5,5,5	1.13	1 (20%)
4	GOL	C	604	-	5,5,5	0.27	0	5,5,5	1.04	0
4	GOL	C	608	-	5,5,5	0.79	0	5,5,5	0.94	0
4	GOL	C	605	-	5,5,5	0.31	0	5,5,5	0.95	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
4	GOL	B	505	-	-	0/4/4/4	-
4	GOL	C	607	-	-	3/4/4/4	-
4	GOL	A	505	-	-	2/4/4/4	-
4	GOL	A	506	-	-	4/4/4/4	-
4	GOL	C	606	-	-	0/4/4/4	-
4	GOL	A	504	-	-	2/4/4/4	-
4	GOL	B	504	-	-	2/4/4/4	-
4	GOL	C	604	-	-	2/4/4/4	-
4	GOL	C	608	-	-	4/4/4/4	-
4	GOL	C	605	-	-	0/4/4/4	-

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	504	GOL	C3-C2-C1	-2.48	102.71	111.80
4	C	607	GOL	O1-C1-C2	-2.38	99.68	110.38
4	A	505	GOL	C3-C2-C1	-2.28	103.44	111.80
4	B	504	GOL	O1-C1-C2	-2.24	100.31	110.38
4	C	607	GOL	O2-C2-C3	2.14	118.05	109.18

There are no chirality outliers.

5 of 19 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	505	GOL	C1-C2-C3-O3
4	A	505	GOL	O2-C2-C3-O3
4	A	506	GOL	C1-C2-C3-O3
4	B	504	GOL	O1-C1-C2-C3
4	C	604	GOL	O1-C1-C2-C3

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	607	GOL	1	0
4	C	608	GOL	1	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^{th} 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	335/342 (97%)	-0.53	0	100	100	14, 32, 51, 80	1 (0%)
1	B	336/342 (98%)	-0.58	2 (0%)	85	85	22, 31, 50, 73	0
1	C	336/342 (98%)	-0.62	2 (0%)	85	85	21, 29, 48, 78	0
All	All	1007/1026 (98%)	-0.58	4 (0%)	88	88	14, 31, 50, 80	1 (0%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	339	GLY	2.8
1	B	339	GLY	2.5
1	B	4	ALA	2.2
1	C	10	ALA	2.1

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 oligosaccharides 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. The B-factors column lists the minimum, median, 95^{th} 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
5	ACY	A	507	4/4	0.68	0.14	50,51,57,59	0
4	GOL	C	608	6/6	0.79	0.14	43,48,50,51	0
4	GOL	A	504	6/6	0.86	0.14	38,45,45,47	0
4	GOL	C	607	6/6	0.86	0.10	48,52,56,61	0
4	GOL	C	605	6/6	0.88	0.08	48,54,56,57	0
3	CL	A	503	1/1	0.88	0.12	63,63,63,63	0
4	GOL	B	504	6/6	0.89	0.12	39,44,46,48	0
4	GOL	C	604	6/6	0.90	0.09	41,44,49,50	0
4	GOL	A	505	6/6	0.90	0.10	47,50,54,58	0
4	GOL	C	606	6/6	0.90	0.14	48,50,53,57	0
4	GOL	A	506	6/6	0.91	0.09	37,44,47,52	0
4	GOL	B	505	6/6	0.91	0.08	33,41,47,48	0
5	ACY	C	609	4/4	0.91	0.10	40,42,45,47	0
3	CL	C	601	1/1	0.92	0.09	53,53,53,53	0
5	ACY	B	506	4/4	0.93	0.08	35,36,37,39	0
3	CL	B	503	1/1	0.97	0.06	49,49,49,49	0
2	CU	C	602	1/1	1.00	0.01	29,29,29,29	0
2	CU	C	603	1/1	1.00	0.01	27,27,27,27	0
2	CU	A	501	1/1	1.00	0.01	30,30,30,30	0
2	CU	A	502	1/1	1.00	0.02	31,31,31,31	0
2	CU	B	501	1/1	1.00	0.01	32,32,32,32	0
2	CU	B	502	1/1	1.00	0.02	30,30,30,30	0

6.5 Other polymers (i)

There are no such residues in this entry.