



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 01:45 am BST

PDB ID : 5D4H  
Title : High-resolution nitrite complex of a copper nitrite reductase determined by synchrotron radiation crystallography  
Authors : Fukuda, Y.; Tse, K.M.; Nakane, T.; Nakatsu, T.; Suzuki, M.; Sugahara, M.; Inoue, S.; Masuda, T.; Yumoto, F.; Matsugaki, N.; Nango, E.; Tono, K.; Joti, Y.; Kameshima, T.; Song, C.; Hatsui, T.; Yabashi, M.; Nureki, O.; Murphy, M.E.P.; Inoue, T.; Iwata, S.; Mizohata, E.  
Deposited on : 2015-08-07  
Resolution : 1.30 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](mailto: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.

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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	:	1.8.5 (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

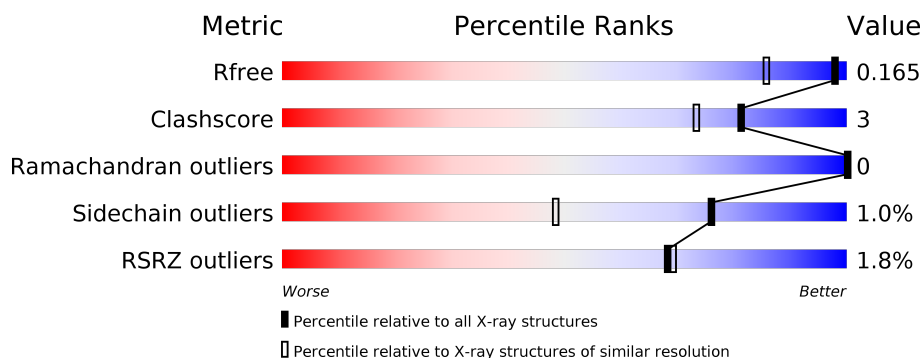
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 1.30 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	1058 (1.30-1.30)
Clashscore	141614	1101 (1.30-1.30)
Ramachandran outliers	138981	1058 (1.30-1.30)
Sidechain outliers	138945	1058 (1.30-1.30)
RSRZ outliers	127900	1029 (1.30-1.30)

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 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	342	<div> <div>2%</div> <div> <div></div> <div>89%</div> <div>8%</div> <div>..</div> </div> </div>
1	B	342	<div> <div>%</div> <div> <div></div> <div>90%</div> <div>9%</div> <div>.</div> </div> </div>
1	C	342	<div> <div>%</div> <div> <div></div> <div>89%</div> <div>10%</div> <div>..</div> </div> </div>

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
3	NO2	B	503[A]	-	-	X	-
4	GOL	A	515	-	X	-	-
4	GOL	C	507	-	X	X	-
4	GOL	C	508	-	X	-	-

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 9007 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	337	Total	C	N	O	S	0	4	0
			2600	1662	439	488	11			
1	B	341	Total	C	N	O	S	0	8	0
			2672	1707	452	502	11			
1	C	339	Total	C	N	O	S	0	9	0
			2661	1701	448	500	12			

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 (three-letter code: CU) (formula: Cu).

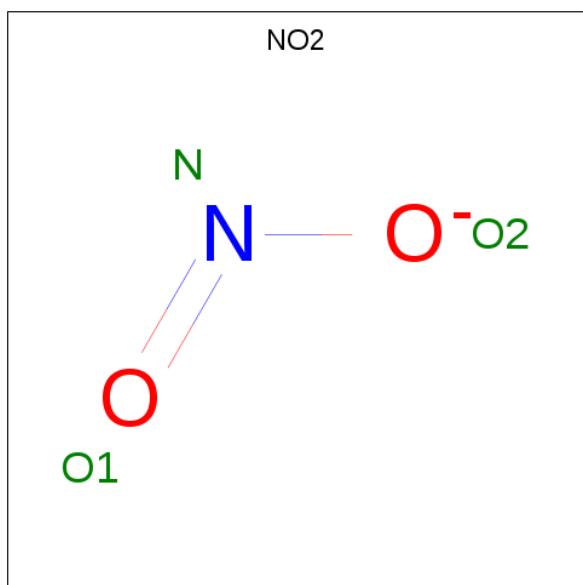
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Cu	0	0
			2	2		

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

- Molecule 3 is NITRITE ION (three-letter code: NO<sub>2</sub>) (formula: NO<sub>2</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	N	O	0	0
			3	1	2		
3	A	1	Total	N	O	0	1
			3	1	2		
3	B	1	Total	N	O	0	1
			3	1	2		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



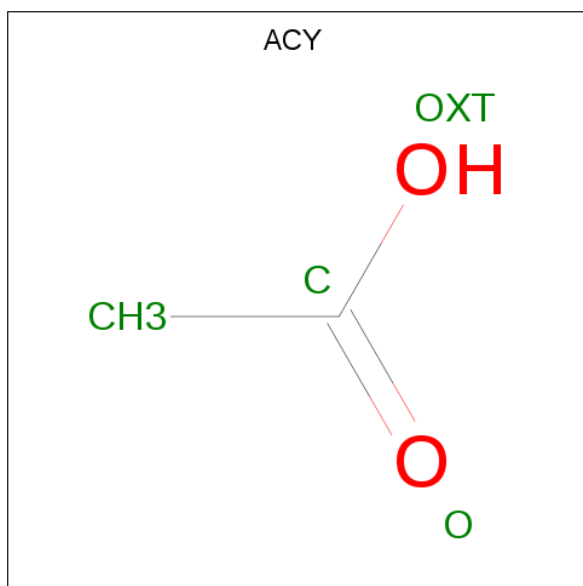
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		
4	B	1	Total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

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

- Molecule 5 is ACETIC ACID (three-letter code: ACY) (formula: C<sub>2</sub>H<sub>4</sub>O<sub>2</sub>).



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

- Molecule 6 is water.

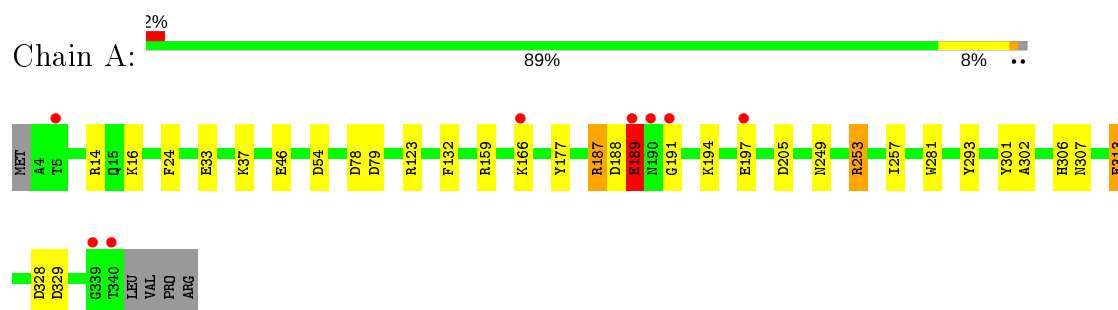
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	314	Total 320	O 320	0	7
6	B	314	Total 315	O 315	0	3
6	C	265	Total 266	O 266	0	1



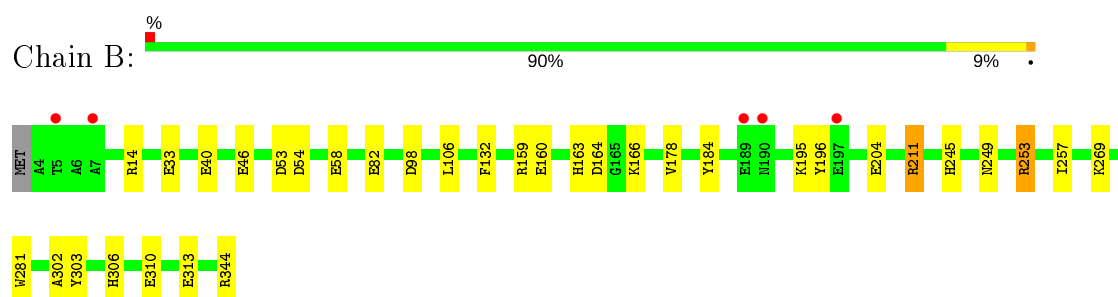
### 3 Residue-property plots [i](#)

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.

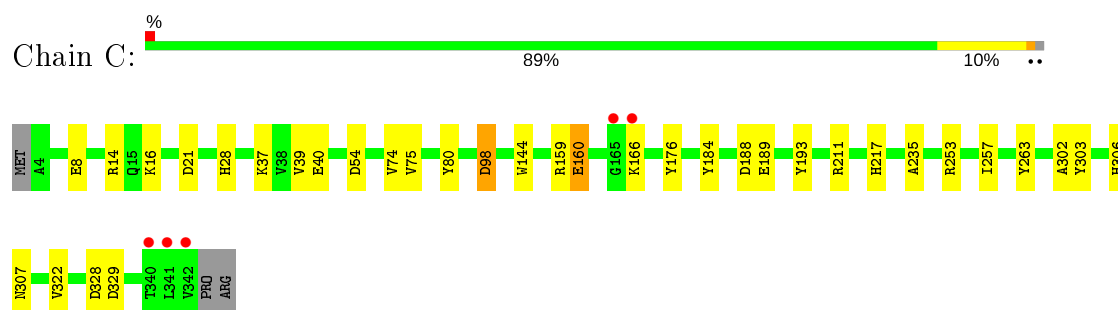
- Molecule 1: Copper-containing nitrite reductase



- Molecule 1: Copper-containing nitrite reductase



- Molecule 1: Copper-containing nitrite reductase



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	61.42Å 102.17Å 145.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.51 – 1.30 23.41 – 1.30	Depositor EDS
% Data completeness (in resolution range)	99.9 (49.51-1.30) 99.9 (23.41-1.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.98 (at 1.30Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, $R_{free}$	0.123 , 0.165 0.123 , 0.165	Depositor DCC
$R_{free}$ test set	11055 reflections (4.92%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	13.8	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 52.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.51$ , $\langle L^2 \rangle = 0.35$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	9007	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	18.0	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.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>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, ACY, NO2, CU

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	1.38	7/2671 (0.3%)	1.25	21/3640 (0.6%)
1	B	1.34	12/2744 (0.4%)	1.21	13/3736 (0.3%)
1	C	1.29	8/2732 (0.3%)	1.25	15/3720 (0.4%)
All	All	1.34	27/8147 (0.3%)	1.24	49/11096 (0.4%)

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 (27) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	82	GLU	CD-OE2	-7.07	1.17	1.25
1	C	40	GLU	CD-OE2	-6.79	1.18	1.25
1	B	196	TYR	CE1-CZ	6.74	1.47	1.38
1	B	313	GLU	CD-OE1	-6.61	1.18	1.25
1	B	160[A]	GLU	CD-OE2	6.52	1.32	1.25
1	B	160[B]	GLU	CD-OE2	6.52	1.32	1.25
1	B	184	TYR	CE1-CZ	6.44	1.47	1.38
1	B	310	GLU	CD-OE1	-6.42	1.18	1.25
1	A	46	GLU	CD-OE2	6.39	1.32	1.25
1	B	46	GLU	CG-CD	6.34	1.61	1.51
1	A	177	TYR	CG-CD1	6.26	1.47	1.39
1	A	293	TYR	CE1-CZ	6.21	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	313	GLU	CG-CD	6.12	1.61	1.51
1	B	313	GLU	CG-CD	5.85	1.60	1.51
1	C	189	GLU	CD-OE1	5.53	1.31	1.25
1	C	8	GLU	CD-OE2	5.49	1.31	1.25
1	B	40	GLU	CD-OE2	-5.45	1.19	1.25
1	A	132	PHE	CE2-CZ	5.43	1.47	1.37
1	A	189	GLU	CD-OE2	5.29	1.31	1.25
1	C	144	TRP	CZ3-CH2	5.24	1.48	1.40
1	C	80	TYR	CG-CD1	5.20	1.46	1.39
1	A	301	TYR	CE2-CZ	5.20	1.45	1.38
1	B	14	ARG	CZ-NH1	5.18	1.39	1.33
1	C	189	GLU	CB-CG	-5.17	1.42	1.52
1	B	40	GLU	CD-OE1	-5.13	1.20	1.25
1	C	303	TYR	CE1-CZ	5.05	1.45	1.38
1	C	193	TYR	CE2-CZ	5.03	1.45	1.38

All (49) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	54	ASP	CB-CG-OD1	9.82	127.14	118.30
1	C	263	TYR	CB-CG-CD1	-9.71	115.18	121.00
1	B	98	ASP	CB-CG-OD1	9.69	127.02	118.30
1	A	253	ARG	NE-CZ-NH2	-9.03	115.78	120.30
1	C	159	ARG	NE-CZ-NH2	-8.71	115.94	120.30
1	A	79	ASP	CB-CG-OD1	8.23	125.71	118.30
1	C	98	ASP	CB-CG-OD1	7.68	125.21	118.30
1	A	328	ASP	CB-CG-OD2	-7.53	111.53	118.30
1	B	344	ARG	NE-CZ-NH1	7.50	124.05	120.30
1	C	159	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	B	164	ASP	CB-CG-OD1	6.93	124.54	118.30
1	A	188	ASP	CB-CG-OD2	-6.93	112.07	118.30
1	B	14	ARG	NE-CZ-NH2	-6.85	116.87	120.30
1	C	14	ARG	NE-CZ-NH2	-6.61	116.99	120.30
1	C	253	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	A	54	ASP	CB-CG-OD1	6.50	124.15	118.30
1	C	328	ASP	CB-CG-OD1	6.46	124.11	118.30
1	B	344	ARG	NE-CZ-NH2	-6.45	117.08	120.30
1	C	329	ASP	CB-CG-OD2	6.45	124.11	118.30
1	B	159	ARG	NE-CZ-NH2	-6.44	117.08	120.30
1	C	54	ASP	CB-CG-OD2	-6.43	112.52	118.30
1	A	329	ASP	CB-CG-OD1	6.30	123.97	118.30
1	A	188	ASP	CB-CG-OD1	6.29	123.97	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	187[A]	ARG	NE-CZ-NH1	-6.24	117.18	120.30
1	A	187[B]	ARG	NE-CZ-NH1	-6.24	117.18	120.30
1	B	253	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	A	159	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	A	79	ASP	CB-CG-OD2	-6.11	112.80	118.30
1	C	188	ASP	CB-CG-OD1	6.04	123.73	118.30
1	C	329	ASP	CB-CG-OD1	-5.86	113.03	118.30
1	A	78	ASP	CB-CG-OD2	-5.70	113.17	118.30
1	B	159	ARG	NE-CZ-NH1	5.64	123.12	120.30
1	A	205	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	A	187[A]	ARG	NE-CZ-NH2	5.46	123.03	120.30
1	A	187[B]	ARG	NE-CZ-NH2	5.46	123.03	120.30
1	A	123	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	A	313	GLU	OE1-CD-OE2	-5.44	116.77	123.30
1	C	21	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	14	ARG	NE-CZ-NH1	-5.37	117.62	120.30
1	B	166	LYS	CD-CE-NZ	-5.30	99.52	111.70
1	B	303	TYR	CG-CD2-CE2	5.22	125.48	121.30
1	C	184	TYR	CD1-CE1-CZ	-5.20	115.12	119.80
1	B	211	ARG	NE-CZ-NH1	-5.15	117.72	120.30
1	B	54	ASP	CB-CG-OD1	5.13	122.92	118.30
1	A	194	LYS	CD-CE-NZ	-5.11	99.95	111.70
1	A	16	LYS	CD-CE-NZ	-5.07	100.03	111.70
1	A	159	ARG	NE-CZ-NH2	-5.07	117.76	120.30
1	B	53	ASP	CB-CG-OD1	5.03	122.82	118.30
1	C	176	TYR	CB-CG-CD2	-5.00	118.00	121.00

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 ⓘ

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	2600	0	2524	10	0
1	B	2672	0	2599	12	0
1	C	2661	0	2587	14	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	6	0	0	1	0
3	B	3	0	0	2	0
4	A	66	0	86	4	0
4	B	30	0	39	2	0
4	C	54	0	70	10	0
5	A	4	0	3	0	0
5	B	4	0	3	1	0
6	A	320	0	0	3	0
6	B	315	0	0	4	0
6	C	266	0	0	5	0
All	All	9007	0	7911	41	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.

All (41) 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)
4:C:508:GOL:H12	6:C:665:HOH:O	1.48	1.10
1:A:187[B]:ARG:HD3	1:A:191:GLY:O	1.82	0.80
4:A:515:GOL:H2	6:A:847:HOH:O	1.81	0.80
1:B:163:HIS:HD2	6:B:615[A]:HOH:O	1.64	0.79
1:B:211:ARG:NH1	6:B:601:HOH:O	2.23	0.70
1:C:257:ILE:HD12	1:C:302:ALA:HB3	1.76	0.68
1:A:189:GLU:H	1:A:189:GLU:CD	1.98	0.67
4:C:505:GOL:O1	4:C:509:GOL:O2	2.04	0.66
1:C:28:HIS:CE1	4:C:506[B]:GOL:H31	2.31	0.66
4:C:506[B]:GOL:H32	6:C:756:HOH:O	1.99	0.62
1:C:74:VAL:O	4:C:507:GOL:H31	2.01	0.61
1:A:257:ILE:HD12	1:A:302:ALA:HB3	1.84	0.60
1:A:33[A]:GLU:O	1:A:37:LYS:NZ	2.34	0.52
1:C:75:VAL:HA	4:C:507:GOL:H31	1.91	0.52
1:C:160:GLU:HG2	6:C:745:HOH:O	2.08	0.52
4:A:515:GOL:C2	6:A:847:HOH:O	2.47	0.52
1:C:160:GLU:CG	6:C:745:HOH:O	2.58	0.51
1:A:24:PHE:HD1	4:A:511:GOL:H2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:58[B]:GLU:HG3	1:B:195:LYS:HE3	1.93	0.49
1:B:257:ILE:HD12	1:B:302:ALA:HB3	1.94	0.49
1:B:204:GLU:HG2	6:B:818:HOH:O	2.12	0.49
4:A:510:GOL:H31	6:A:774:HOH:O	2.11	0.49
1:C:217:HIS:CD2	4:C:508:GOL:H11	2.49	0.47
1:C:39:VAL:HG21	4:C:507:GOL:H12	1.97	0.46
4:C:507:GOL:H32	6:C:615:HOH:O	2.15	0.45
1:B:257:ILE:HG12	3:B:503[A]:NO2:N	2.32	0.45
4:B:507[B]:GOL:O1	4:B:507[B]:GOL:O3	2.30	0.45
3:B:503[A]:NO2:O2	1:C:98:ASP:OD2	2.35	0.44
1:A:253:ARG:HA	1:A:281:TRP:O	2.18	0.43
1:A:307:ASN:HA	1:B:249:ASN:O	2.19	0.42
1:C:235:ALA:O	1:C:322:VAL:HA	2.19	0.42
1:B:132:PHE:CE2	1:B:269:LYS:HE3	2.55	0.42
1:B:253:ARG:HA	1:B:281:TRP:O	2.20	0.42
1:B:178:VAL:O	1:B:245:HIS:HA	2.20	0.42
1:A:257:ILE:HG22	1:B:106:LEU:HA	2.01	0.41
1:C:28:HIS:O	4:C:506[B]:GOL:H11	2.21	0.41
1:B:163:HIS:CD2	6:B:615[A]:HOH:O	2.51	0.41
3:A:503:NO2:N	1:C:257:ILE:HG12	2.36	0.40
4:B:507[B]:GOL:H32	1:C:211:ARG:HH12	1.85	0.40
1:A:249:ASN:O	1:C:307:ASN:HA	2.20	0.40
1:A:313:GLU:OE1	5:B:508:ACY:H1	2.22	0.40

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	339/342 (99%)	336 (99%)	3 (1%)	0	100	100
1	B	347/342 (102%)	345 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	346/342 (101%)	344 (99%)	2 (1%)	0	100	100
All	All	1032/1026 (101%)	1025 (99%)	7 (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	268/270 (99%)	265 (99%)	3 (1%)	73	45
1	B	277/270 (103%)	276 (100%)	1 (0%)	91	76
1	C	276/270 (102%)	272 (99%)	4 (1%)	67	34
All	All	821/810 (101%)	813 (99%)	8 (1%)	76	48

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

Mol	Chain	Res	Type
1	A	166	LYS
1	A	189	GLU
1	A	197	GLU
1	B	33	GLU
1	C	16	LYS
1	C	37	LYS
1	C	160	GLU
1	C	166	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	296	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 ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 36 ligands modelled in this entry, 6 are monoatomic - leaving 30 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$
4	GOL	B	504	-	5,5,5	0.66	0	5,5,5	0.65	0
4	GOL	A	507	-	5,5,5	0.61	0	5,5,5	0.22	0
4	GOL	B	507[B]	-	5,5,5	1.50	2 (40%)	5,5,5	1.63	2 (40%)
5	ACY	B	508	-	1,3,3	6.64	1 (100%)	0,3,3	0.00	-
4	GOL	B	507[A]	-	5,5,5	1.41	1 (20%)	5,5,5	1.46	1 (20%)
4	GOL	A	511	-	5,5,5	0.60	0	5,5,5	1.70	1 (20%)
4	GOL	C	507	-	5,5,5	0.96	0	5,5,5	4.17	5 (100%)
3	NO2	A	504[A]	2	1,2,2	1.29	0	0,1,1	0.00	-
4	GOL	B	505	-	5,5,5	1.69	1 (20%)	5,5,5	1.28	0
4	GOL	A	512	-	5,5,5	1.15	0	5,5,5	1.56	2 (40%)
4	GOL	C	505	-	5,5,5	0.42	0	5,5,5	1.16	0
4	GOL	C	503[A]	-	5,5,5	0.57	0	5,5,5	0.93	0
4	GOL	A	509	-	5,5,5	1.46	1 (20%)	5,5,5	0.94	1 (20%)
4	GOL	C	509	-	5,5,5	1.36	1 (20%)	5,5,5	1.28	1 (20%)
5	ACY	A	516	-	1,3,3	4.95	1 (100%)	0,3,3	0.00	-

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	NO2	A	503	2	1,2,2	0.41	0	0,1,1	0.00	-
4	GOL	A	514	-	5,5,5	0.72	0	5,5,5	1.57	1 (20%)
4	GOL	A	510	-	5,5,5	1.70	1 (20%)	5,5,5	1.00	0
4	GOL	C	504	-	5,5,5	1.10	0	5,5,5	1.28	1 (20%)
4	GOL	B	506	-	5,5,5	0.34	0	5,5,5	0.74	0
4	GOL	C	506[B]	-	5,5,5	0.78	0	5,5,5	0.93	0
4	GOL	A	515	-	5,5,5	1.44	1 (20%)	5,5,5	2.31	4 (80%)
4	GOL	A	506	-	5,5,5	1.83	1 (20%)	5,5,5	1.53	2 (40%)
4	GOL	C	506[A]	-	5,5,5	0.78	0	5,5,5	1.17	0
4	GOL	C	503[B]	-	5,5,5	0.51	0	5,5,5	1.56	1 (20%)
4	GOL	A	513	-	5,5,5	1.02	1 (20%)	5,5,5	1.97	2 (40%)
4	GOL	A	508	-	5,5,5	2.01	2 (40%)	5,5,5	0.82	0
4	GOL	C	508	-	5,5,5	2.44	2 (40%)	5,5,5	3.40	4 (80%)
3	NO2	B	503[A]	2	1,2,2	1.68	0	0,1,1	0.00	-
4	GOL	A	505	-	5,5,5	1.20	1 (20%)	5,5,5	1.11	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	504	-	-	0/4/4/4	-
4	GOL	A	507	-	-	0/4/4/4	-
4	GOL	B	507[B]	-	-	0/4/4/4	-
4	GOL	B	507[A]	-	-	0/4/4/4	-
4	GOL	A	511	-	-	1/4/4/4	-
4	GOL	C	507	-	-	1/4/4/4	-
4	GOL	B	505	-	-	0/4/4/4	-
4	GOL	A	512	-	-	2/4/4/4	-
4	GOL	C	505	-	-	0/4/4/4	-
4	GOL	C	503[A]	-	-	2/4/4/4	-
4	GOL	A	509	-	-	0/4/4/4	-
4	GOL	C	509	-	-	3/4/4/4	-
4	GOL	A	514	-	-	4/4/4/4	-
4	GOL	A	510	-	-	0/4/4/4	-
4	GOL	C	504	-	-	0/4/4/4	-
4	GOL	B	506	-	-	0/4/4/4	-
4	GOL	C	506[B]	-	-	4/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	A	515	-	-	4/4/4/4	-
4	GOL	A	506	-	-	0/4/4/4	-
4	GOL	C	506[A]	-	-	4/4/4/4	-
4	GOL	C	503[B]	-	-	4/4/4/4	-
4	GOL	A	513	-	-	0/4/4/4	-
4	GOL	A	508	-	-	0/4/4/4	-
4	GOL	C	508	-	-	2/4/4/4	-
4	GOL	A	505	-	-	0/4/4/4	-

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	508	ACY	CH3-C	6.64	1.57	1.48
5	A	516	ACY	CH3-C	4.95	1.55	1.48
4	C	508	GOL	O1-C1	-3.94	1.25	1.42
4	B	505	GOL	O2-C2	-3.70	1.32	1.43
4	C	508	GOL	O2-C2	3.60	1.54	1.43
4	A	506	GOL	O2-C2	-3.34	1.33	1.43
4	A	510	GOL	O1-C1	3.24	1.56	1.42
4	A	508	GOL	O3-C3	3.22	1.56	1.42
4	A	509	GOL	C1-C2	2.73	1.63	1.51
4	A	505	GOL	O2-C2	2.58	1.51	1.43
4	C	509	GOL	O2-C2	-2.33	1.36	1.43
4	A	508	GOL	O2-C2	2.33	1.50	1.43
4	A	515	GOL	O1-C1	-2.28	1.32	1.42
4	B	507[A]	GOL	O1-C1	2.16	1.51	1.42
4	A	513	GOL	O2-C2	2.12	1.49	1.43
4	B	507[B]	GOL	O2-C2	-2.11	1.37	1.43
4	B	507[B]	GOL	O1-C1	2.04	1.51	1.42

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	507	GOL	O3-C3-C2	-6.47	79.18	110.20
4	C	508	GOL	O3-C3-C2	-5.38	84.39	110.20
4	C	507	GOL	C3-C2-C1	-4.58	93.90	111.70
4	C	508	GOL	C3-C2-C1	-3.71	97.27	111.70
4	C	507	GOL	O2-C2-C1	-3.36	94.33	109.12
4	A	513	GOL	O1-C1-C2	-3.16	95.05	110.20
4	A	514	GOL	O1-C1-C2	3.15	125.32	110.20
4	A	515	GOL	O2-C2-C3	-3.04	95.73	109.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	508	GOL	O2-C2-C3	2.90	121.89	109.12
4	A	511	GOL	O3-C3-C2	-2.86	96.51	110.20
4	A	513	GOL	O3-C3-C2	-2.85	96.52	110.20
4	C	507	GOL	O2-C2-C3	2.73	121.15	109.12
4	B	507[A]	GOL	O1-C1-C2	2.61	122.72	110.20
4	C	508	GOL	O1-C1-C2	-2.55	97.95	110.20
4	A	512	GOL	O3-C3-C2	-2.46	98.39	110.20
4	C	507	GOL	O1-C1-C2	-2.32	99.07	110.20
4	A	506	GOL	O3-C3-C2	-2.31	99.14	110.20
4	A	515	GOL	O2-C2-C1	2.30	119.26	109.12
4	C	504	GOL	O2-C2-C1	2.25	119.03	109.12
4	B	507[B]	GOL	O2-C2-C1	-2.23	99.31	109.12
4	A	512	GOL	C3-C2-C1	-2.18	103.22	111.70
4	B	507[B]	GOL	O1-C1-C2	2.12	120.37	110.20
4	A	515	GOL	O1-C1-C2	2.12	120.36	110.20
4	C	509	GOL	O3-C3-C2	2.08	120.19	110.20
4	A	515	GOL	C3-C2-C1	-2.04	103.76	111.70
4	A	506	GOL	O2-C2-C1	-2.04	100.14	109.12
4	C	503[B]	GOL	O2-C2-C3	2.02	118.04	109.12
4	A	509	GOL	C3-C2-C1	-2.01	103.88	111.70

There are no chirality outliers.

All (31) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	C	503[A]	GOL	C1-C2-C3-O3
4	A	514	GOL	O1-C1-C2-C3
4	A	514	GOL	C1-C2-C3-O3
4	C	506[B]	GOL	O1-C1-C2-C3
4	A	515	GOL	C1-C2-C3-O3
4	C	506[A]	GOL	O1-C1-C2-C3
4	C	503[B]	GOL	O1-C1-C2-O2
4	C	503[B]	GOL	O1-C1-C2-C3
4	C	503[B]	GOL	C1-C2-C3-O3
4	C	508	GOL	C1-C2-C3-O3
4	A	515	GOL	O2-C2-C3-O3
4	C	506[A]	GOL	O1-C1-C2-O2
4	A	511	GOL	O1-C1-C2-C3
4	A	512	GOL	C1-C2-C3-O3
4	C	509	GOL	O1-C1-C2-C3
4	C	506[B]	GOL	C1-C2-C3-O3
4	A	515	GOL	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
4	C	506[A]	GOL	C1-C2-C3-O3
4	A	512	GOL	O2-C2-C3-O3
4	C	509	GOL	O2-C2-C3-O3
4	A	514	GOL	O1-C1-C2-O2
4	A	515	GOL	O1-C1-C2-O2
4	C	503[B]	GOL	O2-C2-C3-O3
4	C	508	GOL	O2-C2-C3-O3
4	A	514	GOL	O2-C2-C3-O3
4	C	506[B]	GOL	O1-C1-C2-O2
4	C	506[B]	GOL	O2-C2-C3-O3
4	C	506[A]	GOL	O2-C2-C3-O3
4	C	503[A]	GOL	O2-C2-C3-O3
4	C	507	GOL	C1-C2-C3-O3
4	C	509	GOL	C1-C2-C3-O3

There are no ring outliers.

12 monomers are involved in 20 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	507[B]	GOL	2	0
5	B	508	ACY	1	0
4	A	511	GOL	1	0
4	C	507	GOL	4	0
4	C	505	GOL	1	0
4	C	509	GOL	1	0
3	A	503	NO2	1	0
4	A	510	GOL	1	0
4	C	506[B]	GOL	3	0
4	A	515	GOL	2	0
4	C	508	GOL	2	0
3	B	503[A]	NO2	2	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, 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	337/342 (98%)	-0.48	8 (2%) 59 58	11, 16, 32, 74	0
1	B	341/342 (99%)	-0.56	5 (1%) 73 75	11, 15, 32, 69	0
1	C	339/342 (99%)	-0.59	5 (1%) 73 75	10, 14, 29, 56	0
All	All	1017/1026 (99%)	-0.54	18 (1%) 68 69	10, 15, 32, 74	0

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	342	VAL	5.7
1	C	340	THR	5.7
1	C	341	LEU	5.6
1	A	190	ASN	4.4
1	A	189	GLU	4.2
1	A	340	THR	3.7
1	B	7	ALA	3.4
1	B	190	ASN	3.2
1	C	166	LYS	3.1
1	A	197	GLU	2.9
1	B	197	GLU	2.8
1	A	191	GLY	2.7
1	C	165	GLY	2.5
1	A	5	THR	2.5
1	B	5	THR	2.4
1	A	339	GLY	2.4
1	B	189	GLU	2.3
1	A	166	LYS	2.3

### 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

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. 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	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	GOL	C	507	6/6	0.84	0.28	26,28,34,34	0
4	GOL	C	509	6/6	0.85	0.44	30,33,38,40	0
4	GOL	B	507[B]	6/6	0.87	0.11	23,24,29,31	6
4	GOL	B	507[A]	6/6	0.87	0.11	17,24,29,31	6
4	GOL	A	513	6/6	0.87	0.16	32,33,40,43	0
4	GOL	C	506[B]	6/6	0.89	0.19	29,29,32,40	6
4	GOL	C	506[A]	6/6	0.89	0.19	25,29,34,38	6
4	GOL	B	506	6/6	0.89	0.10	28,29,32,43	0
4	GOL	A	514	6/6	0.90	0.18	28,37,39,44	0
4	GOL	C	508	6/6	0.90	0.18	22,28,32,33	0
4	GOL	A	512	6/6	0.91	0.22	26,29,41,42	0
4	GOL	A	515	6/6	0.92	0.28	24,30,34,36	0
4	GOL	C	504	6/6	0.92	0.10	28,32,36,36	0
4	GOL	C	505	6/6	0.93	0.23	26,30,40,42	0
4	GOL	A	510	6/6	0.94	0.17	21,24,25,28	0
3	NO2	A	503	3/3	0.95	0.11	23,23,26,27	0
4	GOL	A	509	6/6	0.95	0.10	21,23,25,25	0
4	GOL	A	511	6/6	0.96	0.09	20,28,34,51	0
5	ACY	B	508	4/4	0.96	0.12	20,25,26,27	0
4	GOL	A	507	6/6	0.97	0.07	33,36,38,40	0
4	GOL	A	506	6/6	0.97	0.08	20,23,25,30	0
5	ACY	A	516	4/4	0.97	0.17	19,25,26,31	0
4	GOL	B	504	6/6	0.97	0.11	26,29,32,33	0
4	GOL	A	508	6/6	0.97	0.07	16,26,34,35	0
4	GOL	B	505	6/6	0.97	0.06	15,26,28,31	0
3	NO2	B	503[A]	3/3	0.97	0.07	19,19,19,20	3
4	GOL	A	505	6/6	0.97	0.04	20,21,21,25	0
4	GOL	C	503[B]	6/6	0.98	0.05	16,23,28,31	6
3	NO2	A	504[A]	3/3	0.98	0.06	19,19,21,21	3
4	GOL	C	503[A]	6/6	0.98	0.05	14,16,18,19	6
2	CU	C	501	1/1	1.00	0.02	11,11,11,11	0
2	CU	A	502	1/1	1.00	0.02	13,13,13,13	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	CU	B	502	1/1	1.00	0.02	12,12,12,12	0
2	CU	A	501	1/1	1.00	0.02	16,16,16,16	0
2	CU	C	502	1/1	1.00	0.01	11,11,11,11	0
2	CU	B	501	1/1	1.00	0.02	13,13,13,13	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.