



# wwPDB X-ray Structure Validation Summary Report ⓘ

Dec 23, 2017 – 10:35 AM EST

PDB ID : 6AQJ  
Title : Crystal structures of Staphylococcus aureus ketol-acid reductoisomerase in complex with two transition state analogs that have biocidal activity.  
Authors : Patel, K.M.; Teran, D.; Zheng, S.; Gracia, M.; Lv, Y.; Schembri, M.A.; McGearry, R.P.; Schenk, G.; Guddat, L.W.  
Deposited on : 2017-08-20  
Resolution : 1.37 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<http://wwpdb.org/validation/2016/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	:	1.7.2 (RC1), CSD as538be (2017)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20030736
Percentile statistics	:	20161228.v01 (using entries in the PDB archive December 28th 2016)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20030736

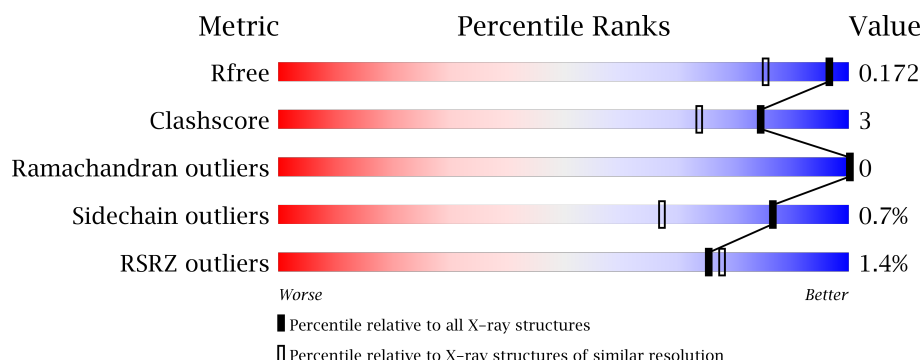
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.37 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))
$R_{free}$	100719	2133 (1.40-1.36)
Clashscore	112137	2266 (1.40-1.36)
Ramachandran outliers	110173	2215 (1.40-1.36)
Sidechain outliers	110143	2214 (1.40-1.36)
RSRZ outliers	101464	2141 (1.40-1.36)

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. 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	339	<div> <div>2%</div> <div>88%</div> <div>7%</div> <div>.</div> </div>
1	B	339	<div> <div>%</div> <div>91%</div> <div>5%</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	40E	A	403[A]	-	-	-	X
4	GOL	A	404	-	-	-	X
4	GOL	A	405	-	-	-	X
4	GOL	A	406	-	-	-	X
4	GOL	B	405	-	-	-	X
6	HIO	A	408[B]	-	-	-	X
7	EDO	B	406	-	-	-	X

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 6237 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 Ketol-acid reductoisomerase (NADP(+)).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	326	Total	C	N	O	S	0	23	0
			2690	1720	453	509	8			
1	B	326	Total	C	N	O	S	0	12	0
			2629	1675	442	501	11			

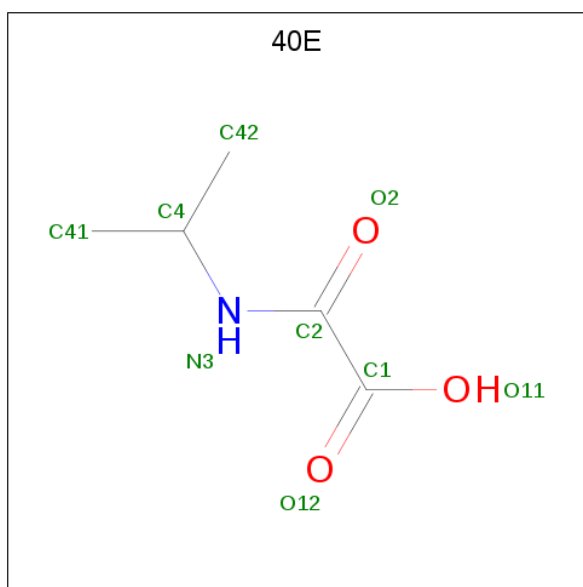
There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	335	HIS	-	expression tag	UNP Q2YUF3
A	336	HIS	-	expression tag	UNP Q2YUF3
A	337	HIS	-	expression tag	UNP Q2YUF3
A	338	HIS	-	expression tag	UNP Q2YUF3
A	339	HIS	-	expression tag	UNP Q2YUF3
A	340	HIS	-	expression tag	UNP Q2YUF3
B	335	HIS	-	expression tag	UNP Q2YUF3
B	336	HIS	-	expression tag	UNP Q2YUF3
B	337	HIS	-	expression tag	UNP Q2YUF3
B	338	HIS	-	expression tag	UNP Q2YUF3
B	339	HIS	-	expression tag	UNP Q2YUF3
B	340	HIS	-	expression tag	UNP Q2YUF3

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	2	Total	Mg	0	0
			2	2		
2	A	2	Total	Mg	0	0
			2	2		

- Molecule 3 is oxo(propan-2-ylamino)acetic acid (three-letter code: 40E) (formula: C<sub>5</sub>H<sub>9</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	1
			9	5	1	3		
3	B	1	Total	C	N	O	0	1
			9	5	1	3		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



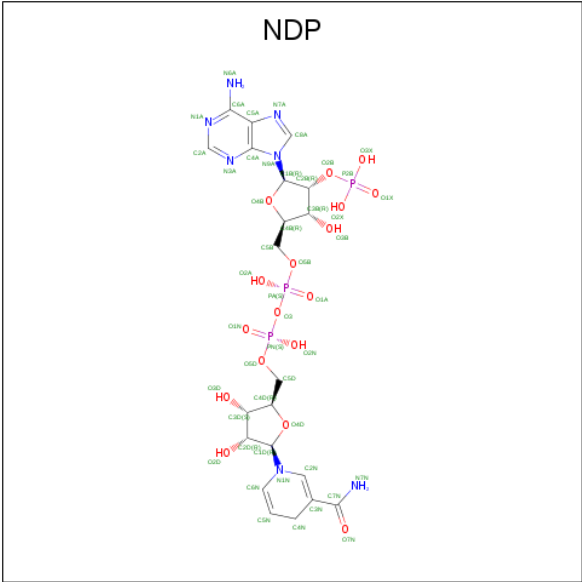
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

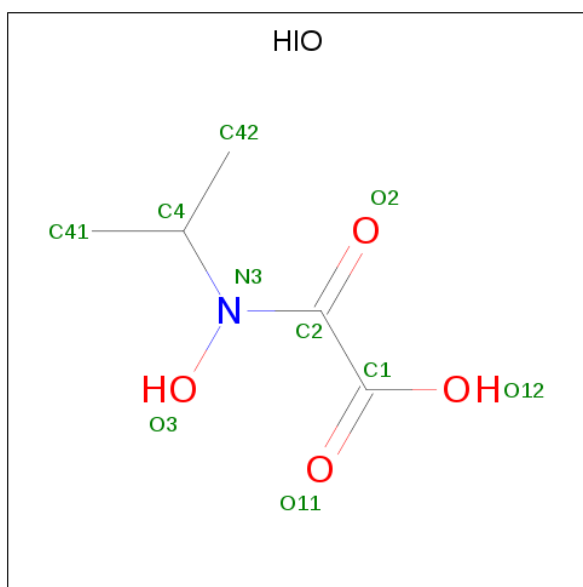
*Continued on next page...*

Continued from previous page...

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

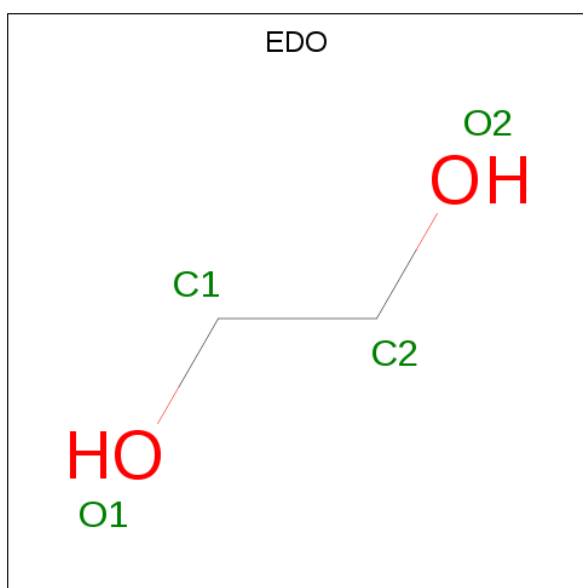
- Molecule 5 is NADPH DIHYDRO-NICOTINAMIDE-ADENINE-DINUCLEOTIDE PHOSPHATE (three-letter code: NDP) (formula: C<sub>21</sub>H<sub>30</sub>N<sub>7</sub>O<sub>17</sub>P<sub>3</sub>).





Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	A	1	Total	C	N	O	0	1
			10	5	1	4		
6	B	1	Total	C	N	O	0	1
			10	5	1	4		

- Molecule 7 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	362	Total 362	O 362	0	0
8	B	386	Total 386	O 386	0	0





- Molecule 1: Ketol-acid reductoisomerase (NADP(+))



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	64.09Å 80.73Å 66.64Å 90.00° 92.58° 90.00°	Depositor
Resolution (Å)	34.52 – 1.37 34.52 – 1.37	Depositor EDS
% Data completeness (in resolution range)	97.9 (34.52-1.37) 97.9 (34.52-1.37)	Depositor EDS
$R_{merge}$	0.06	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.06 (at 1.37Å)	Xtriage
Refinement program	PHENIX 1.11.1_2575	Depositor
R, $R_{free}$	0.154 , 0.172 0.153 , 0.172	Depositor DCC
$R_{free}$ test set	1989 reflections (1.44%)	DCC
Wilson B-factor (Å <sup>2</sup> )	13.7	Xtriage
Anisotropy	0.118	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.39 , 51.5	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.007 for l,k,-h 0.020 for h,-k,-l 0.016 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	6237	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	19.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.13% 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 [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, 40E, MG, EDO, NDP, HIO

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	0.71	0/2809	0.83	3/3790 (0.1%)
1	B	0.76	1/2715 (0.0%)	0.84	2/3665 (0.1%)
All	All	0.74	1/5524 (0.0%)	0.84	5/7455 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	214	VAL	CB-CG2	-5.24	1.41	1.52

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	137	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	B	48	ARG	NE-CZ-NH1	-6.48	117.06	120.30
1	B	258	ASP	CB-CG-OD2	5.52	123.26	118.30
1	A	236	ASP	CB-CG-OD1	5.43	123.19	118.30
1	A	7	ASP	CB-CG-OD1	5.14	122.93	118.30

There are no chirality outliers.

There are no planarity outliers.

### 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	2690	0	2699	17	0
1	B	2629	0	2599	9	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
3	A	9	0	8	1	0
3	B	9	0	8	1	0
4	A	18	0	24	0	0
4	B	6	0	8	0	0
5	A	48	0	26	1	0
5	B	48	0	26	1	0
6	A	10	0	7	1	0
6	B	10	0	7	2	0
7	B	8	0	12	1	0
8	A	362	0	0	1	3
8	B	386	0	0	5	3
All	All	6237	0	5424	29	3

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 29 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:275:LYS:HG3	8:B:516:HOH:O	1.74	0.87
1:A:289:ARG:NH2	1:A:300:GLU:OE2	2.18	0.71
1:B:5:TYR:OH	1:B:161[A]:ARG:NH2	2.25	0.69
7:B:406:EDO:H22	8:B:779:HOH:O	1.93	0.69
6:B:402[B]:HIO:C2	5:B:408:NDP:H41N	2.25	0.66

All (3) 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)
8:A:772:HOH:O	8:B:620:HOH:O[1_556]	2.08	0.12
8:A:762:HOH:O	8:B:778:HOH:O[2_655]	2.12	0.08
8:A:629:HOH:O	8:B:695:HOH:O[2_655]	2.18	0.02

## 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	348/339 (103%)	340 (98%)	8 (2%)	0	100	100
1	B	337/339 (99%)	329 (98%)	8 (2%)	0	100	100
All	All	685/678 (101%)	669 (98%)	16 (2%)	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	293/282 (104%)	290 (99%)	3 (1%)	80	55
1	B	282/282 (100%)	279 (99%)	3 (1%)	78	51
All	All	575/564 (102%)	569 (99%)	6 (1%)	87	55

5 of 6 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	298	PHE
1	B	239[B]	TYR
1	B	90	LYS
1	A	51[B]	ARG
1	B	239[A]	TYR

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

### 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 16 ligands modelled in this entry, 4 are monoatomic - leaving 12 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$
3	40E	A	403[A]	2	5,8,8	1.71	1 (20%)	6,10,10	1.77	3 (50%)
4	GOL	A	404	-	5,5,5	0.36	0	5,5,5	0.63	0
4	GOL	A	405	-	5,5,5	0.32	0	5,5,5	0.77	0
4	GOL	A	406	-	5,5,5	0.44	0	5,5,5	0.35	0
5	NDP	A	407	-	43,52,52	1.24	3 (6%)	49,80,80	1.15	2 (4%)
6	HIO	A	408[B]	2	4,9,9	0.56	0	4,12,12	3.04	2 (50%)
3	40E	B	401[A]	2	5,8,8	1.47	2 (40%)	6,10,10	2.57	4 (66%)
6	HIO	B	402[B]	2	4,9,9	0.83	0	4,12,12	2.14	1 (25%)
4	GOL	B	405	-	5,5,5	0.41	0	5,5,5	0.65	0
7	EDO	B	406	-	3,3,3	0.45	0	2,2,2	0.66	0
7	EDO	B	407	-	3,3,3	0.49	0	2,2,2	0.71	0
5	NDP	B	408	-	43,52,52	1.86	9 (20%)	49,80,80	1.63	8 (16%)

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	40E	A	403[A]	2	-	1/4/8/8	0/0/0/0
4	GOL	A	404	-	-	0/4/4/4	0/0/0/0
4	GOL	A	405	-	-	0/4/4/4	0/0/0/0
4	GOL	A	406	-	-	0/4/4/4	0/0/0/0
5	NDP	A	407	-	-	0/30/77/77	0/5/5/5
6	HIO	A	408[B]	2	-	0/6/12/12	0/0/0/0
3	40E	B	401[A]	2	-	1/4/8/8	0/0/0/0
6	HIO	B	402[B]	2	-	0/6/12/12	0/0/0/0
4	GOL	B	405	-	-	0/4/4/4	0/0/0/0
7	EDO	B	406	-	-	0/1/1/1	0/0/0/0
7	EDO	B	407	-	-	0/1/1/1	0/0/0/0
5	NDP	B	408	-	-	0/30/77/77	0/5/5/5

The worst 5 of 15 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	408	NDP	O5B-C5B	-3.94	1.29	1.44
3	B	401[A]	40E	C4-N3	-2.17	1.42	1.47
5	A	407	NDP	O4D-C1D	2.03	1.46	1.42
3	B	401[A]	40E	C2-N3	2.08	1.38	1.34
5	B	408	NDP	O3B-C3B	2.37	1.48	1.43

The worst 5 of 20 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	408	NDP	N3A-C2A-N1A	-5.71	123.89	128.86
6	A	408[B]	HIO	C41-C4-N3	-4.68	104.90	109.90
3	B	401[A]	40E	C42-C4-N3	-4.10	101.60	109.77
6	B	402[B]	HIO	O2-C2-N3	-3.69	115.88	120.41
5	B	408	NDP	C4B-O4B-C1B	-3.45	106.10	109.77

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	401[A]	40E	C1-C2-N3-C4
3	A	403[A]	40E	C1-C2-N3-C4

There are no ring outliers.

7 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	403[A]	40E	1	0
5	A	407	NDP	1	0
6	A	408[B]	HIO	1	0
3	B	401[A]	40E	1	0
6	B	402[B]	HIO	2	0
7	B	406	EDO	1	0
5	B	408	NDP	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 [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	326/339 (96%)	0.14	7 (2%) 64 67	9, 16, 30, 49	3 (0%)
1	B	326/339 (96%)	-0.05	2 (0%) 89 89	9, 15, 27, 41	2 (0%)
All	All	652/678 (96%)	0.04	9 (1%) 75 78	9, 15, 29, 49	5 (0%)

The worst 5 of 9 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	12	THR	4.4
1	A	327	ILE	3.9
1	B	2	THR	3.7
1	B	327	ILE	3.0
1	A	2	THR	2.7

### 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GOL	A	405	6/6	0.89	0.13	7.64	23,27,27,32	0
4	GOL	A	406	6/6	0.97	0.11	6.52	19,20,21,24	0
7	EDO	B	406	4/4	0.86	0.14	3.71	35,39,47,49	0
4	GOL	A	404	6/6	0.91	0.13	3.30	25,33,36,40	0
3	40E	A	403[A]	9/9	0.98	0.11	3.15	7,9,12,13	9
4	GOL	B	405	6/6	0.93	0.14	2.51	21,27,30,44	0
6	HIO	A	408[B]	10/10	0.98	0.12	2.39	7,8,11,13	10
7	EDO	B	407	4/4	0.85	0.12	1.99	36,42,46,62	0
6	HIO	B	402[B]	10/10	0.98	0.12	1.26	9,11,15,17	10
3	40E	B	401[A]	9/9	0.98	0.11	0.53	10,10,16,16	9
5	NDP	A	407	48/48	0.98	0.07	-0.68	8,11,16,17	0
5	NDP	B	408	48/48	0.98	0.07	-0.69	9,12,21,26	0
2	MG	A	401	1/1	0.99	0.04	-2.45	12,12,12,12	0
2	MG	B	403	1/1	0.99	0.04	-3.94	12,12,12,12	0
2	MG	A	402	1/1	1.00	0.06	-	9,9,9,9	0
2	MG	B	404	1/1	1.00	0.08	-	9,9,9,9	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.