



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 22, 2025 – 03:57 AM EDT

PDB ID : 4YRI / pdb_00004yri
Title : Crystal structure of T. cruzi Histidyl-tRNA synthetase in complex with 1-(3-bromophenyl)methanamine (Chem 166)
Authors : Koh, C.-Y.; Hol, W.G.J.
Deposited on : 2015-03-15
Resolution : 2.00 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 : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0rc1
EDS : 3.0
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4 : 9.0.006 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.42

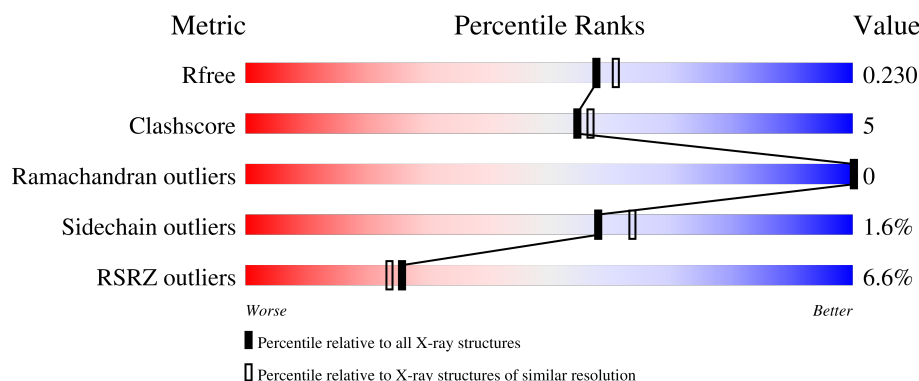
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION


The reported resolution of this entry is 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}	164625	9409 (2.00-2.00)
Clashscore	180529	10737 (2.00-2.00)
Ramachandran outliers	177936	10628 (2.00-2.00)
Sidechain outliers	177891	10627 (2.00-2.00)
RSRZ outliers	164620	9409 (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 $\leq 5\%$. 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	456	

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	4JH	A	502[B]	-	-	X	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	GOL	A	503[B]	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 3416 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.

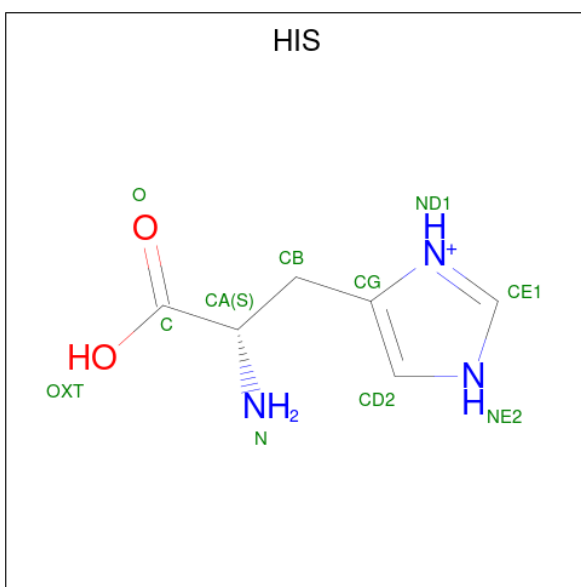
- Molecule 1 is a protein called Histidyl-tRNA synthetase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	408	Total	C	N	O	S	0	2	0
			3154	2005	554	576	19			

There are 22 discrepancies between the modelled and reference sequences:

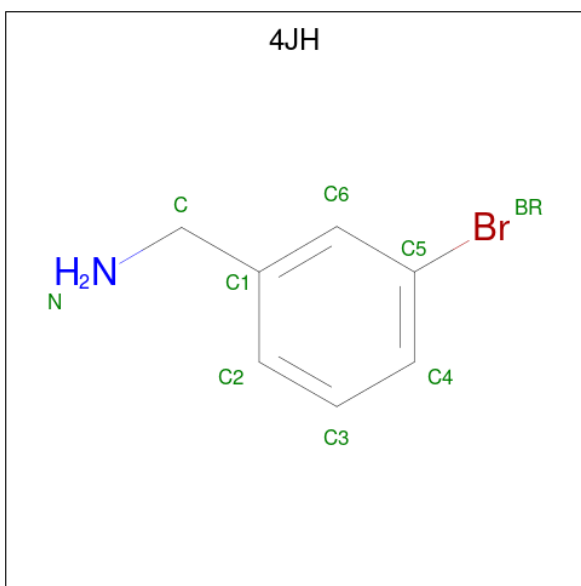
Chain	Residue	Modelled	Actual	Comment	Reference
A	-21	MET	-	initiating methionine	UNP Q4DA54
A	-20	ALA	-	expression tag	UNP Q4DA54
A	-19	HIS	-	expression tag	UNP Q4DA54
A	-18	HIS	-	expression tag	UNP Q4DA54
A	-17	HIS	-	expression tag	UNP Q4DA54
A	-16	HIS	-	expression tag	UNP Q4DA54
A	-15	HIS	-	expression tag	UNP Q4DA54
A	-14	HIS	-	expression tag	UNP Q4DA54
A	-13	MET	-	expression tag	UNP Q4DA54
A	-12	GLY	-	expression tag	UNP Q4DA54
A	-11	THR	-	expression tag	UNP Q4DA54
A	-10	LEU	-	expression tag	UNP Q4DA54
A	-9	GLU	-	expression tag	UNP Q4DA54
A	-8	ALA	-	expression tag	UNP Q4DA54
A	-7	GLN	-	expression tag	UNP Q4DA54
A	-6	THR	-	expression tag	UNP Q4DA54
A	-5	GLN	-	expression tag	UNP Q4DA54
A	-4	GLY	-	expression tag	UNP Q4DA54
A	-3	PRO	-	expression tag	UNP Q4DA54
A	-2	GLY	-	expression tag	UNP Q4DA54
A	-1	SER	-	expression tag	UNP Q4DA54
A	0	MET	-	expression tag	UNP Q4DA54

- Molecule 2 is HISTIDINE (CCD ID: HIS) (formula: C₆H₁₀N₃O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			11	6	3	2		

- Molecule 3 is 1-(3-bromophenyl)methanamine (CCD ID: 4JH) (formula: C₇H₈BrN).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	Br	C	N	0	1
			18	2	14	2		

- Molecule 4 is GLYCEROL (CCD ID: GOL) (formula: C₃H₈O₃).



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

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



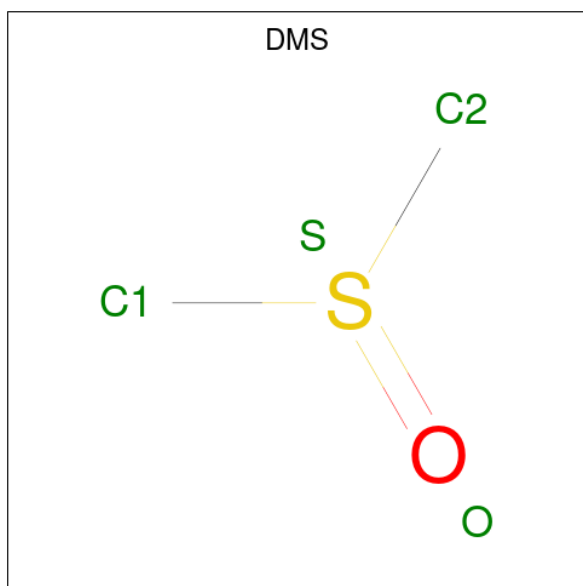
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	O	S	0	0
			5	4	1		
5	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 7 is DIMETHYL SULFOXIDE (CCD ID: DMS) (formula: C_2H_6OS).



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

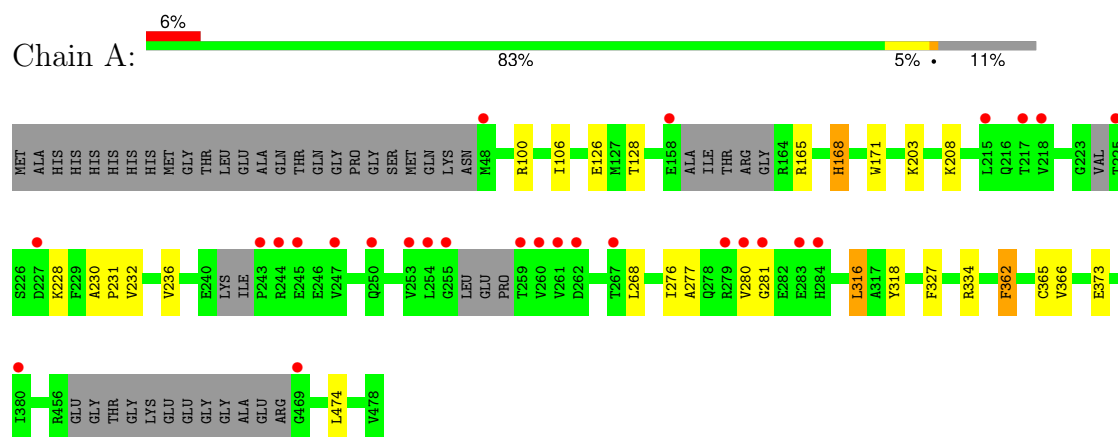
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	199	Total 199	O 199	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: Histidyl-tRNA synthetase, putative



4 Data and refinement statistics

Property	Value	Source
Space group	I 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	64.38Å 118.69Å 66.11Å 90.00° 92.68° 90.00°	Depositor
Resolution (Å)	30.00 – 2.00 30.00 – 2.00	Depositor EDS
% Data completeness (in resolution range)	93.2 (30.00-2.00) 93.2 (30.00-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 2.00Å)	Xtriage
Refinement program	REFMAC refmac _5.8.0073	Depositor
R, R_{free}	0.190 , 0.228 0.195 , 0.230	Depositor DCC
R_{free} test set	1591 reflections (5.11%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.494	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 55.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.001 for l,k,-h 0.028 for h,-k,-l 0.022 for l,-k,h	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	3416	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.41% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, DMS, 4JH, EDO, SO4

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	0.40	0/3222	0.60	0/4360

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 [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	3154	0	3079	23	0
2	A	11	0	6	1	0
3	A	18	0	16	8	0
4	A	12	0	16	13	0
5	A	10	0	0	0	0
6	A	4	0	6	0	0
7	A	8	0	12	2	0
8	A	199	0	0	2	0
All	All	3416	0	3135	30	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 5.

All (30) 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:365[B]:CYS:HB2	4:A:503[B]:GOL:H32	1.50	0.94
1:A:365[A]:CYS:HB3	4:A:503[A]:GOL:H31	1.58	0.86
3:A:502[B]:4JH:C2	4:A:503[B]:GOL:O1	2.26	0.83
3:A:502[B]:4JH:H1	4:A:503[B]:GOL:O1	1.82	0.79
3:A:502[B]:4JH:C2	4:A:503[B]:GOL:HO1	2.00	0.72
3:A:502[B]:4JH:C3	4:A:503[B]:GOL:O1	2.42	0.66
1:A:366:VAL:HG23	4:A:503[B]:GOL:H31	1.82	0.59
1:A:276:ILE:O	1:A:280:VAL:HG22	2.03	0.58
1:A:128:THR:HG1	2:A:501:HIS:N	2.02	0.58
1:A:106:ILE:HD11	1:A:126:GLU:HB3	1.87	0.56
1:A:230:ALA:HB3	1:A:231:PRO:HD3	1.87	0.55
1:A:365[A]:CYS:CB	4:A:503[A]:GOL:H31	2.35	0.55
1:A:236:VAL:HG13	1:A:268:LEU:HD11	1.88	0.55
1:A:100:ARG:HG2	7:A:507:DMS:H12	1.90	0.53
1:A:168:HIS:ND1	4:A:503[B]:GOL:O2	2.30	0.51
1:A:277:ALA:O	1:A:281:GLY:N	2.46	0.49
1:A:365[A]:CYS:HB3	4:A:503[A]:GOL:C3	2.39	0.49
1:A:203:LYS:NZ	8:A:604:HOH:O	2.45	0.49
1:A:100:ARG:HG2	7:A:507:DMS:C1	2.44	0.48
3:A:502[B]:4JH:C3	4:A:503[B]:GOL:HO1	2.23	0.47
3:A:502[B]:4JH:H2	4:A:503[B]:GOL:O1	2.15	0.46
1:A:165:ARG:HB3	3:A:502[B]:4JH:H8	1.81	0.45
1:A:165:ARG:NH2	1:A:365[B]:CYS:SG	2.89	0.45
3:A:502[A]:4JH:N	8:A:601:HOH:O	2.36	0.45
1:A:334:ARG:HH12	4:A:503[B]:GOL:H12	1.81	0.44
1:A:208:LYS:HG3	1:A:327:PHE:CE1	2.52	0.44
1:A:228:LYS:O	1:A:232:VAL:HG23	2.18	0.43
1:A:208:LYS:HG3	1:A:327:PHE:CD1	2.55	0.42
1:A:316:LEU:HD22	1:A:318:TYR:OH	2.20	0.41
1:A:171:TRP:HB3	1:A:362:PHE:HB3	2.03	0.41

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	398/456 (87%)	393 (99%)	5 (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	323/380 (85%)	318 (98%)	5 (2%)	60	66

All (5) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	168	HIS
1	A	316	LEU
1	A	362	PHE
1	A	373	GLU
1	A	474	LEU

Sometimes 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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

10 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	$\# Z > 2$
2	HIS	A	501	-	6,11,11	1.15	1 (16%)	5,14,14	1.54	1 (20%)
4	GOL	A	503[A]	-	5,5,5	0.26	0	5,5,5	0.25	0
6	EDO	A	506	-	3,3,3	0.37	0	2,2,2	0.42	0
3	4JH	A	502[B]	-	9,9,9	0.43	0	11,11,11	0.43	0
5	SO4	A	504	-	4,4,4	0.41	0	6,6,6	0.21	0
4	GOL	A	503[B]	-	5,5,5	0.27	0	5,5,5	0.42	0
7	DMS	A	507	-	3,3,3	0.67	0	3,3,3	0.50	0
7	DMS	A	508	-	3,3,3	0.62	0	3,3,3	0.64	0
3	4JH	A	502[A]	-	9,9,9	0.20	0	11,11,11	0.37	0
5	SO4	A	505	-	4,4,4	0.37	0	6,6,6	0.45	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
2	HIS	A	501	-	-	0/8/8/8	0/1/1/1
4	GOL	A	503[A]	-	-	2/4/4/4	-
6	EDO	A	506	-	-	1/1/1/1	-
3	4JH	A	502[B]	-	-	0/2/2/2	0/1/1/1
4	GOL	A	503[B]	-	-	4/4/4/4	-
3	4JH	A	502[A]	-	-	0/2/2/2	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	HIS	OXT-C	-2.46	1.22	1.30

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	A	501	HIS	CB-CG-CD2	2.06	131.44	127.75

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	503[B]	GOL	O1-C1-C2-C3
4	A	503[B]	GOL	C1-C2-C3-O3
4	A	503[B]	GOL	O2-C2-C3-O3
4	A	503[B]	GOL	O1-C1-C2-O2
4	A	503[A]	GOL	O1-C1-C2-C3
4	A	503[A]	GOL	O1-C1-C2-O2
6	A	506	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	HIS	1	0
4	A	503[A]	GOL	3	0
3	A	502[B]	4JH	7	0
4	A	503[B]	GOL	10	0
7	A	507	DMS	2	0
3	A	502[A]	4JH	1	0

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 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	408/456 (89%)	0.19	27 (6%) 26 24	10, 34, 67, 79	2 (0%)

All (27) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	280	VAL	3.8
1	A	283	GLU	3.6
1	A	279	ARG	3.3
1	A	469	GLY	3.3
1	A	243	PRO	3.0
1	A	253	VAL	3.0
1	A	225	THR	2.9
1	A	245	GLU	2.8
1	A	380	ILE	2.8
1	A	255	GLY	2.7
1	A	259	THR	2.6
1	A	244	ARG	2.5
1	A	227	ASP	2.5
1	A	262	ASP	2.5
1	A	260	VAL	2.4
1	A	215	LEU	2.4
1	A	284	HIS	2.4
1	A	158	GLU	2.3
1	A	48	MET	2.3
1	A	217	THR	2.3
1	A	267	THR	2.3
1	A	250	GLN	2.3
1	A	247	VAL	2.2
1	A	281	GLY	2.2
1	A	254	LEU	2.2
1	A	261	VAL	2.1
1	A	218	VAL	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 monosaccharides 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(\AA^2)	Q<0.9
6	EDO	A	506	4/4	0.81	0.17	45,47,50,54	0
7	DMS	A	507	4/4	0.90	0.15	55,60,60,62	0
5	SO4	A	505	5/5	0.91	0.10	46,46,48,50	0
7	DMS	A	508	4/4	0.92	0.14	44,48,48,49	0
4	GOL	A	503[B]	6/6	0.94	0.08	22,22,23,23	6
5	SO4	A	504	5/5	0.94	0.10	26,28,29,29	5
4	GOL	A	503[A]	6/6	0.94	0.08	25,25,26,27	6
2	HIS	A	501	11/11	0.97	0.05	18,20,21,21	0
3	4JH	A	502[B]	9/9	0.98	0.08	28,31,33,39	9
3	4JH	A	502[A]	9/9	0.98	0.08	26,26,29,31	9

6.5 Other polymers [i](#)

There are no such residues in this entry.