



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 14, 2020 – 06:07 am BST

PDB ID : 1SB7  
Title : Crystal structure of the E.coli pseudouridine synthase TruD  
Authors : Hoang, C.; Ferre-D'Amare, A.R.  
Deposited on : 2004-02-10  
Resolution : 2.20 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

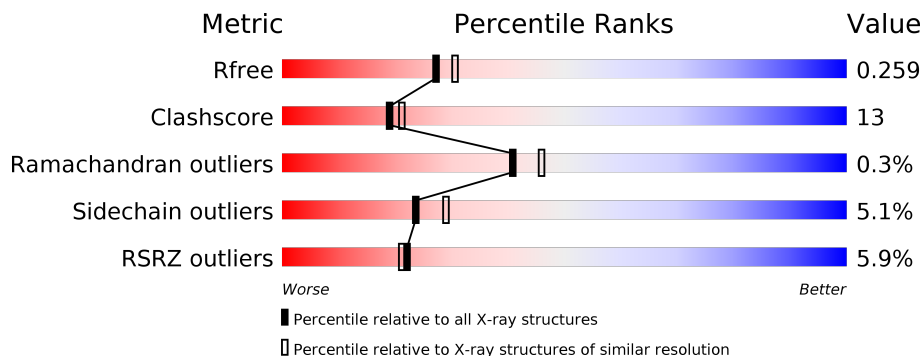
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.20 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	4898 (2.20-2.20)
Clashscore	141614	5594 (2.20-2.20)
Ramachandran outliers	138981	5503 (2.20-2.20)
Sidechain outliers	138945	5504 (2.20-2.20)
RSRZ outliers	127900	4800 (2.20-2.20)

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	368	
1	B	368	

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
2	GOL	A	1202	-	X	-	-
2	GOL	A	1203	-	X	-	-
2	GOL	B	1201	-	X	-	-
2	GOL	B	1204	-	X	-	-
2	GOL	B	1205	-	X	-	-
2	GOL	B	1206	-	X	-	-
3	PO4	B	1301	-	-	X	-

## 2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 5723 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 tRNA pseudouridine synthase D.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	342	2704	1715	486	495	4	4	0	4	0
1	B	344	2720	1718	493	500	5	4	0	6	0

There are 46 discrepancies between the modelled and reference sequences:

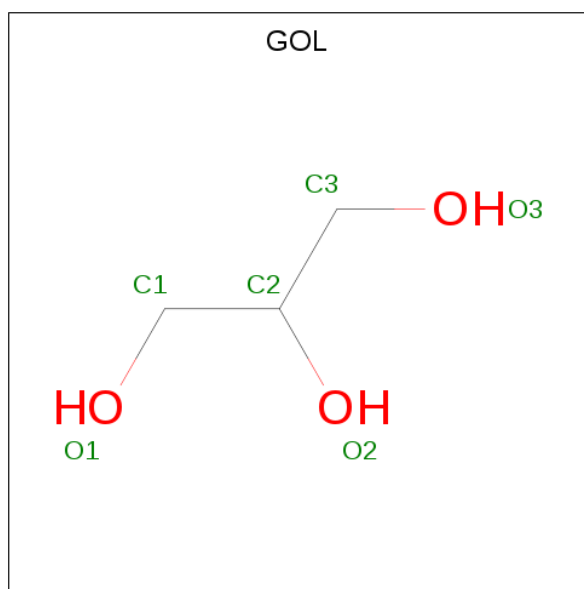
Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	GLY	-	CLONING ARTIFACT	UNP Q57261
A	-17	SER	-	CLONING ARTIFACT	UNP Q57261
A	-16	SER	-	CLONING ARTIFACT	UNP Q57261
A	-15	HIS	-	CLONING ARTIFACT	UNP Q57261
A	-14	HIS	-	CLONING ARTIFACT	UNP Q57261
A	-13	HIS	-	CLONING ARTIFACT	UNP Q57261
A	-12	HIS	-	CLONING ARTIFACT	UNP Q57261
A	-11	HIS	-	CLONING ARTIFACT	UNP Q57261
A	-10	HIS	-	CLONING ARTIFACT	UNP Q57261
A	-9	SER	-	CLONING ARTIFACT	UNP Q57261
A	-8	SER	-	CLONING ARTIFACT	UNP Q57261
A	-7	GLY	-	CLONING ARTIFACT	UNP Q57261
A	-6	LEU	-	CLONING ARTIFACT	UNP Q57261
A	-5	VAL	-	CLONING ARTIFACT	UNP Q57261
A	-4	PRO	-	CLONING ARTIFACT	UNP Q57261
A	-3	ARG	-	CLONING ARTIFACT	UNP Q57261
A	-2	GLY	-	CLONING ARTIFACT	UNP Q57261
A	-1	SER	-	CLONING ARTIFACT	UNP Q57261
A	0	HIS	-	CLONING ARTIFACT	UNP Q57261
A	1	MSE	MET	MODIFIED RESIDUE	UNP Q57261
A	98	MSE	MET	MODIFIED RESIDUE	UNP Q57261
A	254	MSE	MET	MODIFIED RESIDUE	UNP Q57261
A	301	MSE	MET	MODIFIED RESIDUE	UNP Q57261
B	-18	GLY	-	CLONING ARTIFACT	UNP Q57261
B	-17	SER	-	CLONING ARTIFACT	UNP Q57261

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Chain	Residue	Modelled	Actual	Comment	Reference
B	-16	SER	-	CLONING ARTIFACT	UNP Q57261
B	-15	HIS	-	CLONING ARTIFACT	UNP Q57261
B	-14	HIS	-	CLONING ARTIFACT	UNP Q57261
B	-13	HIS	-	CLONING ARTIFACT	UNP Q57261
B	-12	HIS	-	CLONING ARTIFACT	UNP Q57261
B	-11	HIS	-	CLONING ARTIFACT	UNP Q57261
B	-10	HIS	-	CLONING ARTIFACT	UNP Q57261
B	-9	SER	-	CLONING ARTIFACT	UNP Q57261
B	-8	SER	-	CLONING ARTIFACT	UNP Q57261
B	-7	GLY	-	CLONING ARTIFACT	UNP Q57261
B	-6	LEU	-	CLONING ARTIFACT	UNP Q57261
B	-5	VAL	-	CLONING ARTIFACT	UNP Q57261
B	-4	PRO	-	CLONING ARTIFACT	UNP Q57261
B	-3	ARG	-	CLONING ARTIFACT	UNP Q57261
B	-2	GLY	-	CLONING ARTIFACT	UNP Q57261
B	-1	SER	-	CLONING ARTIFACT	UNP Q57261
B	0	HIS	-	CLONING ARTIFACT	UNP Q57261
B	1	MSE	MET	MODIFIED RESIDUE	UNP Q57261
B	98	MSE	MET	MODIFIED RESIDUE	UNP Q57261
B	254	MSE	MET	MODIFIED RESIDUE	UNP Q57261
B	301	MSE	MET	MODIFIED RESIDUE	UNP Q57261

- Molecule 2 is GLYCEROL (three-letter code: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



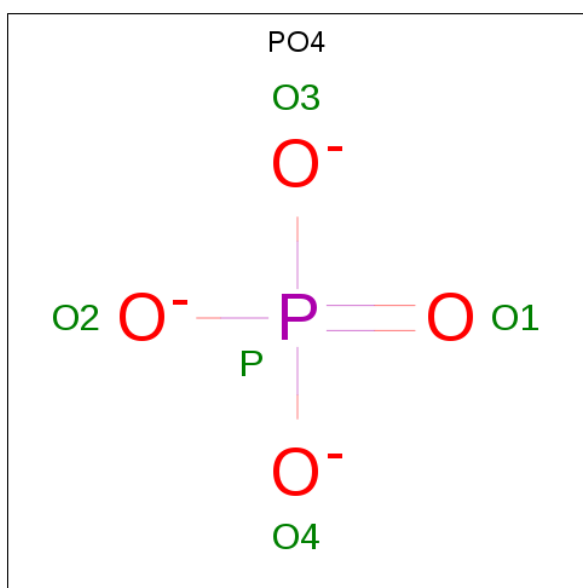
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	O	P	0	0
			5	4	1		

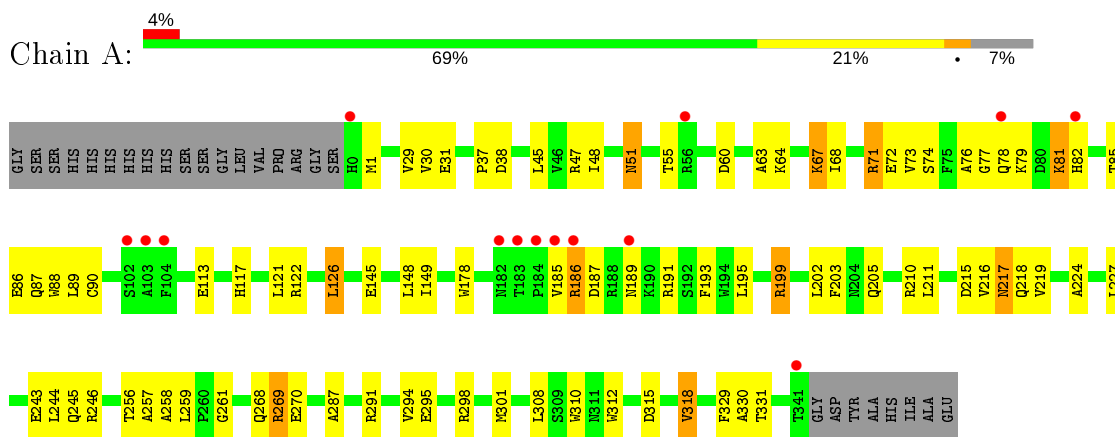
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	133	Total	O	0	0
			133	133		
4	B	125	Total	O	0	0
			125	125		

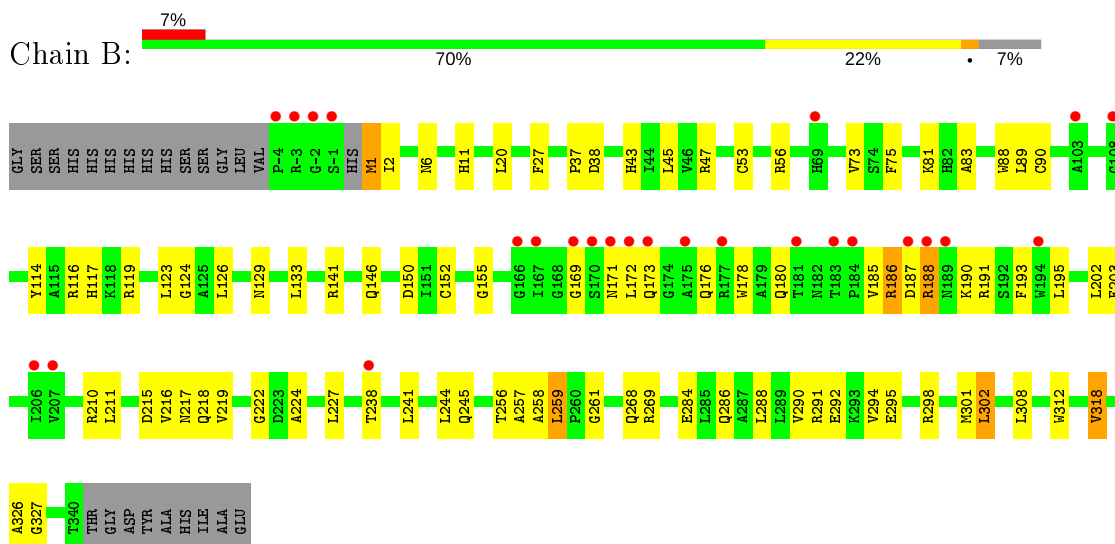
### 3 Residue-property plots [i](#)

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: tRNA pseudouridine synthase D



- Molecule 1: tRNA pseudouridine synthase D



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	63.66Å 108.78Å 111.86Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	27.69 – 2.20 27.69 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.6 (27.69-2.20) 97.8 (27.69-2.20)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	0.07	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	5.82 (at 2.20Å)	Xtrriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.216 , 0.254 0.220 , 0.259	Depositor DCC
$R_{free}$ test set	3938 reflections (9.83%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	35.0	Xtrriage
Anisotropy	0.349	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 41.0	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	0.012 for -h,l,k	Xtrriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	5723	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	40.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.50% 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, PO4

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	0.36	0/2751	0.60	1/3718 (0.0%)
1	B	0.33	0/2770	0.58	1/3748 (0.0%)
All	All	0.35	0/5521	0.59	2/7466 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	259	LEU	N-CA-C	-5.66	95.72	111.00
1	B	259	LEU	N-CA-C	-5.25	96.83	111.00

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	2704	0	2661	74	0
1	B	2720	0	2661	68	0
2	A	12	0	8	3	0
2	B	24	0	16	0	0
3	B	5	0	0	4	0
4	A	133	0	0	6	0
4	B	125	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	5723	0	5346	141	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 13.

All (141) 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:1:MSE:HE1	1:A:202:LEU:HD23	1.39	1.01
1:A:186:ARG:HG2	1:A:187:ASP:H	1.28	0.97
1:B:186:ARG:HD2	1:B:187[B]:ASP:H	1.32	0.91
1:B:186:ARG:HD2	1:B:187[A]:ASP:H	1.33	0.91
1:A:219:VAL:H	1:A:245:GLN:HE22	1.24	0.85
1:B:218:GLN:HA	1:B:245:GLN:HE22	1.46	0.81
1:B:171:ASN:ND2	1:B:193:PHE:HB3	1.95	0.81
1:B:1:MSE:HE1	1:B:202:LEU:HD23	1.64	0.78
1:A:38:ASP:H	1:A:117:HIS:HD2	1.33	0.76
1:B:38:ASP:H	1:B:117:HIS:HD2	1.32	0.75
1:B:186:ARG:HD2	1:B:187[B]:ASP:N	2.03	0.73
1:A:76:ALA:HB3	1:A:126:LEU:HD13	1.71	0.72
1:A:79:LYS:HG3	1:A:85:THR:HG21	1.71	0.71
1:A:186:ARG:HG2	1:A:187:ASP:N	2.06	0.68
1:A:312:TRP:CZ3	1:A:318:VAL:HG22	2.29	0.67
1:B:211:LEU:HD23	1:B:216:VAL:HG11	1.76	0.67
1:B:327:GLY:N	3:B:1301:PO4:O2	2.28	0.66
1:B:211:LEU:HD23	1:B:216:VAL:CG1	2.26	0.66
1:B:224:ALA:CB	1:B:298:ARG:HD2	2.27	0.65
1:A:186:ARG:CD	1:A:186:ARG:H	2.09	0.65
1:A:77:GLY:O	1:A:87:GLN:NE2	2.30	0.65
1:A:37:PRO:HB3	1:A:45:LEU:HD12	1.78	0.64
1:A:295:GLU:HG2	4:A:1066:HOH:O	1.97	0.64
1:A:48:ILE:HD12	1:A:89:LEU:HD12	1.79	0.64
1:B:186:ARG:CD	1:B:187[B]:ASP:H	2.07	0.64
1:B:186:ARG:CD	1:B:187[A]:ASP:H	2.07	0.63
1:A:219:VAL:H	1:A:245:GLN:NE2	1.94	0.63
1:A:186:ARG:CG	1:A:187:ASP:H	2.08	0.62
1:A:31:GLU:O	1:A:47[A]:ARG:NH2	2.32	0.62
1:A:126:LEU:HB2	4:A:1039:HOH:O	2.00	0.62
1:B:171:ASN:HD22	1:B:193:PHE:HB3	1.66	0.61
1:B:126:LEU:HD11	3:B:1301:PO4:O3	2.01	0.60
1:B:312:TRP:CZ3	1:B:318:VAL:HG22	2.36	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:27:PHE:CD1	1:B:133:LEU:HD22	2.37	0.59
1:B:169:GLY:O	1:B:173:GLN:HG3	2.02	0.59
1:A:63:ALA:HA	1:A:68:ILE:HD11	1.85	0.58
1:A:30:VAL:CG1	1:A:47[B]:ARG:HH22	2.17	0.58
1:A:51:ASN:C	1:A:51:ASN:HD22	2.05	0.57
1:B:11:HIS:HE1	1:B:155:GLY:O	1.88	0.57
1:A:215:ASP:OD2	1:A:218:GLN:HB2	2.05	0.57
1:B:129:ASN:ND2	3:B:1301:PO4:O3	2.33	0.56
1:B:53:CYS:N	1:B:81:LYS:HG3	2.20	0.56
1:B:56:ARG:O	1:B:56:ARG:HD3	2.05	0.56
1:A:331:THR:HG23	2:A:1203:GOL:O3	2.05	0.56
1:A:90:CYS:HB2	1:A:121:LEU:HB2	1.87	0.56
1:A:258:ALA:HB2	1:A:298:ARG:NH2	2.20	0.56
1:A:38:ASP:H	1:A:117:HIS:CD2	2.19	0.55
1:B:258:ALA:HB2	1:B:298:ARG:NH2	2.21	0.55
1:B:38:ASP:H	1:B:117:HIS:CD2	2.20	0.55
1:B:286:GLN:O	1:B:290:VAL:HG23	2.07	0.55
1:A:1:MSE:HG3	1:A:205:GLN:OE1	2.07	0.54
1:B:301:MSE:HG2	1:B:302:LEU:HD13	1.89	0.54
1:A:55:THR:HB	1:A:78:GLN:NE2	2.21	0.54
1:B:123:LEU:HD23	1:B:124:GLY:N	2.22	0.54
1:A:47[B]:ARG:HD2	1:A:113:GLU:OE1	2.08	0.54
1:A:195:LEU:O	1:A:199:ARG:HG2	2.07	0.53
1:B:180:GLN:HG2	1:B:284:GLU:OE1	2.10	0.51
1:B:288:LEU:O	1:B:291:ARG:HG2	2.10	0.51
4:A:1141:HOH:O	1:B:295:GLU:HG2	2.11	0.51
1:A:268:GLN:HG3	4:A:1150:HOH:O	2.10	0.51
1:B:312:TRP:CD2	1:B:318:VAL:HG13	2.46	0.51
1:A:68:ILE:HD13	1:A:72:GLU:HB2	1.93	0.50
1:B:45:LEU:O	1:B:114:TYR:HA	2.11	0.50
1:A:189:ASN:O	1:A:193:PHE:HD1	1.94	0.50
1:B:261:GLY:HA3	1:B:294:VAL:O	2.12	0.50
1:A:312:TRP:CD2	1:A:318:VAL:HG13	2.45	0.50
1:B:210:ARG:HG2	1:B:301:MSE:SE	2.62	0.49
1:A:51:ASN:ND2	1:A:51:ASN:C	2.64	0.49
1:B:224:ALA:HB3	1:B:298:ARG:HD2	1.92	0.49
1:A:203:PHE:CE1	1:A:257:ALA:HB3	2.47	0.49
1:A:73:VAL:HA	1:A:90:CYS:O	2.12	0.49
1:B:186:ARG:HD2	1:B:187[A]:ASP:N	2.03	0.49
1:A:30:VAL:HG13	1:A:47[B]:ARG:NH2	2.27	0.49
1:B:126:LEU:H	1:B:126:LEU:HD23	1.76	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:219:VAL:H	1:B:245:GLN:NE2	2.11	0.48
1:A:145[A]:GLU:OE1	1:A:312:TRP:NE1	2.42	0.48
1:A:64:LYS:O	1:A:67:LYS:HD2	2.13	0.48
1:A:71:ARG:NH1	1:A:71:ARG:HG2	2.29	0.48
1:A:78:GLN:NE2	4:A:1140:HOH:O	2.47	0.48
1:A:224:ALA:HB3	1:A:298:ARG:HD2	1.95	0.48
1:A:76:ALA:CB	1:A:126:LEU:HD13	2.43	0.48
1:A:148:LEU:HD13	1:A:310:TRP:CG	2.49	0.47
1:B:215:ASP:OD2	1:B:218:GLN:HB2	2.13	0.47
1:B:211:LEU:CD2	1:B:216:VAL:HG11	2.43	0.47
1:A:186:ARG:CD	1:A:186:ARG:N	2.78	0.47
1:A:287:ALA:O	1:A:291:ARG:HB2	2.14	0.47
1:A:178:TRP:CE2	1:A:185:VAL:HG23	2.50	0.47
1:A:224:ALA:CB	1:A:298:ARG:HD2	2.43	0.47
1:A:211:LEU:HD23	1:A:216:VAL:HG13	1.96	0.47
1:B:141:ARG:HG3	1:B:312:TRP:CH2	2.49	0.47
1:B:2:ILE:HG23	1:B:6[B]:ASN:HD22	1.80	0.47
1:A:38:ASP:N	1:A:117:HIS:HD2	2.09	0.47
1:B:326:ALA:HA	3:B:1301:PO4:O2	2.15	0.46
1:A:312:TRP:CE3	1:A:318:VAL:HG22	2.50	0.46
1:B:178:TRP:CE2	1:B:185:VAL:HG23	2.51	0.46
1:B:218:GLN:HA	1:B:245:GLN:NE2	2.23	0.46
1:A:47[B]:ARG:NH2	1:A:86:GLU:OE1	2.48	0.46
1:B:141:ARG:HG3	1:B:312:TRP:CZ2	2.51	0.46
1:A:270:GLU:HB2	4:A:1003:HOH:O	2.16	0.45
1:A:81:LYS:HG3	1:A:81:LYS:H	1.57	0.45
1:B:256:THR:OG1	1:B:298:ARG:HD3	2.17	0.45
1:B:176:GLN:O	1:B:180:GLN:HG3	2.17	0.45
1:B:222:GLY:HA3	1:B:268:GLN:O	2.17	0.45
1:A:29:VAL:HG11	1:A:79:LYS:HE3	1.99	0.44
1:B:211:LEU:HD23	1:B:216:VAL:HG13	1.99	0.44
1:A:261:GLY:HA3	1:A:294:VAL:O	2.17	0.44
1:B:38:ASP:N	1:B:117:HIS:HD2	2.09	0.44
1:B:187[B]:ASP:HB2	1:B:190:LYS:HB3	1.98	0.44
1:B:47:ARG:HD2	1:B:88:TRP:CZ2	2.52	0.44
1:A:243:GLU:OE1	1:A:246:ARG:NH1	2.50	0.44
1:A:37:PRO:HA	1:A:117:HIS:CD2	2.52	0.44
1:B:185:VAL:HB	1:B:191:ARG:HG3	2.00	0.44
1:B:238:THR:HA	1:B:241:LEU:HG	2.00	0.43
1:B:188:ARG:HD2	1:B:188:ARG:HA	1.74	0.43
1:A:217:ASN:HD22	1:A:217:ASN:HA	1.55	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:30:VAL:HG13	1:A:47[B]:ARG:HH22	1.82	0.43
1:A:71:ARG:HH11	1:A:71:ARG:HG2	1.83	0.43
1:B:27:PHE:O	1:B:83:ALA:HB1	2.18	0.43
1:B:126:LEU:HD23	1:B:126:LEU:N	2.34	0.43
1:A:329:PHE:N	1:A:329:PHE:CD1	2.86	0.43
1:A:63:ALA:HA	1:A:68:ILE:CD1	2.47	0.43
1:B:37:PRO:HA	1:B:117:HIS:CD2	2.53	0.43
1:A:74:SER:OG	1:A:90:CYS:HB3	2.19	0.42
1:A:149:ILE:CD1	1:B:119:ARG:HD3	2.49	0.42
1:B:73:VAL:HA	1:B:90:CYS:O	2.18	0.42
1:A:76:ALA:HA	1:A:122:ARG:O	2.20	0.42
1:B:146[A]:GLN:HE22	1:B:150:ASP:CG	2.23	0.42
1:B:43:HIS:O	1:B:116:ARG:HA	2.20	0.42
1:B:75:PHE:HB3	1:B:89:LEU:HD23	2.02	0.42
1:B:172:LEU:O	1:B:176:GLN:HG3	2.20	0.42
1:B:203:PHE:CE1	1:B:257:ALA:HB3	2.55	0.42
1:A:269:ARG:HB3	1:A:270:GLU:H	1.56	0.41
1:B:191:ARG:NH1	1:B:292:GLU:OE1	2.53	0.41
1:A:330:ALA:H	2:A:1203:GOL:C3	2.32	0.41
1:A:210:ARG:HG2	1:A:301:MSE:SE	2.71	0.41
1:A:45:LEU:HD21	1:A:121:LEU:HD13	2.03	0.41
1:A:47[A]:ARG:HD2	1:A:88:TRP:CZ2	2.55	0.41
1:B:195:LEU:HD21	1:B:292:GLU:HG3	2.02	0.41
1:A:60:ASP:O	1:A:64:LYS:HG2	2.22	0.40
1:A:256:THR:OG1	1:A:298:ARG:HD3	2.21	0.40
1:A:298:ARG:N	2:A:1202:GOL:O3	2.50	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	344/368 (94%)	329 (96%)	13 (4%)	2 (1%)	25	26
1	B	346/368 (94%)	331 (96%)	15 (4%)	0	100	100
All	All	690/736 (94%)	660 (96%)	28 (4%)	2 (0%)	41	46

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	82	HIS
1	A	186	ARG

### 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	270/295 (92%)	256 (95%)	14 (5%)	23	28
1	B	274/295 (93%)	260 (95%)	14 (5%)	24	29
All	All	544/590 (92%)	516 (95%)	28 (5%)	24	29

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ASN
1	A	67	LYS
1	A	71	ARG
1	A	81	LYS
1	A	126	LEU
1	A	191	ARG
1	A	199	ARG
1	A	217	ASN
1	A	227	LEU
1	A	244	LEU
1	A	269	ARG
1	A	308	LEU
1	A	315	ASP
1	A	318	VAL

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Mol	Chain	Res	Type
1	B	1	MSE
1	B	20	LEU
1	B	152[A]	CYS
1	B	152[B]	CYS
1	B	186	ARG
1	B	188	ARG
1	B	217	ASN
1	B	227	LEU
1	B	244	LEU
1	B	259	LEU
1	B	269	ARG
1	B	302	LEU
1	B	308	LEU
1	B	318	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	51	ASN
1	A	78	GLN
1	A	87	GLN
1	A	117	HIS
1	A	217	ASN
1	A	218	GLN
1	A	245	GLN
1	A	286	GLN
1	B	11	HIS
1	B	87	GLN
1	B	117	HIS
1	B	217	ASN
1	B	245	GLN
1	B	268	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

7 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	GOL	B	1205	-	5,5,5	4.44	5 (100%)	5,5,5	5.80	3 (60%)
2	GOL	A	1203	-	5,5,5	4.66	5 (100%)	5,5,5	5.76	3 (60%)
2	GOL	B	1206	-	5,5,5	4.49	5 (100%)	5,5,5	5.78	3 (60%)
2	GOL	B	1201	-	5,5,5	4.48	5 (100%)	5,5,5	5.78	3 (60%)
2	GOL	A	1202	-	5,5,5	4.63	5 (100%)	5,5,5	5.76	3 (60%)
3	PO4	B	1301	-	4,4,4	1.75	2 (50%)	6,6,6	0.44	0
2	GOL	B	1204	-	5,5,5	4.47	5 (100%)	5,5,5	5.79	3 (60%)

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	GOL	B	1205	-	-	2/4/4/4	-
2	GOL	A	1203	-	-	2/4/4/4	-
2	GOL	B	1206	-	-	2/4/4/4	-
2	GOL	B	1201	-	-	2/4/4/4	-
2	GOL	A	1202	-	-	2/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	GOL	B	1204	-	-	2/4/4/4	-

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1202	GOL	C3-C2	-7.98	1.18	1.51
2	A	1203	GOL	C3-C2	-7.81	1.19	1.51
2	B	1206	GOL	C3-C2	-7.31	1.21	1.51
2	B	1201	GOL	C3-C2	-7.30	1.21	1.51
2	B	1204	GOL	C3-C2	-7.29	1.21	1.51
2	B	1205	GOL	C3-C2	-7.21	1.22	1.51
2	A	1203	GOL	O1-C1	4.77	1.62	1.42
2	B	1206	GOL	O1-C1	4.50	1.61	1.42
2	B	1201	GOL	O1-C1	4.49	1.61	1.42
2	B	1204	GOL	O1-C1	4.45	1.61	1.42
2	A	1202	GOL	O1-C1	4.39	1.61	1.42
2	B	1205	GOL	O1-C1	4.38	1.60	1.42
2	B	1201	GOL	O3-C3	3.53	1.57	1.42
2	B	1205	GOL	O3-C3	3.49	1.57	1.42
2	B	1206	GOL	O3-C3	3.47	1.57	1.42
2	B	1204	GOL	O3-C3	3.42	1.56	1.42
2	A	1203	GOL	O3-C3	3.02	1.55	1.42
2	A	1203	GOL	O2-C2	-3.00	1.34	1.43
2	A	1202	GOL	O2-C2	-2.94	1.34	1.43
2	B	1204	GOL	C1-C2	-2.91	1.39	1.51
2	A	1202	GOL	C1-C2	-2.83	1.40	1.51
2	B	1205	GOL	C1-C2	-2.80	1.40	1.51
2	B	1206	GOL	O2-C2	-2.77	1.35	1.43
2	A	1202	GOL	O3-C3	2.76	1.54	1.42
2	B	1206	GOL	C1-C2	-2.73	1.40	1.51
2	B	1205	GOL	O2-C2	-2.72	1.35	1.43
2	B	1201	GOL	C1-C2	-2.70	1.40	1.51
2	B	1201	GOL	O2-C2	-2.64	1.35	1.43
2	B	1204	GOL	O2-C2	-2.60	1.35	1.43
2	A	1203	GOL	C1-C2	-2.58	1.41	1.51
3	B	1301	PO4	P-O2	-2.24	1.47	1.54
3	B	1301	PO4	P-O3	-2.11	1.48	1.54

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1204	GOL	O3-C3-C2	10.56	160.84	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1206	GOL	O3-C3-C2	10.54	160.74	110.20
2	A	1203	GOL	O3-C3-C2	10.51	160.61	110.20
2	B	1205	GOL	O3-C3-C2	10.47	160.38	110.20
2	B	1201	GOL	O3-C3-C2	10.45	160.32	110.20
2	A	1202	GOL	O3-C3-C2	10.40	160.08	110.20
2	B	1201	GOL	O2-C2-C3	6.84	139.24	109.12
2	B	1205	GOL	O2-C2-C3	6.82	139.18	109.12
2	A	1202	GOL	O2-C2-C3	6.80	139.08	109.12
2	B	1204	GOL	O2-C2-C3	6.79	139.04	109.12
2	B	1206	GOL	O2-C2-C3	6.69	138.61	109.12
2	A	1203	GOL	O2-C2-C3	6.56	138.00	109.12
2	A	1203	GOL	O1-C1-C2	3.38	126.43	110.20
2	B	1205	GOL	O1-C1-C2	3.36	126.31	110.20
2	B	1206	GOL	O1-C1-C2	3.26	125.82	110.20
2	A	1202	GOL	O1-C1-C2	3.23	125.70	110.20
2	B	1201	GOL	O1-C1-C2	3.18	125.43	110.20
2	B	1204	GOL	O1-C1-C2	3.08	124.98	110.20

There are no chirality outliers.

All (12) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	1205	GOL	O1-C1-C2-C3
2	B	1205	GOL	C1-C2-C3-O3
2	A	1203	GOL	C1-C2-C3-O3
2	B	1206	GOL	C1-C2-C3-O3
2	B	1201	GOL	C1-C2-C3-O3
2	A	1202	GOL	O1-C1-C2-C3
2	A	1202	GOL	C1-C2-C3-O3
2	B	1204	GOL	C1-C2-C3-O3
2	A	1203	GOL	O1-C1-C2-O2
2	B	1206	GOL	O1-C1-C2-O2
2	B	1204	GOL	O1-C1-C2-O2
2	B	1201	GOL	O1-C1-C2-O2

There are no ring outliers.

3 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1203	GOL	2	0
2	A	1202	GOL	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	1301	PO4	4	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<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	338/368 (91%)	0.04	14 (4%) 37 35	18, 35, 65, 76	0
1	B	340/368 (92%)	0.29	26 (7%) 13 12	20, 39, 70, 80	0
All	All	678/736 (92%)	0.17	40 (5%) 22 21	18, 37, 67, 80	0

All (40) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	-2	GLY	5.7
1	A	341	THR	5.4
1	B	-4	PRO	4.5
1	A	184	PRO	3.9
1	B	-3	ARG	3.7
1	B	167	ILE	3.4
1	A	103	ALA	3.3
1	B	172	LEU	3.3
1	B	187[A]	ASP	3.2
1	B	188	ARG	3.2
1	A	185	VAL	3.1
1	A	56	ARG	3.0
1	A	183	THR	3.0
1	B	194	TRP	3.0
1	B	177	ARG	2.8
1	B	169	GLY	2.8
1	A	189	ASN	2.7
1	A	82	HIS	2.6
1	A	182	ASN	2.6
1	A	186	ARG	2.6
1	B	184	PRO	2.6
1	B	183	THR	2.5
1	A	104	PHE	2.5
1	B	166	GLY	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	206	ILE	2.4
1	B	181	THR	2.4
1	B	171	ASN	2.4
1	B	69[A]	HIS	2.3
1	A	102	SER	2.3
1	B	207	VAL	2.3
1	B	170	SER	2.3
1	B	189	ASN	2.2
1	B	173	GLN	2.2
1	B	108	GLY	2.2
1	A	0	HIS	2.2
1	B	103	ALA	2.2
1	B	175	ALA	2.2
1	B	-1	SER	2.2
1	A	78	GLN	2.1
1	B	238	THR	2.1

## 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. 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
2	GOL	B	1205	6/6	0.65	0.22	58,64,65,65	0
2	GOL	B	1206	6/6	0.71	0.33	66,68,70,70	0
2	GOL	A	1202	6/6	0.72	0.28	49,51,53,53	0
2	GOL	B	1204	6/6	0.76	0.18	67,67,68,68	0
2	GOL	A	1203	6/6	0.80	0.32	66,68,69,69	0
3	PO4	B	1301	5/5	0.81	0.69	50,54,55,55	5
2	GOL	B	1201	6/6	0.83	0.32	39,45,48,52	0

## 6.5 Other polymers

There are no such residues in this entry.