



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:25 PM GMT

PDB ID : 1TLW  
Title : Tsx structure complexed with thymidine  
Authors : Ye, J.; van den Berg, B.  
Deposited on : 2004-06-10  
Resolution : 3.10 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
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) : trunk26865

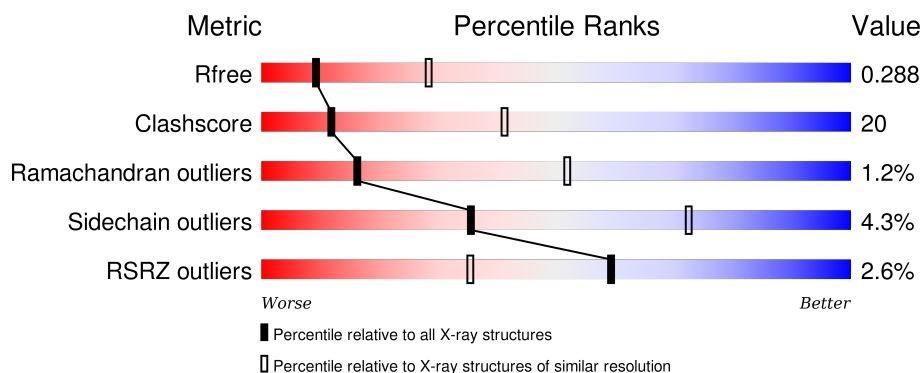
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*


The reported resolution of this entry is 3.10 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))
$R_{free}$	91344	1114 (3.14-3.06)
Clashscore	102246	1222 (3.14-3.06)
Ramachandran outliers	100387	1174 (3.14-3.06)
Sidechain outliers	100360	1174 (3.14-3.06)
RSRZ outliers	91569	1119 (3.14-3.06)

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	278	
1	B	278	

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 4194 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.

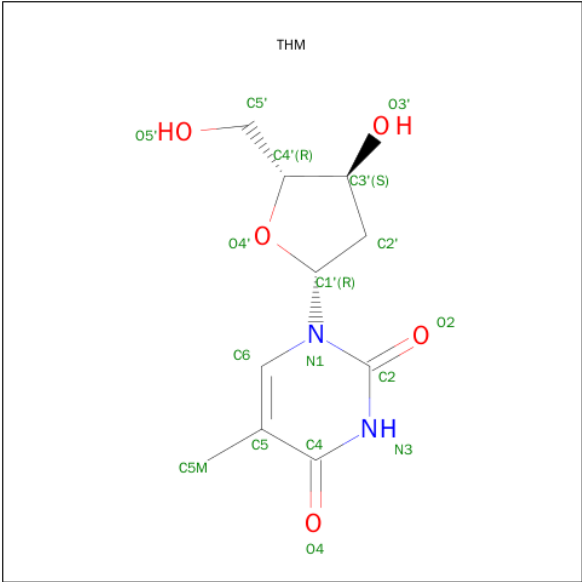
- Molecule 1 is a protein called Nucleoside-specific channel-forming protein tsx.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	251	Total	C	N	O	S	0	0	0
			2078	1340	347	386	5			
1	B	248	Total	C	N	O	S	0	0	0
			2048	1322	338	383	5			

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	273	HIS	-	EXPRESSION TAG	UNP P0A927
A	274	HIS	-	EXPRESSION TAG	UNP P0A927
A	275	HIS	-	EXPRESSION TAG	UNP P0A927
A	276	HIS	-	EXPRESSION TAG	UNP P0A927
A	277	HIS	-	EXPRESSION TAG	UNP P0A927
A	278	HIS	-	EXPRESSION TAG	UNP P0A927
B	273	HIS	-	EXPRESSION TAG	UNP P0A927
B	274	HIS	-	EXPRESSION TAG	UNP P0A927
B	275	HIS	-	EXPRESSION TAG	UNP P0A927
B	276	HIS	-	EXPRESSION TAG	UNP P0A927
B	277	HIS	-	EXPRESSION TAG	UNP P0A927
B	278	HIS	-	EXPRESSION TAG	UNP P0A927

- Molecule 2 is THYMIDINE (three-letter code: THM) (formula: C<sub>10</sub>H<sub>14</sub>N<sub>2</sub>O<sub>5</sub>).

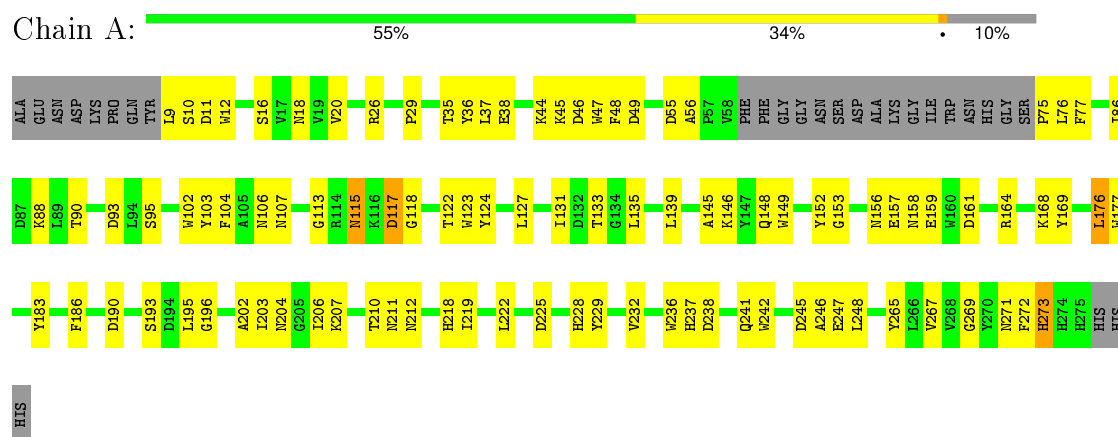


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			17	10	2	5		
2	B	1	Total	C	N	O	0	0
			17	10	2	5		
2	A	1	Total	C	N	O	0	0
			17	10	2	5		
2	B	1	Total	C	N	O	0	0
			17	10	2	5		

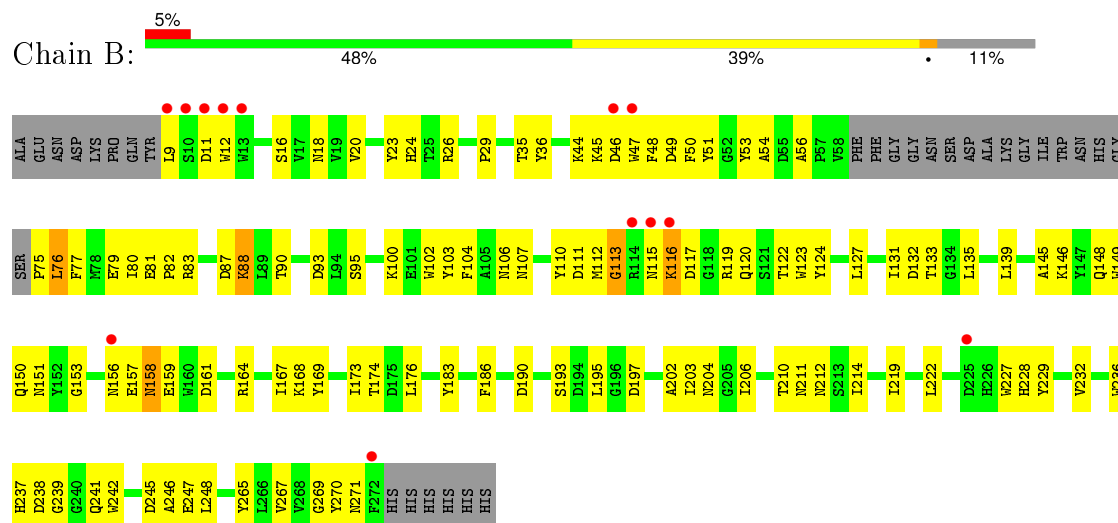
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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: Nucleoside-specific channel-forming protein tsx



- Molecule 1: Nucleoside-specific channel-forming protein tsx



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	149.65Å 149.65Å 119.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.34 – 3.10 44.01 – 3.00	Depositor EDS
% Data completeness (in resolution range)	97.1 (29.34-3.10) 96.2 (44.01-3.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.74 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.269 , 0.297 0.258 , 0.288	Depositor DCC
$R_{free}$ test set	2072 reflections (7.50%)	DCC
Wilson B-factor (Å <sup>2</sup> )	59.6	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.34 , 46.6	EDS
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 31218 reflections	Xtriage
$F_o, F_c$ correlation	0.87	EDS
Total number of atoms	4194	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.62% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: THM

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	0.47	0/2154	0.73	2/2931 (0.1%)
1	B	0.41	0/2121	0.68	2/2886 (0.1%)
All	All	0.44	0/4275	0.71	4/5817 (0.1%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	104	PHE	N-CA-C	-5.74	95.51	111.00
1	A	104	PHE	N-CA-C	-5.59	95.91	111.00
1	B	145	ALA	N-CA-C	-5.27	96.77	111.00
1	A	145	ALA	N-CA-C	-5.05	97.36	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	2078	0	1867	74	0
1	B	2048	0	1846	87	0
2	A	34	0	28	1	0
2	B	34	0	28	2	0
All	All	4194	0	3769	160	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 20.

All (160) 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:B:29:PRO:HG3	1:B:242:TRP:CZ2	2.12	0.84
1:A:106:ASN:HD22	1:A:123:TRP:HE1	1.29	0.80
1:B:210:THR:HG22	1:B:212:ASN:H	1.47	0.80
1:A:29:PRO:HG3	1:A:242:TRP:CZ2	2.20	0.76
1:A:107:ASN:ND2	1:A:164:ARG:HH11	1.85	0.73
1:B:107:ASN:ND2	1:B:164:ARG:HH11	1.88	0.72
1:B:29:PRO:HG3	1:B:242:TRP:CE2	2.25	0.71
1:B:112:MET:HA	1:B:119:ARG:HD2	1.71	0.70
1:A:210:THR:HG22	1:A:212:ASN:H	1.57	0.69
1:B:204:ASN:ND2	1:B:245:ASP:O	2.26	0.68
1:B:146:LYS:HG2	1:B:161:ASP:O	1.94	0.67
1:B:18:ASN:OD1	1:B:269:GLY:HA3	1.94	0.67
1:B:131:ILE:HB	1:B:139:LEU:HD12	1.77	0.66
1:B:106:ASN:HD22	1:B:123:TRP:HE1	1.44	0.65
1:B:9:LEU:HB3	1:B:12:TRP:HE1	1.62	0.65
1:A:210:THR:HG22	1:A:212:ASN:O	1.96	0.65
1:A:36:TYR:HB2	1:A:56:ALA:O	1.96	0.65
1:A:75:PRO:HG2	1:A:76:LEU:H	1.62	0.64
1:A:204:ASN:ND2	1:A:245:ASP:O	2.30	0.64
1:A:146:LYS:HG2	1:A:161:ASP:O	1.97	0.64
1:B:210:THR:HG22	1:B:212:ASN:O	1.99	0.63
1:A:131:ILE:HB	1:A:139:LEU:HD12	1.81	0.62
1:B:111:ASP:O	1:B:119:ARG:HB3	1.99	0.62
1:B:75:PRO:HA	1:B:113:GLY:HA2	1.79	0.62
1:B:36:TYR:HB2	1:B:56:ALA:O	1.98	0.62
1:A:9:LEU:HD12	1:A:10:SER:H	1.64	0.62
1:A:18:ASN:OD1	1:A:269:GLY:HA3	2.01	0.61
1:A:139:LEU:HD23	1:A:169:TYR:HB3	1.81	0.61
1:A:203:ILE:HD12	1:A:247:GLU:HG2	1.83	0.60
1:A:202:ALA:HB1	1:A:247:GLU:O	2.00	0.60
1:A:29:PRO:HG3	1:A:242:TRP:CE2	2.36	0.60
1:B:100:LYS:HD2	1:B:132:ASP:HB2	1.83	0.60
1:B:45:LYS:O	1:B:47:TRP:N	2.35	0.59
1:B:153:GLY:HA2	1:B:157:GLU:OE1	2.02	0.59
1:B:168:LYS:HB3	1:B:186:PHE:HB3	1.84	0.58
1:B:161:ASP:OD2	1:B:193:SER:HA	2.03	0.58
1:A:45:LYS:O	1:A:47:TRP:N	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:GLY:HA2	1:A:157:GLU:OE1	2.04	0.57
1:A:102:TRP:CZ3	1:A:127:LEU:HD11	2.40	0.57
1:B:206:ILE:HD11	1:B:246:ALA:HA	1.87	0.57
1:A:90:THR:O	1:A:90:THR:HG22	2.05	0.56
1:B:107:ASN:HB3	1:B:124:TYR:HB2	1.86	0.56
1:B:210:THR:CG2	1:B:212:ASN:H	2.19	0.56
1:B:210:THR:HG22	1:B:212:ASN:N	2.18	0.56
1:A:122:THR:HG23	1:A:146:LYS:HD2	1.87	0.56
1:B:139:LEU:HD23	1:B:169:TYR:HB3	1.87	0.56
1:A:210:THR:CG2	1:A:212:ASN:O	2.54	0.55
1:B:90:THR:HG22	1:B:90:THR:O	2.06	0.55
1:A:133:THR:C	1:A:135:LEU:H	2.09	0.55
1:A:164:ARG:HB2	1:A:190:ASP:OD2	2.06	0.55
1:B:164:ARG:HB2	1:B:190:ASP:OD2	2.07	0.55
1:A:193:SER:O	1:A:211:ASN:ND2	2.40	0.55
1:B:9:LEU:HG	1:B:11:ASP:H	1.72	0.54
1:A:93:ASP:OD1	1:A:95:SER:HB3	2.07	0.54
1:A:117:ASP:O	1:A:152:TYR:HA	2.07	0.54
1:A:169:TYR:HE1	1:A:183:TYR:HE2	1.57	0.53
1:B:210:THR:CG2	1:B:212:ASN:O	2.57	0.53
1:A:156:ASN:HA	1:A:159:GLU:OE1	2.08	0.53
1:B:133:THR:C	1:B:135:LEU:H	2.12	0.53
1:A:196:GLY:O	1:A:207:LYS:HD3	2.08	0.53
1:B:229:TYR:N	1:B:229:TYR:CD1	2.76	0.53
1:A:210:THR:O	1:A:241:GLN:NE2	2.36	0.52
1:A:204:ASN:HB3	1:A:206:ILE:HG12	1.91	0.52
1:B:204:ASN:HB3	1:B:206:ILE:HG12	1.90	0.52
1:A:183:TYR:OH	1:A:218:HIS:ND1	2.40	0.52
1:A:9:LEU:HD12	1:A:10:SER:N	2.24	0.52
1:A:26:ARG:HB2	1:A:236:TRP:CD2	2.45	0.52
1:B:49:ASP:OD2	1:B:83:ARG:HB2	2.10	0.52
1:A:210:THR:CG2	1:A:212:ASN:H	2.22	0.52
1:A:219:ILE:HG12	1:A:232:VAL:HG22	1.92	0.52
1:B:122:THR:HG23	1:B:146:LYS:HD2	1.91	0.52
1:A:49:ASP:C	1:A:49:ASP:OD2	2.48	0.52
1:B:76:LEU:HG	1:B:77:PHE:N	2.25	0.51
1:B:202:ALA:HB1	1:B:247:GLU:O	2.11	0.51
1:A:210:THR:HG22	1:A:212:ASN:N	2.24	0.51
1:A:161:ASP:OD2	1:A:193:SER:HA	2.11	0.51
1:A:135:LEU:HD21	1:B:214:ILE:HG21	1.93	0.51
1:A:206:ILE:HD11	1:A:246:ALA:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:20:VAL:HB	1:B:36:TYR:CE1	2.46	0.51
1:A:107:ASN:HB3	1:A:124:TYR:HB2	1.91	0.50
1:A:107:ASN:ND2	1:A:164:ARG:NH1	2.57	0.50
1:A:169:TYR:HE1	1:A:183:TYR:CE2	2.30	0.49
1:A:229:TYR:CD1	1:A:229:TYR:N	2.80	0.49
1:B:203:ILE:HD12	1:B:247:GLU:HG2	1.94	0.49
1:B:107:ASN:ND2	1:B:164:ARG:NH1	2.60	0.49
1:A:20:VAL:HG13	1:A:267:VAL:HG22	1.93	0.49
1:B:93:ASP:OD1	1:B:95:SER:HB3	2.12	0.49
1:A:20:VAL:HB	1:A:36:TYR:CE1	2.48	0.49
1:A:237:HIS:O	1:A:238:ASP:HB2	2.12	0.49
1:A:169:TYR:CE1	1:A:183:TYR:HE2	2.30	0.49
1:A:168:LYS:HB3	1:A:186:PHE:HB3	1.95	0.48
1:B:156:ASN:HA	1:B:159:GLU:OE1	2.14	0.48
1:B:23:TYR:CZ	1:B:24:HIS:CE1	3.03	0.47
1:A:146:LYS:HE3	1:A:148:GLN:OE1	2.13	0.47
1:B:204:ASN:HB2	1:B:247:GLU:H	1.78	0.47
1:A:225:ASP:O	1:A:273:HIS:HE1	1.97	0.47
1:B:237:HIS:O	1:B:238:ASP:HB2	2.14	0.47
1:B:102:TRP:CZ3	1:B:127:LEU:HD11	2.50	0.47
1:A:44:LYS:NZ	1:A:103:TYR:OH	2.48	0.47
1:A:77:PHE:CG	2:A:798:THM:H5'2	2.50	0.47
1:B:53:TYR:CE2	2:B:801:THM:H2'1	2.50	0.46
1:B:169:TYR:CE1	1:B:183:TYR:HE2	2.33	0.46
1:B:53:TYR:CE2	1:B:79:GLU:HB3	2.50	0.46
1:A:113:GLY:HA3	1:A:118:GLY:O	2.16	0.46
1:B:148:GLN:O	1:B:158:ASN:HA	2.16	0.46
1:B:193:SER:O	1:B:211:ASN:ND2	2.48	0.46
1:A:272:PHE:O	1:A:273:HIS:HB3	2.16	0.46
1:B:146:LYS:HE3	1:B:148:GLN:OE1	2.15	0.46
1:B:195:LEU:O	1:B:197:ASP:N	2.41	0.46
1:B:54:ALA:HA	1:B:77:PHE:O	2.15	0.46
1:B:169:TYR:HE1	1:B:183:TYR:CE2	2.35	0.45
1:B:133:THR:C	1:B:135:LEU:N	2.70	0.45
1:A:86:ILE:O	1:A:90:THR:HB	2.17	0.45
1:A:115:ASN:C	1:A:117:ASP:N	2.69	0.45
1:B:16:SER:OG	1:B:228:HIS:HE1	2.00	0.45
1:A:176:LEU:HD22	1:A:177:TRP:N	2.32	0.45
1:B:20:VAL:HG13	1:B:267:VAL:HG22	1.99	0.44
1:B:173:ILE:O	1:B:174:THR:HG23	2.17	0.44
1:A:37:LEU:N	1:A:37:LEU:HD22	2.32	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:16:SER:HB2	1:B:271:ASN:OD1	2.17	0.44
1:B:51:TYR:O	1:B:81:GLU:N	2.43	0.44
1:B:169:TYR:HE1	1:B:183:TYR:HE2	1.64	0.44
1:B:20:VAL:O	1:B:35:THR:HA	2.17	0.44
1:B:120:GLN:HA	1:B:150:GLN:O	2.18	0.44
1:A:16:SER:HB2	1:A:271:ASN:OD1	2.17	0.44
1:B:44:LYS:NZ	1:B:103:TYR:OH	2.51	0.44
1:B:88:LYS:N	1:B:88:LYS:HD2	2.32	0.44
1:B:195:LEU:O	1:B:211:ASN:ND2	2.51	0.43
1:B:9:LEU:HB3	1:B:12:TRP:NE1	2.30	0.43
1:B:232:VAL:HB	1:B:265:TYR:HB2	2.01	0.43
1:A:12:TRP:CD1	1:A:12:TRP:N	2.86	0.43
1:A:38:GLU:HG3	1:A:55:ASP:OD1	2.18	0.43
1:A:122:THR:CG2	1:A:146:LYS:HD2	2.48	0.43
1:B:26:ARG:HB2	1:B:236:TRP:CD2	2.53	0.43
1:A:148:GLN:O	1:A:158:ASN:HA	2.19	0.42
1:A:195:LEU:O	1:A:211:ASN:ND2	2.52	0.42
1:A:133:THR:C	1:A:135:LEU:N	2.70	0.42
1:B:77:PHE:CD2	2:B:799:THM:O5'	2.72	0.42
1:B:75:PRO:CA	1:B:113:GLY:HA2	2.45	0.42
1:B:168:LYS:HB3	1:B:186:PHE:CB	2.48	0.42
1:B:112:MET:O	1:B:113:GLY:O	2.38	0.42
1:B:122:THR:CG2	1:B:146:LYS:HD2	2.49	0.42
1:B:50:PHE:HE1	1:B:80:ILE:HB	1.84	0.42
1:B:210:THR:O	1:B:241:GLN:NE2	2.44	0.42
1:B:110:TYR:CZ	1:B:112:MET:HB2	2.54	0.42
1:B:227:TRP:CE2	1:B:270:TYR:HD1	2.38	0.41
1:A:193:SER:HB3	1:A:211:ASN:O	2.19	0.41
1:B:116:LYS:HB3	1:B:117:ASP:H	1.76	0.41
1:A:16:SER:OG	1:A:228:HIS:HE1	2.03	0.41
1:A:20:VAL:O	1:A:35:THR:HA	2.20	0.41
1:B:167:ILE:O	1:B:167:ILE:HG23	2.20	0.41
1:A:11:ASP:HB2	1:A:12:TRP:HD1	1.85	0.41
1:B:193:SER:HB3	1:B:211:ASN:O	2.21	0.41
1:B:50:PHE:HD1	1:B:82:PRO:HB3	1.87	0.41
1:A:44:LYS:HD2	1:A:49:ASP:HB3	2.04	0.40
1:B:49:ASP:C	1:B:49:ASP:OD2	2.59	0.40
1:B:219:ILE:HG12	1:B:232:VAL:HG22	2.02	0.40
1:B:100:LYS:CD	1:B:132:ASP:HB2	2.51	0.40
1:A:232:VAL:HB	1:A:265:TYR:HB2	2.03	0.40
1:B:26:ARG:O	1:B:239:GLY:HA3	2.21	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	247/278 (89%)	227 (92%)	18 (7%)	2 (1%)	24	63
1	B	244/278 (88%)	219 (90%)	21 (9%)	4 (2%)	12	44
All	All	491/556 (88%)	446 (91%)	39 (8%)	6 (1%)	16	52

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	ASP
1	B	46	ASP
1	A	273	HIS
1	B	113	GLY
1	B	116	LYS
1	B	158	ASN

### 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	212/233 (91%)	204 (96%)	8 (4%)	40	76
1	B	209/233 (90%)	199 (95%)	10 (5%)	31	69
All	All	421/466 (90%)	403 (96%)	18 (4%)	35	72

All (18) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	PHE
1	A	88	LYS
1	A	115	ASN
1	A	117	ASP
1	A	149	TRP
1	A	176	LEU
1	A	222	LEU
1	A	248	LEU
1	B	48	PHE
1	B	76	LEU
1	B	87	ASP
1	B	88	LYS
1	B	115	ASN
1	B	149	TRP
1	B	151	ASN
1	B	176	LEU
1	B	222	LEU
1	B	248	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	30	GLN
1	A	91	ASN
1	A	106	ASN
1	A	107	ASN
1	A	151	ASN
1	A	180	GLN
1	A	188	ASN
1	A	211	ASN
1	A	228	HIS
1	A	243	ASN
1	A	273	HIS
1	B	30	GLN
1	B	91	ASN
1	B	106	ASN
1	B	107	ASN
1	B	151	ASN
1	B	180	GLN
1	B	188	ASN
1	B	211	ASN

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Mol	Chain	Res	Type
1	B	243	ASN

### 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](#)

4 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	THM	A	798	-	13,18,18	1.26	3 (23%)	16,26,26	3.98	3 (18%)
2	THM	A	800	-	13,18,18	1.28	2 (15%)	16,26,26	4.05	3 (18%)
2	THM	B	799	-	13,18,18	1.21	2 (15%)	16,26,26	4.03	3 (18%)
2	THM	B	801	-	13,18,18	1.41	2 (15%)	16,26,26	4.02	3 (18%)

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	THM	A	798	-	-	0/2/18/18	0/2/2/2
2	THM	A	800	-	-	0/2/18/18	0/2/2/2
2	THM	B	799	-	-	0/2/18/18	0/2/2/2
2	THM	B	801	-	-	0/2/18/18	0/2/2/2

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	798	THM	C6-C5	-2.56	1.33	1.40
2	A	798	THM	C6-N1	2.18	1.38	1.35
2	A	800	THM	C6-N1	2.32	1.38	1.35
2	B	799	THM	C6-N1	2.48	1.38	1.35
2	A	798	THM	C4-N3	2.86	1.38	1.33
2	B	799	THM	C4-N3	2.87	1.38	1.33
2	B	801	THM	C6-N1	2.87	1.39	1.35
2	A	800	THM	C4-N3	3.44	1.39	1.33
2	B	801	THM	C4-N3	3.80	1.40	1.33

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	800	THM	C5-C4-N3	-9.14	114.97	125.14
2	B	799	THM	C5-C4-N3	-8.86	115.27	125.14
2	B	801	THM	C5-C4-N3	-8.66	115.49	125.14
2	A	798	THM	C5-C4-N3	-8.36	115.83	125.14
2	A	798	THM	C5M-C5-C6	2.02	122.68	118.62
2	B	799	THM	C5M-C5-C6	2.10	122.86	118.62
2	A	800	THM	C5M-C5-C6	2.23	123.11	118.62
2	B	801	THM	C5M-C5-C6	2.27	123.20	118.62
2	A	800	THM	C4-N3-C2	13.09	126.56	115.25
2	B	801	THM	C4-N3-C2	13.17	126.63	115.25
2	B	799	THM	C4-N3-C2	13.19	126.65	115.25
2	A	798	THM	C4-N3-C2	13.25	126.70	115.25

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	798	THM	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	799	THM	1	0
2	B	801	THM	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	251/278 (90%)	-0.29	0 <span style="border: 1px solid blue; padding: 0 2px;">100</span> <span style="border: 1px solid blue; padding: 0 2px;">100</span>	26, 40, 75, 97	0
1	B	248/278 (89%)	0.16	13 (5%) <span style="border: 1px solid red; padding: 0 2px;">31</span> <span style="border: 1px solid red; padding: 0 2px;">13</span>	35, 80, 125, 165	0
All	All	499/556 (89%)	-0.06	13 (2%) <span style="border: 1px solid blue; padding: 0 2px;">59</span> <span style="border: 1px solid red; padding: 0 2px;">35</span>	26, 52, 111, 165	0

All (13) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	115	ASN	3.9
1	B	13	TRP	3.6
1	B	272	PHE	3.4
1	B	11	ASP	3.3
1	B	116	LYS	2.9
1	B	114	ARG	2.8
1	B	12	TRP	2.8
1	B	9	LEU	2.8
1	B	46	ASP	2.7
1	B	10	SER	2.6
1	B	47	TRP	2.4
1	B	225	ASP	2.3
1	B	156	ASN	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 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(Å <sup>2</sup> )	Q<0.9
2	THM	B	799	17/17	0.92	0.31	1.53	58,61,69,71	0
2	THM	A	798	17/17	0.96	0.20	-0.23	34,38,46,47	0
2	THM	A	800	17/17	0.97	0.17	-0.38	25,27,29,33	0
2	THM	B	801	17/17	0.94	0.20	-0.72	51,53,61,65	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.