



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:32 PM UTC

PDB ID : 1TLW / pdb_00001tlw
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

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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

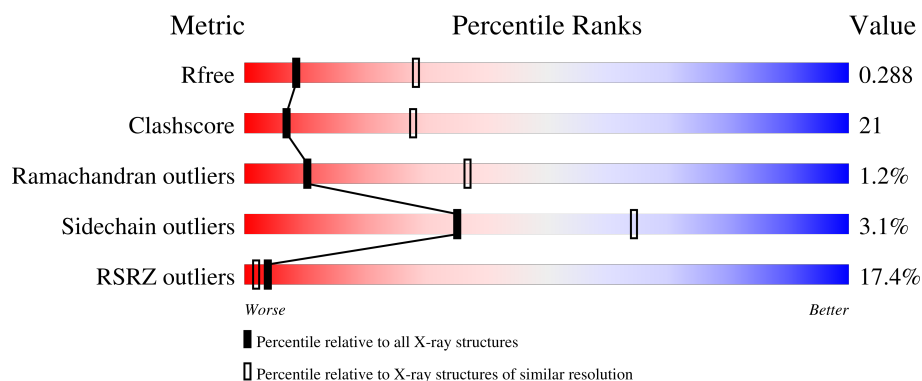
1 Overall quality at a glance

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}	180053	1456 (3.10-3.10)
Clashscore	190562	1539 (3.10-3.10)
Ramachandran outliers	187476	1467 (3.10-3.10)
Sidechain outliers	187428	1467 (3.10-3.10)
RSRZ outliers	180081	1456 (3.10-3.10)

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	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.

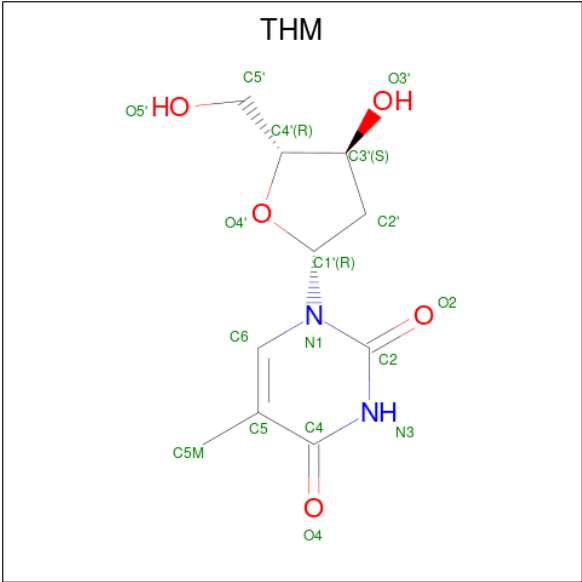
- Molecule 1 is a protein called Nucleoside-specific channel-forming protein tsx.

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 (CCD ID: THM) (formula: C₁₀H₁₄N₂O₅).

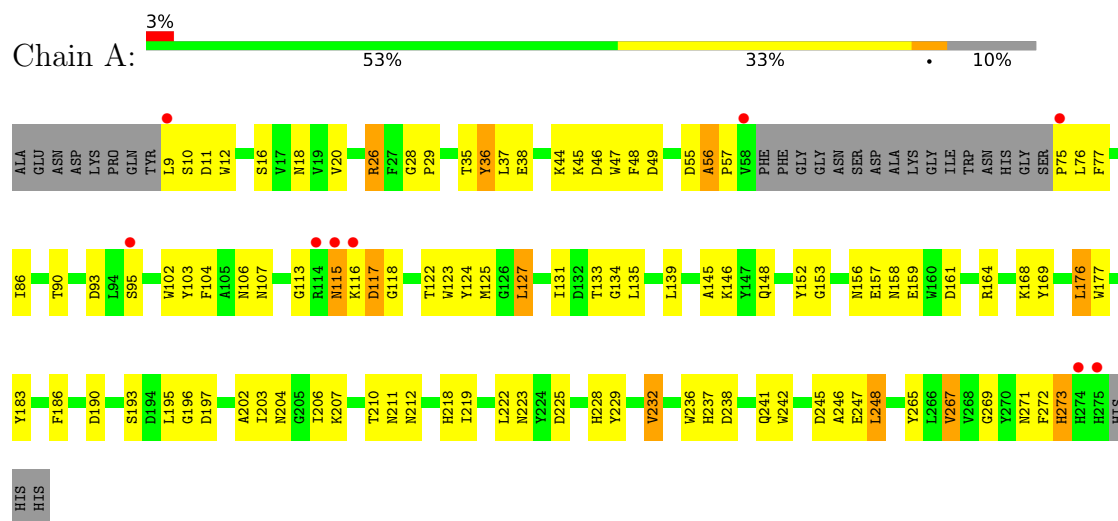


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			17	10	2	5		
2	A	1	Total	C	N	O	0	0
			17	10	2	5		
2	B	1	Total	C	N	O	0	0
			17	10	2	5		
2	B	1	Total	C	N	O	0	0
			17	10	2	5		

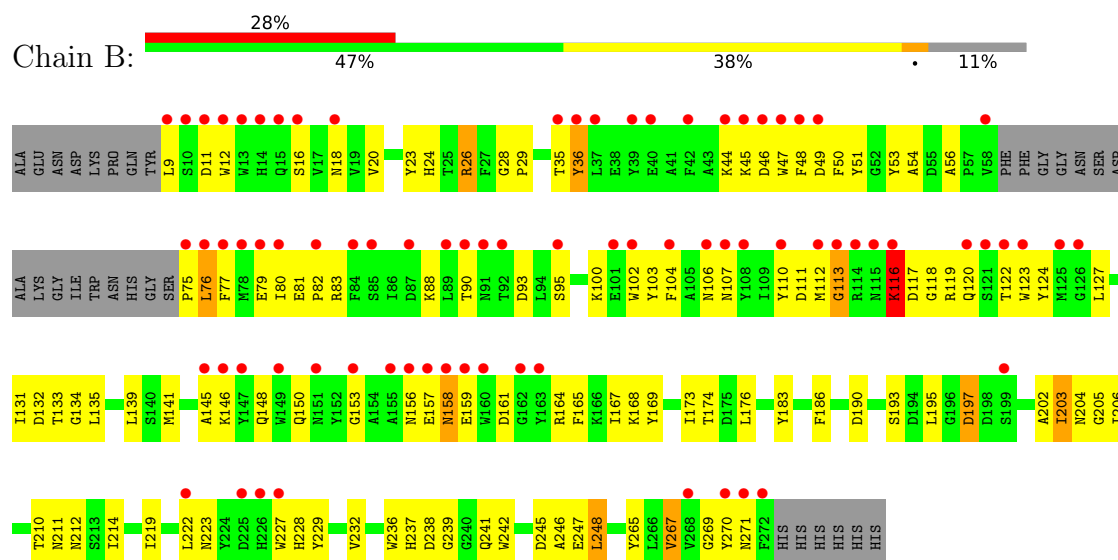
3 Residue-property plots [i](#)

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: 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, α , β , γ	149.65Å 149.65Å 119.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.34 – 3.10 29.34 – 3.10	Depositor EDS
% Data completeness (in resolution range)	97.1 (29.34-3.10) 96.9 (29.34-3.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	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 (6.64%)	wwPDB-VP
Wilson B-factor (Å ²)	59.6	Xtriage
Anisotropy	0.198	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 36.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.026 for -h,-k,l	Xtriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	4194	wwPDB-VP
Average B, all atoms (Å ²)	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.*

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

5.1 Standard geometry

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	0.53	0/2154	1.05	15/2931 (0.5%)
1	B	0.43	0/2121	0.99	13/2886 (0.5%)
All	All	0.48	0/4275	1.02	28/5817 (0.5%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	118	GLY	N-CA-C	8.46	121.85	110.43
1	A	145	ALA	N-CA-C	-8.24	97.36	110.14
1	B	145	ALA	N-CA-C	-8.09	96.77	109.72
1	A	104	PHE	N-CA-C	-7.76	95.91	108.41
1	B	104	PHE	N-CA-C	-7.09	95.51	107.99
1	A	116	LYS	N-CA-C	-6.82	104.69	112.87
1	A	26	ARG	N-CA-C	6.51	120.55	111.56
1	A	28	GLY	CA-C-N	6.29	126.49	119.32
1	A	28	GLY	C-N-CA	6.29	126.49	119.32
1	B	28	GLY	CA-C-N	6.24	125.73	119.24
1	B	28	GLY	C-N-CA	6.24	125.73	119.24
1	B	26	ARG	N-CA-C	6.04	119.90	111.56
1	B	267	VAL	N-CA-C	5.92	116.40	108.11
1	B	197	ASP	N-CA-C	-5.67	105.18	111.36
1	A	267	VAL	N-CA-C	5.64	116.12	107.77
1	A	36	TYR	N-CA-C	5.52	116.53	108.14
1	B	205	GLY	N-CA-C	-5.51	108.14	114.69
1	A	232	VAL	N-CA-C	5.49	115.77	107.75
1	B	203	ILE	N-CA-C	-5.48	104.20	111.05
1	B	134	GLY	N-CA-C	-5.37	108.44	115.47
1	B	36	TYR	N-CA-C	5.32	116.22	108.14
1	A	134	GLY	N-CA-C	-5.26	108.65	115.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	223	ASN	N-CA-C	5.23	117.43	108.90
1	A	56	ALA	CA-C-N	5.20	125.48	119.92
1	A	56	ALA	C-N-CA	5.20	125.48	119.92
1	A	197	ASP	N-CA-C	-5.13	105.60	111.14
1	A	57	PRO	N-CA-C	5.02	119.12	111.34
1	A	223	ASN	N-CA-C	5.01	117.07	108.90

There are no chirality outliers.

There are no planarity outliers.

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	2078	0	1867	79	0
1	B	2048	0	1846	90	0
2	A	34	0	28	1	0
2	B	34	0	28	2	0
All	All	4194	0	3769	168	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 21.

All (168) 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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:B:141:MET:HE2	1:B:165:PHE:HZ	1.62	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:75:PRO:HA	1:B:113:GLY:HA2	1.79	0.62
1:B:111:ASP:O	1:B:119:ARG:HB3	1.99	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:A:133:THR:C	1:A:135:LEU:H	2.09	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
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:49:ASP:C	1:A:49:ASP:OD2	2.48	0.56
1:A:90:THR:HG22	1:A:90:THR:O	2.05	0.56
1:B:107:ASN:HB3	1:B:124:TYR:HB2	1.86	0.56
1:B:133:THR:C	1:B:135:LEU:H	2.12	0.56
1:B:210:THR:CG2	1:B:212:ASN:H	2.19	0.56
1:A:122:THR:HG23	1:A:146:LYS:HD2	1.87	0.56
1:B:210:THR:HG22	1:B:212:ASN:N	2.18	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:THR:HG22	1:B:90:THR:O	2.06	0.55
1:A:164:ARG:HB2	1:A:190:ASP:OD2	2.06	0.55
1:A:193:SER:O	1:A:211:ASN:ND2	2.40	0.55
1:B:164:ARG:HB2	1:B:190:ASP:OD2	2.07	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:A:156:ASN:HA	1:A:159:GLU:OE1	2.08	0.53
1:B:210:THR:CG2	1:B:212:ASN:O	2.57	0.53
1:A:196:GLY:O	1:A:207:LYS:HD3	2.08	0.53
1:B:229:TYR:CD1	1:B:229:TYR:N	2.76	0.53
1:A:204:ASN:HB3	1:A:206:ILE:HG12	1.91	0.52
1:A:210:THR:O	1:A:241:GLN:NE2	2.36	0.52
1:A:9:LEU:HD12	1:A:10:SER:N	2.24	0.52
1:B:204:ASN:HB3	1:B:206:ILE:HG12	1.90	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: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:161:ASP:OD2	1:A:193:SER:HA	2.11	0.51
1:A:210:THR:HG22	1:A:212:ASN:N	2.24	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
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:B:133:THR:C	1:B:135:LEU:N	2.70	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: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:B:107:ASN:ND2	1:B:164:ARG:NH1	2.60	0.49
1:A:115:ASN:C	1:A:117:ASP:N	2.69	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:225:ASP:O	1:A:273:HIS:HE1	1.97	0.47
1:B:204:ASN:HB2	1:B:247:GLU:H	1.78	0.47
1:A:133:THR:C	1:A:135:LEU:N	2.70	0.47
1:A:183:TYR:OH	1:A:218:HIS:ND1	2.40	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:A:12:TRP:CD1	1:A:12:TRP:H	2.34	0.46
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:A:113:GLY:HA3	1:A:118:GLY:O	2.16	0.46
1:B:53:TYR:CE2	1:B:79:GLU:HB3	2.50	0.46
1:B:148:GLN:O	1:B:158:ASN:HA	2.16	0.46
1:A:272:PHE:O	1:A:273:HIS:HB3	2.16	0.46
1:B:193:SER:O	1:B:211:ASN:ND2	2.48	0.46
1:B:54:ALA:HA	1:B:77:PHE:O	2.15	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:169:TYR:HE1	1:B:183:TYR:CE2	2.35	0.45
1:B:49:ASP:OD2	1:B:49:ASP:C	2.59	0.45
1:A:86:ILE:O	1:A:90:THR:HB	2.17	0.45
1:A:176:LEU:HD22	1:A:177:TRP:N	2.32	0.45
1:B:16:SER:OG	1:B:228:HIS:HE1	2.00	0.45
1:A:37:LEU:HD22	1:A:37:LEU:N	2.32	0.44
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: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:A:16:SER:HB2	1:A:271:ASN:OD1	2.17	0.44
1:B:20:VAL:O	1:B:35:THR:HA	2.17	0.44
1:B:44:LYS:NZ	1:B:103:TYR:OH	2.51	0.44
1:B:120:GLN:HA	1:B:150:GLN:O	2.18	0.44
1:B:169:TYR:HE1	1:B:183:TYR:HE2	1.64	0.44
1:B:245:ASP:O	1:B:246:ALA:C	2.59	0.44
1:B:88:LYS:HD2	1:B:88:LYS:N	2.32	0.44
1:B:9:LEU:HB3	1:B:12:TRP:NE1	2.30	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:LEU:O	1:B:211:ASN:ND2	2.51	0.43
1:A:247:GLU:C	1:A:248:LEU:HD13	2.43	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:123:TRP:CD2	1:A:125:MET:HE2	2.54	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:B:77:PHE:CD2	2:B:799:THM:O5'	2.72	0.42
1:A:115:ASN:C	1:A:117:ASP:H	2.26	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:50:PHE:HE1	1:B:80:ILE:HB	1.84	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:110:TYR:CZ	1:B:112:MET:HB2	2.54	0.42
1:B:210:THR:O	1:B:241:GLN:NE2	2.44	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:106:ASN:HD22	1:A:123:TRP:NE1	2.09	0.41
1:B:247:GLU:C	1:B:248:LEU:HD13	2.45	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:219:ILE:HG12	1:B:232:VAL:HG22	2.02	0.40
1:A:232:VAL:HB	1:A:265:TYR:HB2	2.03	0.40
1:B:100:LYS:CD	1:B:132:ASP:HB2	2.51	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

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	247/278 (89%)	227 (92%)	18 (7%)	2 (1%)	16	47
1	B	244/278 (88%)	219 (90%)	21 (9%)	4 (2%)	7	30
All	All	491/556 (88%)	446 (91%)	39 (8%)	6 (1%)	10	37

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

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%)	205 (97%)	7 (3%)	33	63
1	B	209/233 (90%)	203 (97%)	6 (3%)	37	66
All	All	421/466 (90%)	408 (97%)	13 (3%)	35	64

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	48	PHE
1	A	115	ASN
1	A	117	ASP
1	A	127	LEU
1	A	176	LEU
1	A	222	LEU
1	A	248	LEU
1	B	48	PHE
1	B	76	LEU
1	B	116	LYS
1	B	176	LEU
1	B	222	LEU
1	B	248	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	14	HIS
1	A	24	HIS
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	237	HIS
1	A	256	ASN
1	A	273	HIS
1	B	15	GLN
1	B	24	HIS
1	B	30	GLN
1	B	91	ASN
1	B	106	ASN
1	B	107	ASN
1	B	115	ASN
1	B	151	ASN
1	B	180	GLN
1	B	188	ASN
1	B	201	ASN
1	B	211	ASN
1	B	237	HIS

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Mol	Chain	Res	Type
1	B	243	ASN
1	B	256	ASN
1	B	271	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 oligosaccharides 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	800	-	18,18,18	0.34	0	26,26,26	0.37	0
2	THM	A	798	-	18,18,18	0.45	0	26,26,26	0.61	0
2	THM	B	799	-	18,18,18	0.55	0	26,26,26	0.52	0
2	THM	B	801	-	18,18,18	0.86	1 (5%)	26,26,26	0.46	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	THM	A	800	-	-	0/6/18/18	0/2/2/2
2	THM	A	798	-	-	2/6/18/18	0/2/2/2
2	THM	B	799	-	-	0/6/18/18	0/2/2/2
2	THM	B	801	-	-	0/6/18/18	0/2/2/2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	801	THM	C2-N1	2.19	1.41	1.38

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	798	THM	C2'-C1'-N1-C2
2	A	798	THM	C2'-C1'-N1-C6

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
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, 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	251/278 (90%)	0.09	9 (3%) 46 26	26, 40, 75, 97	0
1	B	248/278 (89%)	1.50	78 (31%) 1 1	35, 80, 125, 165	0
All	All	499/556 (89%)	0.79	87 (17%) 4 2	26, 52, 111, 165	0

All (87) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	272	PHE	7.0
1	B	9	LEU	6.2
1	B	75	PRO	5.9
1	B	10	SER	5.9
1	B	47	TRP	5.9
1	B	13	TRP	5.8
1	B	116	LYS	5.7
1	B	48	PHE	5.4
1	B	114	ARG	5.2
1	B	15	GLN	4.6
1	B	44	LYS	4.5
1	B	46	ASP	4.4
1	B	14	HIS	4.2
1	B	155	ALA	4.2
1	A	275	HIS	4.2
1	B	156	ASN	4.1
1	B	12	TRP	3.9
1	B	160	TRP	3.8
1	B	123	TRP	3.8
1	B	108	TYR	3.7
1	B	84	PHE	3.7
1	B	58	VAL	3.6
1	B	89	LEU	3.6
1	B	270	TYR	3.6

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Mol	Chain	Res	Type	RSRZ
1	B	151	ASN	3.5
1	B	162	GLY	3.5
1	A	58	VAL	3.5
1	B	158	ASN	3.5
1	B	271	ASN	3.5
1	B	42	PHE	3.4
1	B	149	TRP	3.4
1	A	9	LEU	3.4
1	B	106	ASN	3.3
1	B	92	THR	3.3
1	B	121	SER	3.2
1	A	75	PRO	3.2
1	B	153	GLY	3.2
1	B	45	LYS	3.1
1	B	39	TYR	3.1
1	B	82	PRO	2.9
1	B	16	SER	2.9
1	B	11	ASP	2.9
1	B	268	VAL	2.8
1	B	115	ASN	2.8
1	B	110	TYR	2.8
1	B	225	ASP	2.8
1	B	125	MET	2.8
1	B	90	THR	2.8
1	B	104	PHE	2.7
1	B	227	TRP	2.7
1	B	122	THR	2.7
1	B	80	ILE	2.6
1	B	120	GLN	2.6
1	B	113	GLY	2.6
1	B	157	GLU	2.6
1	B	95	SER	2.5
1	B	79	GLU	2.5
1	B	107	ASN	2.5
1	A	274	HIS	2.5
1	B	226	HIS	2.5
1	B	85	SER	2.5
1	B	49	ASP	2.5
1	B	199	SER	2.4
1	B	35	THR	2.4
1	B	37	LEU	2.3
1	B	101	GLU	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	163	TYR	2.3
1	B	126	GLY	2.2
1	B	112	MET	2.2
1	A	114	ARG	2.2
1	B	102	TRP	2.2
1	B	147	TYR	2.2
1	B	87	ASP	2.2
1	B	77	PHE	2.2
1	B	40	GLU	2.2
1	A	95	SER	2.1
1	B	145	ALA	2.1
1	B	76	LEU	2.1
1	B	222	LEU	2.1
1	B	18	ASN	2.1
1	B	159	GLU	2.1
1	A	115	ASN	2.1
1	B	146	LYS	2.1
1	B	91	ASN	2.1
1	B	78	MET	2.1
1	A	116	LYS	2.0
1	B	36	TYR	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 oligosaccharides 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($\text{\AA}^2$)	Q<0.9
2	THM	B	799	17/17	0.86	0.16	58,61,69,71	0
2	THM	B	801	17/17	0.89	0.13	51,53,61,65	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	THM	A	798	17/17	0.94	0.12	34,38,46,47	0
2	THM	A	800	17/17	0.96	0.08	25,27,29,33	0

6.5 Other polymers [i](#)

There are no such residues in this entry.