



Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 10:25 PM GMT

PDB ID : 1TLY
Title : Tsx structure
Authors : Ye, J.; van den Berg, B.
Deposited on : 2004-06-10
Resolution : 3.01 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
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (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

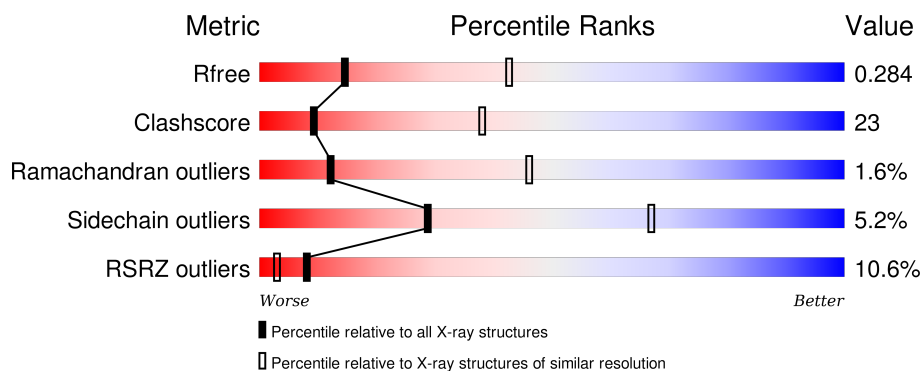
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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	1773 (3.04-3.00)
Clashscore	102246	2117 (3.04-3.00)
Ramachandran outliers	100387	2050 (3.04-3.00)
Sidechain outliers	100360	2053 (3.04-3.00)
RSRZ outliers	91569	1788 (3.04-3.00)

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 on the lower bar indicate the fraction of residues that contain outliers for ≥ 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 is only 1 type of molecule in this entry. The entry contains 4126 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			

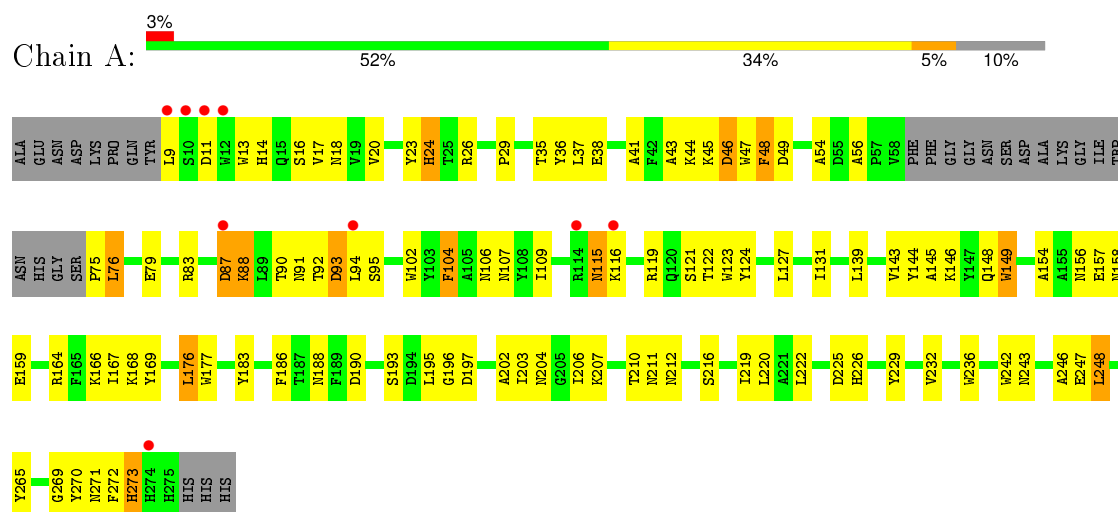
There are 12 discrepancies between the modelled and reference sequences:

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

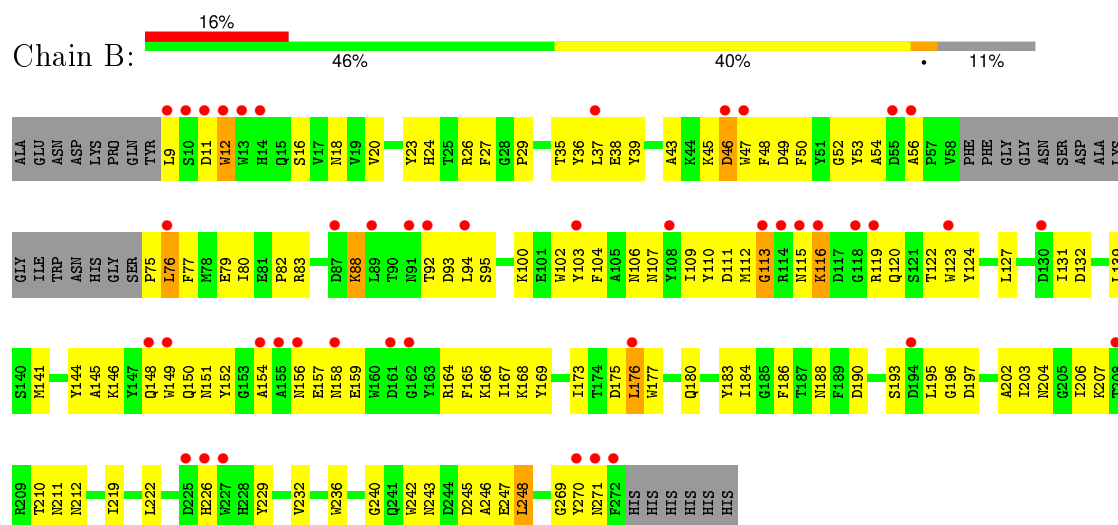
3 Residue-property plots

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, α , β , γ	149.78Å 149.78Å 120.89Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	29.76 – 3.01 49.03 – 3.01	Depositor EDS
% Data completeness (in resolution range)	97.1 (29.76-3.01) 98.5 (49.03-3.01)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.16 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.262 , 0.288 0.263 , 0.284	Depositor DCC
R_{free} test set	2287 reflections (7.39%)	DCC
Wilson B-factor (Å ²)	60.2	Xtriage
Anisotropy	0.213	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.39 , 68.8	EDS
Estimated twinning fraction	0.018 for -h,-k,l	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 60045 reflections	Xtriage
F_o, F_c correlation	0.86	EDS
Total number of atoms	4126	wwPDB-VP
Average B, all atoms (Å ²)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.10% 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, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

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	0.48	0/2154	0.72	2/2931 (0.1%)
1	B	0.38	0/2121	0.66	2/2886 (0.1%)
All	All	0.43	0/4275	0.69	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	-5.67	95.68	111.00
1	B	145	ALA	N-CA-C	-5.35	96.56	111.00
1	A	145	ALA	N-CA-C	-5.28	96.75	111.00
1	A	104	PHE	N-CA-C	-5.11	97.21	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	81	0
1	B	2048	0	1846	98	0
All	All	4126	0	3713	179	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 23.

All (179) 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:75:PRO:HA	1:B:113:GLY:HA2	1.39	1.03
1:A:106:ASN:HD22	1:A:123:TRP:HE1	1.13	0.91
1:B:29:PRO:HG3	1:B:242:TRP:CZ2	2.09	0.88
1:B:112:MET:HA	1:B:119:ARG:HD2	1.59	0.82
1:B:210:THR:HG22	1:B:212:ASN:H	1.44	0.81
1:A:210:THR:HG22	1:A:212:ASN:H	1.47	0.79
1:A:29:PRO:HG3	1:A:242:TRP:CZ2	2.19	0.77
1:B:131:ILE:HB	1:B:139:LEU:HD12	1.67	0.76
1:B:9:LEU:HG	1:B:11:ASP:H	1.52	0.73
1:B:29:PRO:HG3	1:B:242:TRP:CE2	2.24	0.72
1:B:106:ASN:HD22	1:B:123:TRP:HE1	1.35	0.71
1:B:111:ASP:O	1:B:119:ARG:HB3	1.89	0.71
1:B:107:ASN:ND2	1:B:164:ARG:HH11	1.88	0.70
1:A:204:ASN:HB2	1:A:247:GLU:H	1.56	0.69
1:A:131:ILE:HB	1:A:139:LEU:HD12	1.73	0.69
1:B:100:LYS:CG	1:B:132:ASP:HB2	2.23	0.68
1:B:204:ASN:HB2	1:B:247:GLU:H	1.56	0.68
1:A:16:SER:HB2	1:A:271:ASN:OD1	1.92	0.67
1:B:79:GLU:HG3	1:B:109:ILE:HG13	1.76	0.66
1:B:112:MET:HG3	1:B:119:ARG:HH11	1.59	0.66
1:A:102:TRP:CZ3	1:A:127:LEU:HD11	2.30	0.66
1:A:107:ASN:ND2	1:A:164:ARG:HH11	1.94	0.65
1:A:79:GLU:HG3	1:A:109:ILE:HG13	1.78	0.65
1:B:76:LEU:HG	1:B:77:PHE:N	2.12	0.64
1:B:196:GLY:O	1:B:207:LYS:HD3	1.97	0.64
1:A:219:ILE:HG12	1:A:232:VAL:HG22	1.80	0.63
1:B:49:ASP:OD2	1:B:83:ARG:HB2	2.00	0.62
1:A:206:ILE:HD12	1:A:243:ASN:ND2	2.15	0.62
1:A:193:SER:O	1:A:211:ASN:ND2	2.34	0.61
1:A:20:VAL:O	1:A:35:THR:HA	2.01	0.60
1:A:225:ASP:O	1:A:273:HIS:HE1	1.84	0.60
1:B:219:ILE:HG12	1:B:232:VAL:HG22	1.82	0.60
1:A:196:GLY:O	1:A:207:LYS:HD3	2.02	0.59
1:B:18:ASN:OD1	1:B:269:GLY:HA3	2.02	0.58
1:A:210:THR:HG22	1:A:212:ASN:N	2.17	0.58
1:B:100:LYS:HD2	1:B:132:ASP:HB2	1.86	0.58
1:A:17:VAL:HG23	1:A:272:PHE:HE1	1.69	0.57
1:A:45:LYS:O	1:A:47:TRP:N	2.38	0.56
1:B:210:THR:HG22	1:B:212:ASN:N	2.18	0.56
1:A:210:THR:HG22	1:A:212:ASN:O	2.04	0.56
1:B:12:TRP:O	1:B:43:ALA:HA	2.05	0.56

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:18:ASN:OD1	1:A:269:GLY:HA3	2.05	0.56
1:B:16:SER:HB2	1:B:271:ASN:OD1	2.07	0.55
1:B:20:VAL:O	1:B:35:THR:HA	2.05	0.55
1:A:169:TYR:HE1	1:A:183:TYR:HE2	1.53	0.55
1:B:204:ASN:ND2	1:B:245:ASP:O	2.40	0.55
1:B:169:TYR:HE1	1:B:183:TYR:HE2	1.56	0.54
1:B:206:ILE:HD11	1:B:246:ALA:HA	1.89	0.54
1:B:164:ARG:HB2	1:B:190:ASP:OD2	2.08	0.54
1:B:195:LEU:O	1:B:197:ASP:N	2.40	0.53
1:B:110:TYR:CZ	1:B:112:MET:HB2	2.43	0.53
1:A:36:TYR:HB2	1:A:56:ALA:O	2.09	0.53
1:A:102:TRP:CE3	1:A:127:LEU:HD11	2.44	0.53
1:A:210:THR:CG2	1:A:212:ASN:O	2.56	0.53
1:A:131:ILE:HD13	1:A:139:LEU:CD1	2.39	0.52
1:B:206:ILE:HD12	1:B:243:ASN:ND2	2.24	0.52
1:B:100:LYS:HG3	1:B:132:ASP:HB2	1.90	0.52
1:B:45:LYS:O	1:B:47:TRP:N	2.43	0.52
1:B:166:LYS:HD3	1:B:168:LYS:HE3	1.92	0.52
1:B:122:THR:HG23	1:B:146:LYS:HD2	1.92	0.51
1:B:107:ASN:HB3	1:B:124:TYR:HB2	1.92	0.51
1:B:75:PRO:CA	1:B:113:GLY:HA2	2.28	0.51
1:B:9:LEU:HB3	1:B:12:TRP:HE1	1.75	0.51
1:A:272:PHE:O	1:A:273:HIS:HB3	2.11	0.51
1:A:93:ASP:OD1	1:A:95:SER:HB3	2.10	0.51
1:B:139:LEU:HD23	1:B:169:TYR:HB3	1.93	0.50
1:B:100:LYS:CD	1:B:132:ASP:HB2	2.41	0.50
1:A:106:ASN:ND2	1:A:123:TRP:HE1	1.95	0.50
1:B:210:THR:HG22	1:B:212:ASN:O	2.11	0.50
1:A:202:ALA:HB1	1:A:247:GLU:O	2.12	0.50
1:A:109:ILE:N	1:A:109:ILE:HD12	2.27	0.50
1:A:226:HIS:HB3	1:A:270:TYR:CE1	2.47	0.50
1:B:93:ASP:OD1	1:B:95:SER:HB3	2.12	0.50
1:A:203:ILE:HD12	1:A:247:GLU:HG2	1.95	0.49
1:B:193:SER:O	1:B:211:ASN:ND2	2.45	0.49
1:B:156:ASN:HA	1:B:159:GLU:OE1	2.13	0.49
1:A:176:LEU:HD22	1:A:177:TRP:N	2.27	0.49
1:A:102:TRP:HZ3	1:A:127:LEU:HD11	1.75	0.49
1:B:27:PHE:O	1:B:240:GLY:HA3	2.13	0.49
1:B:36:TYR:HB2	1:B:56:ALA:O	2.12	0.49
1:B:107:ASN:HD21	1:B:164:ARG:HH11	1.57	0.49
1:A:131:ILE:HD13	1:A:139:LEU:HD13	1.95	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:156:ASN:HA	1:A:159:GLU:OE1	2.12	0.49
1:B:176:LEU:HD22	1:B:177:TRP:N	2.28	0.48
1:A:23:TYR:O	1:A:24:HIS:HB2	2.12	0.48
1:B:9:LEU:HD21	1:B:11:ASP:HB2	1.94	0.48
1:A:195:LEU:O	1:A:211:ASN:ND2	2.47	0.48
1:B:131:ILE:CB	1:B:139:LEU:HD12	2.40	0.48
1:B:46:ASP:O	1:B:88:LYS:HG2	2.13	0.48
1:B:148:GLN:O	1:B:158:ASN:HA	2.14	0.48
1:B:50:PHE:HE1	1:B:80:ILE:HB	1.79	0.48
1:A:17:VAL:HG23	1:A:272:PHE:CE1	2.49	0.48
1:B:107:ASN:ND2	1:B:164:ARG:NH1	2.61	0.48
1:B:229:TYR:N	1:B:229:TYR:CD1	2.81	0.48
1:A:139:LEU:HD23	1:A:169:TYR:HB3	1.94	0.47
1:A:169:TYR:HE1	1:A:183:TYR:CE2	2.32	0.47
1:A:166:LYS:HD3	1:A:168:LYS:HE3	1.97	0.47
1:B:169:TYR:HE1	1:B:183:TYR:CE2	2.32	0.47
1:B:109:ILE:HD12	1:B:109:ILE:N	2.30	0.47
1:B:38:GLU:HA	1:B:54:ALA:O	2.14	0.47
1:B:103:TYR:O	1:B:127:LEU:HD22	2.15	0.47
1:A:48:PHE:CD2	1:A:48:PHE:O	2.68	0.47
1:A:210:THR:CG2	1:A:212:ASN:H	2.23	0.47
1:B:226:HIS:HB3	1:B:270:TYR:CE1	2.49	0.47
1:A:46:ASP:O	1:A:88:LYS:HG2	2.15	0.47
1:B:23:TYR:O	1:B:24:HIS:HB2	2.15	0.46
1:A:206:ILE:HD11	1:A:246:ALA:HA	1.97	0.46
1:A:26:ARG:HB2	1:A:236:TRP:CD2	2.51	0.46
1:A:92:THR:O	1:A:94:LEU:HG	2.16	0.46
1:A:49:ASP:OD2	1:A:83:ARG:HB2	2.15	0.46
1:B:169:TYR:CE1	1:B:183:TYR:HE2	2.34	0.46
1:B:168:LYS:HB3	1:B:186:PHE:HB3	1.97	0.46
1:A:75:PRO:HG2	1:A:76:LEU:H	1.79	0.46
1:B:115:ASN:ND2	1:B:152:TYR:CD2	2.84	0.46
1:A:154:ALA:O	1:A:157:GLU:HG3	2.15	0.46
1:B:210:THR:CG2	1:B:212:ASN:O	2.64	0.46
1:A:29:PRO:HG3	1:A:242:TRP:CE2	2.50	0.46
1:A:107:ASN:HB3	1:A:124:TYR:HB2	1.97	0.46
1:A:13:TRP:CE3	1:A:43:ALA:HB2	2.51	0.46
1:B:52:GLY:HA2	1:B:79:GLU:O	2.16	0.46
1:A:164:ARG:HB2	1:A:190:ASP:OD2	2.16	0.45
1:A:87:ASP:O	1:A:91:ASN:N	2.49	0.45
1:B:131:ILE:HD13	1:B:139:LEU:HD13	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:26:ARG:HB2	1:B:236:TRP:CD2	2.52	0.45
1:A:38:GLU:HA	1:A:54:ALA:O	2.16	0.45
1:B:76:LEU:HD23	1:B:112:MET:HB3	1.97	0.45
1:A:220:LEU:HD12	1:A:220:LEU:HA	1.84	0.45
1:B:203:ILE:HD12	1:B:247:GLU:HG2	1.99	0.45
1:B:175:ASP:OD1	1:B:180:GLN:HG2	2.17	0.45
1:B:124:TYR:CD2	1:B:146:LYS:HB3	2.52	0.45
1:A:232:VAL:HB	1:A:265:TYR:HB2	1.99	0.44
1:A:169:TYR:CE1	1:A:183:TYR:HE2	2.35	0.44
1:A:148:GLN:O	1:A:158:ASN:HA	2.17	0.44
1:B:107:ASN:HD21	1:B:164:ARG:NH1	2.14	0.44
1:A:37:LEU:N	1:A:37:LEU:HD22	2.32	0.44
1:B:23:TYR:CZ	1:B:24:HIS:CE1	3.06	0.44
1:B:247:GLU:C	1:B:248:LEU:HD13	2.38	0.44
1:B:110:TYR:CE1	1:B:112:MET:HB2	2.53	0.44
1:A:166:LYS:HG3	1:A:188:ASN:HD21	1.83	0.43
1:B:167:ILE:O	1:B:167:ILE:HG23	2.17	0.43
1:B:120:GLN:HA	1:B:150:GLN:O	2.18	0.43
1:B:112:MET:O	1:B:113:GLY:O	2.36	0.43
1:B:202:ALA:HB1	1:B:247:GLU:O	2.19	0.43
1:A:195:LEU:O	1:A:197:ASP:N	2.50	0.43
1:B:195:LEU:O	1:B:211:ASN:ND2	2.52	0.43
1:B:9:LEU:CD2	1:B:11:ASP:HB2	2.49	0.43
1:A:167:ILE:O	1:A:186:PHE:HA	2.18	0.43
1:A:116:LYS:HA	1:A:119:ARG:HH11	1.83	0.43
1:B:39:TYR:O	1:B:53:TYR:HA	2.19	0.43
1:B:122:THR:CG2	1:B:146:LYS:HD2	2.48	0.42
1:B:206:ILE:HD11	1:B:246:ALA:CA	2.50	0.42
1:A:122:THR:HG23	1:A:146:LYS:HD2	2.01	0.42
1:A:9:LEU:HG	1:A:11:ASP:H	1.85	0.42
1:A:14:HIS:O	1:A:41:ALA:HA	2.19	0.42
1:A:229:TYR:N	1:A:229:TYR:CD1	2.87	0.42
1:B:102:TRP:CZ3	1:B:127:LEU:HD11	2.54	0.42
1:B:82:PRO:HG2	1:B:106:ASN:HB2	2.01	0.42
1:B:167:ILE:O	1:B:186:PHE:HA	2.20	0.42
1:B:115:ASN:O	1:B:116:LYS:C	2.57	0.42
1:B:184:ILE:HB	1:B:219:ILE:HB	2.02	0.42
1:A:44:LYS:HD2	1:A:49:ASP:HB3	2.02	0.42
1:A:166:LYS:HG3	1:A:188:ASN:ND2	2.35	0.41
1:A:131:ILE:CB	1:A:139:LEU:HD12	2.46	0.41
1:A:204:ASN:HB2	1:A:247:GLU:HB3	2.01	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:247:GLU:C	1:A:248:LEU:HD13	2.41	0.41
1:A:168:LYS:CB	1:A:186:PHE:HB3	2.50	0.41
1:B:166:LYS:HG3	1:B:188:ASN:ND2	2.36	0.41
1:B:166:LYS:HG3	1:B:188:ASN:HD21	1.84	0.41
1:B:154:ALA:O	1:B:157:GLU:HG3	2.20	0.41
1:A:176:LEU:HD22	1:A:177:TRP:CD1	2.56	0.41
1:A:121:SER:HB3	1:A:149:TRP:HB2	2.03	0.41
1:A:115:ASN:N	1:A:115:ASN:ND2	2.67	0.41
1:B:37:LEU:HD22	1:B:37:LEU:N	2.36	0.41
1:B:203:ILE:HG13	1:B:203:ILE:H	1.74	0.41
1:A:90:THR:HG22	1:A:92:THR:OG1	2.20	0.41
1:B:92:THR:O	1:B:94:LEU:HG	2.20	0.40
1:B:173:ILE:HD11	1:B:183:TYR:HB2	2.01	0.40
1:B:141:MET:HE3	1:B:165:PHE:HZ	1.85	0.40
1:A:49:ASP:C	1:A:49:ASP:OD2	2.60	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%)	226 (92%)	17 (7%)	4 (2%)	12	46
1	B	244/278 (88%)	220 (90%)	20 (8%)	4 (2%)	12	46
All	All	491/556 (88%)	446 (91%)	37 (8%)	8 (2%)	12	46

All (8) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	46	ASP
1	B	46	ASP
1	B	113	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	116	LYS
1	A	93	ASP
1	A	273	HIS
1	B	12	TRP
1	A	76	LEU

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%)	199 (94%)	13 (6%)	23	60
1	B	209/233 (90%)	200 (96%)	9 (4%)	35	74
All	All	421/466 (90%)	399 (95%)	22 (5%)	29	67

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	HIS
1	A	48	PHE
1	A	87	ASP
1	A	88	LYS
1	A	104	PHE
1	A	115	ASN
1	A	143	VAL
1	A	144	TYR
1	A	149	TRP
1	A	176	LEU
1	A	216	SER
1	A	222	LEU
1	A	248	LEU
1	B	48	PHE
1	B	76	LEU
1	B	88	LYS
1	B	144	TYR
1	B	149	TRP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
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 (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	15	GLN
1	A	91	ASN
1	A	106	ASN
1	A	107	ASN
1	A	115	ASN
1	A	151	ASN
1	A	180	GLN
1	A	188	ASN
1	A	211	ASN
1	A	243	ASN
1	A	273	HIS
1	B	15	GLN
1	B	91	ASN
1	B	106	ASN
1	B	107	ASN
1	B	115	ASN
1	B	151	ASN
1	B	158	ASN
1	B	180	GLN
1	B	188	ASN
1	B	211	ASN

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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

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, 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%)	0.23	9 (3%) 46 19	27, 44, 80, 101	0
1	B	248/278 (89%)	1.02	44 (17%) 2 1	40, 84, 131, 172	0
All	All	499/556 (89%)	0.62	53 (10%) 8 3	27, 57, 118, 172	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	9	LEU	11.6
1	B	10	SER	10.5
1	B	11	ASP	6.9
1	B	114	ARG	6.5
1	B	271	ASN	5.3
1	A	11	ASP	5.1
1	B	272	PHE	4.7
1	B	76	LEU	4.2
1	A	9	LEU	4.2
1	B	12	TRP	4.1
1	B	14	HIS	4.1
1	B	225	ASP	4.0
1	A	10	SER	3.7
1	B	37	LEU	3.5
1	B	227	TRP	3.5
1	B	148	GLN	3.5
1	B	56	ALA	3.5
1	B	226	HIS	3.4
1	B	46	ASP	3.4
1	B	13	TRP	3.3
1	B	118	GLY	3.3
1	A	12	TRP	3.3
1	B	115	ASN	3.3
1	B	47	TRP	3.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	B	89	LEU	3.2
1	B	162	GLY	3.2
1	B	91	ASN	3.0
1	B	92	THR	3.0
1	B	87	ASP	3.0
1	B	158	ASN	2.9
1	B	119	ARG	2.8
1	B	156	ASN	2.6
1	A	114	ARG	2.5
1	B	130	ASP	2.5
1	A	87	ASP	2.5
1	B	116	LYS	2.5
1	B	154	ALA	2.4
1	B	161	ASP	2.4
1	B	55	ASP	2.4
1	B	176	LEU	2.4
1	B	270	TYR	2.4
1	B	108	TYR	2.4
1	B	123	TRP	2.3
1	B	103	TYR	2.3
1	B	155	ALA	2.3
1	B	194	ASP	2.2
1	A	94	LEU	2.2
1	B	149	TRP	2.2
1	B	94	LEU	2.2
1	B	208	THR	2.1
1	A	274	HIS	2.1
1	A	116	LYS	2.1
1	B	113	GLY	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands ⓘ

There are no ligands in this entry.

6.5 Other polymers [i](#)

There are no such residues in this entry.