



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 06:22 PM UTC

PDB ID : 2FP9 / pdb_00002fp9
Title : Crystal structure of Native Strictosidine Synthase
Authors : Panjikar, S.
Deposited on : 2006-01-16
Resolution : 2.96 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

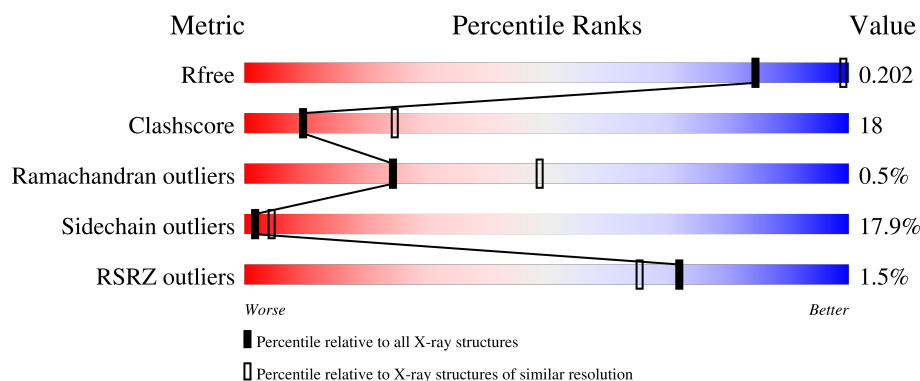
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.96 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	322	
1	B	322	

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	TLA	A	345	-	X	-	-
2	TLA	B	1	-	X	-	-

2 Entry composition [i](#)

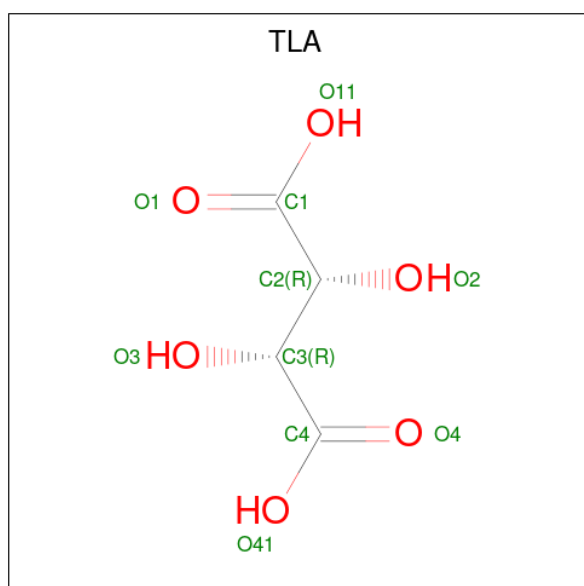
There are 3 unique types of molecules in this entry. The entry contains 4929 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Strictosidine synthase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	305	Total	C	N	O	S	0	0	0
			2405	1546	391	463	5			
1	B	305	Total	C	N	O	S	0	0	0
			2405	1546	391	463	5			

- Molecule 2 is L(+)-TARTARIC ACID (CCD ID: TLA) (formula: C₄H₆O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			10	4	6		
2	B	1	Total	C	O	0	0
			10	4	6		

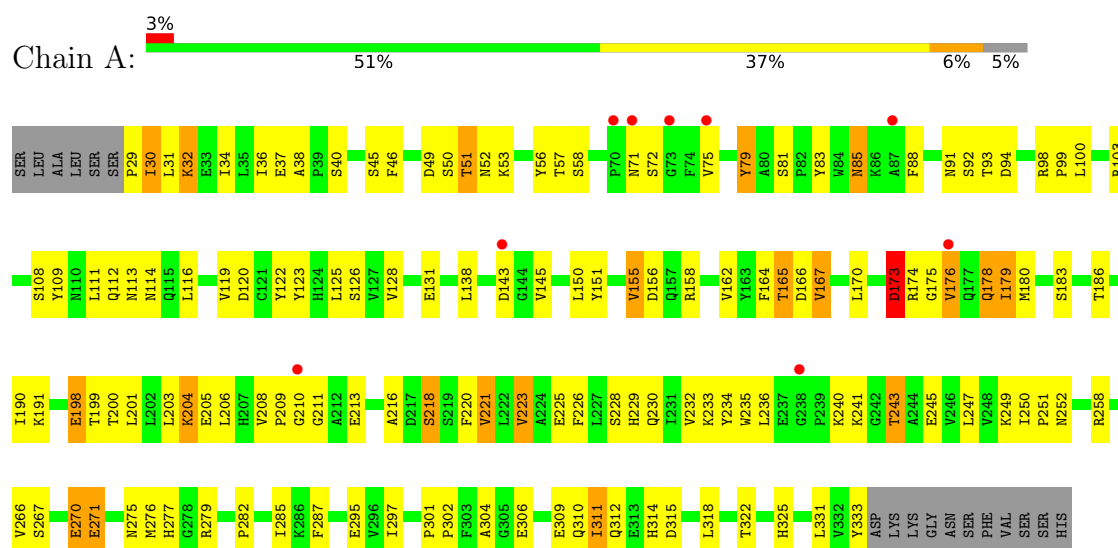
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	41	Total 41	O 41	0	0
3	B	58	Total 58	O 58	0	0

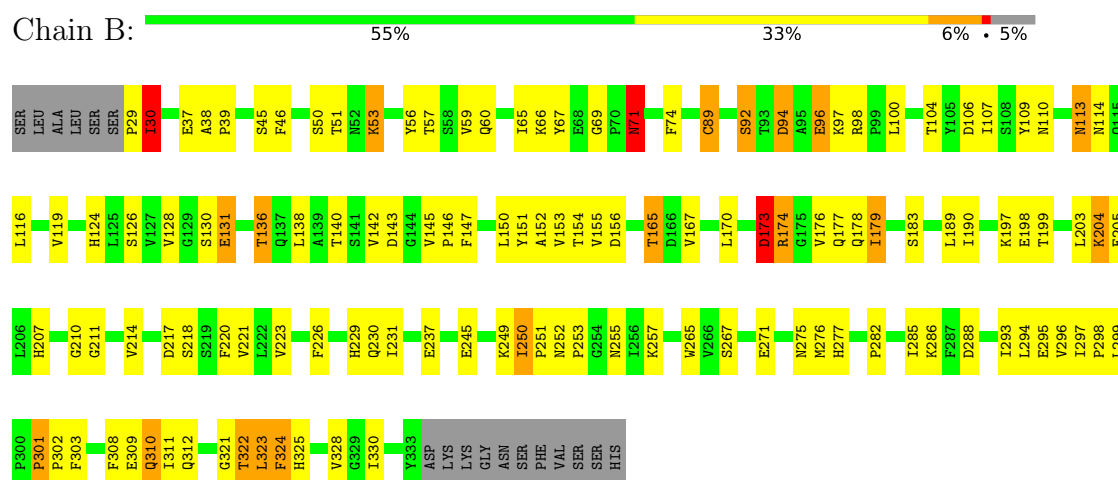
3 Residue-property plots

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: Strictosidine synthase



• Molecule 1: Strictosidine synthase



4 Data and refinement statistics

Property	Value	Source
Space group	H 3	Depositor
Cell constants a, b, c, α , β , γ	150.28Å 150.28Å 122.40Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.96 20.00 – 2.96	Depositor EDS
% Data completeness (in resolution range)	98.5 (20.00-2.96) 98.1 (20.00-2.96)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.13 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.189 , 0.237 (Not available) , 0.202	Depositor DCC
R_{free} test set	1053 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	66.2	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.30 , 47.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.027 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4929	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.83% 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: TLA

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	1.13	6/2471 (0.2%)	1.26	6/3362 (0.2%)
1	B	1.24	7/2471 (0.3%)	1.32	12/3362 (0.4%)
All	All	1.19	13/4942 (0.3%)	1.29	18/6724 (0.3%)

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	30	ILE	CA-CB	9.09	1.65	1.54
1	A	276	MET	SD-CE	7.35	1.98	1.79
1	B	179	ILE	CA-CB	-7.22	1.46	1.54
1	B	330	ILE	CA-CB	-6.52	1.46	1.54
1	A	30	ILE	CA-CB	6.40	1.62	1.54
1	A	176	VAL	CA-CB	6.06	1.61	1.54
1	A	297	ILE	CA-CB	5.65	1.59	1.54
1	A	38	ALA	CA-CB	-5.37	1.45	1.53
1	A	36	ILE	CA-CB	-5.37	1.47	1.54
1	B	301	PRO	CA-C	5.35	1.57	1.52
1	B	37	GLU	CA-C	-5.14	1.46	1.52
1	B	324	PHE	CA-C	-5.13	1.46	1.52
1	B	30	ILE	CA-C	5.12	1.58	1.52

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
1	A	198	GLU	N-CA-C	9.51	122.27	108.86
1	B	30	ILE	N-CA-C	6.63	117.83	108.36
1	B	69	GLY	CA-C-N	6.37	125.87	119.24
1	B	69	GLY	C-N-CA	6.37	125.87	119.24
1	B	328	VAL	N-CA-C	-6.15	99.72	108.58
1	A	210	GLY	N-CA-C	6.13	120.31	112.83

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	173	ASP	N-CA-C	6.03	123.64	110.80
1	B	322	THR	CB-CA-C	-5.93	99.25	111.22
1	B	323	LEU	N-CA-C	-5.83	104.87	113.61
1	B	210	GLY	N-CA-C	5.63	119.70	112.83
1	B	89	CYS	N-CA-C	5.61	120.14	113.12
1	B	198	GLU	N-CA-C	5.49	118.50	109.72
1	B	59	VAL	N-CA-C	5.47	115.49	108.82
1	A	270	GLU	N-CA-CB	5.39	118.03	109.51
1	A	111	LEU	N-CA-C	5.32	117.77	111.33
1	B	173	ASP	N-CA-C	5.32	122.13	110.80
1	A	221	VAL	CB-CA-C	-5.24	102.68	110.33
1	B	146	PRO	CA-C-O	-5.18	115.62	121.43

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	2405	0	2317	82	0
1	B	2405	0	2317	88	0
2	A	10	0	4	0	0
2	B	10	0	4	0	0
3	A	41	0	0	9	0
3	B	58	0	0	8	0
All	All	4929	0	4642	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 18.

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:A:83:TYR:HD2	3:A:382:HOH:O	1.39	1.06
1:A:85:ASN:C	1:A:85:ASN:HD22	1.74	0.96

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:229:HIS:HD2	1:A:252:ASN:H	1.01	0.95
1:B:229:HIS:HD2	1:B:252:ASN:H	1.14	0.94
1:A:311:ILE:HD11	1:A:318:LEU:HD22	1.52	0.92
1:A:49:ASP:OD1	1:A:51:THR:HG22	1.69	0.92
1:A:204:LYS:H	1:A:204:LYS:HD2	1.33	0.91
1:A:229:HIS:CD2	1:A:252:ASN:H	1.88	0.91
1:B:96:GLU:OE1	1:B:96:GLU:N	2.07	0.88
1:B:229:HIS:CD2	1:B:252:ASN:H	1.93	0.86
1:A:83:TYR:CD2	3:A:382:HOH:O	2.21	0.82
1:B:131:GLU:OE2	1:B:131:GLU:N	2.10	0.82
1:B:302:PRO:HD2	1:B:303:PHE:CE2	2.15	0.82
1:A:45:SER:HB2	3:A:355:HOH:O	1.79	0.81
1:B:174:ARG:HG3	1:B:174:ARG:HH11	1.48	0.79
1:A:29:PRO:HG3	1:B:298:PRO:HD2	1.66	0.78
1:A:229:HIS:HD2	1:A:252:ASN:N	1.81	0.75
1:B:288:ASP:HB3	1:B:294:LEU:HD11	1.69	0.75
1:A:85:ASN:C	1:A:85:ASN:ND2	2.45	0.74
1:A:206:LEU:HB2	1:A:209:PRO:HG3	1.69	0.74
1:B:322:THR:HG21	1:B:325:HIS:HD2	1.53	0.74
1:B:71:ASN:HB3	3:B:386:HOH:O	1.86	0.74
1:B:98:ARG:HD3	1:B:173:ASP:OD1	1.88	0.72
1:A:151:TYR:OH	1:A:309:GLU:OE1	2.07	0.72
1:B:131:GLU:H	1:B:131:GLU:CD	2.00	0.70
1:A:204:LYS:HD2	1:A:204:LYS:N	2.01	0.70
1:B:275:ASN:HD22	1:B:277:HIS:H	1.40	0.69
1:B:275:ASN:ND2	1:B:277:HIS:H	1.90	0.69
1:B:301:PRO:HA	3:B:370:HOH:O	1.93	0.67
1:B:94:ASP:N	1:B:94:ASP:OD1	2.28	0.65
1:A:51:THR:HG21	3:A:348:HOH:O	1.98	0.64
1:A:93:THR:HG21	3:A:383:HOH:O	1.98	0.64
1:B:286:LYS:HE3	3:B:350:HOH:O	1.97	0.63
1:A:322:THR:HG21	1:A:325:HIS:HB2	1.81	0.62
1:B:147:PHE:CD2	1:B:150:LEU:HD11	2.34	0.62
1:A:114:ASN:HB3	3:A:371:HOH:O	1.99	0.62
1:B:286:LYS:HB3	1:B:295:GLU:HB2	1.81	0.62
1:A:186:THR:HA	1:A:205:GLU:HA	1.81	0.61
1:B:229:HIS:HD2	1:B:252:ASN:N	1.92	0.61
1:B:276:MET:HE3	1:B:277:HIS:NE2	2.15	0.61
1:A:322:THR:HG21	1:A:325:HIS:CB	2.31	0.60
1:B:309:GLU:HA	1:B:309:GLU:OE1	2.00	0.60
1:B:152:ALA:H	1:B:165:THR:HG22	1.67	0.60

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:217:ASP:O	1:B:218:SER:HB2	2.03	0.59
1:B:249:LYS:C	1:B:250:ILE:HD13	2.27	0.59
1:B:322:THR:HB	1:B:324:PHE:H	1.68	0.59
1:B:67:TYR:HB2	1:B:74:PHE:CE2	2.38	0.58
1:A:213:GLU:OE2	1:A:213:GLU:HA	2.02	0.58
1:A:203:LEU:HB3	1:A:206:LEU:HD21	1.85	0.58
1:A:116:LEU:C	1:A:116:LEU:HD23	2.29	0.58
1:B:257:LYS:HE3	3:B:359:HOH:O	2.02	0.58
1:B:124:HIS:HD2	1:B:140:THR:HG22	1.69	0.57
1:B:282:PRO:HB2	1:B:299:LEU:HD12	1.86	0.56
1:B:204:LYS:HD3	1:B:205:GLU:HB2	1.87	0.56
1:A:122:TYR:HE2	1:A:173:ASP:OD1	1.88	0.56
1:A:208:VAL:HG12	1:A:208:VAL:O	2.04	0.56
1:B:126:SER:HB2	1:B:136:THR:O	2.06	0.56
1:B:226:PHE:HA	1:B:253:PRO:HD2	1.88	0.56
1:A:40:SER:HA	1:A:91:ASN:HD22	1.70	0.55
1:A:310:GLN:NE2	1:A:312:GLN:OE1	2.39	0.55
1:A:93:THR:CG2	3:A:383:HOH:O	2.53	0.55
1:B:110:ASN:OD1	1:B:110:ASN:C	2.50	0.54
1:A:229:HIS:CD2	1:A:251:PRO:HA	2.42	0.54
1:A:226:PHE:CE1	1:A:252:ASN:HB3	2.43	0.54
1:B:124:HIS:CD2	1:B:140:THR:HG22	2.41	0.54
1:B:310:GLN:HE21	1:B:312:GLN:HB3	1.72	0.54
1:B:106:ASP:HB3	1:B:153:VAL:HG12	1.91	0.53
1:B:251:PRO:O	1:B:252:ASN:C	2.50	0.53
1:B:309:GLU:HB2	1:B:321:GLY:O	2.08	0.53
1:B:174:ARG:HG3	1:B:174:ARG:NH1	2.19	0.53
1:B:39:PRO:HA	3:B:399:HOH:O	2.09	0.52
1:A:85:ASN:HD21	1:A:88:PHE:H	1.57	0.52
1:B:231:ILE:N	1:B:231:ILE:HD13	2.25	0.52
1:A:108:SER:OG	1:A:155:VAL:HG23	2.10	0.51
1:A:165:THR:HG21	1:A:209:PRO:O	2.10	0.51
1:A:252:ASN:ND2	1:A:271:GLU:H	2.09	0.51
1:A:233:LYS:HE3	1:A:247:LEU:HD13	1.93	0.51
1:B:46:PHE:HA	1:B:56:TYR:O	2.11	0.51
1:B:45:SER:O	1:B:57:THR:HA	2.11	0.51
1:B:110:ASN:CG	1:B:113:ASN:HD21	2.19	0.51
1:B:71:ASN:HD22	1:B:71:ASN:H	1.59	0.50
1:B:89:CYS:O	1:B:92:SER:HB3	2.10	0.50
1:A:167:VAL:HA	1:A:209:PRO:HD2	1.93	0.50
1:B:142:VAL:HB	1:B:199:THR:HG21	1.94	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:ASN:ND2	1:B:271:GLU:H	2.09	0.50
1:B:252:ASN:HD21	1:B:271:GLU:H	1.59	0.50
1:A:295:GLU:OE2	1:A:333:TYR:OH	2.29	0.50
1:B:302:PRO:HD2	1:B:303:PHE:CD2	2.47	0.50
1:A:81:SER:HB2	1:A:123:TYR:CE2	2.47	0.49
1:A:211:GLY:O	1:A:223:VAL:HA	2.12	0.49
1:B:38:ALA:HB1	1:B:39:PRO:HD2	1.94	0.49
1:A:234:TYR:CD2	1:A:234:TYR:C	2.91	0.49
1:A:243:THR:HG22	3:A:364:HOH:O	2.13	0.49
1:B:109:TYR:HE2	1:B:114:ASN:HD22	1.61	0.47
1:A:155:VAL:HG13	1:A:162:VAL:HG22	1.96	0.47
1:B:151:TYR:OH	1:B:309:GLU:OE1	2.31	0.47
1:B:109:TYR:HE2	1:B:114:ASN:ND2	2.12	0.47
1:B:265:TRP:CH2	1:B:297:ILE:HD12	2.50	0.47
1:A:150:LEU:HD23	1:A:166:ASP:HB2	1.97	0.47
1:A:46:PHE:HA	1:A:56:TYR:O	2.15	0.47
1:A:235:TRP:HB3	1:A:241:LYS:HA	1.97	0.46
1:B:220:PHE:CD1	1:B:220:PHE:C	2.93	0.46
1:B:189:LEU:C	1:B:190:ILE:HG13	2.40	0.46
1:B:130:SER:N	1:B:131:GLU:OE2	2.49	0.46
1:B:189:LEU:HB3	1:B:203:LEU:HB2	1.96	0.46
1:A:266:VAL:CG2	1:A:267:SER:N	2.79	0.45
1:B:71:ASN:H	1:B:71:ASN:ND2	2.13	0.45
1:A:314:HIS:O	1:A:315:ASP:C	2.60	0.45
1:B:293:ILE:HD13	1:B:293:ILE:N	2.31	0.45
1:B:96:GLU:H	1:B:96:GLU:CD	2.07	0.45
1:A:282:PRO:HG3	1:A:304:ALA:HA	1.98	0.45
1:A:318:LEU:HB2	1:A:331:LEU:HB2	1.99	0.44
1:B:153:VAL:HG22	1:B:154:THR:N	2.32	0.44
1:A:225:GLU:O	1:A:226:PHE:C	2.59	0.44
1:A:266:VAL:HG22	1:A:267:SER:N	2.30	0.44
1:B:250:ILE:HD13	1:B:250:ILE:N	2.31	0.44
1:A:119:VAL:HB	1:A:150:LEU:HB3	2.00	0.44
1:A:175:GLY:HA2	1:A:178:GLN:HE22	1.83	0.44
1:B:249:LYS:O	1:B:250:ILE:HD13	2.18	0.43
1:A:98:ARG:O	1:A:99:PRO:C	2.60	0.43
1:B:119:VAL:O	1:B:119:VAL:HG23	2.18	0.43
1:B:53:LYS:HB2	1:B:53:LYS:HZ3	1.83	0.43
1:A:252:ASN:HD21	1:A:271:GLU:H	1.66	0.43
1:B:107:ILE:HB	1:B:116:LEU:HD21	1.99	0.43
1:B:116:LEU:C	1:B:116:LEU:HD23	2.42	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:288:ASP:C	1:B:288:ASP:OD1	2.61	0.43
1:A:125:LEU:HG	1:A:138:LEU:HB2	2.00	0.43
1:B:29:PRO:HA	3:B:392:HOH:O	2.18	0.43
1:A:266:VAL:HG12	1:A:287:PHE:HE2	1.84	0.43
1:A:266:VAL:CG1	1:A:287:PHE:HE2	2.31	0.43
1:B:267:SER:HB2	1:B:308:PHE:CZ	2.54	0.43
1:A:243:THR:HB	3:A:374:HOH:O	2.18	0.43
1:B:178:GLN:O	1:B:179:ILE:C	2.59	0.42
1:B:322:THR:HG21	1:B:325:HIS:CD2	2.43	0.42
1:A:203:LEU:HD23	1:A:203:LEU:HA	1.91	0.42
1:B:113:ASN:C	1:B:113:ASN:HD22	2.27	0.42
1:A:310:GLN:HE21	1:A:312:GLN:HB2	1.85	0.42
1:B:116:LEU:HB3	1:B:128:VAL:HG12	2.02	0.42
1:A:322:THR:HG21	1:A:325:HIS:HB3	2.01	0.42
1:B:113:ASN:H	1:B:113:ASN:ND2	2.18	0.42
1:A:156:ASP:OD2	1:A:218:SER:HB3	2.19	0.42
1:A:164:PHE:CZ	1:A:190:ILE:CG2	3.03	0.42
1:A:216:ALA:HB2	1:A:258:ARG:HD2	2.02	0.42
1:B:142:VAL:HG13	3:B:368:HOH:O	2.19	0.42
1:A:252:ASN:HD22	1:A:270:GLU:HA	1.84	0.42
1:A:45:SER:O	1:A:57:THR:HA	2.20	0.41
1:A:103:ARG:C	1:A:120:ASP:OD1	2.63	0.41
1:A:301:PRO:HA	1:A:302:PRO:HA	1.84	0.41
1:B:138:LEU:HD23	1:B:138:LEU:HA	1.88	0.41
1:A:226:PHE:CZ	1:A:252:ASN:HB3	2.55	0.41
1:A:79:TYR:CD1	1:A:79:TYR:N	2.88	0.41
1:A:85:ASN:ND2	1:A:88:PHE:H	2.18	0.41
1:A:178:GLN:O	1:A:179:ILE:C	2.64	0.41
1:A:250:ILE:HG23	1:A:285:ILE:HD12	2.02	0.41
1:B:211:GLY:HA3	1:B:255:ASN:HA	2.02	0.41
1:A:279:ARG:HE	1:A:279:ARG:HB2	1.69	0.41
1:B:110:ASN:CG	1:B:113:ASN:ND2	2.79	0.41
1:A:251:PRO:O	1:A:252:ASN:C	2.64	0.41
1:A:275:ASN:ND2	1:A:277:HIS:H	2.19	0.41
1:A:213:GLU:OE2	1:A:213:GLU:CA	2.68	0.40
1:A:223:VAL:HG13	1:A:232:VAL:HB	2.02	0.40
1:B:143:ASP:HB2	3:B:368:HOH:O	2.20	0.40
1:A:32:LYS:HG3	1:B:30:ILE:CD1	2.51	0.40
1:B:156:ASP:OD1	1:B:156:ASP:C	2.65	0.40
1:B:109:TYR:CE2	1:B:114:ASN:ND2	2.87	0.40
1:B:176:VAL:O	1:B:177:GLN:C	2.64	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:220:PHE:CD1	1:A:220:PHE:C	3.00	0.40
1:B:285:ILE:HG12	1:B:296:VAL:HG13	2.03	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	303/322 (94%)	284 (94%)	18 (6%)	1 (0%)	36	59
1	B	303/322 (94%)	286 (94%)	15 (5%)	2 (1%)	18	40
All	All	606/644 (94%)	570 (94%)	33 (5%)	3 (0%)	24	49

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	173	ASP
1	B	173	ASP
1	B	71	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	263/278 (95%)	207 (79%)	56 (21%)	1	2

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	263/278 (95%)	225 (86%)	38 (14%)	3	9
All	All	526/556 (95%)	432 (82%)	94 (18%)	2	4

All (94) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	30	ILE
1	A	31	LEU
1	A	32	LYS
1	A	34	ILE
1	A	37	GLU
1	A	50	SER
1	A	51	THR
1	A	52	ASN
1	A	53	LYS
1	A	58	SER
1	A	71	ASN
1	A	72	SER
1	A	75	VAL
1	A	79	TYR
1	A	85	ASN
1	A	92	SER
1	A	94	ASP
1	A	100	LEU
1	A	109	TYR
1	A	112	GLN
1	A	113	ASN
1	A	126	SER
1	A	128	VAL
1	A	131	GLU
1	A	143	ASP
1	A	145	VAL
1	A	155	VAL
1	A	158	ARG
1	A	165	THR
1	A	167	VAL
1	A	170	LEU
1	A	174	ARG
1	A	176	VAL
1	A	178	GLN
1	A	179	ILE
1	A	180	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	183	SER
1	A	191	LYS
1	A	198	GLU
1	A	199	THR
1	A	200	THR
1	A	201	LEU
1	A	204	LYS
1	A	218	SER
1	A	221	VAL
1	A	223	VAL
1	A	228	SER
1	A	230	GLN
1	A	236	LEU
1	A	240	LYS
1	A	243	THR
1	A	245	GLU
1	A	249	LYS
1	A	271	GLU
1	A	306	GLU
1	A	311	ILE
1	B	30	ILE
1	B	50	SER
1	B	51	THR
1	B	53	LYS
1	B	60	GLN
1	B	65	ILE
1	B	66	LYS
1	B	71	ASN
1	B	92	SER
1	B	94	ASP
1	B	96	GLU
1	B	97	LYS
1	B	100	LEU
1	B	104	THR
1	B	113	ASN
1	B	131	GLU
1	B	136	THR
1	B	145	VAL
1	B	155	VAL
1	B	165	THR
1	B	167	VAL
1	B	170	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	173	ASP
1	B	174	ARG
1	B	183	SER
1	B	197	LYS
1	B	204	LYS
1	B	207	HIS
1	B	214	VAL
1	B	221	VAL
1	B	223	VAL
1	B	230	GLN
1	B	237	GLU
1	B	245	GLU
1	B	250	ILE
1	B	310	GLN
1	B	311	ILE
1	B	323	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	52	ASN
1	A	85	ASN
1	A	91	ASN
1	A	112	GLN
1	A	113	ASN
1	A	178	GLN
1	A	229	HIS
1	A	252	ASN
1	A	255	ASN
1	A	275	ASN
1	A	292	ASN
1	A	310	GLN
1	A	312	GLN
1	B	71	ASN
1	B	113	ASN
1	B	137	GLN
1	B	177	GLN
1	B	207	HIS
1	B	229	HIS
1	B	230	GLN
1	B	252	ASN
1	B	259	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	275	ASN
1	B	292	ASN
1	B	310	GLN
1	B	312	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

2 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	TLA	A	345	-	9,9,9	2.98	4 (44%)	12,12,12	1.96	5 (41%)
2	TLA	B	1	-	9,9,9	3.44	7 (77%)	12,12,12	2.00	4 (33%)

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	TLA	A	345	-	-	7/12/12/12	-
2	TLA	B	1	-	-	3/12/12/12	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	TLA	C2-C1	6.39	1.61	1.52
2	A	345	TLA	C2-C1	6.02	1.61	1.52
2	B	1	TLA	O2-C2	4.42	1.50	1.42
2	A	345	TLA	O2-C2	3.99	1.50	1.42
2	B	1	TLA	C3-C4	3.99	1.58	1.52
2	A	345	TLA	C3-C4	3.92	1.58	1.52
2	B	1	TLA	C3-C2	3.34	1.63	1.53
2	B	1	TLA	O3-C3	2.40	1.46	1.42
2	B	1	TLA	O1-C1	2.36	1.29	1.22
2	B	1	TLA	O4-C4	2.32	1.29	1.22
2	A	345	TLA	O4-C4	2.29	1.28	1.22

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	TLA	C2-C3-C4	4.26	119.25	109.82
2	A	345	TLA	C2-C3-C4	3.86	118.37	109.82
2	A	345	TLA	C3-C2-C1	3.24	116.99	109.82
2	B	1	TLA	O3-C3-C4	-3.08	104.10	110.69
2	A	345	TLA	O11-C1-C2	2.67	120.73	113.31
2	B	1	TLA	C3-C2-C1	2.46	115.28	109.82
2	B	1	TLA	O2-C2-C3	2.28	114.81	110.17
2	A	345	TLA	O1-C1-C2	-2.14	115.91	121.62
2	A	345	TLA	O3-C3-C2	-2.08	105.92	110.17

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	345	TLA	C1-C2-C3-C4
2	A	345	TLA	O1-C1-C2-O2
2	A	345	TLA	O11-C1-C2-O2
2	A	345	TLA	O1-C1-C2-C3
2	A	345	TLA	O11-C1-C2-C3
2	A	345	TLA	C1-C2-C3-O3
2	B	1	TLA	C1-C2-C3-O3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
2	A	345	TLA	O2-C2-C3-C4
2	B	1	TLA	O2-C2-C3-C4
2	B	1	TLA	C1-C2-C3-C4

There are no ring outliers.

No monomer is involved in short contacts.

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	305/322 (94%)	0.22	9 (2%) 52 45	12, 20, 27, 66	0
1	B	305/322 (94%)	-0.79	0 100 100	12, 20, 26, 67	0
All	All	610/644 (94%)	-0.28	9 (1%) 72 65	12, 20, 27, 67	0

All (9) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	210	GLY	3.1
1	A	71	ASN	2.9
1	A	73	GLY	2.6
1	A	70	PRO	2.5
1	A	238	GLY	2.5
1	A	75	VAL	2.3
1	A	176	VAL	2.2
1	A	87	ALA	2.1
1	A	143	ASP	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	TLA	B	1	10/10	0.88	0.12	55,66,72,73	0
2	TLA	A	345	10/10	0.90	0.13	74,76,82,83	0

6.5 Other polymers [i](#)

There are no such residues in this entry.