



Full wwPDB X-ray Structure Validation Report

Feb 28, 2014 – 11:17 AM GMT

PDB ID : 2FP9
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 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/ValidationPDFNotes.html>

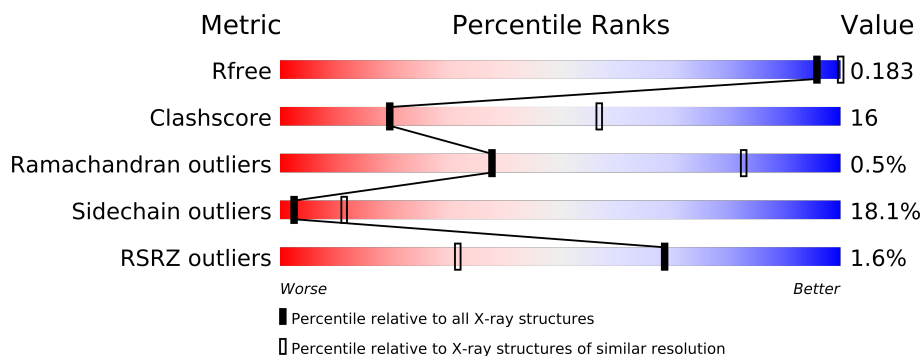
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	1587 (3.00-2.92)
Clashscore	79885	2029 (3.00-2.92)
Ramachandran outliers	78287	1955 (3.00-2.92)
Sidechain outliers	78261	1958 (3.00-2.92)
RSRZ outliers	66119	1588 (3.00-2.92)

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. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	322	
1	B	322	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	TAR	A	345	-	X
2	TAR	B	1	-	X

2 Entry composition i

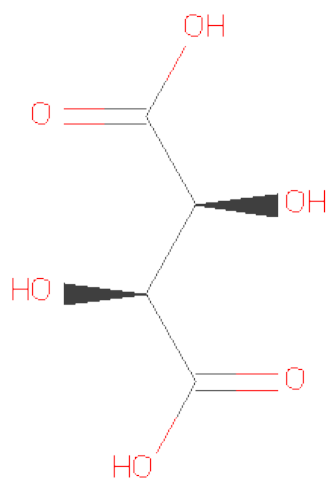
There are 3 unique types of molecules in this entry. The entry contains 4929 atoms, of which 0 are hydrogen and 0 are deuterium.

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 D(-)-TARTARIC ACID (three-letter code: TAR) (formula: C₄H₆O₆).



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

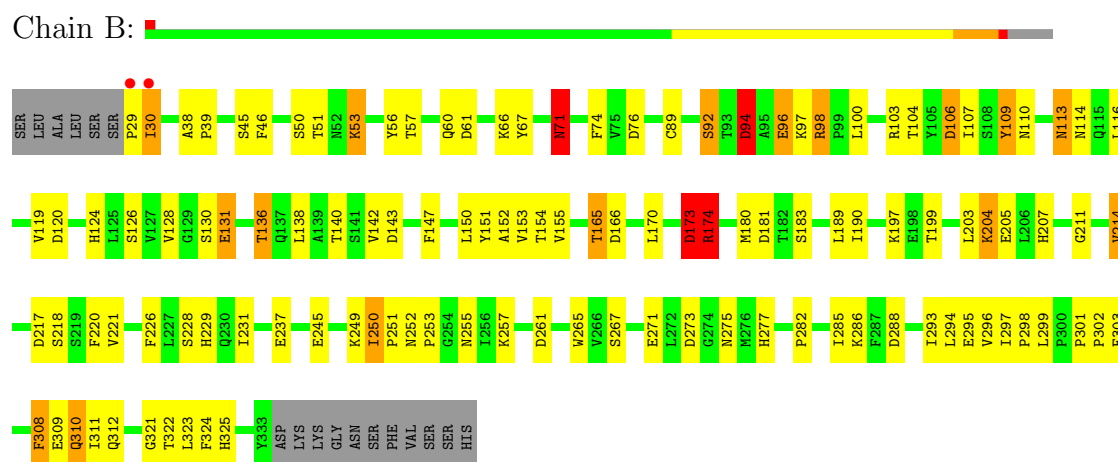
3 Residue-property plots

These plots are drawn for all protein, RNA 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: 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 19.83 – 2.96	Depositor EDS
% Data completeness (in resolution range)	98.5 (20.00-2.96) 98.5 (19.83-2.96)	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 0.190 , 0.183	Depositor DCC
R_{free} test set	1053 reflections (5.25%)	DCC
Wilson B-factor (Å ²)	66.2	Xtriage
Anisotropy	0.084	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 26.2	EDS
Estimated twinning fraction	0.027 for h,-h-k,-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 21097 reflections	Xtriage
F_o, F_c correlation	0.95	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.

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: TAR

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	0.93	0/2471	1.04	7/3362 (0.2%)
1	B	1.00	2/2471 (0.1%)	1.09	12/3362 (0.4%)
All	All	0.96	2/4942 (0.0%)	1.07	19/6724 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	71	ASN	CB-CG	5.31	1.63	1.51
1	B	214	VAL	CB-CG2	-5.07	1.42	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	174	ARG	NE-CZ-NH1	8.67	124.64	120.30
1	A	172	ASP	CB-CG-OD2	7.88	125.39	118.30
1	B	106	ASP	CB-CG-OD2	6.92	124.53	118.30
1	A	261	ASP	CB-CG-OD2	6.92	124.52	118.30
1	B	61	ASP	CB-CG-OD1	6.63	124.26	118.30
1	A	181	ASP	CB-CG-OD2	6.59	124.23	118.30
1	A	61	ASP	CB-CG-OD2	6.55	124.19	118.30
1	B	174	ARG	NE-CZ-NH2	-6.38	117.11	120.30
1	A	106	ASP	CB-CG-OD2	5.80	123.52	118.30
1	B	120	ASP	CB-CG-OD2	5.78	123.50	118.30
1	B	94	ASP	CB-CG-OD2	5.64	123.38	118.30
1	A	143	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	184	ASP	CB-CG-OD2	5.36	123.12	118.30
1	B	273	ASP	CB-CG-OD2	5.31	123.08	118.30
1	B	261	ASP	CB-CG-OD2	5.29	123.06	118.30
1	B	166	ASP	CB-CG-OD2	5.19	122.97	118.30
1	B	180	MET	CG-SD-CE	5.17	108.47	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	98	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	181	ASP	CB-CG-OD2	5.07	122.87	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2405	0	2317	76	0
1	B	2405	0	2317	79	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	153	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 16.

All (153) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:83:TYR:HD2	3:A:382:HOH:O	1.39	1.06
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:85:ASN:C	1:A:85:ASN:HD22	1.74	0.92
1:A:204:LYS:HD2	1:A:204:LYS:H	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:N	1:B:131:GLU:OE2	2.10	0.82

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:B:322:THR:HG21	1:B:325:HIS:HD2	1.53	0.74
1:A:206:LEU:HB2	1:A:209:PRO:HG3	1.69	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:A:85:ASN:C	1:A:85:ASN:ND2	2.45	0.70
1:A:204:LYS:N	1:A:204:LYS:HD2	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:OD1	1:B:94:ASP:N	2.28	0.65
1:B:131:GLU:CD	1:B:131:GLU:H	2.00	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: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
1:B:217:ASP:O	1:B:218:SER:HB2	2.03	0.59
1:B:322:THR:HB	1:B:324:PHE:H	1.68	0.59
1:A:213:GLU:OE2	1:A:213:GLU:HA	2.02	0.58
1:B:67:TYR:HB2	1:B:74:PHE:CE2	2.38	0.58
1:A:203:LEU:HB3	1:A:206:LEU:HD21	1.85	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:B:126:SER:HB2	1:B:136:THR:O	2.06	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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: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:249:LYS:C	1:B:250:ILE:HD13	2.27	0.54
1:B:310:GLN:HE21	1:B:312:GLN:HB3	1.72	0.54
1:B:309:GLU:HB2	1:B:321:GLY:O	2.08	0.53
1:B:106:ASP:HB3	1:B:153:VAL:HG12	1.91	0.53
1:A:116:LEU:C	1:A:116:LEU:HD23	2.29	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:HD13	1:B:231:ILE:N	2.25	0.52
1:A:108:SER:OG	1:A:155:VAL:HG23	2.10	0.51
1:A:252:ASN:ND2	1:A:271:GLU:H	2.09	0.51
1:A:165:THR:HG21	1:A:209:PRO:O	2.10	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: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
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:B:110:ASN:OD1	1:B:110:ASN:C	2.50	0.50
1:A:81:SER:HB2	1:A:123:TYR:CE2	2.47	0.49
1:B:251:PRO:O	1:B:252:ASN:C	2.50	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: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:B:151:TYR:OH	1:B:309:GLU:OE1	2.31	0.47
1:A:155:VAL:HG13	1:A:162:VAL:HG22	1.96	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

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
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:130:SER:N	1:B:131:GLU:OE2	2.49	0.46
1:B:110:ASN:CG	1:B:113:ASN:HD21	2.19	0.46
1:B:189:LEU:HB3	1:B:203:LEU:HB2	1.96	0.46
1:B:71:ASN:ND2	1:B:71:ASN:H	2.13	0.45
1:A:266:VAL:CG2	1:A:267:SER:N	2.79	0.45
1:B:293:ILE:HD13	1:B:293:ILE:N	2.31	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:234:TYR:CD2	1:A:234:TYR:C	2.91	0.44
1:B:250:ILE:N	1:B:250:ILE:HD13	2.31	0.44
1:A:266:VAL:HG22	1:A:267:SER:N	2.30	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:B:119:VAL:O	1:B:119:VAL:HG23	2.18	0.43
1:B:53:LYS:HZ3	1:B:53:LYS:HB2	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: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:322:THR:HG21	1:B:325:HIS:CD2	2.43	0.42
1:A:203:LEU:HA	1:A:203:LEU:HD23	1.91	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:ND2	1:B:113:ASN:H	2.18	0.42
1:B:142:VAL:HG13	3:B:368:HOH:O	2.19	0.42
1:A:156:ASP:OD2	1:A:218:SER:HB3	2.19	0.42
1:A:216:ALA:HB2	1:A:258:ARG:HD2	2.02	0.42
1:A:164:PHE:CZ	1:A:190:ILE:CG2	3.03	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:301:PRO:HA	1:A:302:PRO:HA	1.84	0.41
1:B:220:PHE:CD1	1:B:220:PHE:C	2.93	0.41
1:B:138:LEU:HA	1:B:138:LEU:HD23	1.88	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:226:PHE:CZ	1:A:252:ASN:HB3	2.55	0.41
1:A:85:ASN:ND2	1:A:88:PHE:H	2.18	0.41
1:B:189:LEU:C	1:B:190:ILE:HG13	2.40	0.41
1:A:79:TYR:N	1:A:79:TYR:CD1	2.88	0.41
1:B:211:GLY:HA3	1:B:255:ASN:HA	2.02	0.41
1:A:250:ILE:HG23	1:A:285:ILE:HD12	2.02	0.41
1:A:279:ARG:HB2	1:A:279:ARG:HE	1.69	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:B:143:ASP:HB2	3:B:368:HOH:O	2.20	0.40
1:A:223:VAL:HG13	1:A:232:VAL:HB	2.02	0.40
1:A:314:HIS:O	1:A:315:ASP:C	2.60	0.40
1:A:32:LYS:HG3	1:B:30:ILE:CD1	2.51	0.40
1:B:109:TYR:CE2	1:B:114:ASN:ND2	2.87	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

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	303/322 (94%)	284 (94%)	18 (6%)	1 (0%)	50	88
1	B	303/322 (94%)	286 (94%)	15 (5%)	2 (1%)	30	76
All	All	606/644 (94%)	570 (94%)	33 (5%)	3 (0%)	38	83

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 ⓘ

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%)	206 (78%)	57 (22%)	1	6
1	B	263/278 (95%)	225 (86%)	38 (14%)	5	20
All	All	526/556 (95%)	431 (82%)	95 (18%)	2	11

All (95) 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	71	ASN
1	A	72	SER
1	A	75	VAL
1	A	79	TYR
1	A	83	TYR
1	A	85	ASN
1	A	92	SER
1	A	94	ASP
1	A	100	LEU
1	A	103	ARG
1	A	109	TYR
1	A	112	GLN
1	A	113	ASN
1	A	114	ASN
1	A	126	SER
1	A	131	GLU
1	A	143	ASP
1	A	145	VAL
1	A	155	VAL
1	A	158	ARG

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Mol	Chain	Res	Type
1	A	165	THR
1	A	173	ASP
1	A	174	ARG
1	A	176	VAL
1	A	178	GLN
1	A	180	MET
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	207	HIS
1	A	218	SER
1	A	221	VAL
1	A	223	VAL
1	A	228	SER
1	A	230	GLN
1	A	235	TRP
1	A	236	LEU
1	A	243	THR
1	A	245	GLU
1	A	249	LYS
1	A	255	ASN
1	A	306	GLU
1	A	308	PHE
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	66	LYS
1	B	71	ASN
1	B	76	ASP
1	B	92	SER
1	B	94	ASP
1	B	96	GLU
1	B	97	LYS
1	B	100	LEU
1	B	103	ARG

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Mol	Chain	Res	Type
1	B	104	THR
1	B	109	TYR
1	B	113	ASN
1	B	131	GLU
1	B	136	THR
1	B	155	VAL
1	B	165	THR
1	B	170	LEU
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	228	SER
1	B	237	GLU
1	B	245	GLU
1	B	250	ILE
1	B	308	PHE
1	B	310	GLN
1	B	311	ILE
1	B	323	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	ASN
1	A	91	ASN
1	A	113	ASN
1	A	124	HIS
1	A	178	GLN
1	A	207	HIS
1	A	229	HIS
1	A	252	ASN
1	A	255	ASN
1	A	275	ASN
1	A	310	GLN
1	A	312	GLN
1	B	71	ASN
1	B	113	ASN

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Mol	Chain	Res	Type
1	B	207	HIS
1	B	229	HIS
1	B	230	GLN
1	B	252	ASN
1	B	275	ASN
1	B	292	ASN
1	B	310	GLN
1	B	312	GLN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry ⓘ

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	TAR	A	345	-	9,9,9	3.02	3 (33%)	12,12,12	1.50	3 (25%)
2	TAR	B	1	-	9,9,9	3.85	6 (66%)	12,12,12	1.70	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	TAR	A	345	-	2/2/4/4	0/12/12/12	0/0/0/0
2	TAR	B	1	-	2/2/4/4	0/12/12/12	0/0/0/0

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1	TAR	C2-C1	6.65	1.61	1.52
2	A	345	TAR	C2-C1	6.26	1.61	1.52
2	B	1	TAR	C3-C2	6.12	1.63	1.53
2	B	1	TAR	O2-C2	4.32	1.50	1.42
2	B	1	TAR	C3-C4	4.10	1.58	1.52
2	A	345	TAR	C3-C4	4.04	1.58	1.52
2	A	345	TAR	O2-C2	3.90	1.50	1.42
2	B	1	TAR	O3-C3	2.35	1.46	1.42
2	B	1	TAR	O1-C1	2.31	1.30	1.22

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1	TAR	C2-C3-C4	3.56	119.25	109.90
2	A	345	TAR	C2-C3-C4	3.22	118.37	109.90
2	B	1	TAR	O3-C3-C4	-3.09	104.10	110.73
2	A	345	TAR	C3-C2-C1	2.70	116.99	109.90
2	B	1	TAR	O2-C2-C3	2.23	114.81	110.19
2	A	345	TAR	O3-C3-C2	-2.06	105.92	110.19
2	B	1	TAR	C3-C2-C1	2.05	115.28	109.90

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	1	TAR	C2
2	B	1	TAR	C3
2	A	345	TAR	C2
2	A	345	TAR	C3

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

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	305/322 (94%)	-0.32	8 (2%)	53 24	12, 20, 27, 66	0
1	B	305/322 (94%)	-0.59	2 (0%)	84 44	12, 20, 26, 67	0
All	All	610/644 (94%)	-0.46	10 (1%)	68 32	12, 20, 27, 67	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	112	GLN	2.9
1	A	275	ASN	2.9
1	A	158	ARG	2.9
1	A	143	ASP	2.4
1	A	274	GLY	2.4
1	A	238	GLY	2.4
1	B	29	PRO	2.1
1	B	30	ILE	2.1
1	A	279	ARG	2.0
1	A	51	THR	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 ⓘ

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	TAR	A	345	10/10	0.28	3.05	74,76,82,83	0
2	TAR	B	1	10/10	0.20	2.78	55,66,72,73	0

6.5 Other polymers ⓘ

There are no such residues in this entry.