



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 02:06 AM GMT

PDB ID : 2FPC  
Title : Structure of Strictosidine Synthase, the Biosynthetic Entry to the Monoterpenoid Indole Alkaloid Family  
Authors : Panjikar, S.  
Deposited on : 2006-01-16  
Resolution : 3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.  
We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>  
with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

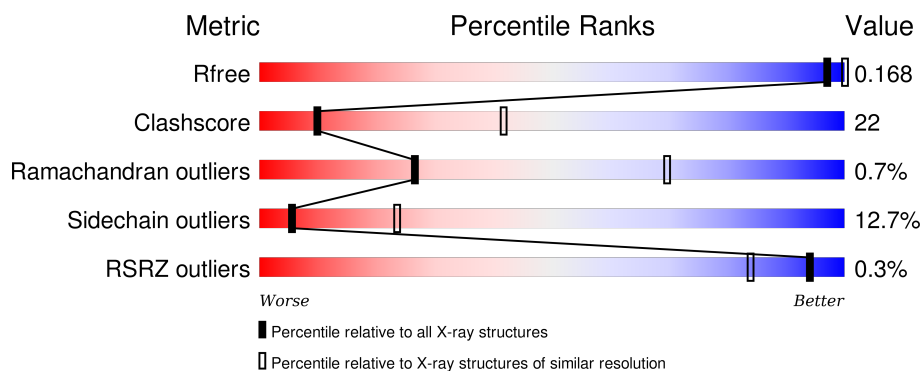
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*



The reported resolution of this entry is 3.00 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	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	322	 49% 38% 7% 6%
1	B	322	 53% 36% 6% 5%

## 2 Entry composition [i](#)

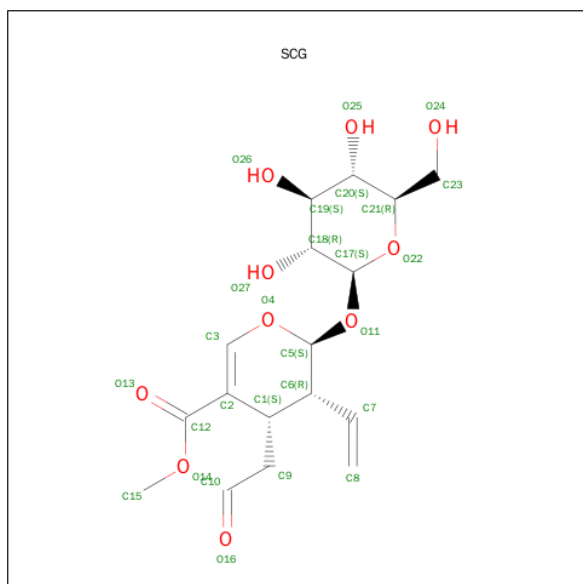
There are 3 unique types of molecules in this entry. The entry contains 4920 atoms, of which 0 are hydrogens and 0 are deuteriums.

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	302	Total	C	N	O	S	0	0	0
			2382	1529	388	460	5			
1	B	302	Total	C	N	O	S	0	0	0
			2382	1529	388	460	5			

- Molecule 2 is SUGAR (METHYL (2S,3R,4S)-2-(BETA-D-GLUCOPYRANOSYLOXY)-4-(2-OXOETHYL)-3-VINYL-3,4-DIHYDRO-2H-PYRAN-5-CARBOXYLATE) (three-letter code: SCG) (formula: C<sub>17</sub>H<sub>24</sub>O<sub>10</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			27	17	10		
2	B	1	Total	C	O	0	0
			27	17	10		

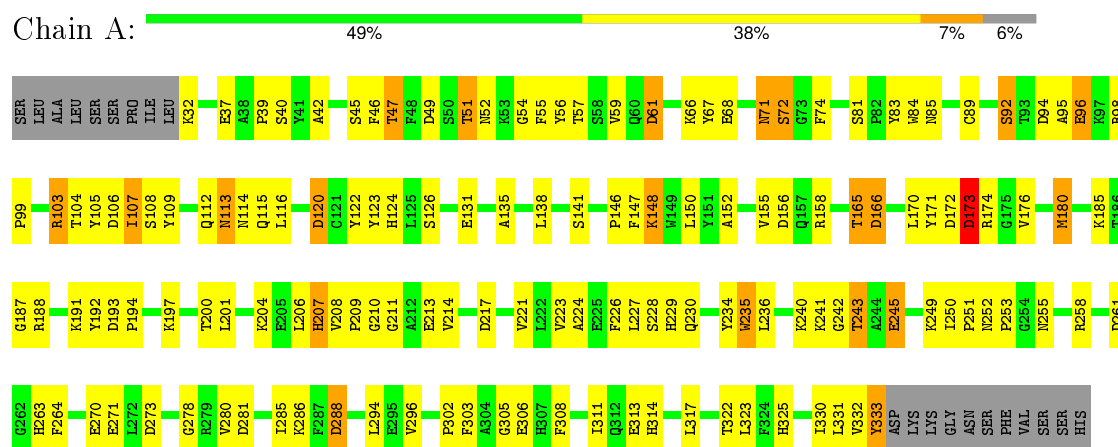
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	55	Total 55	O 55	0	0
3	B	47	Total 47	O 47	0	0

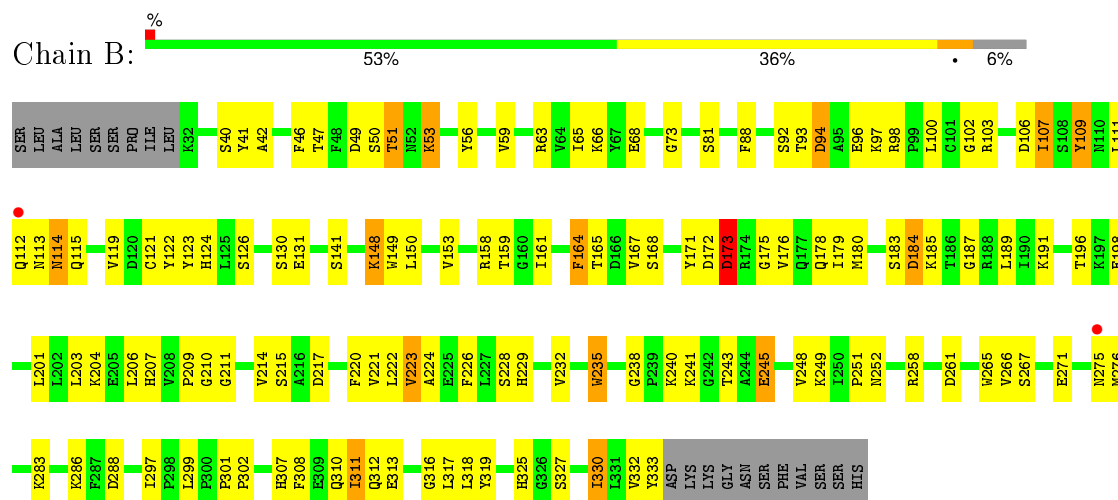
### 3 Residue-property plots

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, $\alpha$ , $\beta$ , $\gamma$	148.61Å 148.61Å 121.07Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.00 19.97 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-3.00) 100.0 (19.97-3.00)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	4.26 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, $R_{free}$	0.186 , 0.240 0.170 , 0.168	Depositor DCC
$R_{free}$ test set	773 reflections (4.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	55.7	Xtriage
Anisotropy	0.734	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 61.2	EDS
Estimated twinning fraction	0.024 for h,-h-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	0 of 19901 reflections	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	4920	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.15% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: SCG

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	0.95	1/2447 (0.0%)	1.01	9/3329 (0.3%)
1	B	0.83	1/2447 (0.0%)	0.97	8/3329 (0.2%)
All	All	0.90	2/4894 (0.0%)	0.99	17/6658 (0.3%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	180	MET	SD-CE	7.74	2.21	1.77
1	B	59	VAL	CB-CG1	-5.01	1.42	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	63	ARG	NE-CZ-NH1	-6.69	116.95	120.30
1	A	120	ASP	CB-CG-OD2	6.64	124.27	118.30
1	A	106	ASP	CB-CG-OD2	6.42	124.08	118.30
1	B	94	ASP	CB-CG-OD2	6.34	124.01	118.30
1	A	288	ASP	CB-CG-OD2	6.14	123.83	118.30
1	A	193	ASP	CB-CG-OD2	6.11	123.79	118.30
1	A	61	ASP	CB-CG-OD2	5.97	123.68	118.30
1	B	288	ASP	CB-CG-OD2	5.93	123.64	118.30
1	B	261	ASP	CB-CG-OD2	5.80	123.52	118.30
1	B	217	ASP	CB-CG-OD2	5.70	123.43	118.30
1	A	261	ASP	CB-CG-OD2	5.40	123.16	118.30
1	B	106	ASP	CB-CG-OD2	5.31	123.08	118.30
1	B	172	ASP	CB-CG-OD2	5.30	123.07	118.30
1	B	184	ASP	CB-CG-OD2	5.21	122.99	118.30
1	A	166	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	156	ASP	CB-CG-OD2	5.15	122.94	118.30
1	A	217	ASP	CB-CG-OD2	5.12	122.91	118.30

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	2382	0	2287	116	0
1	B	2382	0	2287	92	0
2	A	27	0	24	2	0
2	B	27	0	24	5	0
3	A	55	0	0	4	0
3	B	47	0	0	4	0
All	All	4920	0	4622	209	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 22.

All (209) 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:180:MET:CE	1:A:180:MET:SD	2.21	1.28
1:B:229:HIS:HD2	1:B:252:ASN:H	1.13	0.94
1:A:240:LYS:O	1:A:243:THR:HB	1.69	0.93
1:B:122:TYR:OH	1:B:173:ASP:HB2	1.69	0.91
1:A:288:ASP:HB3	1:A:294:LEU:HD11	1.51	0.91
1:A:229:HIS:HD2	1:A:252:ASN:H	1.20	0.89
1:A:229:HIS:CD2	1:A:252:ASN:H	1.92	0.88
1:B:229:HIS:CD2	1:B:252:ASN:H	1.93	0.86
1:B:240:LYS:O	1:B:243:THR:HB	1.73	0.86
1:A:49:ASP:OD1	1:A:51:THR:HG22	1.75	0.84
1:B:201:LEU:HD21	1:B:204:LYS:HB3	1.62	0.81
1:A:103:ARG:HD2	1:A:105:TYR:CE2	2.16	0.81
1:B:313:GLU:HB2	1:B:318:LEU:HD23	1.63	0.80
1:A:122:TYR:OH	1:A:173:ASP:HB2	1.84	0.78
1:A:96:GLU:OE1	1:A:96:GLU:N	2.16	0.78
1:B:51:THR:HG23	1:B:53:LYS:HB2	1.64	0.77
1:A:230:GLN:HE21	1:A:249:LYS:HE3	1.50	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:167:VAL:HA	1:B:209:PRO:HD2	1.67	0.75
1:B:301:PRO:HA	3:B:2044:HOH:O	1.87	0.74
1:B:175:GLY:O	1:B:178:GLN:HB2	1.88	0.73
1:A:322:THR:HG21	1:A:325:HIS:HB2	1.71	0.72
1:B:229:HIS:HD2	1:B:252:ASN:N	1.87	0.72
1:A:71:ASN:HD22	1:A:72:SER:HB2	1.55	0.71
1:B:235:TRP:HZ3	1:B:245:GLU:CD	1.93	0.71
1:B:94:ASP:HB3	1:B:97:LYS:HG3	1.74	0.69
1:A:47:THR:HB	1:A:107:ILE:HG13	1.74	0.69
1:B:226:PHE:CE1	1:B:252:ASN:HB3	2.29	0.68
1:B:159:THR:OG1	1:B:161:ILE:HG12	1.95	0.67
1:B:252:ASN:ND2	1:B:271:GLU:H	1.93	0.67
1:A:67:TYR:HB2	1:A:74:PHE:CE2	2.30	0.66
1:B:211:GLY:H	1:B:224:ALA:HB3	1.61	0.66
1:A:152:ALA:H	1:A:165:THR:HG22	1.60	0.66
1:A:187:GLY:HA3	1:A:209:PRO:CD	2.26	0.66
1:A:235:TRP:HZ3	1:A:245:GLU:CD	1.99	0.66
1:A:263:HIS:HD2	3:A:1022:HOH:O	1.79	0.65
1:B:47:THR:CG2	1:B:107:ILE:HG13	2.26	0.65
1:B:327:SER:O	3:B:2033:HOH:O	2.14	0.65
1:B:47:THR:HG22	1:B:107:ILE:HG13	1.79	0.64
1:B:317:LEU:HD13	1:B:330:ILE:HG21	1.80	0.63
1:A:147:PHE:CD2	1:A:150:LEU:HD11	2.33	0.63
1:A:158:ARG:CB	1:A:158:ARG:HH11	2.11	0.63
1:A:71:ASN:HB2	3:A:1016:HOH:O	1.98	0.63
1:A:229:HIS:HD2	1:A:252:ASN:N	1.95	0.62
1:B:122:TYR:OH	1:B:173:ASP:CB	2.45	0.62
1:A:56:TYR:CE1	1:A:66:LYS:HD2	2.35	0.62
1:A:52:ASN:OD1	1:A:314:HIS:NE2	2.31	0.62
1:B:235:TRP:CZ3	1:B:245:GLU:CD	2.74	0.61
1:B:189:LEU:HB3	1:B:203:LEU:HB2	1.82	0.61
2:B:2001:SCG:H10	3:B:2002:HOH:O	1.98	0.61
1:B:98:ARG:HD3	1:B:173:ASP:OD1	2.01	0.61
1:B:235:TRP:HZ3	1:B:245:GLU:CG	2.14	0.61
1:A:158:ARG:HB2	1:A:158:ARG:NH1	2.15	0.60
1:A:71:ASN:ND2	1:A:72:SER:HB2	2.16	0.60
1:B:176:VAL:O	1:B:180:MET:HG2	2.01	0.60
1:B:41:TYR:CD2	1:B:42:ALA:HB2	2.36	0.60
1:A:141:SER:HB3	1:A:146:PRO:HA	1.84	0.60
1:A:187:GLY:HA3	1:A:209:PRO:HD3	1.83	0.60
1:B:109:TYR:HE2	1:B:114:ASN:HA	1.66	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:187:GLY:HA3	1:B:209:PRO:HD3	1.84	0.59
1:A:56:TYR:CZ	1:A:66:LYS:HD2	2.38	0.59
1:B:229:HIS:CD2	1:B:251:PRO:HA	2.37	0.59
1:A:108:SER:HB3	1:A:155:VAL:HG23	1.84	0.59
1:B:171:TYR:HB2	1:B:179:ILE:HD11	1.85	0.58
1:B:313:GLU:HB2	1:B:318:LEU:CD2	2.30	0.58
1:B:98:ARG:HH11	1:B:173:ASP:HB3	1.69	0.57
1:A:42:ALA:HB1	1:A:323:LEU:HA	1.87	0.57
1:B:49:ASP:OD1	1:B:51:THR:HG22	2.04	0.57
1:B:307:HIS:CD2	2:B:2001:SCG:H81	2.40	0.57
1:A:158:ARG:HB2	1:A:158:ARG:HH11	1.69	0.56
2:A:1001:SCG:H10	3:A:1005:HOH:O	2.05	0.55
1:A:95:ALA:O	1:A:98:ARG:HG3	2.07	0.55
1:A:96:GLU:CD	1:A:96:GLU:H	2.07	0.55
1:B:187:GLY:HA3	1:B:209:PRO:CD	2.37	0.55
1:A:47:THR:HB	1:A:107:ILE:CG1	2.36	0.55
1:A:235:TRP:CZ3	1:A:240:LYS:HD2	2.43	0.54
1:B:122:TYR:HH	1:B:173:ASP:HB2	1.73	0.54
1:A:85:ASN:O	1:A:89:CYS:HB2	2.07	0.54
1:A:98:ARG:N	1:A:99:PRO:CD	2.70	0.54
1:B:56:TYR:CZ	1:B:66:LYS:HD2	2.43	0.54
1:A:191:LYS:HG2	1:A:200:THR:HB	1.90	0.53
1:B:121:CYS:HB3	1:B:122:TYR:CD2	2.43	0.53
1:B:196:THR:OG1	1:B:198:GLU:HB2	2.08	0.53
1:B:56:TYR:CE1	1:B:66:LYS:HD2	2.44	0.53
1:A:313:GLU:CD	1:A:333:TYR:HE2	2.12	0.53
1:A:252:ASN:ND2	1:A:271:GLU:H	2.07	0.53
1:B:109:TYR:CE2	1:B:114:ASN:HA	2.44	0.53
1:A:113:ASN:ND2	1:A:115:GLN:HG3	2.24	0.53
1:B:229:HIS:HD2	1:B:251:PRO:HA	1.74	0.53
1:A:211:GLY:HA3	1:A:255:ASN:HA	1.90	0.52
1:B:121:CYS:HB3	1:B:122:TYR:CE2	2.44	0.52
1:A:81:SER:C	1:A:83:TYR:H	2.13	0.52
1:A:306:GLU:OE2	1:A:325:HIS:NE2	2.40	0.52
1:B:94:ASP:CG	1:B:96:GLU:OE1	2.47	0.52
1:B:276:MET:HE2	2:B:2001:SCG:O11	2.10	0.52
1:A:39:PRO:HA	3:A:1033:HOH:O	2.09	0.52
1:B:153:VAL:HG23	1:B:164:PHE:HB3	1.92	0.52
1:A:104:THR:HA	1:A:120:ASP:HA	1.92	0.51
1:B:41:TYR:HD2	1:B:42:ALA:HB2	1.75	0.51
1:A:191:LYS:CG	1:A:200:THR:HB	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:LEU:HD21	1:A:204:LYS:HB3	1.93	0.51
1:B:265:TRP:HB3	1:B:311:ILE:HG23	1.93	0.51
1:A:46:PHE:HA	1:A:56:TYR:O	2.11	0.51
1:B:319:TYR:CE1	1:B:330:ILE:HD13	2.46	0.51
1:B:307:HIS:HD2	2:B:2001:SCG:O22	1.94	0.50
1:B:308:PHE:HE1	1:B:311:ILE:HB	1.76	0.50
1:A:109:TYR:OH	1:A:114:ASN:ND2	2.32	0.50
1:A:302:PRO:HD2	1:A:303:PHE:CE2	2.46	0.50
1:A:147:PHE:CG	1:A:150:LEU:HD21	2.46	0.50
1:A:148:LYS:HE3	1:A:172:ASP:HB3	1.94	0.50
1:A:264:PHE:O	1:A:286:LYS:HA	2.12	0.50
1:A:229:HIS:HD2	1:A:251:PRO:HA	1.77	0.50
1:B:149:TRP:CH2	2:B:2001:SCG:H152	2.47	0.50
1:A:71:ASN:HD22	1:A:72:SER:CB	2.24	0.50
1:A:214:VAL:O	1:A:258:ARG:NH1	2.45	0.50
1:A:124:HIS:HA	1:A:150:LEU:HD12	1.93	0.49
1:A:313:GLU:CD	1:A:333:TYR:CE2	2.85	0.49
1:A:230:GLN:HB3	1:A:249:LYS:HG2	1.94	0.49
1:A:107:ILE:HB	1:A:116:LEU:HD11	1.94	0.49
1:A:94:ASP:HB3	1:A:96:GLU:OE1	2.12	0.49
1:B:209:PRO:HA	1:B:224:ALA:O	2.12	0.49
1:A:180:MET:CE	1:A:227:LEU:HD21	2.43	0.49
1:A:221:VAL:CG2	1:A:236:LEU:HD11	2.43	0.49
1:A:226:PHE:HA	1:A:253:PRO:HD2	1.95	0.49
1:A:270:GLU:HB3	1:A:281:ASP:HB3	1.95	0.49
1:A:166:ASP:OD2	1:A:188:ARG:NH2	2.39	0.48
1:B:46:PHE:HA	1:B:56:TYR:O	2.14	0.48
1:B:252:ASN:HD22	1:B:271:GLU:H	1.62	0.48
1:A:317:LEU:HD13	1:A:330:ILE:HG21	1.94	0.48
1:A:234:TYR:CZ	1:A:242:GLY:HA2	2.49	0.48
1:A:84:TRP:O	1:A:85:ASN:ND2	2.46	0.48
1:B:265:TRP:HH2	1:B:297:ILE:HD12	1.78	0.48
1:B:94:ASP:OD2	1:B:96:GLU:OE1	2.32	0.48
1:A:138:LEU:HD13	1:A:192:TYR:CE2	2.49	0.47
1:A:40:SER:HB3	1:A:59:VAL:HB	1.97	0.47
1:A:71:ASN:ND2	1:A:72:SER:N	2.63	0.47
1:A:103:ARG:HD2	1:A:105:TYR:CZ	2.49	0.47
1:B:215:SER:HB3	1:B:220:PHE:CZ	2.50	0.47
1:B:187:GLY:HA3	1:B:209:PRO:HG3	1.97	0.47
1:B:124:HIS:HA	1:B:150:LEU:HD12	1.97	0.46
1:B:164:PHE:CD2	1:B:164:PHE:N	2.83	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:VAL:HG12	1:B:332:VAL:O	2.15	0.46
1:B:215:SER:HB3	1:B:220:PHE:CE2	2.51	0.46
1:A:98:ARG:HH11	1:A:173:ASP:HB3	1.80	0.46
1:A:192:TYR:O	1:A:194:PRO:HD3	2.16	0.46
1:A:252:ASN:HD22	1:A:270:GLU:HA	1.80	0.46
1:B:302:PRO:HB2	1:B:325:HIS:CE1	2.50	0.46
1:A:229:HIS:CD2	1:A:251:PRO:HA	2.52	0.45
1:B:98:ARG:O	1:B:102:GLY:N	2.39	0.45
1:A:81:SER:C	1:A:83:TYR:N	2.70	0.45
1:A:54:GLY:HA3	1:A:67:TYR:O	2.17	0.45
1:A:213:GLU:HG2	1:A:258:ARG:HB2	1.99	0.45
1:B:168:SER:OG	1:B:184:ASP:OD2	2.22	0.45
1:A:126:SER:HB2	1:A:135:ALA:HB1	1.97	0.45
1:B:214:VAL:O	1:B:258:ARG:NH1	2.50	0.44
1:A:273:ASP:HB2	1:A:278:GLY:HA3	2.00	0.44
1:A:221:VAL:HG23	1:A:236:LEU:HD11	1.99	0.44
1:B:316:GLY:O	1:B:317:LEU:HD23	2.17	0.44
1:B:81:SER:HB2	1:B:123:TYR:CE2	2.53	0.44
1:A:49:ASP:OD1	1:A:49:ASP:C	2.56	0.44
1:B:299:LEU:HD11	1:B:308:PHE:CD1	2.52	0.44
1:A:45:SER:O	1:A:57:THR:HA	2.17	0.44
1:A:235:TRP:CZ3	1:A:245:GLU:CD	2.87	0.44
1:A:71:ASN:ND2	1:A:72:SER:H	2.15	0.44
1:A:37:GLU:HG3	1:B:73:GLY:HA3	1.99	0.44
1:A:61:ASP:OD1	1:A:61:ASP:C	2.56	0.44
1:B:235:TRP:HZ3	1:B:245:GLU:HG2	1.83	0.43
1:A:138:LEU:HD23	1:A:138:LEU:HA	1.57	0.43
1:A:170:LEU:HD12	1:A:171:TYR:CE2	2.53	0.43
1:A:89:CYS:O	1:A:92:SER:HB3	2.17	0.43
1:B:119:VAL:HG22	1:B:153:VAL:HB	2.01	0.43
1:B:206:LEU:HD13	1:B:223:VAL:HG21	1.99	0.43
1:B:238:GLY:O	1:B:241:LYS:HB2	2.18	0.43
1:B:235:TRP:CZ3	1:B:245:GLU:CG	2.97	0.43
1:A:230:GLN:NE2	1:A:249:LYS:HE3	2.26	0.43
1:A:158:ARG:CB	1:A:158:ARG:NH1	2.77	0.43
1:A:123:TYR:CD2	1:A:123:TYR:N	2.86	0.43
1:A:71:ASN:HD22	1:A:72:SER:N	2.17	0.43
1:B:88:PHE:CE1	1:B:97:LYS:HD3	2.54	0.43
1:A:209:PRO:HA	1:A:224:ALA:O	2.19	0.43
1:B:222:LEU:HA	1:B:232:VAL:O	2.18	0.43
1:A:288:ASP:C	1:A:288:ASP:OD1	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:313:GLU:HA	1:B:317:LEU:O	2.19	0.42
1:B:223:VAL:HG13	1:B:232:VAL:HB	2.00	0.42
1:B:187:GLY:HA3	1:B:209:PRO:CG	2.49	0.42
1:B:302:PRO:HA	3:B:2044:HOH:O	2.18	0.42
1:A:150:LEU:HD23	1:A:166:ASP:HB2	2.02	0.42
1:B:310:GLN:NE2	1:B:312:GLN:OE1	2.53	0.42
1:B:266:VAL:HG22	1:B:267:SER:O	2.20	0.42
1:B:119:VAL:CG2	1:B:153:VAL:HB	2.50	0.42
1:A:32:LYS:HD3	1:A:332:VAL:HG21	2.01	0.42
1:B:148:LYS:HD2	1:B:148:LYS:HA	1.44	0.42
1:A:206:LEU:HD13	1:A:223:VAL:HG21	2.02	0.42
1:A:280:VAL:HB	1:A:305:GLY:O	2.19	0.41
1:A:285:ILE:HG12	1:A:296:VAL:HG22	2.01	0.41
1:B:111:LEU:H	1:B:111:LEU:HG	1.74	0.41
1:A:55:PHE:CE2	1:A:67:TYR:CD2	3.08	0.41
1:B:286:LYS:NZ	1:B:333:TYR:OH	2.53	0.41
1:A:207:HIS:O	1:A:208:VAL:HB	2.20	0.41
1:A:235:TRP:HZ3	1:A:245:GLU:CG	2.33	0.41
1:A:226:PHE:CE1	1:A:252:ASN:HB3	2.55	0.41
1:A:207:HIS:HD2	1:A:228:SER:OG	2.04	0.41
1:A:249:LYS:O	1:A:250:ILE:HD13	2.20	0.41
1:B:40:SER:OG	1:B:41:TYR:N	2.53	0.41
1:A:208:VAL:HG21	1:A:227:LEU:HG	2.02	0.41
1:A:124:HIS:CA	1:A:150:LEU:HD12	2.51	0.40
1:A:85:ASN:HA	1:A:85:ASN:HD22	1.47	0.40
1:A:98:ARG:N	1:A:99:PRO:HD2	2.36	0.40
1:B:175:GLY:HA2	1:B:178:GLN:OE1	2.21	0.40
1:A:176:VAL:HG11	2:A:1001:SCG:H6	2.02	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	300/322 (93%)	280 (93%)	18 (6%)	2 (1%)	26	70
1	B	300/322 (93%)	280 (93%)	18 (6%)	2 (1%)	26	70
All	All	600/644 (93%)	560 (93%)	36 (6%)	4 (1%)	26	70

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	173	ASP
1	A	210	GLY
1	A	173	ASP
1	B	210	GLY

### 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	260/278 (94%)	233 (90%)	27 (10%)	9	32
1	B	260/278 (94%)	221 (85%)	39 (15%)	3	17
All	All	520/556 (94%)	454 (87%)	66 (13%)	5	23

All (66) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	THR
1	A	51	THR
1	A	68	GLU
1	A	71	ASN
1	A	72	SER
1	A	92	SER
1	A	96	GLU
1	A	103	ARG
1	A	107	ILE
1	A	112	GLN
1	A	113	ASN
1	A	131	GLU

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Mol	Chain	Res	Type
1	A	148	LYS
1	A	165	THR
1	A	173	ASP
1	A	174	ARG
1	A	185	LYS
1	A	197	LYS
1	A	207	HIS
1	A	235	TRP
1	A	241	LYS
1	A	243	THR
1	A	245	GLU
1	A	308	PHE
1	A	311	ILE
1	A	331	LEU
1	A	333	TYR
1	B	50	SER
1	B	51	THR
1	B	53	LYS
1	B	65	ILE
1	B	68	GLU
1	B	92	SER
1	B	93	THR
1	B	100	LEU
1	B	103	ARG
1	B	107	ILE
1	B	109	TYR
1	B	112	GLN
1	B	113	ASN
1	B	114	ASN
1	B	115	GLN
1	B	126	SER
1	B	130	SER
1	B	131	GLU
1	B	141	SER
1	B	148	LYS
1	B	158	ARG
1	B	164	PHE
1	B	165	THR
1	B	173	ASP
1	B	183	SER
1	B	185	LYS
1	B	191	LYS

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Mol	Chain	Res	Type
1	B	207	HIS
1	B	221	VAL
1	B	223	VAL
1	B	228	SER
1	B	235	TRP
1	B	245	GLU
1	B	248	VAL
1	B	249	LYS
1	B	275	ASN
1	B	283	LYS
1	B	311	ILE
1	B	330	ILE

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	71	ASN
1	A	85	ASN
1	A	91	ASN
1	A	112	GLN
1	A	113	ASN
1	A	114	ASN
1	A	207	HIS
1	A	229	HIS
1	A	230	GLN
1	A	252	ASN
1	A	263	HIS
1	A	275	ASN
1	A	292	ASN
1	B	91	ASN
1	B	113	ASN
1	B	207	HIS
1	B	229	HIS
1	B	252	ASN
1	B	292	ASN
1	B	307	HIS
1	B	310	GLN
1	B	312	GLN



### 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 ⓘ

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	SCG	A	1001	-	27,28,28	1.48	3 (11%)	30,39,39	1.56	6 (20%)
2	SCG	B	2001	-	27,28,28	2.03	3 (11%)	30,39,39	2.14	8 (26%)

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	SCG	A	1001	-	-	0/17/54/54	0/2/2/2
2	SCG	B	2001	-	-	0/17/54/54	0/2/2/2

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1001	SCG	C6-C1	-2.83	1.51	1.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	2001	SCG	C6-C7	3.19	1.54	1.50
2	A	1001	SCG	O14-C12	3.95	1.42	1.33
2	A	1001	SCG	O4-C3	4.88	1.45	1.35
2	B	2001	SCG	O4-C3	5.80	1.46	1.35
2	B	2001	SCG	O14-C12	6.87	1.49	1.33

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	2001	SCG	O13-C12-C2	-4.57	118.02	124.37
2	B	2001	SCG	O4-C3-C2	-3.22	119.92	125.74
2	A	1001	SCG	O14-C12-O13	-2.76	118.06	123.56
2	A	1001	SCG	O4-C3-C2	-2.45	121.32	125.74
2	B	2001	SCG	O16-C10-C9	-2.41	116.44	125.24
2	A	1001	SCG	O11-C17-O22	-2.04	105.51	110.68
2	B	2001	SCG	C17-O22-C21	2.02	117.67	113.75
2	B	2001	SCG	O26-C19-C18	2.85	116.76	110.34
2	A	1001	SCG	C5-O4-C3	2.95	120.61	116.17
2	A	1001	SCG	C15-O14-C12	3.21	121.94	115.90
2	A	1001	SCG	O14-C12-C2	3.81	117.93	112.66
2	B	2001	SCG	O14-C12-C2	4.36	118.69	112.66
2	B	2001	SCG	C5-O4-C3	4.65	123.17	116.17
2	B	2001	SCG	C15-O14-C12	5.45	126.14	115.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1001	SCG	2	0
2	B	2001	SCG	5	0

## 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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å <sup>2</sup> )	Q<0.9
1	A	302/322 (93%)	-0.75	0	100   100	20, 26, 31, 44	0
1	B	302/322 (93%)	-0.54	2 (0%)	89   70	20, 26, 31, 39	0
All	All	604/644 (93%)	-0.64	2 (0%)	94   84	20, 26, 32, 44	0

All (2) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	275	ASN	4.2
1	B	112	GLN	2.3

### 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

### 6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

### 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled ‘Q< 0.9’ lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
2	SCG	B	2001	27/27	0.84	0.26	1.56	56,63,71,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
2	SCG	A	1001	27/27	0.92	0.16	0.41	48,54,63,67	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.