



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 03:45 AM UTC

PDB ID : 2V91 / pdb_00002v91
Title : STRUCTURE OF STRICTOSIDINE SYNTHASE IN COMPLEX WITH
STRICTOSIDINE
Authors : Loris, E.A.; Panjikar, S.; Ruppert, M.; Barleben, L.; Unger, M.; Stoeckigt, J.
Deposited on : 2007-08-16
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

<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
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

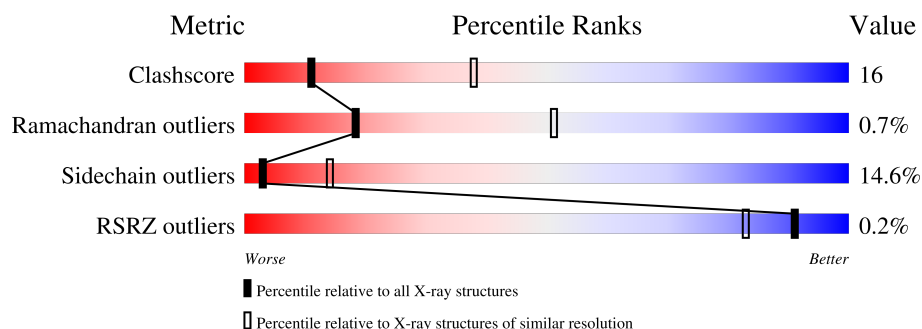
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.01 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))
Clashscore	190562	3444 (3.04-3.00)
Ramachandran outliers	187476	3319 (3.04-3.00)
Sidechain outliers	187428	3322 (3.04-3.00)
RSRZ outliers	180081	3130 (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 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	302	
1	B	302	

2 Entry composition [i](#)

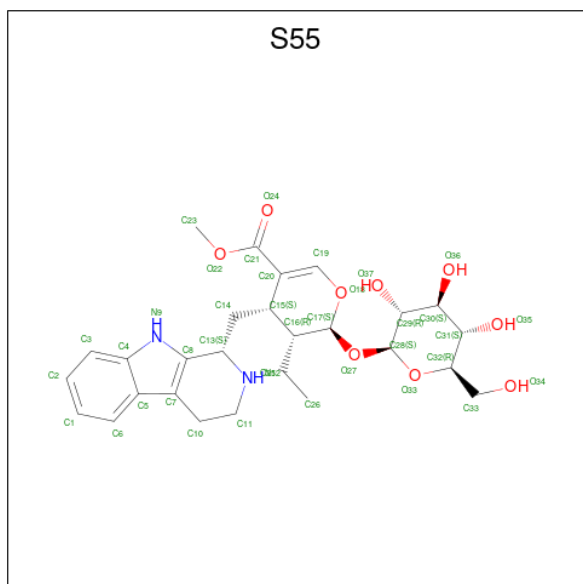
There are 3 unique types of molecules in this entry. The entry contains 4858 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			2363	1511	388	459	5			
1	B	302	Total	C	N	O	S	0	0	0
			2364	1512	388	459	5			

- Molecule 2 is METHYL (2S,3R,4S)-3-ETHYL-2-(BETA-D-GLUCOPYRANOSYLOXY)-4-[(1S)-2,3,4,9-TETRAHYDRO-1H-BETA-CARBOLIN-1-YLMETHYL]-3,4-DIHYDRO-2H-PYRAN-5-CARBOXYLATE (CCD ID: S55) (formula: C₂₇H₃₆N₂O₉).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			38	27	2	9		
2	B	1	Total	C	N	O	0	0
			38	27	2	9		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	35	Total 35	O 35	0	0
3	B	20	Total 20	O 20	0	0

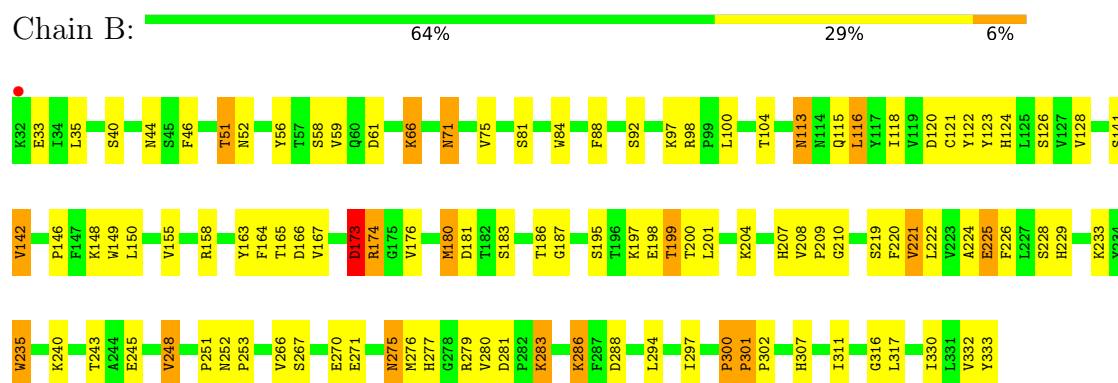
3 Residue-property plots

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	150.18Å 150.18Å 121.71Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 3.01 20.00 – 3.01	Depositor EDS
% Data completeness (in resolution range)	100.0 (20.00-3.01) 99.7 (20.00-3.01)	Depositor EDS
R_{merge}	0.13	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.47 (at 2.98Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.192 , 0.235 0.181 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	60.4	Xtriage
Anisotropy	0.758	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 38.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	4858	wwPDB-VP
Average B, all atoms (Å ²)	27.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: S55

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	1.05	2/2428 (0.1%)	1.20	9/3309 (0.3%)
1	B	0.99	5/2429 (0.2%)	1.15	8/3311 (0.2%)
All	All	1.02	7/4857 (0.1%)	1.17	17/6620 (0.3%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	180	MET	SD-CE	11.54	2.08	1.79
1	B	180	MET	SD-CE	8.48	2.00	1.79
1	B	297	ILE	CA-CB	8.22	1.62	1.53
1	A	250	ILE	CA-CB	5.97	1.61	1.54
1	B	311	ILE	CA-CB	5.72	1.61	1.54
1	B	248	VAL	CA-CB	5.48	1.61	1.55
1	B	164	PHE	CA-C	-5.25	1.46	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	301	PRO	N-CA-C	11.11	124.26	110.70
1	B	301	PRO	N-CA-C	9.44	122.21	110.70
1	A	300	PRO	CA-C-N	6.50	127.08	120.38
1	A	300	PRO	C-N-CA	6.50	127.08	120.38
1	B	174	ARG	N-CA-C	-6.47	105.01	113.17
1	A	315	ASP	CB-CA-C	-6.20	103.09	111.89
1	B	300	PRO	CA-C-N	5.86	126.42	120.38
1	B	300	PRO	C-N-CA	5.86	126.42	120.38
1	B	221	VAL	CB-CA-C	-5.76	101.95	110.82
1	A	301	PRO	CA-C-O	-5.61	112.43	120.56
1	B	198	GLU	N-CA-C	5.42	118.31	109.59
1	B	311	ILE	N-CA-C	-5.36	100.61	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	302	PRO	N-CA-C	-5.30	106.49	113.65
1	A	257	LYS	N-CA-C	5.29	117.01	108.34
1	A	222	LEU	N-CA-C	-5.12	101.81	109.95
1	B	173	ASP	N-CA-C	5.09	121.64	110.80
1	A	89	CYS	N-CA-C	5.04	119.39	112.68

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	2363	0	2201	75	0
1	B	2364	0	2202	70	0
2	A	38	0	36	7	0
2	B	38	0	36	5	0
3	A	35	0	0	3	0
3	B	20	0	0	0	0
All	All	4858	0	4475	152	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 16.

All (152) 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	2.08	1.41
2:A:1334:S55:H263	2:A:1334:S55:H13	1.26	1.13
1:B:229:HIS:CD2	1:B:252:ASN:H	1.91	0.88
2:B:1334:S55:H263	2:B:1334:S55:H13	1.63	0.80
1:B:141:SER:HB3	1:B:146:PRO:HA	1.65	0.79
1:B:229:HIS:HD2	1:B:251:PRO:HA	1.49	0.77
1:A:229:HIS:CD2	1:A:252:ASN:H	2.03	0.77
1:A:221:VAL:HG22	1:A:236:LEU:HD11	1.68	0.76
1:A:131:GLU:H	1:A:131:GLU:CD	1.97	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:142:VAL:HG23	1:B:199:THR:HB	1.69	0.72
1:B:252:ASN:ND2	1:B:271:GLU:H	1.87	0.72
1:B:124:HIS:HA	1:B:150:LEU:HD12	1.73	0.71
1:A:116:LEU:HD12	1:A:117:TYR:N	2.05	0.70
1:B:229:HIS:HD2	1:B:252:ASN:H	1.38	0.69
1:A:141:SER:HB2	1:A:146:PRO:HA	1.74	0.68
1:B:229:HIS:CD2	1:B:251:PRO:HA	2.29	0.67
1:A:308:PHE:O	2:A:1334:S55:H112	1.93	0.67
1:A:252:ASN:ND2	1:A:271:GLU:H	1.93	0.65
1:B:280:VAL:HG21	1:B:307:HIS:CE1	2.32	0.64
1:A:80:ALA:HB1	3:A:2018:HOH:O	1.96	0.64
1:A:191:LYS:HD3	1:A:200:THR:HB	1.80	0.64
1:A:288:ASP:HB3	1:A:294:LEU:HD11	1.80	0.64
1:A:158:ARG:HH11	1:A:158:ARG:CB	2.11	0.63
1:B:276:MET:HE3	2:B:1334:S55:H252	1.80	0.63
1:A:71:ASN:HD22	1:A:72:SER:HB2	1.63	0.62
1:A:158:ARG:HH11	1:A:158:ARG:HB2	1.64	0.62
1:B:252:ASN:HD22	1:B:270:GLU:HA	1.66	0.61
2:A:1334:S55:H15	2:A:1334:S55:H9	1.66	0.60
1:A:165:THR:HG21	1:A:210:GLY:O	2.01	0.60
1:A:230:GLN:HE21	1:A:249:LYS:HE3	1.67	0.60
1:A:142:VAL:HG23	1:A:199:THR:HG22	1.83	0.60
2:A:1334:S55:H263	2:A:1334:S55:C13	2.18	0.59
1:B:229:HIS:HD2	1:B:252:ASN:N	2.01	0.59
1:A:180:MET:HB3	1:A:180:MET:HE3	1.83	0.59
1:A:158:ARG:HB2	1:A:158:ARG:NH1	2.18	0.57
1:A:326:GLY:H	1:B:71:ASN:HA	1.69	0.57
1:A:243:THR:HG21	3:A:2031:HOH:O	2.05	0.57
1:A:275:ASN:ND2	1:A:277:HIS:H	2.02	0.56
1:A:116:LEU:HD12	1:A:116:LEU:C	2.30	0.56
1:B:316:GLY:O	1:B:317:LEU:HD23	2.05	0.56
1:B:240:LYS:O	1:B:243:THR:HB	2.05	0.56
1:A:113:ASN:ND2	1:A:115:GLN:HG3	2.20	0.56
1:B:208:VAL:O	1:B:208:VAL:HG12	2.05	0.56
1:A:180:MET:CE	1:A:180:MET:HB3	2.36	0.55
1:A:180:MET:CE	1:A:180:MET:CG	2.84	0.55
1:A:71:ASN:ND2	1:A:72:SER:HB2	2.22	0.54
1:A:187:GLY:HA3	1:A:209:PRO:CD	2.38	0.54
1:A:252:ASN:HD22	1:A:270:GLU:HA	1.72	0.54
1:A:202:LEU:O	1:A:203:LEU:HD23	2.08	0.53
2:A:1334:S55:H15	2:A:1334:S55:N9	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:235:TRP:HZ3	1:B:245:GLU:CG	2.22	0.53
1:A:275:ASN:HD22	1:A:277:HIS:H	1.55	0.53
2:A:1334:S55:H13	2:A:1334:S55:C26	2.19	0.53
1:B:141:SER:CB	1:B:146:PRO:HA	2.36	0.53
1:B:116:LEU:HD23	1:B:118:ILE:CG1	2.38	0.53
1:B:235:TRP:HZ3	1:B:245:GLU:CD	2.17	0.53
1:B:300:PRO:HB2	1:B:301:PRO:HD2	1.91	0.53
1:A:180:MET:CE	1:A:227:LEU:HD21	2.39	0.52
1:A:252:ASN:HD21	1:A:271:GLU:H	1.57	0.52
1:A:229:HIS:HD2	1:A:252:ASN:H	1.56	0.52
1:B:207:HIS:H	1:B:225:GLU:HG2	1.74	0.52
1:B:176:VAL:O	1:B:180:MET:HG2	2.09	0.52
1:B:226:PHE:CE1	1:B:252:ASN:HB3	2.45	0.51
1:B:201:LEU:HD21	1:B:204:LYS:HB3	1.93	0.51
1:A:138:LEU:HD13	1:A:192:TYR:CE2	2.46	0.50
1:B:40:SER:HB3	1:B:59:VAL:HB	1.93	0.50
1:B:150:LEU:HD23	1:B:166:ASP:HB2	1.93	0.50
1:A:141:SER:CB	1:A:146:PRO:HA	2.40	0.50
1:B:56:TYR:CE1	1:B:66:LYS:HD3	2.47	0.50
1:B:187:GLY:HA3	1:B:209:PRO:CD	2.41	0.50
1:A:226:PHE:CE1	2:A:1334:S55:H101	2.46	0.49
1:B:317:LEU:HD13	1:B:330:ILE:HG21	1.93	0.49
1:A:126:SER:HB2	1:A:136:THR:O	2.13	0.49
1:B:286:LYS:HG2	1:B:294:LEU:HB2	1.95	0.48
1:A:131:GLU:CD	1:A:131:GLU:N	2.69	0.48
1:A:229:HIS:HD2	1:A:251:PRO:HA	1.78	0.48
1:A:241:LYS:HE3	3:A:2030:HOH:O	2.14	0.48
1:B:122:TYR:OH	1:B:173:ASP:HB2	2.14	0.48
1:B:220:PHE:CE1	1:B:222:LEU:HD21	2.48	0.48
1:A:40:SER:HB3	1:A:59:VAL:HB	1.94	0.47
1:A:211:GLY:CA	1:A:255:ASN:HA	2.43	0.47
1:B:209:PRO:HA	1:B:224:ALA:O	2.14	0.47
1:A:221:VAL:CG2	1:A:236:LEU:HD11	2.41	0.47
1:A:49:ASP:OD1	1:A:49:ASP:C	2.57	0.47
2:B:1334:S55:H9	2:B:1334:S55:H15	1.79	0.47
1:B:266:VAL:HG22	1:B:267:SER:N	2.29	0.47
1:A:96:GLU:OE1	1:A:96:GLU:N	2.39	0.47
1:A:94:ASP:N	1:A:94:ASP:OD1	2.46	0.46
1:A:113:ASN:C	1:A:113:ASN:HD22	2.23	0.46
1:A:98:ARG:N	1:A:99:PRO:CD	2.79	0.46
1:B:149:TRP:CD1	1:B:150:LEU:O	2.68	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:332:VAL:O	1:B:332:VAL:HG12	2.15	0.46
1:A:189:LEU:HD13	1:A:223:VAL:HB	1.96	0.46
1:B:81:SER:HB2	1:B:123:TYR:CE2	2.51	0.46
1:A:67:TYR:CE2	1:A:69:GLY:HA2	2.51	0.46
1:B:226:PHE:HA	1:B:253:PRO:HD2	1.98	0.45
1:A:108:SER:OG	1:A:155:VAL:HG23	2.17	0.45
1:B:229:HIS:CD2	1:B:252:ASN:N	2.70	0.45
1:B:207:HIS:HD2	1:B:228:SER:OG	2.00	0.45
1:A:251:PRO:O	1:A:252:ASN:C	2.60	0.45
1:B:253:PRO:HA	1:B:267:SER:O	2.16	0.45
1:B:288:ASP:C	1:B:288:ASP:OD1	2.60	0.44
1:A:180:MET:HE1	1:A:226:PHE:HE2	1.82	0.44
1:A:46:PHE:HA	1:A:56:TYR:O	2.18	0.44
1:B:56:TYR:CD1	1:B:66:LYS:HB2	2.53	0.44
1:B:113:ASN:ND2	1:B:115:GLN:HG3	2.33	0.44
1:B:44:ASN:OD1	1:B:58:SER:OG	2.36	0.43
1:B:71:ASN:ND2	1:B:71:ASN:H	2.15	0.43
1:B:301:PRO:O	1:B:302:PRO:C	2.60	0.43
1:A:265:TRP:CD2	1:A:286:LYS:HB2	2.53	0.43
1:B:233:LYS:HD3	1:B:235:TRP:CZ2	2.53	0.43
1:A:138:LEU:HD23	1:A:138:LEU:HA	1.81	0.43
1:A:180:MET:HE1	1:A:227:LEU:HD21	2.00	0.43
1:A:83:TYR:O	1:A:84:TRP:C	2.58	0.43
1:B:51:THR:O	1:B:52:ASN:C	2.61	0.43
1:B:163:TYR:CD2	1:B:163:TYR:N	2.86	0.43
1:B:46:PHE:HA	1:B:56:TYR:O	2.19	0.43
1:B:121:CYS:HB3	1:B:122:TYR:CD2	2.54	0.43
1:B:275:ASN:HD22	1:B:277:HIS:H	1.66	0.42
1:A:95:ALA:HB1	1:A:174:ARG:HD2	2.01	0.42
1:A:230:GLN:HE21	1:A:230:GLN:HB3	1.66	0.42
1:A:214:VAL:HG13	1:A:215:SER:O	2.19	0.42
1:A:322:THR:HG21	1:A:325:HIS:HB2	2.01	0.42
1:B:88:PHE:CE1	1:B:97:LYS:HD3	2.53	0.42
1:B:281:ASP:HB3	1:B:283:LYS:NZ	2.33	0.42
1:B:61:ASP:O	1:B:84:TRP:NE1	2.45	0.42
1:A:276:MET:HE2	1:A:277:HIS:CE1	2.54	0.42
1:B:210:GLY:CA	2:B:1334:S55:H1	2.49	0.42
1:A:89:CYS:O	1:A:92:SER:HB3	2.20	0.42
1:A:149:TRP:C	1:A:149:TRP:CD1	2.98	0.42
1:B:229:HIS:HD2	1:B:251:PRO:CA	2.25	0.42
1:A:84:TRP:O	1:A:85:ASN:ND2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:178:GLN:O	1:A:179:ILE:C	2.63	0.41
1:A:235:TRP:HZ3	1:A:245:GLU:OE2	2.03	0.41
1:B:235:TRP:HZ3	1:B:245:GLU:HG2	1.84	0.41
1:A:96:GLU:H	1:A:96:GLU:CD	2.26	0.41
1:B:233:LYS:HD3	1:B:235:TRP:CH2	2.55	0.41
1:A:142:VAL:CG2	1:A:199:THR:HG22	2.48	0.41
1:B:149:TRP:CD1	1:B:149:TRP:C	2.97	0.41
1:B:266:VAL:CG2	1:B:267:SER:N	2.84	0.41
1:B:98:ARG:HD3	1:B:173:ASP:OD1	2.20	0.41
1:B:279:ARG:HE	1:B:279:ARG:HB2	1.67	0.41
1:B:300:PRO:CB	1:B:301:PRO:HD2	2.50	0.41
1:A:189:LEU:HB3	1:A:203:LEU:HB2	2.01	0.41
2:B:1334:S55:H15	2:B:1334:S55:N9	2.36	0.41
1:B:120:ASP:O	1:B:121:CYS:C	2.64	0.41
1:B:316:GLY:C	1:B:317:LEU:HD23	2.46	0.41
1:A:215:SER:HB3	1:A:220:PHE:CZ	2.56	0.40
1:A:220:PHE:CD1	1:A:220:PHE:C	2.99	0.40
1:B:113:ASN:ND2	1:B:115:GLN:CG	2.84	0.40
1:A:253:PRO:HA	1:A:267:SER:O	2.22	0.40
1:B:251:PRO:O	1:B:252:ASN:C	2.65	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	300/302 (99%)	281 (94%)	16 (5%)	3 (1%)	12	43
1	B	300/302 (99%)	282 (94%)	17 (6%)	1 (0%)	36	68
All	All	600/604 (99%)	563 (94%)	33 (6%)	4 (1%)	18	51

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	173	ASP
1	A	173	ASP
1	A	71	ASN
1	A	301	PRO

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	243/260 (94%)	208 (86%)	35 (14%)	3	14
1	B	243/260 (94%)	207 (85%)	36 (15%)	3	14
All	All	486/520 (94%)	415 (85%)	71 (15%)	3	14

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	32	LYS
1	A	47	THR
1	A	53	LYS
1	A	68	GLU
1	A	72	SER
1	A	86	LYS
1	A	92	SER
1	A	96	GLU
1	A	111	LEU
1	A	113	ASN
1	A	131	GLU
1	A	136	THR
1	A	141	SER
1	A	142	VAL
1	A	155	VAL
1	A	158	ARG
1	A	165	THR
1	A	167	VAL
1	A	170	LEU
1	A	173	ASP

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Mol	Chain	Res	Type
1	A	174	ARG
1	A	176	VAL
1	A	191	LYS
1	A	203	LEU
1	A	205	GLU
1	A	207	HIS
1	A	214	VAL
1	A	221	VAL
1	A	235	TRP
1	A	240	LYS
1	A	276	MET
1	A	283	LYS
1	A	286	LYS
1	A	295	GLU
1	A	301	PRO
1	B	33	GLU
1	B	35	LEU
1	B	51	THR
1	B	66	LYS
1	B	71	ASN
1	B	75	VAL
1	B	92	SER
1	B	100	LEU
1	B	104	THR
1	B	113	ASN
1	B	116	LEU
1	B	126	SER
1	B	128	VAL
1	B	142	VAL
1	B	148	LYS
1	B	155	VAL
1	B	158	ARG
1	B	165	THR
1	B	167	VAL
1	B	174	ARG
1	B	181	ASP
1	B	183	SER
1	B	186	THR
1	B	195	SER
1	B	197	LYS
1	B	199	THR
1	B	200	THR

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Mol	Chain	Res	Type
1	B	219	SER
1	B	221	VAL
1	B	225	GLU
1	B	235	TRP
1	B	248	VAL
1	B	275	ASN
1	B	283	LYS
1	B	286	LYS
1	B	333	TYR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (21) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	71	ASN
1	A	85	ASN
1	A	91	ASN
1	A	113	ASN
1	A	178	GLN
1	A	229	HIS
1	A	230	GLN
1	A	252	ASN
1	A	275	ASN
1	A	277	HIS
1	A	292	ASN
1	A	310	GLN
1	A	312	GLN
1	B	113	ASN
1	B	177	GLN
1	B	207	HIS
1	B	229	HIS
1	B	230	GLN
1	B	252	ASN
1	B	275	ASN
1	B	292	ASN

5.3.3 RNA ⓘ

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	S55	A	1334	-	41,42,42	1.65	5 (12%)	48,61,61	2.35	16 (33%)
2	S55	B	1334	-	41,42,42	1.88	5 (12%)	48,61,61	1.92	11 (22%)

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	S55	A	1334	-	-	2/18/65/65	0/5/5/5
2	S55	B	1334	-	-	1/18/65/65	0/5/5/5

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1334	S55	O18-C19	6.76	1.48	1.35
2	B	1334	S55	O22-C21	6.19	1.46	1.33
2	A	1334	S55	O18-C19	6.07	1.46	1.35
2	A	1334	S55	O22-C21	5.86	1.46	1.33
2	B	1334	S55	C8-N9	-3.59	1.34	1.38
2	B	1334	S55	C5-C7	-3.27	1.38	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1334	S55	C5-C7	-3.25	1.38	1.44
2	A	1334	S55	C8-N9	-2.65	1.35	1.38
2	B	1334	S55	C17-C16	2.19	1.55	1.52
2	A	1334	S55	C4-N9	-2.10	1.35	1.38

All (27) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1334	S55	O22-C21-C20	9.24	124.52	112.65
2	B	1334	S55	O22-C21-C20	6.49	120.98	112.65
2	A	1334	S55	O24-C21-C20	-4.40	118.67	124.32
2	A	1334	S55	C23-O22-C21	4.33	123.87	115.85
2	A	1334	S55	C16-C15-C20	-4.14	104.30	108.78
2	B	1334	S55	C3-C4-C5	-4.04	118.28	122.19
2	B	1334	S55	C23-O22-C21	3.85	123.00	115.85
2	A	1334	S55	O22-C21-O24	-3.55	116.72	123.50
2	B	1334	S55	C6-C5-C4	3.50	122.47	118.84
2	A	1334	S55	C6-C5-C4	3.26	122.22	118.84
2	A	1334	S55	C3-C4-C5	-3.15	119.14	122.19
2	B	1334	S55	C10-C7-C8	3.13	125.78	122.07
2	A	1334	S55	C17-O18-C19	3.12	122.69	116.41
2	A	1334	S55	O18-C19-C20	-2.99	120.90	125.60
2	B	1334	S55	O22-C21-O24	-2.96	117.86	123.50
2	B	1334	S55	C17-O18-C19	2.75	121.95	116.41
2	A	1334	S55	C10-C7-C8	2.70	125.26	122.07
2	A	1334	S55	C28-O33-C32	2.62	118.84	113.72
2	B	1334	S55	O36-C30-C31	-2.51	104.47	110.38
2	B	1334	S55	O24-C21-C20	-2.46	121.16	124.32
2	B	1334	S55	O27-C28-O33	-2.40	104.37	110.69
2	A	1334	S55	O33-C32-C33	2.37	112.32	106.44
2	A	1334	S55	C10-C11-N12	2.31	115.00	109.98
2	B	1334	S55	O18-C19-C20	-2.29	122.00	125.60
2	A	1334	S55	O35-C31-C32	-2.25	103.77	109.32
2	A	1334	S55	C6-C5-C7	-2.24	129.92	133.73
2	A	1334	S55	O35-C31-C30	-2.05	105.54	110.38

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	1334	S55	O24-C21-O22-C23
2	A	1334	S55	C20-C21-O22-C23

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Mol	Chain	Res	Type	Atoms
2	B	1334	S55	C15-C16-C25-C26

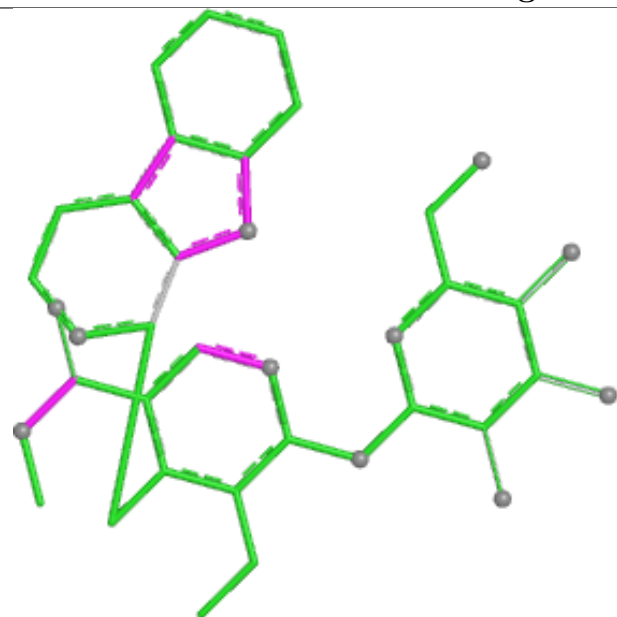
There are no ring outliers.

2 monomers are involved in 12 short contacts:

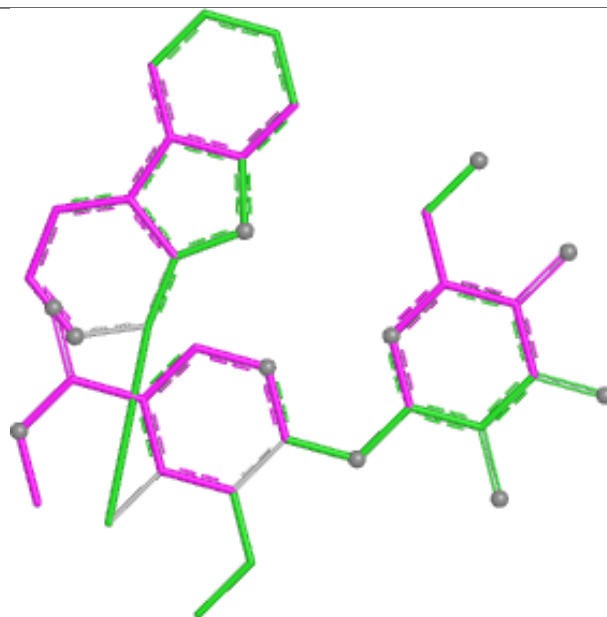
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1334	S55	7	0
2	B	1334	S55	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

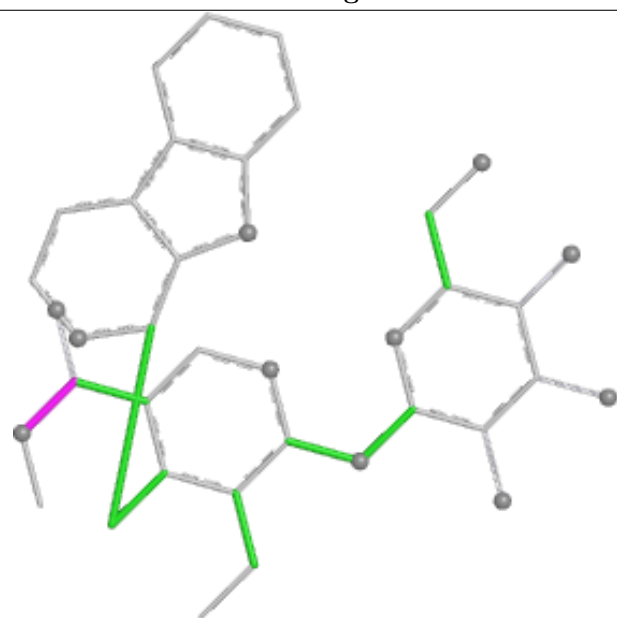
Ligand S55 A 1334



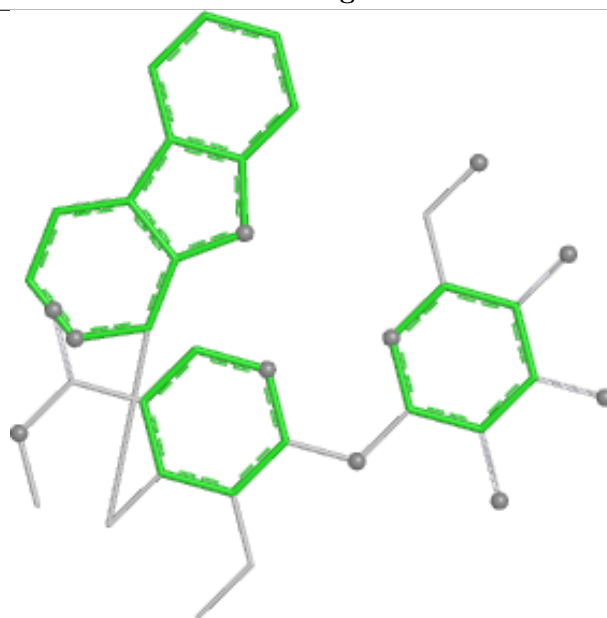
Bond lengths



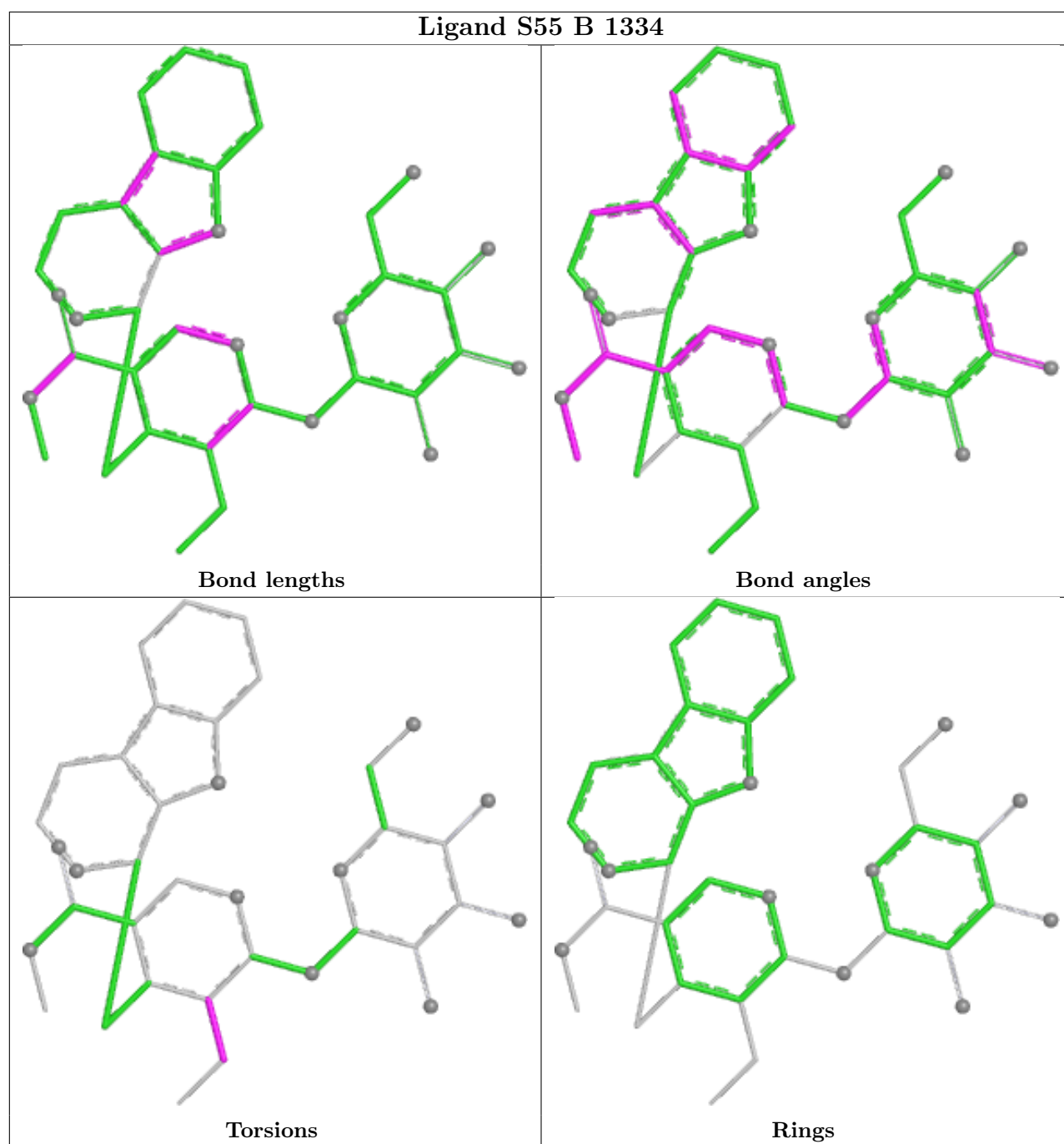
Bond angles



Torsions



Rings



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	302/302 (100%)	-0.73	0 100 100	21, 26, 31, 42	0
1	B	302/302 (100%)	-0.13	1 (0%) 90 79	20, 26, 31, 35	0
All	All	604/604 (100%)	-0.43	1 (0%) 91 83	20, 26, 31, 42	0

All (1) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	32	LYS	3.0

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.

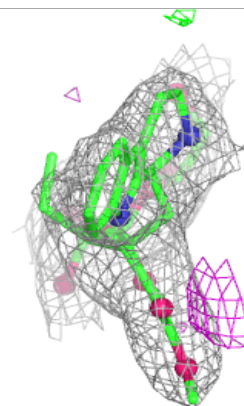
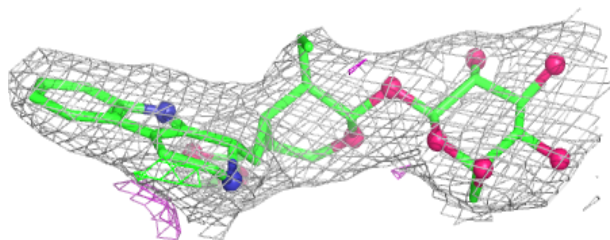
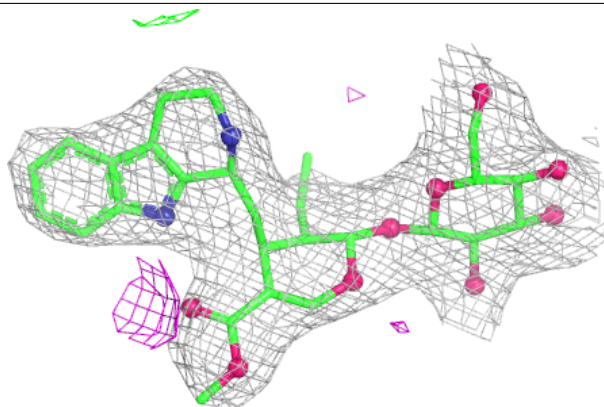
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	S55	B	1334	38/38	0.95	0.07	45,53,62,64	0
2	S55	A	1334	38/38	0.97	0.07	42,48,56,58	0

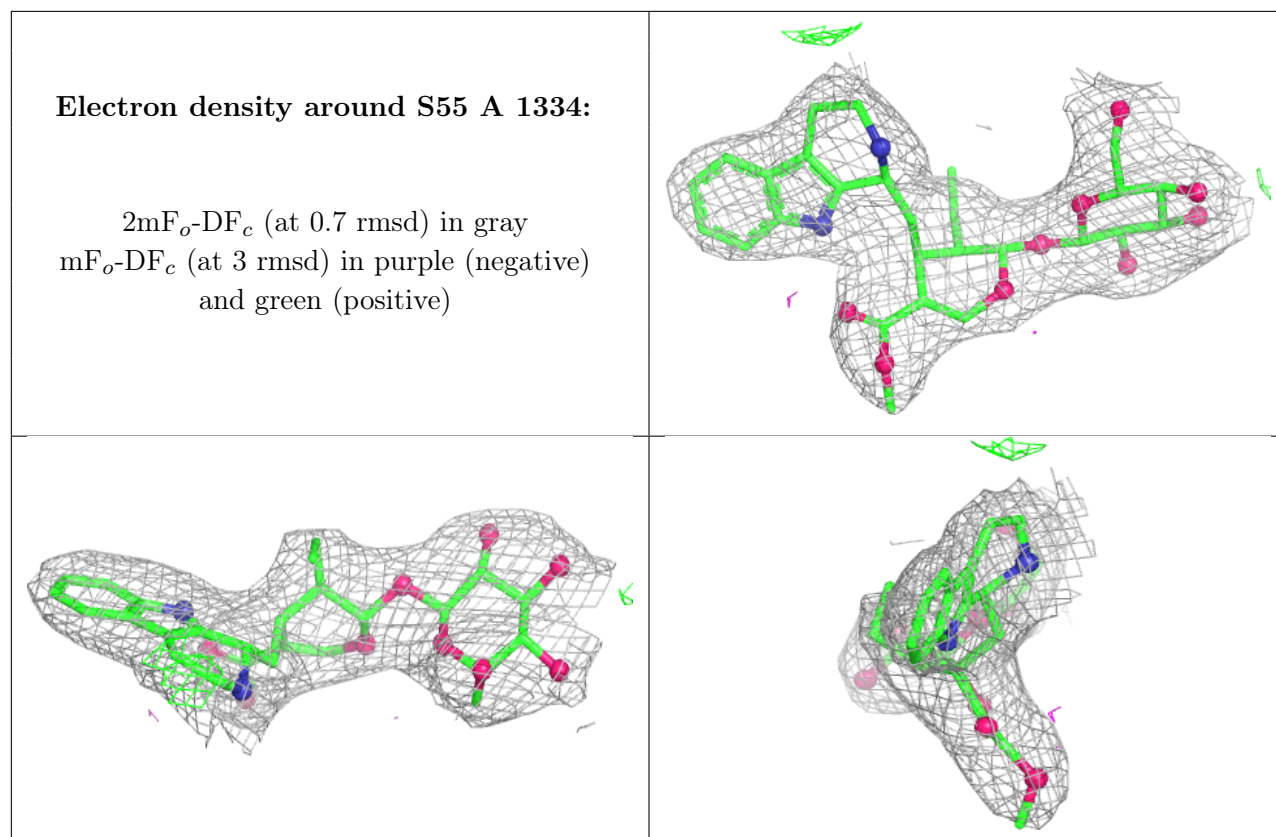
The following is a graphical depiction of the model fit to experimental electron density of all

instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around S55 B 1334:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





6.5 Other polymers [i](#)

There are no such residues in this entry.