



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 16, 2026 – 10:23 AM UTC

PDB ID : 1W96 / pdb_00001w96
Title : Crystal Structure of Biotin Carboxylase Domain of Acetyl-coenzyme A Carboxylase from *Saccharomyces cerevisiae* in Complex with Soraphen A
Authors : Shen, Y.; Volrath, S.L.; Weatherly, S.C.; Elich, T.D.; Tong, L.
Deposited on : 2004-10-06
Resolution : 1.80 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

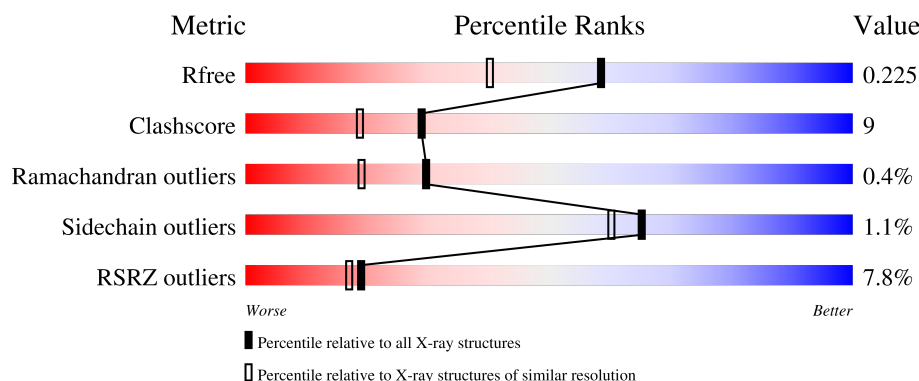
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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	554	7% 80% 19% .
1	B	554	8% 82% 15% ..
1	C	554	8% 78% 18% ..

2 Entry composition [i](#)

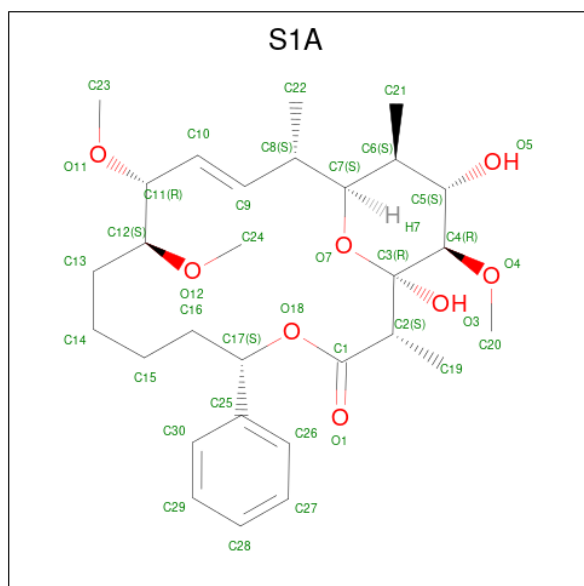
There are 3 unique types of molecules in this entry. The entry contains 14282 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 ACETYL-COENZYME A CARBOXYLASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	549	Total	C	N	O	S	0	0	0
			4290	2697	751	824	18			
1	B	542	Total	C	N	O	S	0	0	0
			4249	2674	746	811	18			
1	C	537	Total	C	N	O	S	0	0	1
			4187	2632	740	797	18			

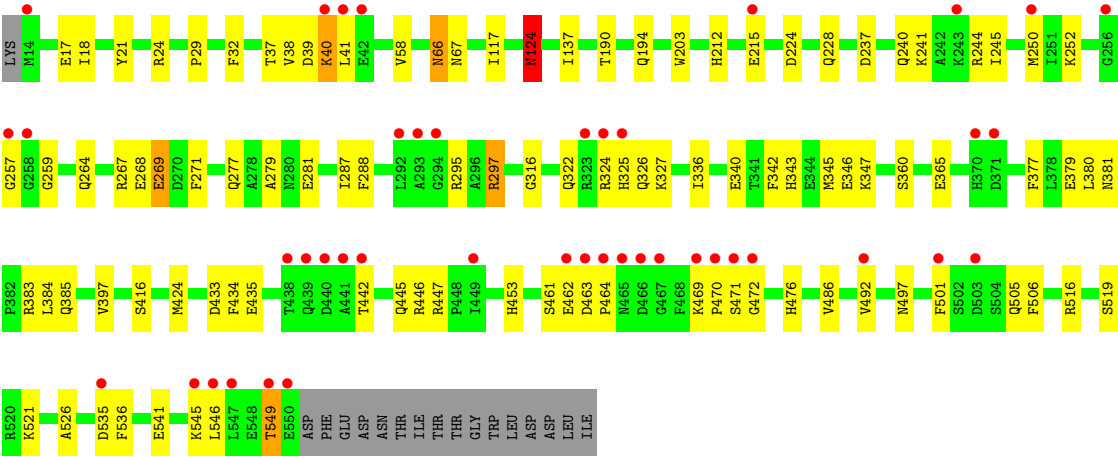
- Molecule 2 is SORAPHEN A (CCD ID: S1A) (formula: $C_{29}H_{44}O_8$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			37	29	8		
2	B	1	Total	C	O	0	0
			37	29	8		
2	C	1	Total	C	O	0	0
			37	29	8		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	454	Total 454	O 454	0	0
3	B	510	Total 510	O 510	0	0
3	C	481	Total 481	O 481	0	0



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	63.83Å 96.52Å 139.95Å 90.00° 96.82° 90.00°	Depositor
Resolution (Å)	29.20 – 1.80 29.20 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.3 (29.20-1.80) 96.3 (29.20-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 1.79Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.195 , 0.230 0.190 , 0.225	Depositor DCC
R_{free} test set	11694 reflections (7.49%)	wwPDB-VP
Wilson B-factor (Å ²)	19.2	Xtriage
Anisotropy	0.251	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14282	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.41% 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: S1A

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	0.34	0/4381	0.83	7/5927 (0.1%)
1	B	0.37	0/4338	0.82	8/5867 (0.1%)
1	C	0.35	1/4277 (0.0%)	0.83	9/5786 (0.2%)
All	All	0.35	1/12996 (0.0%)	0.83	24/17580 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	549	THR	C-N	-5.62	1.25	1.33

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	18	ILE	N-CA-C	8.10	120.78	108.71
1	B	18	ILE	N-CA-C	8.06	120.72	108.71
1	C	18	ILE	N-CA-C	7.57	119.98	108.71
1	C	325	HIS	N-CA-C	-7.13	103.74	113.30
1	B	124	ASN	N-CA-C	6.70	120.55	112.38
1	C	384	LEU	N-CA-C	-6.38	101.94	110.55
1	C	271	PHE	N-CA-C	6.21	118.59	111.02
1	A	384	LEU	N-CA-C	-6.20	101.30	110.48
1	B	367	LEU	N-CA-C	-6.19	99.15	109.24
1	B	384	LEU	N-CA-C	-6.10	101.45	110.48
1	A	124	ASN	N-CA-C	5.86	119.52	112.38
1	C	124	ASN	N-CA-C	5.84	119.51	112.38
1	C	416	SER	N-CA-C	5.70	117.94	111.11
1	B	271	PHE	N-CA-C	5.64	117.11	110.97
1	A	271	PHE	N-CA-C	5.59	117.84	111.02
1	B	17	GLU	N-CA-C	-5.47	102.18	110.28
1	C	38	VAL	N-CA-C	5.31	116.67	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	416	SER	N-CA-C	5.26	117.42	111.11
1	B	131	VAL	N-CA-C	5.20	115.82	110.36
1	A	416	SER	N-CA-C	5.15	117.29	111.11
1	C	397	VAL	N-CA-C	5.09	115.91	108.58
1	A	367	LEU	N-CA-C	-5.04	100.51	108.73
1	A	17	GLU	N-CA-C	-5.00	102.87	110.28
1	C	17	GLU	N-CA-C	-5.00	102.88	110.28

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	4290	0	4199	80	0
1	B	4249	0	4173	67	0
1	C	4187	0	4112	79	0
2	A	37	0	44	1	0
2	B	37	0	44	1	0
2	C	37	0	44	0	0
3	A	454	0	0	9	0
3	B	510	0	0	12	0
3	C	481	0	0	11	0
All	All	14282	0	12616	221	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 9.

All (221) 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:C:66:ASN:HD22	1:C:67:ASN:H	1.18	0.91
1:A:433:ASP:H	1:A:445:GLN:HE22	1.14	0.90
1:B:66:ASN:HD22	1:B:67:ASN:H	1.16	0.88
1:A:66:ASN:HD22	1:A:67:ASN:H	1.17	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:ASP:H	1:B:445:GLN:HE22	1.23	0.86
1:C:433:ASP:H	1:C:445:GLN:HE22	1.24	0.85
1:A:319:CYS:HB3	1:A:330:GLU:OE2	1.78	0.83
1:A:43:GLU:HA	3:A:2056:HOH:O	1.82	0.77
1:A:443:LYS:HD2	1:C:244:ARG:NH2	2.00	0.76
1:C:462:GLU:HG2	1:C:464:PRO:HD3	1.70	0.74
1:A:47:ARG:HD2	3:A:2056:HOH:O	1.89	0.72
1:A:250:MET:HE3	1:A:252:LYS:NZ	2.05	0.72
1:A:433:ASP:H	1:A:445:GLN:NE2	1.87	0.72
1:C:279:ALA:HB2	1:C:287:ILE:HD11	1.72	0.70
1:A:269:GLU:CD	1:A:269:GLU:H	1.98	0.70
1:B:23:GLU:HG3	1:B:24:ARG:N	2.07	0.69
1:B:253:ALA:HA	1:B:287:ILE:HD13	1.73	0.69
1:B:250:MET:SD	1:B:264:GLN:HG2	2.32	0.69
1:B:433:ASP:H	1:B:445:GLN:NE2	1.91	0.69
1:B:528:LYS:O	1:B:532:ILE:HD13	1.92	0.69
1:C:383:ARG:HH12	1:C:385:GLN:HG2	1.59	0.68
1:B:117:ILE:HD12	1:B:137:ILE:HG23	1.75	0.67
1:C:124:ASN:HD21	1:C:497:ASN:HD22	1.45	0.65
1:C:250:MET:HB3	1:C:252:LYS:HZ3	1.60	0.64
1:C:250:MET:SD	1:C:264:GLN:HG2	2.38	0.64
1:A:250:MET:HB3	1:A:252:LYS:HZ3	1.61	0.63
1:C:117:ILE:HD12	1:C:137:ILE:HG23	1.80	0.63
1:B:224:ASP:HB2	1:C:215:GLU:OE1	1.99	0.63
1:B:545:LYS:O	1:B:549:THR:HG23	1.99	0.62
1:B:537:ARG:O	1:B:541:GLU:HB2	2.00	0.62
1:C:267:ARG:HB3	1:C:269:GLU:OE2	2.00	0.62
1:C:433:ASP:H	1:C:445:GLN:NE2	1.93	0.62
1:C:442:THR:HG23	3:C:2406:HOH:O	2.00	0.62
1:C:463:ASP:HB2	1:C:505:GLN:NE2	2.15	0.61
1:A:250:MET:HE3	1:A:252:LYS:HZ1	1.66	0.61
1:A:321:VAL:HG12	3:A:2280:HOH:O	2.01	0.61
1:B:250:MET:HE3	1:B:252:LYS:HZ3	1.66	0.61
1:B:212:HIS:HD2	3:C:2270:HOH:O	1.84	0.60
1:B:23:GLU:HG3	1:B:24:ARG:H	1.65	0.60
1:B:540:VAL:O	1:B:544:ILE:HG13	2.02	0.60
1:C:250:MET:HE1	1:C:264:GLN:HG2	1.82	0.60
1:C:40:LYS:HB2	1:C:40:LYS:NZ	2.17	0.60
1:A:532:ILE:HG22	1:A:532:ILE:O	2.02	0.59
1:C:277:GLN:O	1:C:281:GLU:HG3	2.02	0.59
1:A:117:ILE:HD12	1:A:137:ILE:HG23	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:B:2279:HOH:O	1:C:212:HIS:HD2	1.85	0.59
1:B:492:VAL:HG12	1:B:505:GLN:HG2	1.84	0.58
1:A:267:ARG:HB3	1:A:269:GLU:OE2	2.04	0.58
1:A:446:ARG:HG2	1:A:446:ARG:HH11	1.68	0.58
1:B:240:GLN:HG3	1:B:241:LYS:N	2.18	0.58
1:C:424:MET:SD	1:C:445:GLN:HG2	2.44	0.58
1:A:250:MET:SD	1:A:264:GLN:HG2	2.44	0.57
1:B:490:PHE:CE1	1:B:505:GLN:HB2	2.39	0.57
1:C:461:SER:HB3	1:C:536:PHE:CZ	2.40	0.56
1:A:460:THR:O	1:A:539:THR:HG23	2.05	0.56
1:B:483:SER:HB3	3:B:2482:HOH:O	2.06	0.56
1:C:269:GLU:H	1:C:269:GLU:CD	2.13	0.56
1:C:383:ARG:NH1	1:C:385:GLN:HG2	2.20	0.56
1:B:95:VAL:HG22	1:B:115:GLN:HG3	1.87	0.56
1:A:277:GLN:O	1:A:281:GLU:HG3	2.05	0.56
1:C:501:PHE:HA	3:C:2447:HOH:O	2.06	0.56
1:B:194:GLN:NE2	1:B:203:TRP:HE1	2.04	0.55
1:A:190:THR:O	1:A:194:GLN:HG3	2.05	0.55
1:B:542:TYR:HA	1:B:545:LYS:HD2	1.86	0.55
1:B:66:ASN:HD22	1:B:67:ASN:N	1.96	0.55
1:B:541:GLU:O	1:B:545:LYS:HG3	2.06	0.55
1:A:27:GLU:CD	1:B:229:LYS:HE2	2.31	0.55
1:A:545:LYS:O	1:A:549:THR:HG23	2.07	0.55
1:A:250:MET:HE1	1:A:264:GLN:HE21	1.72	0.55
1:C:463:ASP:HB2	1:C:505:GLN:HE21	1.71	0.54
1:A:256:GLY:HA2	1:A:282:ILE:HG13	1.90	0.54
1:B:250:MET:SD	1:B:292:LEU:HD13	2.48	0.54
1:A:194:GLN:NE2	1:A:203:TRP:HE1	2.06	0.54
1:B:250:MET:HE3	1:B:252:LYS:NZ	2.22	0.54
1:C:240:GLN:HG3	1:C:241:LYS:N	2.23	0.54
1:A:393:MET:HE2	2:A:1567:S1A:C26	2.38	0.53
1:B:269:GLU:CD	1:B:269:GLU:H	2.15	0.53
1:B:194:GLN:HE22	1:B:203:TRP:HE1	1.55	0.53
1:B:277:GLN:O	1:B:281:GLU:HG3	2.09	0.53
1:A:323:ARG:HB2	1:A:562:LEU:HD23	1.91	0.53
1:C:66:ASN:HD22	1:C:67:ASN:N	1.98	0.53
1:C:41:LEU:HD12	3:C:2063:HOH:O	2.08	0.53
1:C:250:MET:CE	1:C:264:GLN:HG2	2.39	0.53
1:A:80:LYS:O	1:A:84:GLU:HG3	2.09	0.53
1:C:462:GLU:C	1:C:464:PRO:HD3	2.33	0.52
1:A:460:THR:HG22	1:A:506:PHE:HD2	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:PRO:HG3	3:A:2397:HOH:O	2.08	0.52
1:C:462:GLU:HG2	1:C:464:PRO:CD	2.38	0.52
1:B:124:ASN:HB3	1:B:495:ASN:O	2.09	0.52
1:C:324:ARG:HB2	3:C:2337:HOH:O	2.09	0.52
1:C:342:PHE:HA	1:C:345:MET:HE3	1.92	0.52
1:C:447:ARG:HG3	3:C:2414:HOH:O	2.09	0.52
1:C:194:GLN:NE2	1:C:203:TRP:HE1	2.08	0.51
1:B:350:VAL:CG1	1:B:354:LYS:HE2	2.41	0.51
1:C:279:ALA:HB2	1:C:287:ILE:CD1	2.40	0.51
1:C:521:LYS:HD3	1:C:521:LYS:C	2.36	0.51
1:B:124:ASN:HD21	1:B:497:ASN:HD22	1.59	0.50
1:C:194:GLN:HE22	1:C:203:TRP:HE1	1.59	0.50
1:B:393:MET:HE2	2:B:1567:S1A:C26	2.41	0.50
1:A:319:CYS:HB3	1:A:330:GLU:CD	2.37	0.50
1:A:440:ASP:OD1	1:A:444:LYS:HE3	2.11	0.50
1:B:225:ASP:OD1	1:B:226:ILE:HG12	2.11	0.50
1:A:328:ILE:HB	3:A:2280:HOH:O	2.12	0.50
1:B:536:PHE:HB2	1:B:540:VAL:HG13	1.94	0.50
1:C:237:ASP:O	1:C:240:GLN:HG2	2.11	0.50
1:C:343:HIS:O	1:C:347:LYS:HG3	2.11	0.50
1:C:461:SER:HB3	1:C:536:PHE:CE2	2.47	0.50
1:C:380:LEU:C	1:C:380:LEU:HD23	2.36	0.50
1:A:66:ASN:HD22	1:A:67:ASN:N	1.97	0.49
1:A:243:LYS:HE3	1:A:268:GLU:OE1	2.13	0.49
1:A:297:ARG:NH2	1:A:555:ASN:O	2.45	0.49
1:A:557:ILE:HD12	1:A:557:ILE:C	2.37	0.49
1:C:377:PHE:CZ	1:C:379:GLU:HA	2.47	0.49
1:A:350:VAL:CG1	1:A:354:LYS:HE2	2.43	0.49
1:A:527:LEU:HD22	1:A:540:VAL:HB	1.94	0.49
1:C:37:THR:OG1	1:C:40:LYS:HG2	2.12	0.49
1:A:413:HIS:HE1	3:A:2360:HOH:O	1.95	0.49
1:B:536:PHE:O	1:B:540:VAL:HG22	2.12	0.49
1:C:492:VAL:HG22	3:C:2447:HOH:O	2.12	0.49
1:C:279:ALA:CB	1:C:287:ILE:HD11	2.40	0.48
1:C:486:VAL:HG11	1:C:526:ALA:CB	2.43	0.48
1:B:321:VAL:CG2	1:B:557:ILE:HD12	2.42	0.48
1:C:471:SER:HB2	1:C:476:HIS:CE1	2.48	0.47
1:A:194:GLN:HE22	1:A:203:TRP:HE1	1.61	0.47
1:A:377:PHE:CZ	1:A:379:GLU:HA	2.49	0.47
1:C:316:GLY:HA3	1:C:342:PHE:HZ	1.79	0.47
1:A:204:SER:HB2	1:A:241:LYS:HD3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:282:ILE:HG22	1:A:285:SER:HB2	1.97	0.47
1:B:549:THR:O	1:B:553:GLU:HG3	2.15	0.47
1:A:459:ILE:HD13	1:A:509:ILE:HG13	1.97	0.46
1:A:124:ASN:HD21	1:A:497:ASN:HD22	1.64	0.46
1:C:252:LYS:HD2	1:C:288:PHE:CZ	2.51	0.46
1:B:342:PHE:HA	1:B:345:MET:HE3	1.98	0.46
1:B:380:LEU:HD23	1:B:380:LEU:C	2.41	0.46
1:C:268:GLU:HG3	3:C:2297:HOH:O	2.14	0.46
1:A:108:GLU:O	1:A:112:MET:HG3	2.16	0.46
1:A:27:GLU:OE1	1:B:229:LYS:HE2	2.16	0.46
1:A:380:LEU:C	1:A:380:LEU:HD23	2.41	0.46
1:C:433:ASP:C	1:C:435:GLU:H	2.24	0.46
1:B:295:ARG:HG3	3:B:2322:HOH:O	2.15	0.46
1:B:350:VAL:HG12	1:B:354:LYS:HE2	1.97	0.46
1:B:413:HIS:HE1	3:B:2013:HOH:O	1.98	0.46
1:B:490:PHE:CD1	1:B:536:PHE:HE2	2.33	0.46
1:A:250:MET:SD	1:A:292:LEU:HD13	2.56	0.46
1:A:435:GLU:HB2	1:A:437:LYS:HG3	1.98	0.45
1:B:21:TYR:CD2	1:B:24:ARG:HD2	2.51	0.45
1:C:297:ARG:HG3	1:C:336:ILE:HD13	1.99	0.45
1:C:453:HIS:HD2	1:C:519:SER:OG	1.99	0.45
1:C:501:PHE:CD1	1:C:501:PHE:C	2.95	0.45
1:C:541:GLU:CG	1:C:545:LYS:HE3	2.46	0.45
1:B:117:ILE:CD1	1:B:137:ILE:HG23	2.45	0.45
1:A:324:ARG:O	1:A:325:HIS:HB2	2.16	0.45
1:C:365:GLU:OE2	1:C:381:ASN:OD1	2.34	0.45
1:C:446:ARG:HG2	1:C:446:ARG:HH11	1.81	0.44
1:B:260:LYS:HE3	3:B:2304:HOH:O	2.16	0.44
1:C:546:LEU:O	1:C:549:THR:HG22	2.18	0.44
1:A:21:TYR:CE2	1:A:24:ARG:HD2	2.51	0.44
1:C:190:THR:O	1:C:194:GLN:HG3	2.18	0.44
1:B:347:LYS:NZ	3:B:2358:HOH:O	2.51	0.44
1:A:446:ARG:HG2	1:A:446:ARG:NH1	2.32	0.44
1:A:550:GLU:HB2	3:A:2441:HOH:O	2.17	0.44
1:B:267:ARG:HB3	1:B:269:GLU:OE2	2.17	0.44
1:B:542:TYR:O	1:B:546:LEU:HG	2.17	0.44
1:C:462:GLU:HG2	1:C:464:PRO:CG	2.48	0.44
1:A:42:GLU:HG2	1:A:43:GLU:N	2.32	0.44
1:A:250:MET:CE	1:A:264:GLN:HE21	2.30	0.44
1:A:466:ASP:OD1	1:A:468:PHE:HB2	2.17	0.44
1:B:377:PHE:CZ	1:B:379:GLU:HA	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:ARG:NH1	1:A:520:ARG:HH21	2.16	0.43
1:B:435:GLU:HB2	1:B:437:LYS:HG3	2.00	0.43
1:B:178:ASN:ND2	3:B:2226:HOH:O	2.50	0.43
1:B:272:ILE:HG12	3:B:2308:HOH:O	2.18	0.43
1:A:48:ASP:OD1	3:A:2056:HOH:O	2.21	0.43
1:B:195:SER:HA	1:B:209:ASP:HB2	2.00	0.43
1:C:326:GLN:OE1	1:C:326:GLN:HA	2.17	0.43
1:C:469:LYS:HA	1:C:470:PRO:HD3	1.89	0.43
1:A:29:PRO:HD2	1:A:32:PHE:CD2	2.53	0.42
1:A:95:VAL:HG22	1:A:115:GLN:CG	2.49	0.42
1:B:520:ARG:NH2	3:B:2481:HOH:O	2.52	0.42
1:C:21:TYR:CD2	1:C:24:ARG:HD2	2.55	0.42
1:A:95:VAL:HG22	1:A:115:GLN:HG2	2.01	0.42
1:A:302:GLN:HG2	1:A:391:THR:HG21	2.01	0.42
1:A:439:GLN:NE2	1:C:245:ILE:HG13	2.33	0.42
1:C:41:LEU:HD23	1:C:58:VAL:HG21	2.02	0.42
1:A:530:LEU:HD23	1:A:540:VAL:HG11	2.01	0.42
1:B:317:ARG:CZ	3:B:2335:HOH:O	2.66	0.42
1:B:552:PHE:CD1	1:B:557:ILE:HD13	2.55	0.42
1:A:124:ASN:HB3	1:A:495:ASN:O	2.19	0.42
1:A:323:ARG:O	1:A:324:ARG:HB2	2.19	0.42
1:A:195:SER:HA	1:A:209:ASP:HB2	2.01	0.42
1:A:383:ARG:NH1	1:A:385:GLN:HG2	2.35	0.42
1:C:342:PHE:O	1:C:346:GLU:HG3	2.19	0.42
1:C:453:HIS:HE1	3:C:2338:HOH:O	2.03	0.42
1:A:61:LYS:HE2	1:A:95:VAL:CG2	2.50	0.42
1:A:342:PHE:HA	1:A:345:MET:HE3	2.01	0.41
1:A:460:THR:HG22	1:A:506:PHE:CD2	2.53	0.41
1:A:566:ILE:HG22	1:A:566:ILE:O	2.20	0.41
1:B:327:LYS:HD3	1:B:330:GLU:OE2	2.20	0.41
1:C:541:GLU:HG2	1:C:545:LYS:HE3	2.02	0.41
1:A:250:MET:HB3	1:A:252:LYS:NZ	2.32	0.41
1:C:257:GLY:C	1:C:259:GLY:H	2.27	0.41
1:B:483:SER:HB3	3:B:2455:HOH:O	2.21	0.41
1:A:135:VAL:O	1:A:139:GLU:HG3	2.20	0.41
1:C:322:GLN:HG2	1:C:327:LYS:HA	2.02	0.41
1:C:224:ASP:O	1:C:228:GLN:HG2	2.21	0.41
1:A:41:LEU:HD23	1:A:58:VAL:HG21	2.03	0.41
1:C:39:ASP:HB2	3:C:2052:HOH:O	2.20	0.41
1:C:250:MET:CE	1:C:264:GLN:HE21	2.34	0.41
1:C:472:GLY:HA2	3:C:2427:HOH:O	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:338:LYS:HG2	3:A:2293:HOH:O	2.21	0.40
1:B:358:TYR:OH	1:B:382:PRO:HA	2.21	0.40
1:A:350:VAL:HG12	1:A:354:LYS:HE2	2.03	0.40
1:B:21:TYR:CE2	1:B:24:ARG:HD2	2.56	0.40
1:C:453:HIS:CD2	1:C:516:ARG:HA	2.57	0.40
1:A:342:PHE:O	1:A:346:GLU:HG3	2.21	0.40
1:B:383:ARG:NH1	1:B:385:GLN:HG2	2.37	0.40
1:B:427:HIS:HD2	3:B:2011:HOH:O	2.05	0.40
1:B:501:PHE:CD1	1:B:501:PHE:C	2.99	0.40
1:C:29:PRO:HD2	1:C:32:PHE:CD2	2.56	0.40
1:C:295:ARG:N	1:C:295:ARG:HD2	2.36	0.40
1:C:506:PHE:CD1	1:C:506:PHE:N	2.88	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	545/554 (98%)	523 (96%)	21 (4%)	1 (0%)	43	31
1	B	538/554 (97%)	519 (96%)	16 (3%)	3 (1%)	21	11
1	C	535/554 (97%)	516 (96%)	17 (3%)	2 (0%)	30	19
All	All	1618/1662 (97%)	1558 (96%)	54 (3%)	6 (0%)	30	19

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	258	GLY
1	A	360	SER
1	B	360	SER
1	C	360	SER
1	C	434	PHE

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Mol	Chain	Res	Type
1	B	257	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	462/467 (99%)	459 (99%)	3 (1%)	78	77
1	B	457/467 (98%)	452 (99%)	5 (1%)	65	60
1	C	450/467 (96%)	443 (98%)	7 (2%)	55	47
All	All	1369/1401 (98%)	1354 (99%)	15 (1%)	65	60

All (15) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	66	ASN
1	A	124	ASN
1	A	269	GLU
1	B	66	ASN
1	B	124	ASN
1	B	240	GLN
1	B	269	GLU
1	B	295	ARG
1	C	40	LYS
1	C	66	ASN
1	C	124	ASN
1	C	269	GLU
1	C	297	ARG
1	C	340	GLU
1	C	535	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	36	ASN

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Mol	Chain	Res	Type
1	A	66	ASN
1	A	106	ASN
1	A	124	ASN
1	A	152	HIS
1	A	194	GLN
1	A	228	GLN
1	A	264	GLN
1	A	280	ASN
1	A	307	GLN
1	A	381	ASN
1	A	385	GLN
1	A	413	HIS
1	A	427	HIS
1	A	445	GLN
1	A	453	HIS
1	B	31	HIS
1	B	66	ASN
1	B	106	ASN
1	B	124	ASN
1	B	126	ASN
1	B	152	HIS
1	B	178	ASN
1	B	194	GLN
1	B	212	HIS
1	B	228	GLN
1	B	280	ASN
1	B	370	HIS
1	B	381	ASN
1	B	385	GLN
1	B	413	HIS
1	B	427	HIS
1	B	445	GLN
1	B	453	HIS
1	B	476	HIS
1	B	479	ASN
1	B	495	ASN
1	C	66	ASN
1	C	93	GLN
1	C	106	ASN
1	C	124	ASN
1	C	126	ASN
1	C	152	HIS

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Mol	Chain	Res	Type
1	C	194	GLN
1	C	212	HIS
1	C	228	GLN
1	C	264	GLN
1	C	276	HIS
1	C	277	GLN
1	C	381	ASN
1	C	385	GLN
1	C	439	GLN
1	C	445	GLN
1	C	453	HIS
1	C	476	HIS
1	C	485	ASN
1	C	505	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](#)

3 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	S1A	A	1567	-	39,39,39	1.05	3 (7%)	46,55,55	1.33	8 (17%)
2	S1A	B	1567	-	39,39,39	1.12	4 (10%)	46,55,55	1.26	4 (8%)
2	S1A	C	1550	-	39,39,39	1.08	3 (7%)	46,55,55	1.36	9 (19%)

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	S1A	A	1567	-	-	3/44/67/67	0/2/3/3
2	S1A	B	1567	-	-	3/44/67/67	0/2/3/3
2	S1A	C	1550	-	-	5/44/67/67	0/2/3/3

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1550	S1A	C10-C9	2.57	1.39	1.32
2	B	1567	S1A	C25-C17	2.56	1.55	1.51
2	B	1567	S1A	C3-C4	2.56	1.57	1.53
2	B	1567	S1A	C5-C4	2.48	1.58	1.53
2	A	1567	S1A	C10-C9	2.46	1.39	1.32
2	A	1567	S1A	C3-C4	2.25	1.56	1.53
2	C	1550	S1A	C3-C4	2.25	1.56	1.53
2	B	1567	S1A	C10-C9	2.22	1.38	1.32
2	A	1567	S1A	C5-C4	2.18	1.57	1.53
2	C	1550	S1A	C8-C9	2.05	1.55	1.51

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	1550	S1A	O18-C1-O1	-4.23	116.31	123.95
2	A	1567	S1A	O18-C1-O1	-4.13	116.49	123.95
2	B	1567	S1A	O18-C1-O1	-3.98	116.77	123.95
2	A	1567	S1A	C8-C7-C6	-3.13	110.51	115.56
2	C	1550	S1A	C8-C7-C6	-2.93	110.83	115.56
2	B	1567	S1A	C8-C7-C6	-2.87	110.93	115.56
2	C	1550	S1A	C20-O4-C4	-2.71	109.88	114.46
2	B	1567	S1A	C20-O4-C4	-2.63	110.01	114.46
2	A	1567	S1A	C20-O4-C4	-2.57	110.12	114.46
2	C	1550	S1A	C11-C10-C9	-2.44	119.84	124.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1567	S1A	C11-C10-C9	-2.41	119.89	124.62
2	B	1567	S1A	C11-C10-C9	-2.31	120.09	124.62
2	C	1550	S1A	C17-O18-C1	-2.30	112.63	116.65
2	C	1550	S1A	O11-C11-C12	2.22	109.51	105.57
2	C	1550	S1A	C2-C3-C4	-2.20	109.46	113.00
2	C	1550	S1A	C3-O7-C7	-2.18	111.15	114.45
2	C	1550	S1A	O1-C1-C2	2.13	129.82	124.97
2	A	1567	S1A	O1-C1-C2	2.10	129.74	124.97
2	A	1567	S1A	C17-O18-C1	-2.06	113.04	116.65
2	A	1567	S1A	O11-C11-C12	2.03	109.17	105.57
2	A	1567	S1A	C2-C3-C4	-2.03	109.74	113.00

There are no chirality outliers.

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1550	S1A	C10-C11-O11-C23
2	C	1550	S1A	C12-C11-O11-C23
2	A	1567	S1A	O1-C1-C2-C19
2	B	1567	S1A	O1-C1-C2-C19
2	C	1550	S1A	O1-C1-C2-C19
2	A	1567	S1A	O18-C1-C2-C19
2	A	1567	S1A	C22-C8-C9-C10
2	B	1567	S1A	C22-C8-C9-C10
2	C	1550	S1A	C22-C8-C9-C10
2	B	1567	S1A	O18-C1-C2-C19
2	C	1550	S1A	O18-C1-C2-C19

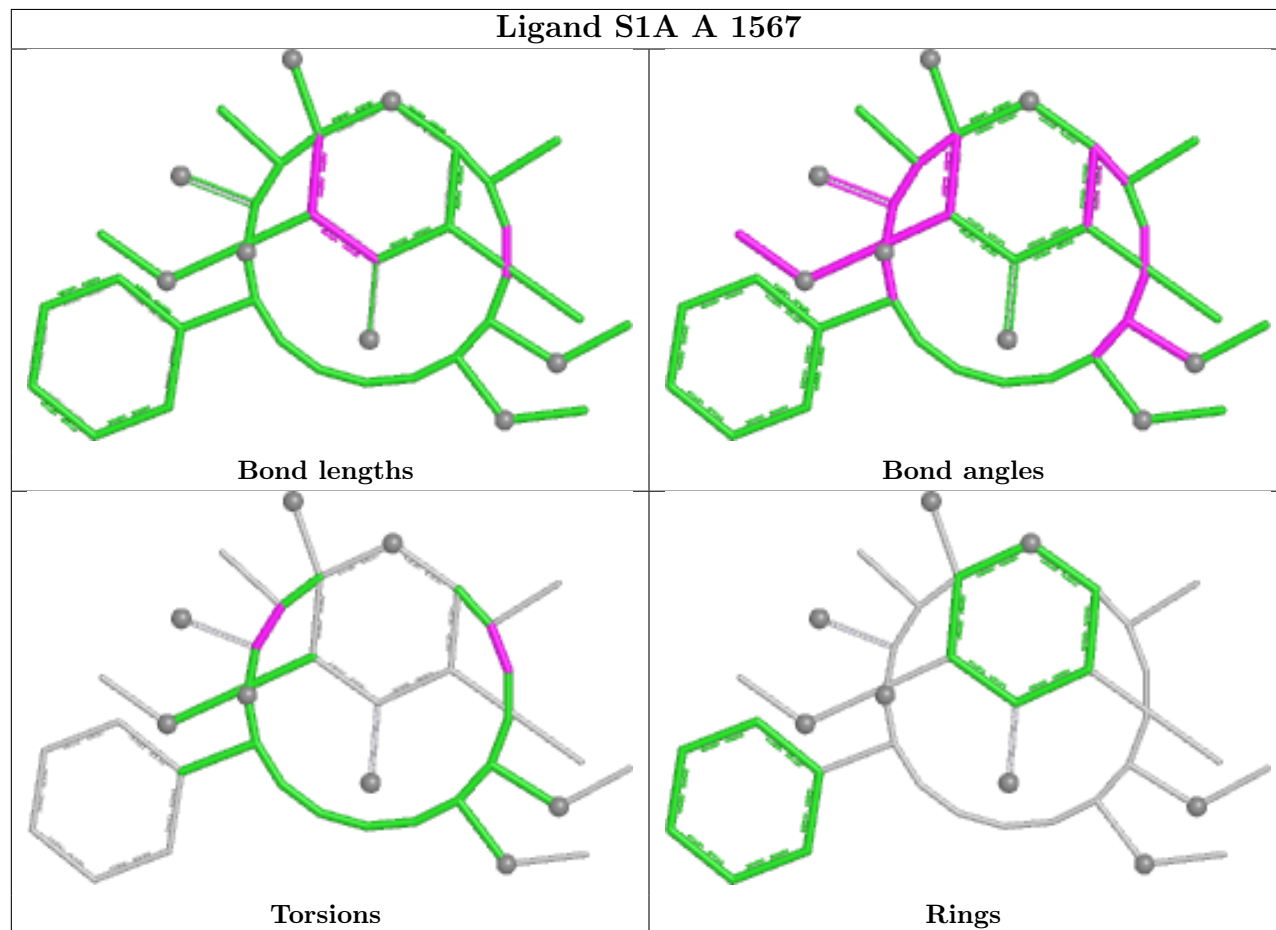
There are no ring outliers.

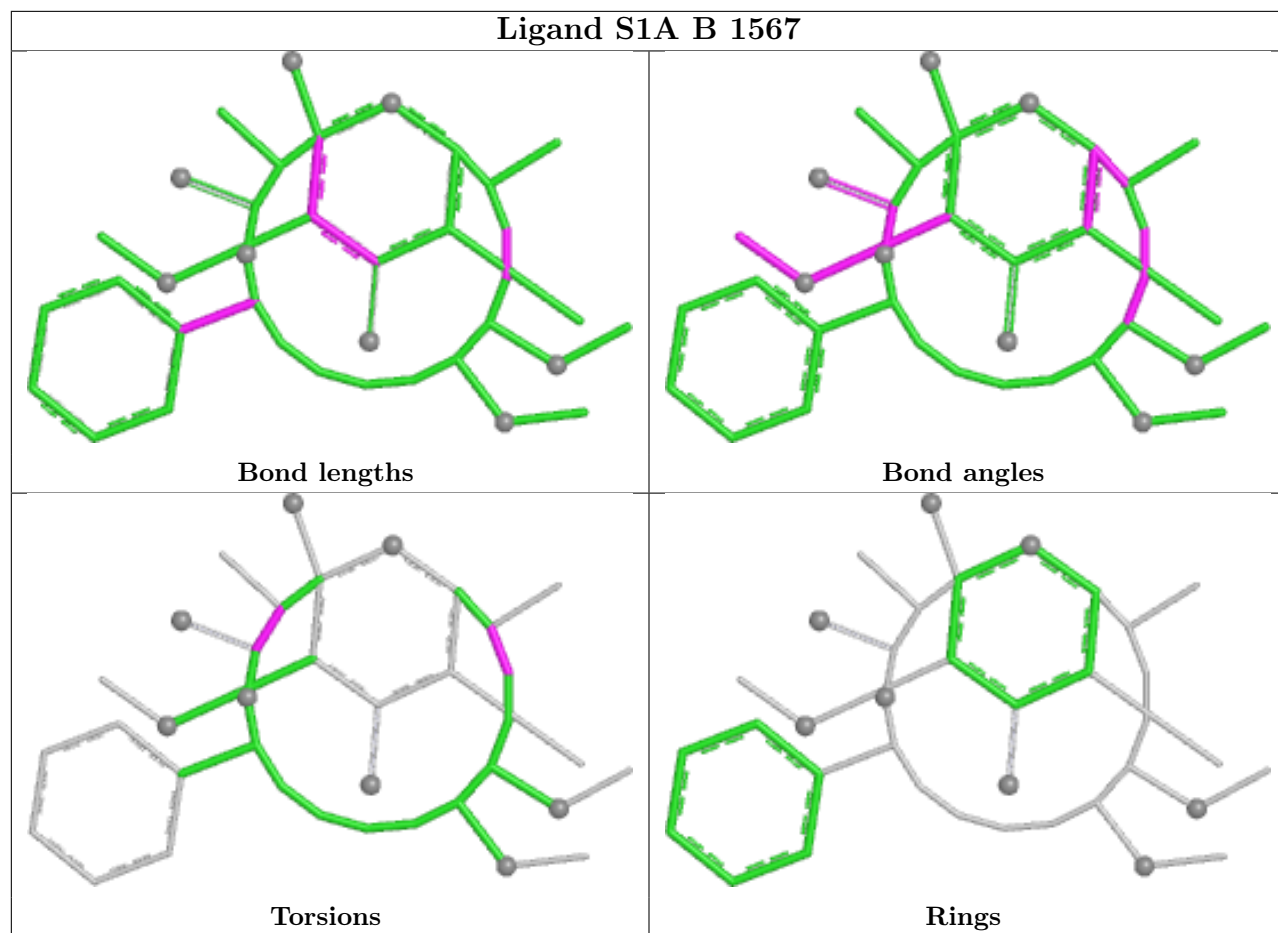
2 monomers are involved in 2 short contacts:

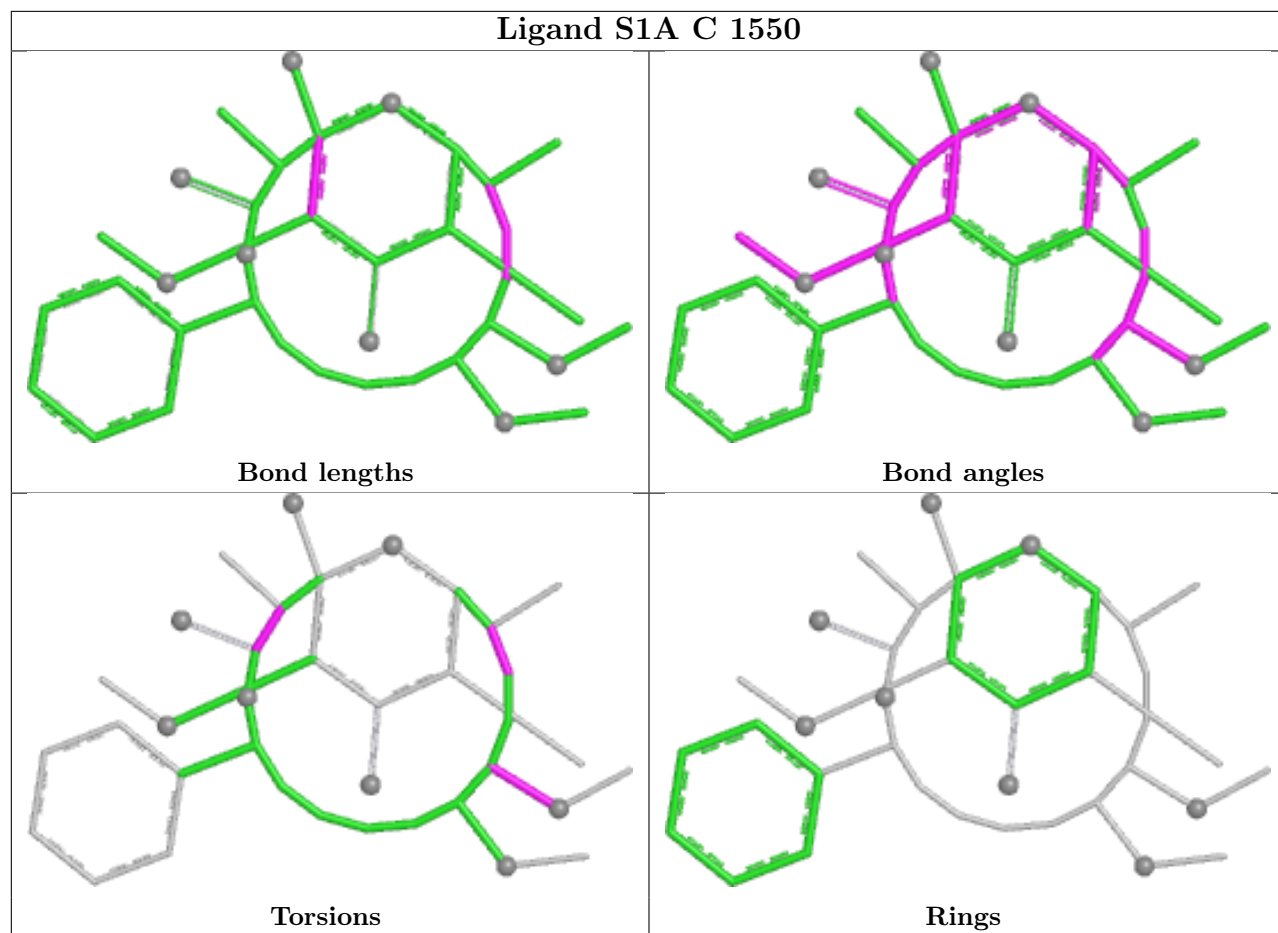
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1567	S1A	1	0
2	B	1567	S1A	1	0

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.







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å ²)	Q<0.9
1	A	549/554 (99%)	0.34	41 (7%)	20	18	10, 24, 47, 57	0
1	B	542/554 (97%)	0.25	43 (7%)	18	16	9, 21, 45, 55	0
1	C	537/554 (96%)	0.35	43 (8%)	18	16	12, 23, 48, 60	0
All	All	1628/1662 (97%)	0.31	127 (7%)	19	17	9, 23, 47, 60	0

All (127) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	483	SER	4.9
1	A	467	GLY	4.9
1	B	484	SER	4.7
1	C	294	GLY	4.1
1	C	258	GLY	4.0
1	B	479	ASN	4.0
1	C	325	HIS	3.9
1	B	257	GLY	3.8
1	B	501	PHE	3.7
1	B	490	PHE	3.6
1	B	23	GLU	3.6
1	C	501	PHE	3.6
1	A	483	SER	3.6
1	C	472	GLY	3.6
1	A	257	GLY	3.5
1	A	14	MET	3.5
1	C	466	ASP	3.4
1	A	225	ASP	3.4
1	B	532	ILE	3.3
1	B	441	ALA	3.3
1	C	464	PRO	3.2
1	B	473	GLY	3.2
1	A	186	LYS	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	565	LEU	3.1
1	C	323	ARG	3.1
1	B	476	HIS	3.1
1	C	40	LYS	3.1
1	C	469	LYS	3.1
1	A	319	CYS	3.1
1	A	470	PRO	3.1
1	C	257	GLY	3.0
1	A	540	VAL	3.0
1	B	542	TYR	3.0
1	C	371	ASP	3.0
1	B	258	GLY	3.0
1	A	532	ILE	3.0
1	B	115	GLN	2.9
1	C	41	LEU	2.9
1	A	471	SER	2.9
1	A	468	PHE	2.8
1	B	536	PHE	2.8
1	C	438	THR	2.8
1	B	106	ASN	2.8
1	A	256	GLY	2.7
1	C	462	GLU	2.7
1	C	439	GLN	2.7
1	A	40	LYS	2.7
1	A	539	THR	2.7
1	C	14	MET	2.7
1	C	546	LEU	2.7
1	C	440	ASP	2.7
1	C	503	ASP	2.7
1	A	549	THR	2.7
1	A	533	ARG	2.7
1	A	479	ASN	2.7
1	B	566	ILE	2.7
1	B	440	ASP	2.6
1	A	463	ASP	2.6
1	B	534	GLY	2.6
1	C	550	GLU	2.6
1	B	256	GLY	2.6
1	B	22	SER	2.6
1	C	250	MET	2.5
1	B	250	MET	2.5
1	B	505	GLN	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	215	GLU	2.5
1	C	470	PRO	2.5
1	B	506	PHE	2.5
1	C	547	LEU	2.5
1	A	294	GLY	2.5
1	C	449	ILE	2.5
1	A	324	ARG	2.5
1	B	550	GLU	2.5
1	C	442	THR	2.5
1	B	503	ASP	2.5
1	B	535	ASP	2.5
1	A	258	GLY	2.5
1	A	506	PHE	2.5
1	B	482	SER	2.5
1	B	538	THR	2.5
1	C	535	ASP	2.5
1	A	183	LEU	2.4
1	C	471	SER	2.4
1	A	293	ALA	2.4
1	C	441	ALA	2.4
1	C	42	GLU	2.4
1	B	371	ASP	2.4
1	B	438	THR	2.4
1	B	504	SER	2.4
1	A	542	TYR	2.4
1	B	225	ASP	2.4
1	C	256	GLY	2.4
1	C	293	ALA	2.3
1	A	482	SER	2.3
1	C	549	THR	2.3
1	A	250	MET	2.3
1	A	534	GLY	2.3
1	C	463	ASP	2.3
1	A	565	LEU	2.3
1	B	442	THR	2.3
1	A	566	ILE	2.3
1	B	324	ARG	2.2
1	A	465	ASN	2.2
1	C	243	LYS	2.2
1	C	324	ARG	2.2
1	C	215	GLU	2.2
1	B	259	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	A	550	GLU	2.2
1	B	475	LEU	2.2
1	A	469	LYS	2.2
1	C	492	VAL	2.2
1	C	370	HIS	2.1
1	B	43	GLU	2.1
1	B	436	PHE	2.1
1	A	41	LEU	2.1
1	B	533	ARG	2.1
1	C	292	LEU	2.1
1	A	216	LYS	2.1
1	B	493	GLY	2.1
1	C	545	LYS	2.1
1	A	478	LEU	2.1
1	A	462	GLU	2.1
1	C	465	ASN	2.1
1	A	461	SER	2.0
1	A	440	ASP	2.0
1	A	240	GLN	2.0
1	C	467	GLY	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](#)

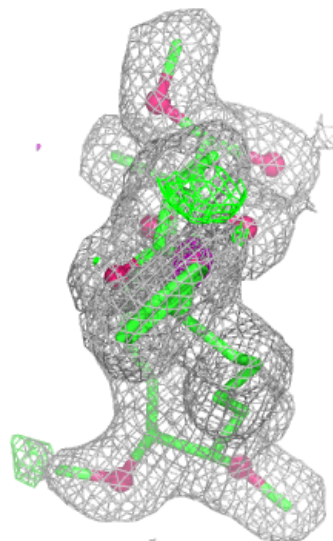
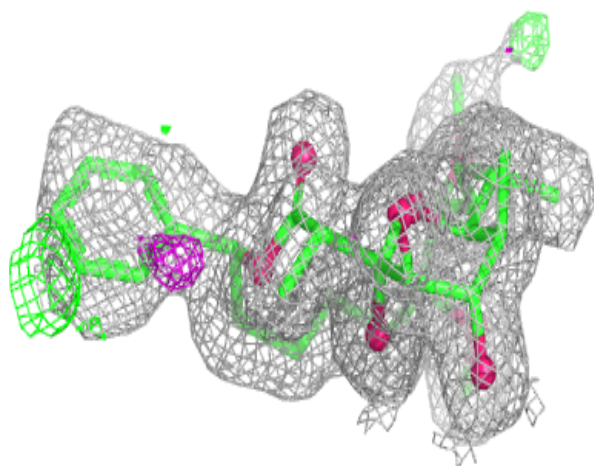
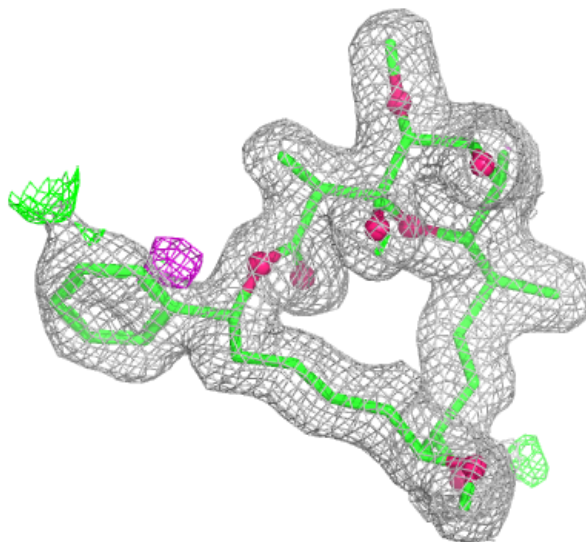
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	S1A	A	1567	37/37	0.94	0.07	13,17,24,26	0
2	S1A	C	1550	37/37	0.95	0.07	14,18,24,24	0
2	S1A	B	1567	37/37	0.96	0.06	9,13,22,23	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.

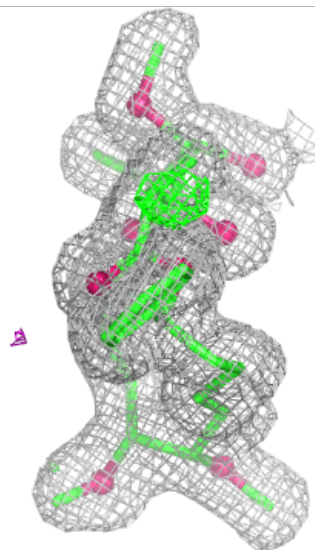
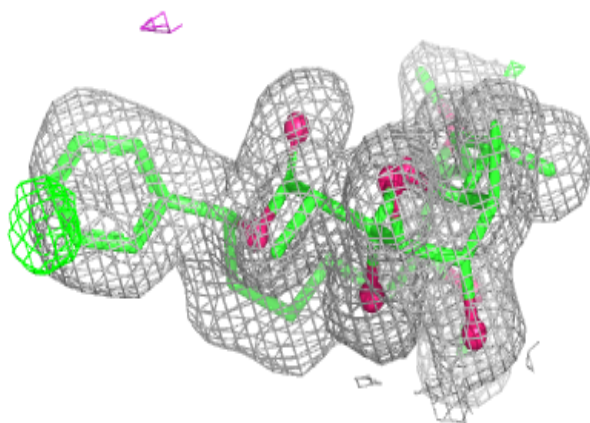
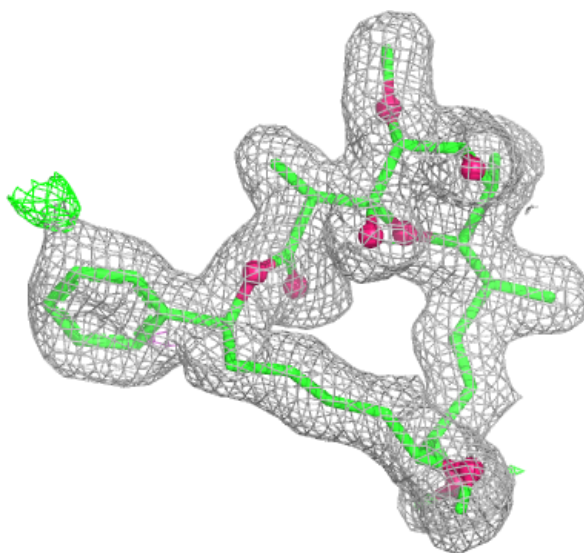
Electron density around S1A A 1567:

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



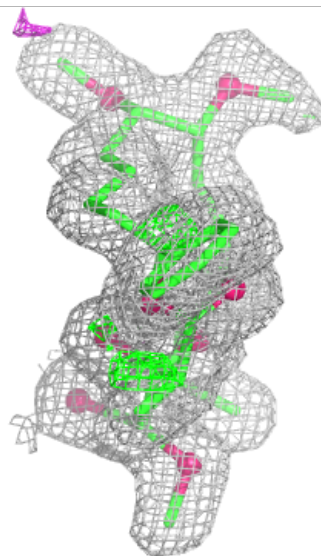
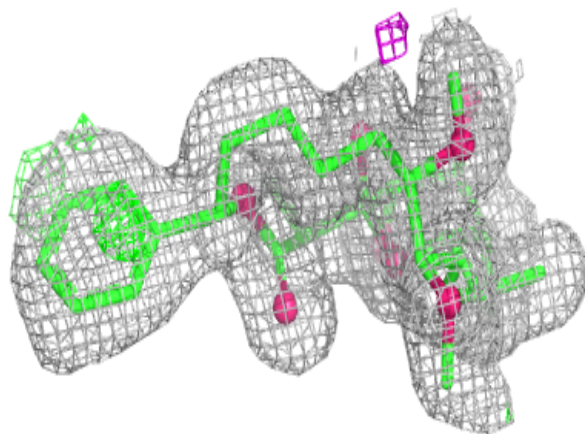
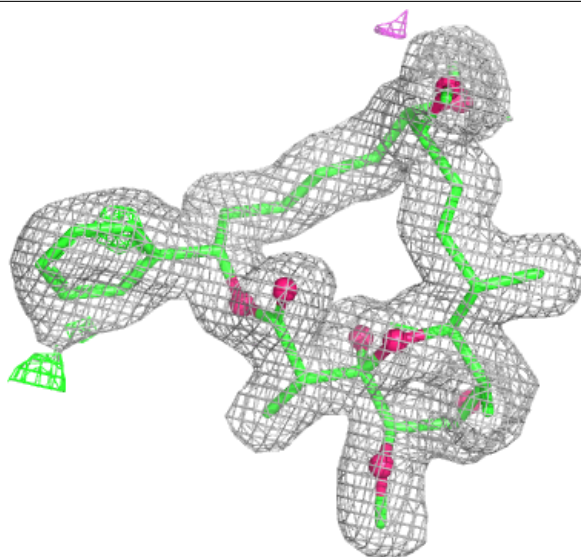
Electron density around S1A C 1550:

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



Electron density around S1A B 1567:

$2mF_o-DF_c$ (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.