



# Full wwPDB X-ray Structure Validation Report ⓘ

May 14, 2020 – 01:46 am BST

PDB ID : 3GID  
Title : The biotin carboxylase (BC) domain of human Acetyl-CoA Carboxylase 2 (ACC2) in complex with Soraphen A  
Authors : Price, A.; Kulathila, R.  
Deposited on : 2009-03-05  
Resolution : 2.30 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

<https://www.wwpdb.org/validation/2017/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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

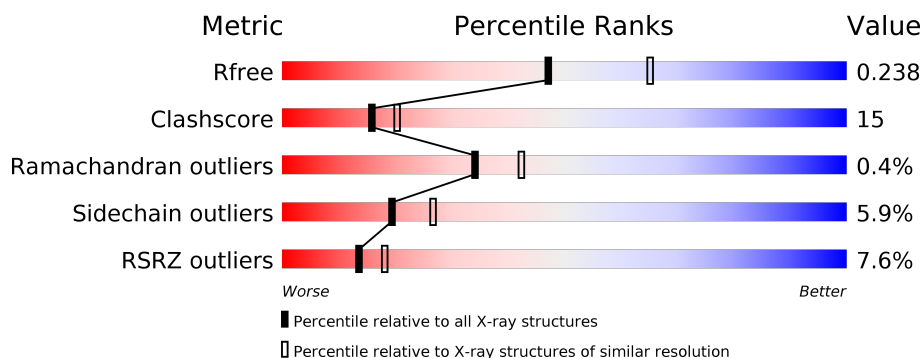
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.30 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))
$R_{free}$	130704	5042 (2.30-2.30)
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 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	540	<div> <div>7%</div> <div> <div></div> <div>61%</div> <div>22%</div> <div>•</div> <div>15%</div> </div> </div>
1	B	540	<div> <div>6%</div> <div> <div></div> <div>59%</div> <div>24%</div> <div>•</div> <div>15%</div> </div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7413 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-CoA carboxylase 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	460	Total	C	N	O	S	0	0	0
			3582	2287	616	661	18			
1	B	457	Total	C	N	O	S	0	0	0
			3560	2275	613	654	18			

There are 34 discrepancies between the modelled and reference sequences:

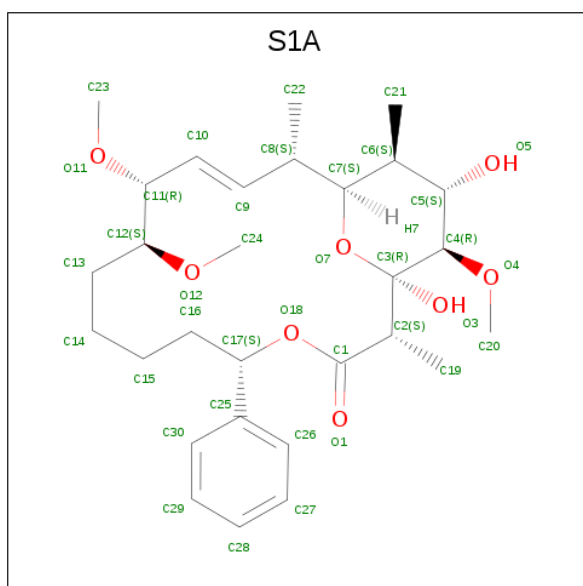
Chain	Residue	Modelled	Actual	Comment	Reference
A	221	MET	-	EXPRESSION TAG	UNP O00763
A	222	GLY	-	EXPRESSION TAG	UNP O00763
A	223	SER	-	EXPRESSION TAG	UNP O00763
A	224	SER	-	EXPRESSION TAG	UNP O00763
A	225	HIS	-	EXPRESSION TAG	UNP O00763
A	226	HIS	-	EXPRESSION TAG	UNP O00763
A	227	HIS	-	EXPRESSION TAG	UNP O00763
A	228	HIS	-	EXPRESSION TAG	UNP O00763
A	229	HIS	-	EXPRESSION TAG	UNP O00763
A	230	HIS	-	EXPRESSION TAG	UNP O00763
A	231	GLU	-	EXPRESSION TAG	UNP O00763
A	232	ASN	-	EXPRESSION TAG	UNP O00763
A	233	LEU	-	EXPRESSION TAG	UNP O00763
A	234	TYR	-	EXPRESSION TAG	UNP O00763
A	235	PHE	-	EXPRESSION TAG	UNP O00763
A	236	GLN	-	EXPRESSION TAG	UNP O00763
A	237	GLY	-	EXPRESSION TAG	UNP O00763
B	221	MET	-	EXPRESSION TAG	UNP O00763
B	222	GLY	-	EXPRESSION TAG	UNP O00763
B	223	SER	-	EXPRESSION TAG	UNP O00763
B	224	SER	-	EXPRESSION TAG	UNP O00763
B	225	HIS	-	EXPRESSION TAG	UNP O00763
B	226	HIS	-	EXPRESSION TAG	UNP O00763
B	227	HIS	-	EXPRESSION TAG	UNP O00763
B	228	HIS	-	EXPRESSION TAG	UNP O00763

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Chain	Residue	Modelled	Actual	Comment	Reference
B	229	HIS	-	EXPRESSION TAG	UNP O00763
B	230	HIS	-	EXPRESSION TAG	UNP O00763
B	231	GLU	-	EXPRESSION TAG	UNP O00763
B	232	ASN	-	EXPRESSION TAG	UNP O00763
B	233	LEU	-	EXPRESSION TAG	UNP O00763
B	234	TYR	-	EXPRESSION TAG	UNP O00763
B	235	PHE	-	EXPRESSION TAG	UNP O00763
B	236	GLN	-	EXPRESSION TAG	UNP O00763
B	237	GLY	-	EXPRESSION TAG	UNP O00763

- Molecule 2 is SORAPHEN A (three-letter code: S1A) (formula: C<sub>29</sub>H<sub>44</sub>O<sub>8</sub>).



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

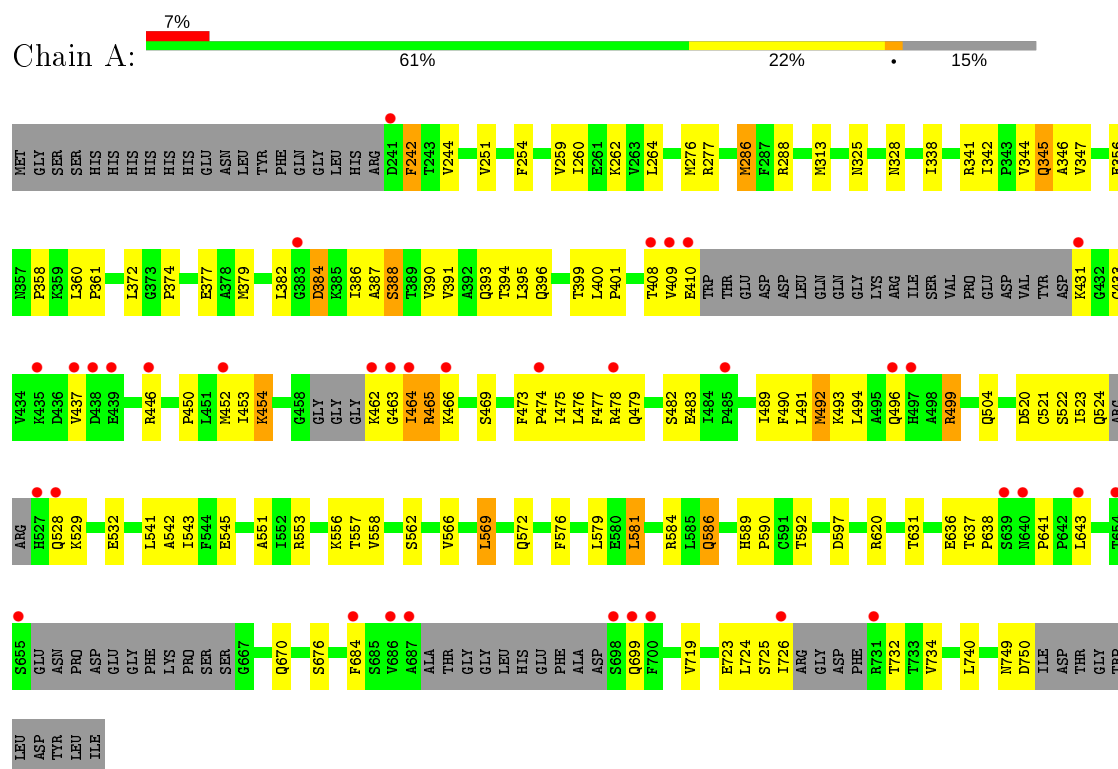
- Molecule 3 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	100	Total O 100 100	0	0
3	B	97	Total O 97 97	0	0

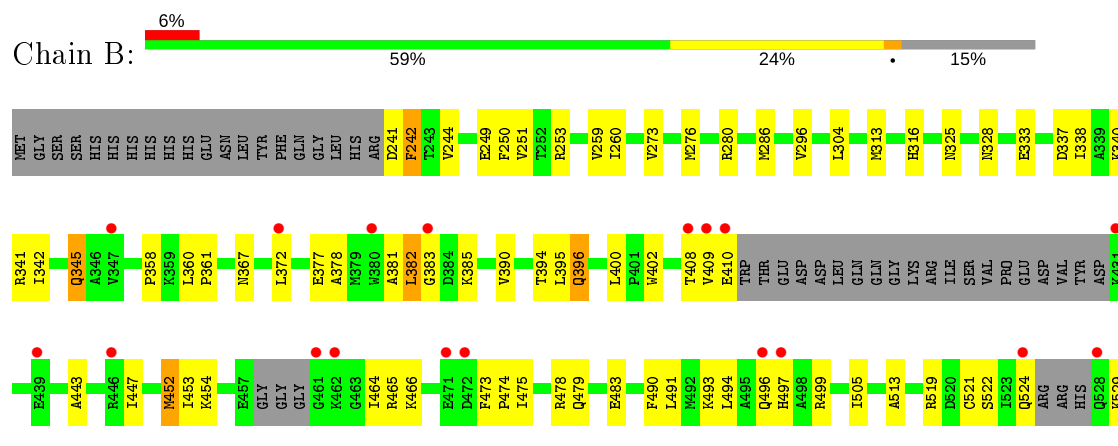
### 3 Residue-property plots [i](#)

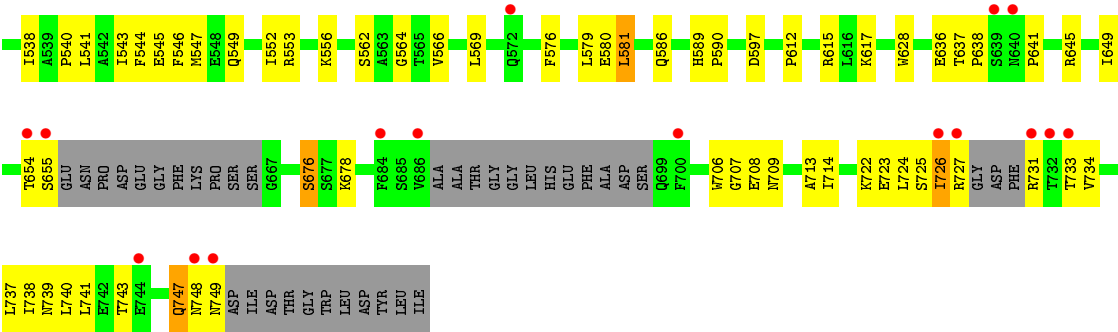
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Acetyl-CoA carboxylase 2



#### • Molecule 1: Acetyl-CoA carboxylase 2





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	138.34Å 141.00Å 123.61Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	26.80 – 2.30 26.79 – 2.30	Depositor EDS
% Data completeness (in resolution range)	93.3 (26.80-2.30) 93.4 (26.79-2.30)	Depositor EDS
$R_{merge}$	0.09	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.89 (at 2.31Å)	Xtriage
Refinement program	CNX	Depositor
R, $R_{free}$	0.200 , 0.242 0.196 , 0.238	Depositor DCC
$R_{free}$ test set	2603 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	31.8	Xtriage
Anisotropy	0.072	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.40 , 50.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	0.036 for -k,-h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7413	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.28% 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, 0.333 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	0.47	0/3660	0.58	0/4965
1	B	0.46	0/3637	0.63	0/4933
All	All	0.47	0/7297	0.61	0/9898

There are no bond length outliers.

There are no bond angle outliers.

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	3582	0	3557	103	0
1	B	3560	0	3543	110	0
2	A	37	0	44	0	0
2	B	37	0	44	0	0
3	A	100	0	0	3	0
3	B	97	0	0	2	0
All	All	7413	0	7188	210	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 15.

All (210) 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:499:ARG:HH11	1:A:499:ARG:HG3	1.14	1.13
1:B:727:ARG:HA	1:B:731:ARG:HD3	1.00	1.00
1:B:727:ARG:CA	1:B:731:ARG:HD3	1.92	1.00
1:B:409:VAL:HG22	1:B:410:GLU:H	1.25	0.99
1:B:727:ARG:HA	1:B:731:ARG:CD	1.92	0.98
1:A:522:SER:O	1:A:523:ILE:HG13	1.69	0.92
1:B:260:ILE:HA	1:B:345:GLN:HG3	1.51	0.91
1:A:553:ARG:O	1:A:557:THR:HG23	1.72	0.90
1:A:499:ARG:CG	1:A:499:ARG:HH11	1.84	0.90
1:A:260:ILE:HA	1:A:345:GLN:HG3	1.54	0.88
1:A:620:ARG:HH22	1:A:631:THR:HG22	1.39	0.88
1:A:584:ARG:HG3	1:A:584:ARG:HH11	1.37	0.87
1:A:382:LEU:HD13	1:A:581:LEU:HG	1.59	0.84
1:A:523:ILE:HD13	1:A:740:LEU:HD21	1.60	0.83
1:A:409:VAL:HG12	1:A:410:GLU:H	1.44	0.83
1:A:262:LYS:HG2	1:A:344:VAL:HG12	1.60	0.83
1:A:499:ARG:HG3	1:A:499:ARG:NH1	1.85	0.82
1:A:452:MET:HB3	1:A:454:LYS:HE3	1.60	0.81
1:B:452:MET:HB3	1:B:494:LEU:HD21	1.60	0.81
1:A:452:MET:SD	1:A:466:LYS:HG2	2.22	0.80
1:B:382:LEU:HD13	1:B:581:LEU:HG	1.66	0.76
1:B:273:VAL:HA	1:B:313:MET:HE1	1.68	0.74
1:A:584:ARG:HG3	1:A:584:ARG:NH1	2.03	0.74
1:A:584:ARG:HH12	1:A:586:GLN:HG3	1.53	0.73
1:B:654:THR:HG22	1:B:733:THR:HG21	1.70	0.73
1:B:409:VAL:HG22	1:B:410:GLU:N	2.02	0.73
1:B:475:ILE:O	1:B:479:GLN:HG3	1.89	0.72
1:A:409:VAL:HG12	1:A:410:GLU:N	2.05	0.72
1:B:748:ASN:O	1:B:749:ASN:HB2	1.90	0.72
1:B:394:THR:HG22	1:B:408:THR:HA	1.70	0.71
1:B:654:THR:O	1:B:655:SER:HB2	1.90	0.71
1:A:390:VAL:O	1:A:394:THR:HG23	1.89	0.71
1:B:337:ASP:O	1:B:341:ARG:HG3	1.92	0.70
1:B:377:GLU:HG2	1:B:378:ALA:N	2.05	0.70
1:B:566:VAL:HG22	1:B:581:LEU:HD23	1.73	0.70
1:A:387:ALA:O	1:A:391:VAL:HG23	1.91	0.69
1:A:394:THR:HG22	1:A:408:THR:HA	1.74	0.69
1:A:566:VAL:HG22	1:A:581:LEU:HD22	1.74	0.69
1:B:381:ALA:C	1:B:383:GLY:H	1.95	0.69
1:A:523:ILE:HG21	1:A:740:LEU:HD21	1.75	0.68
1:B:360:LEU:HB3	1:B:361:PRO:HD3	1.78	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:452:MET:HB3	1:A:454:LYS:CE	2.27	0.65
1:B:649:ILE:HD11	1:B:714:ILE:HG13	1.78	0.65
1:B:543:ILE:HD11	1:B:576:PHE:CE1	2.32	0.64
1:A:620:ARG:HH22	1:A:631:THR:CG2	2.08	0.64
1:A:450:PRO:HD3	1:A:496:GLN:HE21	1.63	0.63
1:A:523:ILE:HD13	1:A:740:LEU:CD2	2.26	0.63
1:A:360:LEU:HB3	1:A:361:PRO:HD3	1.81	0.62
1:A:676:SER:HB3	1:A:719:VAL:HG12	1.81	0.62
1:B:579:LEU:HD22	1:B:580:GLU:HG2	1.82	0.62
1:B:544:PHE:HD1	1:B:547:MET:HE3	1.65	0.62
1:B:649:ILE:CD1	1:B:714:ILE:HG13	2.30	0.61
1:A:325:ASN:HA	1:A:328:ASN:OD1	2.02	0.60
1:B:566:VAL:HG22	1:B:581:LEU:CD2	2.33	0.59
1:B:654:THR:HG22	1:B:733:THR:CG2	2.33	0.58
1:A:409:VAL:CG1	1:A:410:GLU:H	2.14	0.58
1:A:475:ILE:HG13	1:A:476:LEU:N	2.19	0.58
1:B:325:ASN:HA	1:B:328:ASN:OD1	2.04	0.58
1:A:475:ILE:O	1:A:479:GLN:HG3	2.03	0.57
1:B:543:ILE:HD11	1:B:576:PHE:HE1	1.68	0.57
1:B:390:VAL:O	1:B:394:THR:HG23	2.03	0.57
1:A:670:GLN:NE2	3:A:178:HOH:O	2.37	0.57
1:B:377:GLU:HB3	3:B:133:HOH:O	2.04	0.57
1:B:727:ARG:HG2	1:B:731:ARG:NH1	2.20	0.56
1:A:446:ARG:O	1:B:493:LYS:NZ	2.37	0.56
1:A:475:ILE:HG13	1:A:476:LEU:H	1.70	0.56
1:A:356:GLU:HG3	1:A:584:ARG:HD3	1.86	0.56
1:B:242:PHE:HB3	1:B:628:TRP:CE2	2.40	0.56
1:A:541:LEU:O	1:A:545:GLU:HG3	2.06	0.56
1:A:584:ARG:NH1	1:A:586:GLN:HG3	2.21	0.56
1:B:394:THR:HG21	1:B:409:VAL:H	1.71	0.56
1:A:499:ARG:HE	1:A:522:SER:HA	1.71	0.55
1:A:450:PRO:CD	1:A:496:GLN:HE21	2.18	0.55
1:A:386:ILE:HD11	1:A:490:PHE:CD1	2.42	0.55
1:B:473:PHE:HB3	1:B:474:PRO:HD3	1.89	0.54
1:A:395:LEU:O	1:A:396:GLN:HB2	2.08	0.54
1:B:338:ILE:O	1:B:342:ILE:HD12	2.07	0.54
1:B:654:THR:O	1:B:655:SER:CB	2.55	0.54
1:B:654:THR:H	1:B:733:THR:HG21	1.73	0.54
1:B:734:VAL:O	1:B:738:ILE:HG13	2.07	0.54
1:B:377:GLU:HG2	1:B:378:ALA:H	1.72	0.53
1:B:465:ARG:NH2	1:B:483:GLU:OE1	2.42	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:SER:C	1:A:523:ILE:HG13	2.28	0.53
1:A:374:PRO:HG2	1:A:379:MET:CE	2.39	0.53
1:A:566:VAL:HG22	1:A:581:LEU:CD2	2.39	0.53
1:B:544:PHE:CD1	1:B:547:MET:HE3	2.43	0.53
1:B:385:LYS:NZ	1:B:579:LEU:HD23	2.24	0.52
1:B:541:LEU:O	1:B:545:GLU:HG3	2.09	0.52
1:B:381:ALA:C	1:B:383:GLY:N	2.63	0.52
1:B:544:PHE:HA	1:B:547:MET:CE	2.40	0.52
1:B:540:PRO:O	1:B:543:ILE:HG22	2.10	0.52
1:A:377:GLU:H	1:A:377:GLU:CD	2.08	0.52
1:A:725:SER:HB3	1:A:734:VAL:HG21	1.91	0.52
1:B:612:PRO:HG2	1:B:615:ARG:HG2	1.90	0.52
1:A:453:ILE:HG12	1:A:491:LEU:CD2	2.40	0.51
1:B:409:VAL:CG2	1:B:410:GLU:H	2.08	0.51
1:B:708:GLU:HG2	1:B:709:ASN:ND2	2.26	0.51
1:A:394:THR:HG21	1:A:409:VAL:H	1.76	0.51
1:A:358:PRO:O	1:A:361:PRO:HD2	2.10	0.51
1:B:544:PHE:HA	1:B:547:MET:HE3	1.93	0.51
1:A:569:LEU:O	1:A:576:PHE:HA	2.12	0.50
1:B:276:MET:HB2	1:B:313:MET:CE	2.41	0.50
1:A:521:CYS:SG	1:A:524:GLN:HG2	2.51	0.50
1:A:684:PHE:CE2	1:A:699:GLN:NE2	2.80	0.50
1:B:276:MET:O	1:B:280:ARG:HG3	2.11	0.50
1:B:340:LYS:HD3	1:B:367:ASN:OD1	2.11	0.50
1:A:450:PRO:HD3	1:A:496:GLN:NE2	2.26	0.49
1:A:382:LEU:HD11	1:A:558:VAL:HG21	1.94	0.49
1:B:402:TRP:HB2	1:B:491:LEU:O	2.12	0.49
1:A:723:GLU:O	1:A:726:ILE:HG23	2.11	0.49
1:B:737:LEU:O	1:B:741:LEU:HG	2.12	0.49
1:A:277:ARG:NE	3:A:101:HOH:O	2.45	0.49
1:B:340:LYS:HD3	1:B:367:ASN:CG	2.33	0.49
1:A:676:SER:HB3	1:A:719:VAL:CG1	2.43	0.49
1:B:519:ARG:NH2	1:B:586:GLN:OE1	2.46	0.48
1:A:620:ARG:NH2	1:A:631:THR:HG22	2.18	0.48
1:A:377:GLU:OE1	1:A:377:GLU:N	2.44	0.48
1:B:443:ALA:O	1:B:447:ILE:HG13	2.14	0.48
1:A:394:THR:CG2	1:A:409:VAL:H	2.26	0.48
1:A:464:ILE:HG12	1:A:465:ARG:N	2.28	0.48
1:A:393:GLN:HG3	1:A:399:THR:HG21	1.96	0.48
1:B:505:ILE:HG13	1:B:564:GLY:O	2.14	0.47
1:A:504:GLN:HG2	1:A:592:THR:HG21	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:496:GLN:O	1:B:497:HIS:HB2	2.15	0.47
1:B:553:ARG:NE	3:B:159:HOH:O	2.47	0.47
1:A:523:ILE:HD13	1:A:740:LEU:CG	2.45	0.47
1:A:740:LEU:HD12	1:A:740:LEU:O	2.14	0.47
1:B:382:LEU:HD13	1:B:581:LEU:CG	2.42	0.47
1:B:654:THR:OG1	1:B:655:SER:N	2.48	0.46
1:A:453:ILE:HG12	1:A:491:LEU:HD22	1.97	0.46
1:B:513:ALA:HB3	1:B:552:ILE:HG23	1.96	0.46
1:B:569:LEU:CD2	1:B:579:LEU:HB2	2.45	0.46
1:B:649:ILE:HD12	1:B:713:ALA:CB	2.45	0.46
1:A:437:VAL:HG22	1:A:477:PHE:HD2	1.81	0.46
1:A:431:LYS:C	1:A:433:CYS:H	2.19	0.46
1:B:408:THR:HG22	1:B:409:VAL:N	2.31	0.46
1:B:747:GLN:HE21	1:B:747:GLN:HB2	1.48	0.46
1:A:493:LYS:HG3	1:A:494:LEU:N	2.31	0.46
1:B:453:ILE:O	1:B:464:ILE:HA	2.16	0.45
1:B:638:PRO:HG2	1:B:641:PRO:HG3	1.98	0.45
1:B:408:THR:HG22	1:B:409:VAL:O	2.16	0.45
1:A:400:LEU:HD23	1:A:401:PRO:HD2	1.97	0.45
1:B:249:GLU:OE1	1:B:253:ARG:NH1	2.44	0.45
1:A:473:PHE:N	1:A:474:PRO:HD2	2.32	0.45
1:A:520:ASP:OD1	1:A:521:CYS:N	2.50	0.45
1:B:276:MET:HB2	1:B:313:MET:HE2	1.98	0.45
1:A:356:GLU:CG	1:A:584:ARG:HD3	2.47	0.45
1:B:409:VAL:HG22	1:B:410:GLU:HG3	2.00	0.45
1:B:474:PRO:O	1:B:478:ARG:HG3	2.17	0.44
1:A:454:LYS:HG3	1:A:490:PHE:CZ	2.52	0.44
1:A:589:HIS:N	1:A:590:PRO:CD	2.81	0.44
1:B:612:PRO:HG2	1:B:615:ARG:CG	2.47	0.44
1:A:584:ARG:NH1	1:A:584:ARG:CG	2.76	0.44
1:A:542:ALA:HB2	1:B:549:GLN:HE22	1.83	0.44
1:A:529:LYS:HD2	1:A:532:GLU:OE2	2.17	0.44
1:A:556:LYS:NZ	1:A:636:GLU:OE1	2.42	0.44
1:B:244:VAL:HG21	1:B:250:PHE:HB2	1.98	0.44
1:A:638:PRO:HG2	1:A:641:PRO:HG3	2.00	0.44
1:A:465:ARG:NH2	1:A:483:GLU:OE2	2.50	0.44
1:B:377:GLU:CG	1:B:378:ALA:N	2.79	0.44
1:B:524:GLN:HG2	1:B:529:LYS:HA	2.00	0.43
1:B:740:LEU:O	1:B:740:LEU:HD23	2.18	0.43
1:A:452:MET:HB3	1:A:454:LYS:NZ	2.33	0.43
1:B:296:VAL:HA	1:B:316:HIS:O	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:569:LEU:HD21	1:B:579:LEU:HD12	1.99	0.43
1:A:465:ARG:HD2	1:A:476:LEU:O	2.18	0.43
1:A:254:PHE:CZ	1:A:286:MET:HE1	2.54	0.43
1:A:462:LYS:HB3	1:A:463:GLY:H	1.56	0.43
1:B:521:CYS:HB3	1:B:529:LYS:CD	2.49	0.43
1:A:462:LYS:HD3	1:A:464:ILE:CG2	2.48	0.43
1:B:538:ILE:HD13	1:B:749:ASN:HB3	2.00	0.43
1:B:242:PHE:C	1:B:242:PHE:CD1	2.90	0.43
1:B:454:LYS:HG2	1:B:490:PHE:CE1	2.54	0.43
1:B:400:LEU:HD13	1:B:493:LYS:O	2.18	0.42
1:A:551:ALA:HB1	1:A:566:VAL:HG21	2.01	0.42
1:B:725:SER:HB3	1:B:734:VAL:HG21	2.01	0.42
1:A:384:ASP:O	1:A:388:SER:HB2	2.18	0.42
1:A:382:LEU:CD1	1:A:581:LEU:HG	2.39	0.42
1:B:338:ILE:O	1:B:342:ILE:CD1	2.67	0.42
1:A:264:LEU:HB3	1:A:347:VAL:HG22	2.01	0.42
1:A:242:PHE:HE2	1:A:244:VAL:CG1	2.33	0.42
1:A:251:VAL:HG21	1:A:259:VAL:HA	2.01	0.42
1:B:394:THR:CG2	1:B:409:VAL:H	2.32	0.42
1:A:260:ILE:HD13	1:A:346:ALA:HB2	2.01	0.42
1:B:395:LEU:O	1:B:396:GLN:CB	2.65	0.42
1:B:589:HIS:N	1:B:590:PRO:CD	2.83	0.42
1:A:276:MET:HB2	1:A:313:MET:CE	2.49	0.42
1:A:338:ILE:O	1:A:342:ILE:HG12	2.20	0.42
1:B:706:TRP:CG	1:B:707:GLY:N	2.88	0.41
1:A:474:PRO:O	1:A:478:ARG:HG3	2.20	0.41
1:B:333:GLU:CD	1:B:333:GLU:H	2.23	0.41
1:B:726:ILE:O	1:B:727:ARG:CB	2.67	0.41
1:A:286:MET:HE2	3:A:22:HOH:O	2.20	0.41
1:B:722:LYS:CG	1:B:738:ILE:HD13	2.50	0.41
1:B:345:GLN:HB3	1:B:345:GLN:HE21	1.69	0.41
1:B:556:LYS:NZ	1:B:636:GLU:HG3	2.36	0.41
1:B:676:SER:HB2	1:B:723:GLU:OE1	2.21	0.41
1:A:374:PRO:HG2	1:A:379:MET:HE2	2.02	0.41
1:B:739:ASN:O	1:B:743:THR:HG23	2.20	0.41
1:A:400:LEU:CD2	1:A:401:PRO:HD2	2.50	0.41
1:A:492:MET:HE2	1:A:492:MET:HB2	1.90	0.41
1:B:358:PRO:O	1:B:361:PRO:HD2	2.20	0.41
1:B:499:ARG:HB3	1:B:522:SER:OG	2.21	0.41
1:B:566:VAL:CG2	1:B:581:LEU:CD2	2.98	0.41
1:B:649:ILE:HD12	1:B:713:ALA:HB1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:466:LYS:HG2	1:B:494:LEU:HD11	2.03	0.40
1:A:543:ILE:HD12	1:B:546:PHE:CE2	2.55	0.40
1:A:637:THR:HG23	1:A:637:THR:O	2.21	0.40
1:B:251:VAL:HG21	1:B:259:VAL:HA	2.03	0.40
1:B:395:LEU:O	1:B:553:ARG:NH2	2.54	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	446/540 (83%)	430 (96%)	14 (3%)	2 (0%)	34	42
1	B	443/540 (82%)	425 (96%)	16 (4%)	2 (0%)	29	35
All	All	889/1080 (82%)	855 (96%)	30 (3%)	4 (0%)	34	42

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	562	SER
1	B	562	SER
1	A	749	ASN
1	B	382	LEU

### 5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	383/450 (85%)	356 (93%)	27 (7%)	15	19
1	B	380/450 (84%)	362 (95%)	18 (5%)	26	37
All	All	763/900 (85%)	718 (94%)	45 (6%)	19	27

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	242	PHE
1	A	286	MET
1	A	288	ARG
1	A	341	ARG
1	A	345	GLN
1	A	372	LEU
1	A	384	ASP
1	A	388	SER
1	A	454	LYS
1	A	464	ILE
1	A	465	ARG
1	A	469	SER
1	A	482	SER
1	A	489	ILE
1	A	492	MET
1	A	499	ARG
1	A	528	GLN
1	A	569	LEU
1	A	572	GLN
1	A	579	LEU
1	A	581	LEU
1	A	586	GLN
1	A	597	ASP
1	A	643	LEU
1	A	724	LEU
1	A	732	THR
1	A	750	ASP
1	B	241	ASP
1	B	242	PHE
1	B	286	MET
1	B	304	LEU
1	B	345	GLN
1	B	372	LEU
1	B	396	GLN
1	B	452	MET

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Mol	Chain	Res	Type
1	B	581	LEU
1	B	597	ASP
1	B	617	LYS
1	B	637	THR
1	B	645	ARG
1	B	676	SER
1	B	678	LYS
1	B	724	LEU
1	B	726	ILE
1	B	747	GLN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	496	GLN
1	A	586	GLN
1	A	699	GLN
1	A	747	GLN
1	B	549	GLN
1	B	747	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 carbohydrates 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	S1A	B	1000	-	39,39,39	2.03	17 (43%)	45,55,55	1.04	3 (6%)
2	S1A	A	1000	-	39,39,39	1.87	9 (23%)	45,55,55	1.03	4 (8%)

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	B	1000	-	-	1/44/67/67	0/2/3/3
2	S1A	A	1000	-	-	4/44/67/67	0/2/3/3

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000	S1A	C3-C4	5.40	1.61	1.53
2	B	1000	S1A	C3-C4	5.36	1.61	1.53
2	B	1000	S1A	C6-C7	3.48	1.60	1.53
2	A	1000	S1A	C6-C7	3.44	1.60	1.53
2	B	1000	S1A	C26-C25	3.26	1.44	1.39
2	B	1000	S1A	C25-C17	3.05	1.56	1.51
2	B	1000	S1A	C5-C4	2.76	1.59	1.53
2	A	1000	S1A	C5-C4	2.72	1.58	1.53
2	B	1000	S1A	C21-C6	2.70	1.59	1.53
2	B	1000	S1A	C30-C25	2.69	1.43	1.39
2	A	1000	S1A	O7-C3	2.57	1.47	1.43
2	A	1000	S1A	C26-C25	2.55	1.43	1.39
2	A	1000	S1A	O7-C7	2.49	1.47	1.44
2	B	1000	S1A	C19-C2	2.40	1.57	1.53
2	B	1000	S1A	C12-C11	2.32	1.57	1.52
2	B	1000	S1A	O7-C3	2.29	1.47	1.43
2	B	1000	S1A	C6-C5	2.27	1.57	1.53
2	B	1000	S1A	O18-C1	2.19	1.39	1.34
2	A	1000	S1A	C13-C12	2.18	1.56	1.52
2	B	1000	S1A	O7-C7	2.17	1.47	1.44
2	B	1000	S1A	C28-C27	2.14	1.43	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	1000	S1A	C29-C30	2.09	1.43	1.38
2	A	1000	S1A	C19-C2	2.07	1.57	1.53
2	A	1000	S1A	C12-C11	2.05	1.56	1.52
2	B	1000	S1A	C27-C26	2.04	1.43	1.38
2	B	1000	S1A	C13-C12	2.02	1.56	1.52

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000	S1A	O18-C17-C16	3.67	110.60	105.34
2	B	1000	S1A	C16-C17-C25	-3.31	106.63	112.62
2	A	1000	S1A	C16-C17-C25	-2.93	107.33	112.62
2	B	1000	S1A	O18-C17-C16	2.86	109.44	105.34
2	A	1000	S1A	O4-C4-C5	2.53	114.04	109.33
2	B	1000	S1A	O1-C1-C2	-2.47	119.16	124.90
2	A	1000	S1A	O1-C1-C2	-2.31	119.53	124.90

There are no chirality outliers.

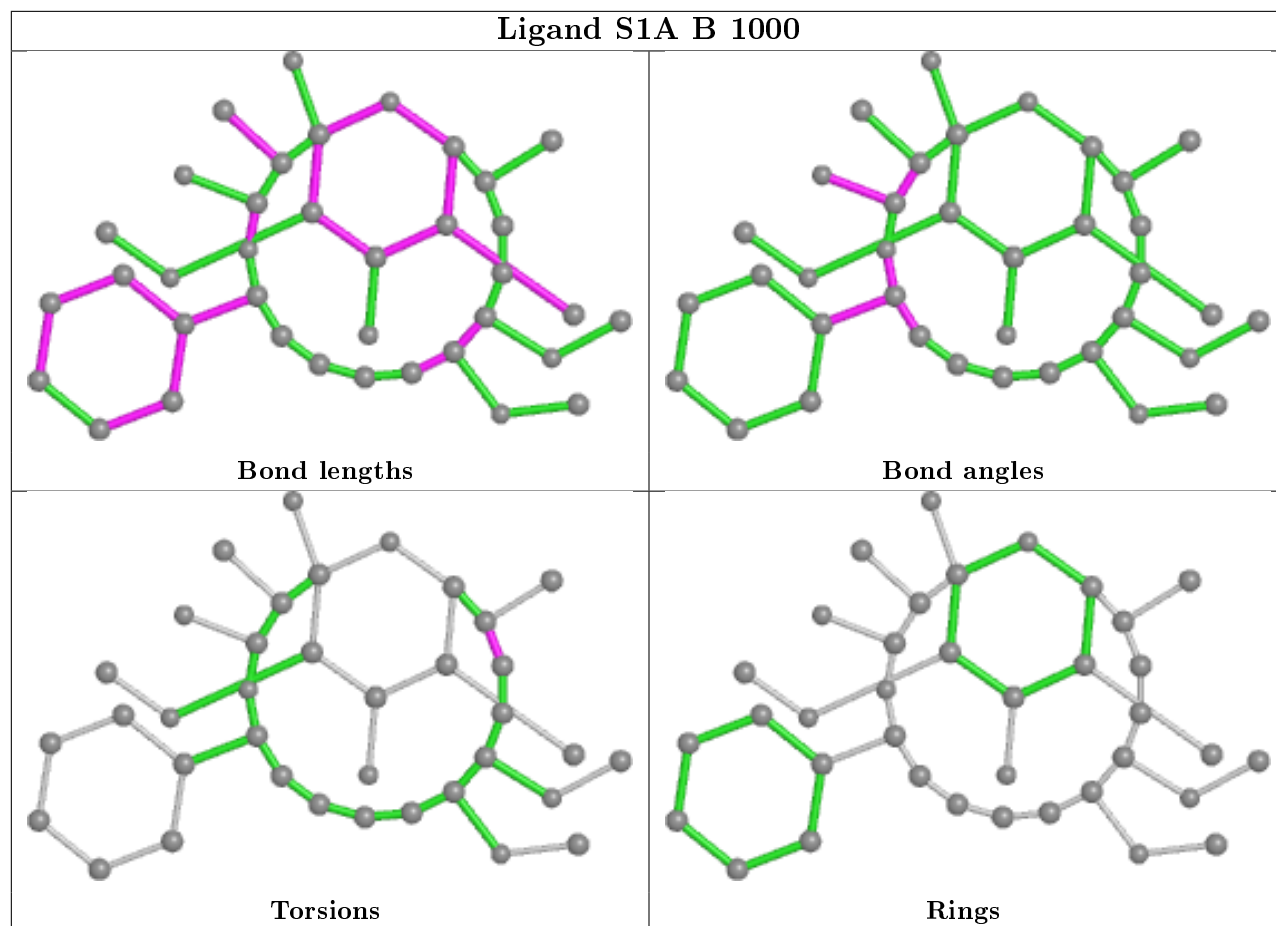
All (5) torsion outliers are listed below:

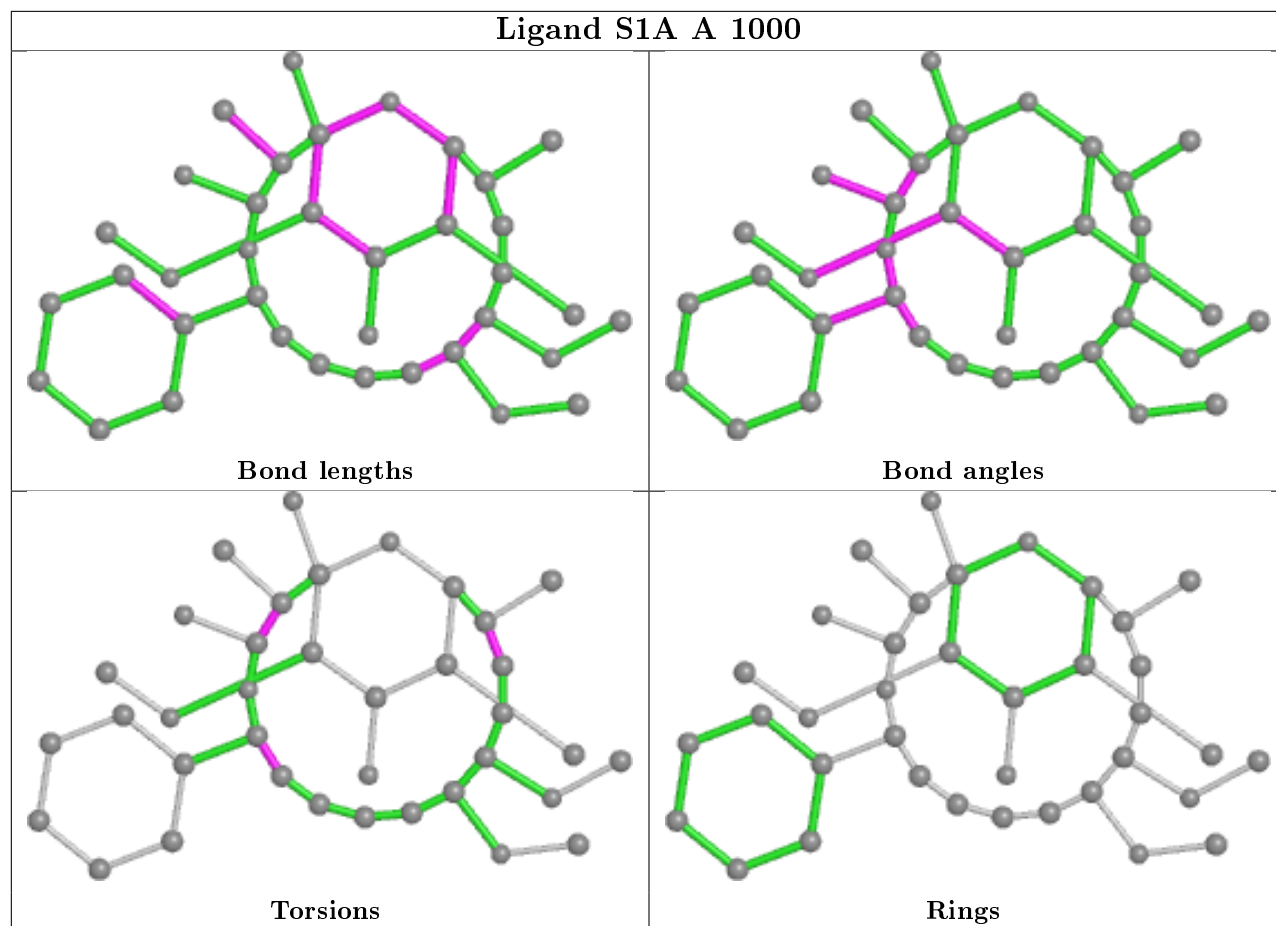
Mol	Chain	Res	Type	Atoms
2	A	1000	S1A	C22-C8-C9-C10
2	B	1000	S1A	C22-C8-C9-C10
2	A	1000	S1A	O1-C1-C2-C19
2	A	1000	S1A	O18-C1-C2-C19
2	A	1000	S1A	C15-C16-C17-O18

There are no ring outliers.

No monomer is involved in short contacts.

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, 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	460/540 (85%)	0.20	36 (7%)	13 17	16, 32, 67, 88	0
1	B	457/540 (84%)	0.16	34 (7%)	14 19	15, 33, 61, 83	0
All	All	917/1080 (84%)	0.18	70 (7%)	13 18	15, 33, 64, 88	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	431	LYS	6.4
1	A	731	ARG	6.3
1	A	435	LYS	6.1
1	A	698	SER	6.0
1	B	431	LYS	5.3
1	B	686	VAL	5.3
1	A	497	HIS	5.0
1	B	727	ARG	4.9
1	B	655	SER	4.7
1	A	496	GLN	4.5
1	B	726	ILE	4.4
1	B	639	SER	4.2
1	B	496	GLN	4.2
1	B	409	VAL	3.8
1	B	640	ASN	3.7
1	B	380	TRP	3.7
1	A	527	HIS	3.6
1	A	452	MET	3.6
1	A	655	SER	3.6
1	A	462	LYS	3.6
1	B	572	GLN	3.5
1	B	497	HIS	3.5
1	B	654	THR	3.4
1	B	731	ARG	3.1

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Mol	Chain	Res	Type	RSRZ
1	B	684	PHE	3.1
1	B	462	LYS	3.1
1	A	410	GLU	3.1
1	B	744	GLU	3.1
1	A	528	GLN	3.0
1	B	446	ARG	3.0
1	B	410	GLU	3.0
1	A	700	PHE	2.9
1	B	524	GLN	2.9
1	B	461	GLY	2.8
1	A	409	VAL	2.8
1	A	463	GLY	2.6
1	B	372	LEU	2.6
1	B	700	PHE	2.6
1	A	439	GLU	2.5
1	B	528	GLN	2.5
1	A	474	PRO	2.5
1	B	383	GLY	2.5
1	B	471	GLU	2.5
1	A	446	ARG	2.4
1	A	438	ASP	2.4
1	B	748	ASN	2.4
1	B	733	THR	2.4
1	A	640	ASN	2.4
1	A	466	LYS	2.4
1	A	408	THR	2.4
1	A	383	GLY	2.4
1	A	687	ALA	2.3
1	A	699	GLN	2.3
1	B	732	THR	2.3
1	A	726	ILE	2.2
1	A	478	ARG	2.2
1	B	749	ASN	2.1
1	A	639	SER	2.1
1	B	439	GLU	2.1
1	A	437	VAL	2.1
1	A	684	PHE	2.1
1	B	472	ASP	2.1
1	B	347	VAL	2.1
1	A	485	PRO	2.1
1	A	654	THR	2.1
1	A	241	ASP	2.0

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Mol	Chain	Res	Type	RSRZ
1	B	408	THR	2.0
1	A	643	LEU	2.0
1	A	686	VAL	2.0
1	A	464	ILE	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 carbohydrates in this entry.

## 6.4 Ligands [i](#)

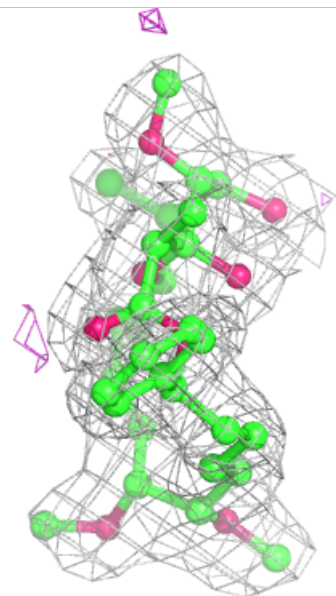
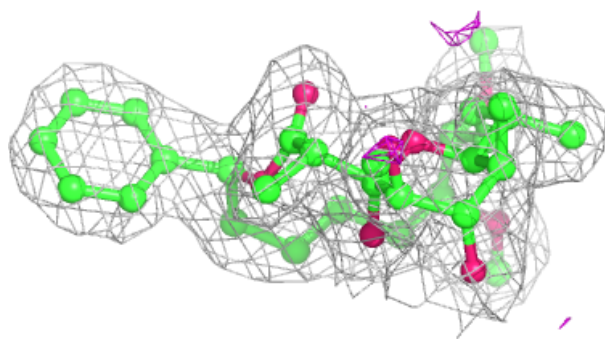
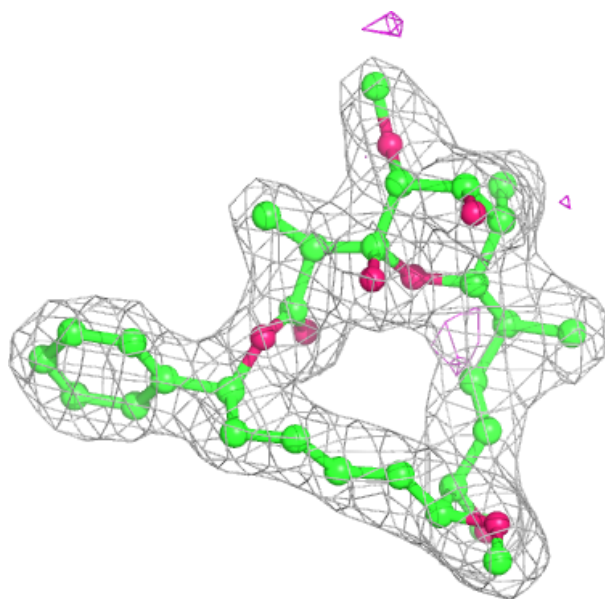
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	S1A	B	1000	37/37	0.96	0.11	18,23,27,35	0
2	S1A	A	1000	37/37	0.97	0.11	15,21,26,32	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 B 1000:**

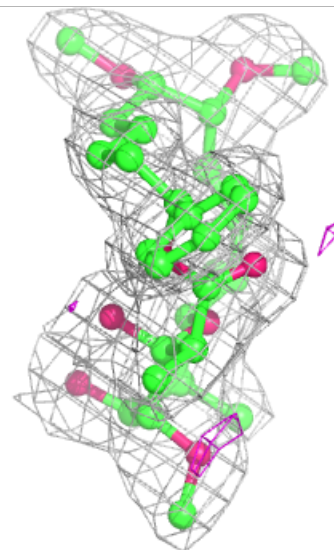
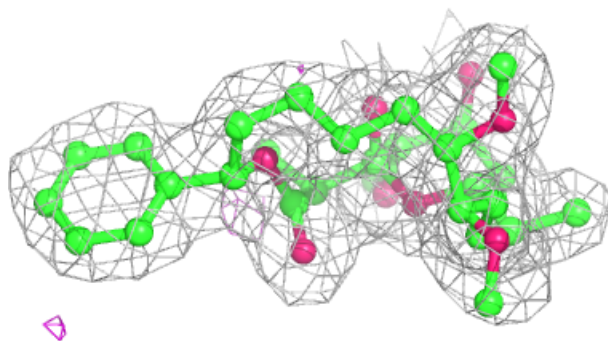
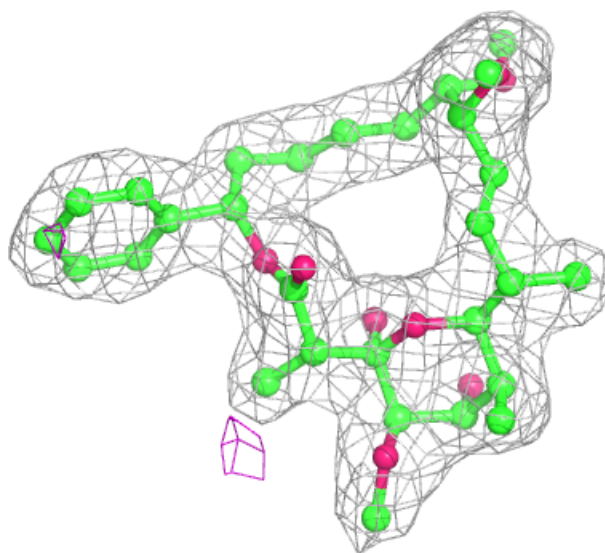
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around S1A A 1000:**

$2mF_o-DF_c$  (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.