



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 9, 2020 – 04:27 PM BST

PDB ID : 2BRP  
Title : Crystal structure of S. pneumoniae hyaluronate lyase in complex with W249b  
Authors : Rigden, D.J.; Jedrzejewski, M.J.  
Deposited on : 2005-05-10  
Resolution : 2.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<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 : 2.13.1  
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) : 2.13.1

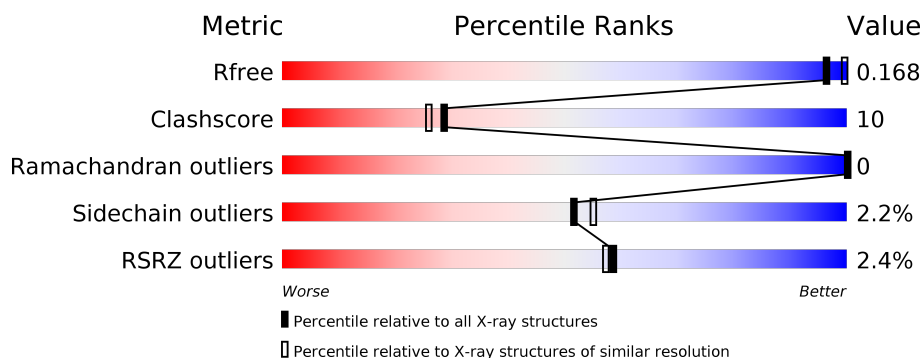
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria 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	731	<div> <div>2%</div> <div>85%</div> <div>12%</div> <div>..</div> </div>

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SIE	A	1000[A]	-	-	X	X
2	SIE	A	1000[B]	-	-	-	X

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	XLS	A	1101	-	X	-	-
3	XLS	A	1102	X	X	-	-

## 2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 6509 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.

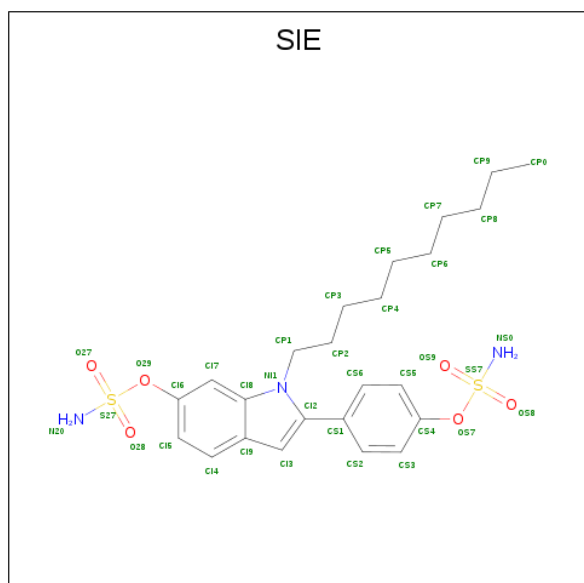
- Molecule 1 is a protein called HYALURONATE LYASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	721	5824	3665	975	1161	23	0	4	0

There are 8 discrepancies between the modelled and reference sequences:

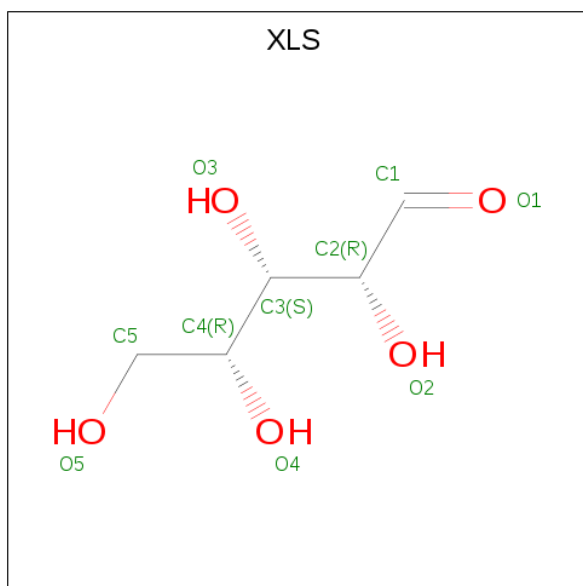
Chain	Residue	Modelled	Actual	Comment	Reference
A	173	THR	ALA	conflict	UNP Q54873
A	196	ASP	GLU	conflict	UNP Q54873
A	223	ILE	THR	conflict	UNP Q54873
A	496	ARG	CYS	conflict	UNP Q54873
A	541	THR	PRO	conflict	UNP Q54873
A	704	SER	GLY	conflict	UNP Q54873
A	736	SER	PHE	conflict	UNP Q54873
A	790	GLY	ARG	conflict	UNP Q54873

- Molecule 2 is SULFAMIC ACID 1-DECYL-2-(4-SULFAMOYLOXYPHENYL)-1H-INDOL-6-YL ESTER (three-letter code: SIE) (formula: C<sub>24</sub>H<sub>33</sub>N<sub>3</sub>O<sub>6</sub>S<sub>2</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	1
			70	48	6	12	4		

- Molecule 3 is D-xylose (three-letter code: XLS) (formula:  $C_5H_{10}O_5$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			10	5	5		
3	A	1	Total	C	O	0	0
			10	5	5		
3	A	1	Total	C	O	0	0
			10	5	5		

- Molecule 4 is SULFATE ION (three-letter code: SO4) (formula:  $O_4S$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		
4	A	1	Total	O	S	0	0
			5	4	1		

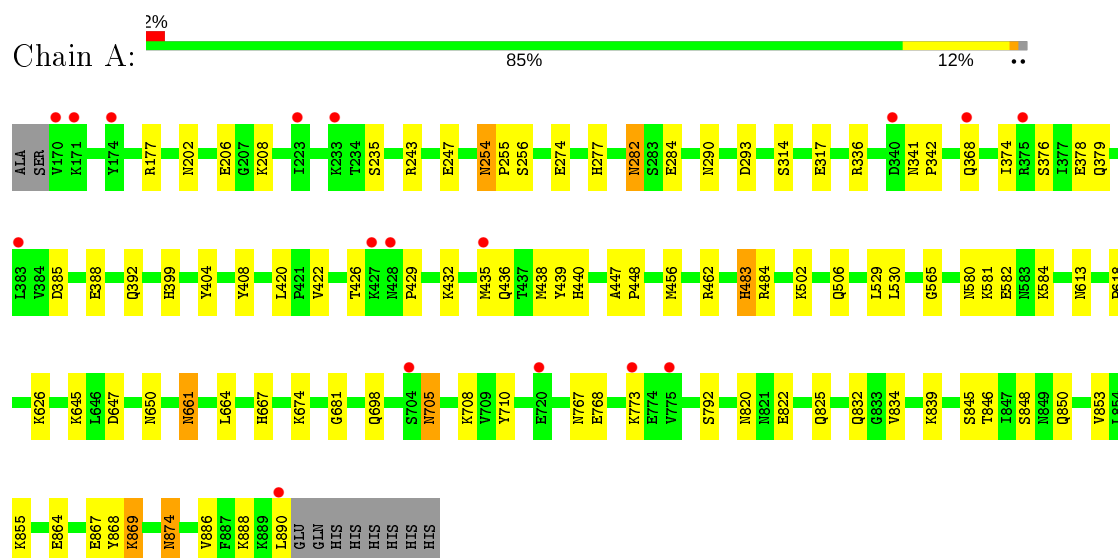
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	560	Total	O	0	0
			560	560		

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

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: HYALURONATE LYASE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	84.19 Å   103.27 Å   103.26 Å 90.00°   90.00°   90.00°	Depositor
Resolution (Å)	44.02 – 2.00 46.18 – 2.00	Depositor EDS
% Data completeness (in resolution range)	43.9 (44.02-2.00) 43.8 (46.18-2.00)	Depositor EDS
$R_{merge}$	0.12	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.29 (at 2.00 Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.178 , 0.202 0.170 , 0.168	Depositor DCC
$R_{free}$ test set	1361 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	29.3	Xtriage
Anisotropy	0.545	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 45.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.015 for -h,l,k	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	6509	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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: XLS, SO4, SIE

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	0.31	0/5945	0.59	0/8028

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	5824	0	5643	96	0
2	A	70	0	62	41	0
3	A	30	0	30	0	0
4	A	25	0	0	1	0
5	A	560	0	0	10	0
All	All	6509	0	5735	113	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 10.

All (113) 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)
2:A:1000[B]:SIE:O29	2:A:1000[B]:SIE:CI6	1.64	1.44
2:A:1000[A]:SIE:CI6	2:A:1000[A]:SIE:O29	1.64	1.42
2:A:1000[B]:SIE:CS4	2:A:1000[B]:SIE:OS7	1.64	1.42
2:A:1000[A]:SIE:OS7	2:A:1000[A]:SIE:CS4	1.65	1.41
1:A:613:ASN:H	1:A:698:GLN:HE22	1.11	0.98
1:A:290:ASN:HD21	2:A:1000[B]:SIE:HI3	1.31	0.94
1:A:869:LYS:N	1:A:869:LYS:HE3	1.88	0.89
1:A:290:ASN:HD21	2:A:1000[A]:SIE:HI3	1.41	0.84
2:A:1000[A]:SIE:SS7	2:A:1000[A]:SIE:CS4	2.66	0.82
2:A:1000[B]:SIE:CS4	2:A:1000[B]:SIE:SS7	2.68	0.80
1:A:290:ASN:ND2	2:A:1000[B]:SIE:HI3	1.97	0.80
2:A:1000[B]:SIE:S27	2:A:1000[B]:SIE:CI6	2.71	0.79
1:A:290:ASN:ND2	2:A:1000[A]:SIE:HI3	2.00	0.76
2:A:1000[A]:SIE:S27	2:A:1000[A]:SIE:CI6	2.75	0.75
1:A:855:LYS:HD3	1:A:886:VAL:HG12	1.70	0.74
1:A:282:ASN:HD22	1:A:284:GLU:H	1.36	0.73
1:A:388:GLU:OE2	2:A:1000[A]:SIE:HP92	1.89	0.73
1:A:388:GLU:OE2	2:A:1000[B]:SIE:HP92	1.89	0.72
1:A:864:GLU:HB2	1:A:869:LYS:HZ3	1.56	0.71
1:A:392:GLN:HG2	5:A:2298:HOH:O	1.91	0.70
1:A:864:GLU:HB2	1:A:869:LYS:NZ	2.07	0.69
2:A:1000[A]:SIE:HP21	2:A:1000[A]:SIE:HS2	1.76	0.68
1:A:243:ARG:O	1:A:247:GLU:HG3	1.98	0.64
1:A:399:HIS:HA	2:A:1000[B]:SIE:HP91	1.82	0.62
1:A:399:HIS:HA	2:A:1000[A]:SIE:HP91	1.82	0.62
1:A:399:HIS:HD2	2:A:1000[A]:SIE:HP91	1.64	0.61
1:A:874:ASN:HD22	1:A:874:ASN:C	2.03	0.61
2:A:1000[A]:SIE:CP2	2:A:1000[A]:SIE:HS2	2.32	0.60
1:A:399:HIS:HD2	2:A:1000[B]:SIE:HP91	1.64	0.60
1:A:483[A]:HIS:HD2	1:A:484:ARG:N	2.03	0.56
1:A:868:TYR:C	1:A:869:LYS:HE3	2.25	0.56
1:A:580:ASN:HD21	2:A:1000[A]:SIE:CI2	2.19	0.56
1:A:529:LEU:HD23	1:A:529:LEU:C	2.27	0.55
1:A:435:MET:HA	1:A:438:MET:HE2	1.89	0.55
2:A:1000[A]:SIE:CS2	2:A:1000[A]:SIE:HP21	2.37	0.54
1:A:483[B]:HIS:CE1	5:A:2235:HOH:O	2.61	0.54
1:A:456:MET:HE3	1:A:565:GLY:HA3	1.91	0.53
1:A:440:HIS:HE1	5:A:2172:HOH:O	1.91	0.53
1:A:447:ALA:HB3	1:A:448:PRO:HD3	1.90	0.53
1:A:254:ASN:HD22	1:A:254:ASN:C	2.12	0.52
1:A:408:TYR:OH	2:A:1000[B]:SIE:HI7	2.09	0.52
2:A:1000[B]:SIE:CP2	2:A:1000[B]:SIE:HS2	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:399:HIS:CD2	2:A:1000[A]:SIE:HP91	2.43	0.51
1:A:399:HIS:CD2	2:A:1000[B]:SIE:HP91	2.43	0.51
1:A:581:LYS:HB3	1:A:768:GLU:HB2	1.92	0.51
1:A:820:ASN:HD22	1:A:825:GLN:HG2	1.75	0.51
1:A:408:TYR:OH	2:A:1000[A]:SIE:HI7	2.10	0.51
1:A:705:ASN:N	1:A:705:ASN:HD22	2.08	0.51
1:A:282:ASN:HD22	1:A:284:GLU:N	2.07	0.50
1:A:399:HIS:HA	2:A:1000[A]:SIE:HP71	1.91	0.50
1:A:399:HIS:HA	2:A:1000[B]:SIE:HP71	1.91	0.50
2:A:1000[B]:SIE:HS2	2:A:1000[B]:SIE:HP21	1.94	0.50
1:A:436:GLN:HA	1:A:439:TYR:HD2	1.77	0.50
1:A:667:HIS:HD2	5:A:2503:HOH:O	1.93	0.49
1:A:314:SER:OG	1:A:317:GLU:HG3	2.13	0.49
1:A:483[B]:HIS:CE1	1:A:529:LEU:HD12	2.47	0.49
1:A:664:LEU:C	1:A:664:LEU:HD23	2.34	0.48
1:A:290:ASN:CG	2:A:1000[B]:SIE:HS6	2.33	0.48
1:A:845:SER:HB2	1:A:853:VAL:HG23	1.95	0.48
1:A:426:THR:O	1:A:429:PRO:HD3	2.14	0.47
1:A:661:ASN:HD22	1:A:661:ASN:C	2.17	0.47
1:A:282:ASN:ND2	1:A:284:GLU:H	2.08	0.47
2:A:1000[A]:SIE:HP82	2:A:1000[A]:SIE:HP52	1.63	0.47
1:A:645:LYS:HE3	1:A:647:ASP:O	2.15	0.47
1:A:440:HIS:CE1	5:A:2172:HOH:O	2.66	0.46
1:A:768:GLU:HG3	5:A:2555:HOH:O	2.16	0.45
1:A:848:SER:O	1:A:850:GLN:HG3	2.17	0.45
1:A:674[A]:LYS:HE3	5:A:2403:HOH:O	2.17	0.44
1:A:422:VAL:HA	5:A:2008:HOH:O	2.17	0.44
1:A:177:ARG:NE	1:A:177:ARG:HA	2.33	0.44
1:A:399:HIS:NE2	2:A:1000[A]:SIE:HP32	2.32	0.44
1:A:432:LYS:O	1:A:432:LYS:HG2	2.17	0.44
1:A:650:ASN:HD21	1:A:832:GLN:HE22	1.64	0.44
1:A:290:ASN:HD21	2:A:1000[B]:SIE:CI3	2.15	0.44
1:A:436:GLN:HA	1:A:439:TYR:CD2	2.52	0.44
1:A:502:LYS:O	1:A:506:GLN:HG3	2.18	0.44
1:A:580:ASN:HD21	2:A:1000[B]:SIE:CI2	2.30	0.43
1:A:202:ASN:O	1:A:206:GLU:HG2	2.18	0.43
1:A:254:ASN:ND2	1:A:256:SER:H	2.17	0.43
1:A:277:HIS:HD2	5:A:2087:HOH:O	2.00	0.43
1:A:208:LYS:HD3	1:A:247:GLU:OE2	2.18	0.43
1:A:839:LYS:HD2	1:A:853:VAL:HG23	2.01	0.43
2:A:1000[B]:SIE:HS2	2:A:1000[B]:SIE:CP1	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:462:ARG:HH22	2:A:1000[A]:SIE:CI8	2.31	0.43
1:A:584:LYS:HE2	4:A:1200:SO4:O1	2.18	0.43
1:A:846:THR:HG23	1:A:890:LEU:HD11	2.00	0.43
1:A:874:ASN:ND2	1:A:874:ASN:C	2.72	0.43
1:A:399:HIS:NE2	2:A:1000[B]:SIE:HP32	2.33	0.43
1:A:708:LYS:HE3	1:A:710:TYR:OH	2.20	0.42
1:A:235:SER:HB2	1:A:293:ASP:HB2	2.02	0.42
2:A:1000[B]:SIE:HP21	2:A:1000[B]:SIE:CS2	2.49	0.42
1:A:254:ASN:ND2	1:A:254:ASN:C	2.73	0.42
2:A:1000[A]:SIE:HP41	2:A:1000[A]:SIE:HS2	2.02	0.42
1:A:483[A]:HIS:CD2	1:A:484:ARG:N	2.84	0.42
1:A:374:ILE:O	1:A:378:GLU:HG3	2.20	0.42
1:A:274:GLU:OE1	1:A:274:GLU:HA	2.20	0.42
1:A:341:ASN:N	1:A:342:PRO:HD3	2.34	0.42
1:A:435:MET:HG2	1:A:438:MET:CE	2.49	0.42
1:A:376:SER:O	1:A:379:GLN:HG3	2.19	0.42
1:A:832:GLN:HB3	1:A:834:VAL:HG23	2.02	0.42
1:A:336:ARG:O	1:A:342:PRO:HG3	2.20	0.42
1:A:582:GLU:HG2	1:A:767:ASN:ND2	2.35	0.42
1:A:681:GLY:O	1:A:792:SER:HB2	2.19	0.41
1:A:420:LEU:HA	1:A:420:LEU:HD23	1.80	0.41
1:A:529:LEU:HD23	1:A:530:LEU:N	2.34	0.41
1:A:235:SER:OG	1:A:290:ASN:HB3	2.20	0.41
1:A:864:GLU:O	1:A:867:GLU:HB2	2.20	0.41
1:A:435:MET:HG2	1:A:438:MET:HE1	2.03	0.41
1:A:618[A]:PRO:HG2	5:A:2353:HOH:O	2.20	0.41
1:A:254:ASN:HD22	1:A:255:PRO:N	2.18	0.40
1:A:581:LYS:HD3	1:A:768:GLU:HG3	2.04	0.40
1:A:456:MET:CE	1:A:565:GLY:HA3	2.50	0.40
1:A:399:HIS:HA	2:A:1000[A]:SIE:CP9	2.48	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	723/731 (99%)	686 (95%)	37 (5%)	0	100	100

There are no Ramachandran outliers to report.

### 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	644/649 (99%)	629 (98%)	15 (2%)	50	53

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

Mol	Chain	Res	Type
1	A	254	ASN
1	A	282	ASN
1	A	368	GLN
1	A	385	ASP
1	A	404	TYR
1	A	483[A]	HIS
1	A	483[B]	HIS
1	A	626	LYS
1	A	661	ASN
1	A	705	ASN
1	A	773	LYS
1	A	822	GLU
1	A	869	LYS
1	A	874	ASN
1	A	888	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (25) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	202	ASN

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Mol	Chain	Res	Type
1	A	237	ASN
1	A	254	ASN
1	A	261	GLN
1	A	277	HIS
1	A	282	ASN
1	A	341	ASN
1	A	349	ASN
1	A	368	GLN
1	A	386	GLN
1	A	418	GLN
1	A	440	HIS
1	A	580	ASN
1	A	661	ASN
1	A	667	HIS
1	A	683	ASN
1	A	698	GLN
1	A	705	ASN
1	A	759	GLN
1	A	788	GLN
1	A	820	ASN
1	A	825	GLN
1	A	832	GLN
1	A	874	ASN
1	A	878	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 monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

10 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$
4	SO4	A	1204	-	4,4,4	0.14	0	6,6,6	0.07	0
3	XLS	A	1100	-	8,9,9	2.38	4 (50%)	10,11,11	2.12	5 (50%)
4	SO4	A	1201	-	4,4,4	0.17	0	6,6,6	0.06	0
2	SIE	A	1000[B]	-	35,37,37	6.51	18 (51%)	45,52,52	3.17	7 (15%)
3	XLS	A	1101	-	8,9,9	2.14	4 (50%)	10,11,11	2.13	6 (60%)
2	SIE	A	1000[A]	-	35,37,37	6.27	18 (51%)	45,52,52	2.02	10 (22%)
3	XLS	A	1102	-	8,9,9	2.51	4 (50%)	10,11,11	2.11	6 (60%)
4	SO4	A	1202	-	4,4,4	0.16	0	6,6,6	0.10	0
4	SO4	A	1200	-	4,4,4	0.20	0	6,6,6	0.05	0
4	SO4	A	1203	-	4,4,4	0.18	0	6,6,6	0.06	0

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	SIE	A	1000[B]	-	-	14/24/24/24	0/3/3/3
3	XLS	A	1101	-	-	4/10/12/12	-
3	XLS	A	1100	-	-	1/10/12/12	-
3	XLS	A	1102	-	1/1/3/4	4/10/12/12	-
2	SIE	A	1000[A]	-	-	15/24/24/24	0/3/3/3

All (48) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000[A]	SIE	OS7-SS7	-17.13	1.40	1.61
2	A	1000[B]	SIE	O29-S27	-15.49	1.42	1.61
2	A	1000[B]	SIE	OS7-SS7	-15.38	1.42	1.61
2	A	1000[A]	SIE	CS1-CI2	14.42	1.72	1.48
2	A	1000[A]	SIE	O29-S27	-14.03	1.44	1.61
2	A	1000[A]	SIE	OS7-CS4	13.92	1.65	1.42
2	A	1000[A]	SIE	O29-CI6	13.52	1.64	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1000[B]	SIE	O29-CI6	13.35	1.64	1.42
2	A	1000[B]	SIE	CS1-CI2	13.33	1.70	1.48
2	A	1000[B]	SIE	OS7-CS4	13.13	1.64	1.42
2	A	1000[B]	SIE	S27-N20	-12.84	1.44	1.58
2	A	1000[A]	SIE	CS5-CS4	8.01	1.54	1.38
2	A	1000[B]	SIE	O27-S27	7.93	1.48	1.42
2	A	1000[A]	SIE	S27-N20	-7.85	1.50	1.58
2	A	1000[B]	SIE	CS5-CS4	7.70	1.54	1.38
2	A	1000[B]	SIE	SS7-NS0	-7.63	1.50	1.58
2	A	1000[A]	SIE	SS7-NS0	-6.06	1.52	1.58
3	A	1102	XLS	C3-C2	-5.54	1.44	1.53
2	A	1000[B]	SIE	CS3-CS4	5.21	1.49	1.38
3	A	1100	XLS	C3-C2	-5.15	1.45	1.53
2	A	1000[A]	SIE	CS3-CS4	4.96	1.48	1.38
2	A	1000[B]	SIE	CS3-CS2	4.86	1.47	1.38
2	A	1000[A]	SIE	CS6-CS5	4.16	1.46	1.38
3	A	1101	XLS	C3-C2	-3.99	1.47	1.53
2	A	1000[B]	SIE	OS8-SS7	3.85	1.45	1.42
2	A	1000[A]	SIE	CS3-CS2	3.78	1.45	1.38
2	A	1000[A]	SIE	CS6-CS1	3.68	1.47	1.39
2	A	1000[B]	SIE	CS6-CS5	3.68	1.45	1.38
2	A	1000[A]	SIE	OS8-SS7	3.49	1.45	1.42
2	A	1000[A]	SIE	O27-S27	-3.27	1.39	1.42
2	A	1000[A]	SIE	CI7-CI6	3.22	1.42	1.37
2	A	1000[B]	SIE	CS2-CS1	3.06	1.45	1.39
3	A	1101	XLS	C4-C3	-3.00	1.47	1.53
2	A	1000[B]	SIE	CI7-CI6	2.96	1.42	1.37
2	A	1000[B]	SIE	CI3-CI2	-2.84	1.35	1.39
3	A	1102	XLS	O2-C2	-2.72	1.38	1.43
3	A	1100	XLS	O2-C2	-2.70	1.38	1.43
2	A	1000[A]	SIE	O28-S27	2.67	1.44	1.42
2	A	1000[B]	SIE	O28-S27	-2.64	1.40	1.42
3	A	1102	XLS	C4-C3	-2.63	1.48	1.53
3	A	1100	XLS	C4-C3	-2.63	1.48	1.53
2	A	1000[A]	SIE	CI3-CI2	-2.60	1.35	1.39
2	A	1000[B]	SIE	CS6-CS1	2.60	1.44	1.39
2	A	1000[A]	SIE	OS9-SS7	-2.57	1.40	1.42
3	A	1101	XLS	O2-C2	-2.50	1.38	1.43
3	A	1101	XLS	O1-C1	2.20	1.28	1.19
3	A	1102	XLS	O1-C1	2.17	1.28	1.19
3	A	1100	XLS	O1-C1	2.05	1.28	1.19

All (34) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1000[B]	SIE	O28-S27-O27	-13.46	107.24	119.97
2	A	1000[B]	SIE	OS9-SS7-OS8	-12.21	108.42	119.97
2	A	1000[A]	SIE	OS9-SS7-OS8	-8.29	112.13	119.97
2	A	1000[B]	SIE	O28-S27-N20	5.34	117.20	109.14
2	A	1000[A]	SIE	CI3-CI2-CS1	-5.27	119.71	128.10
2	A	1000[B]	SIE	CI3-CI2-CS1	-5.13	119.93	128.10
2	A	1000[B]	SIE	OS7-SS7-OS8	4.31	118.35	105.27
2	A	1000[A]	SIE	CI6-O29-S27	3.71	126.16	118.69
3	A	1100	XLS	C4-C3-C2	3.53	122.28	112.97
2	A	1000[A]	SIE	OS7-SS7-OS8	3.45	115.76	105.27
3	A	1102	XLS	C4-C3-C2	3.35	121.81	112.97
3	A	1101	XLS	C4-C3-C2	3.21	121.43	112.97
3	A	1101	XLS	C3-C2-C1	2.99	120.50	111.10
3	A	1100	XLS	C3-C2-C1	2.97	120.45	111.10
3	A	1102	XLS	O5-C5-C4	2.95	117.51	111.07
3	A	1101	XLS	O3-C3-C2	2.93	114.53	109.17
3	A	1100	XLS	O5-C5-C4	2.80	117.18	111.07
2	A	1000[B]	SIE	CI6-O29-S27	2.78	124.28	118.69
3	A	1101	XLS	O5-C5-C4	2.72	117.00	111.07
3	A	1102	XLS	C3-C2-C1	2.67	119.50	111.10
2	A	1000[B]	SIE	CS5-CS4-CS3	-2.66	116.08	120.18
2	A	1000[A]	SIE	CI3-CI9-CI8	2.56	108.50	106.27
2	A	1000[A]	SIE	CS5-CS4-CS3	-2.50	116.32	120.18
3	A	1102	XLS	C5-C4-C3	2.37	117.55	112.41
2	A	1000[A]	SIE	CS1-CI2-NI1	2.30	127.01	122.79
3	A	1100	XLS	O3-C3-C2	2.28	113.36	109.17
2	A	1000[A]	SIE	CS6-CS1-CI2	-2.24	116.73	120.74
2	A	1000[A]	SIE	O28-S27-O27	-2.17	117.91	119.97
3	A	1102	XLS	O4-C4-C3	2.13	114.27	109.10
3	A	1101	XLS	C5-C4-C3	2.11	116.99	112.41
3	A	1100	XLS	C5-C4-C3	2.11	116.99	112.41
2	A	1000[A]	SIE	OS7-CS4-CS3	2.08	122.73	118.64
3	A	1102	XLS	O3-C3-C2	2.06	112.95	109.17
3	A	1101	XLS	O4-C4-C3	2.04	114.06	109.10

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1102	XLS	C4

All (38) torsion outliers are listed below:

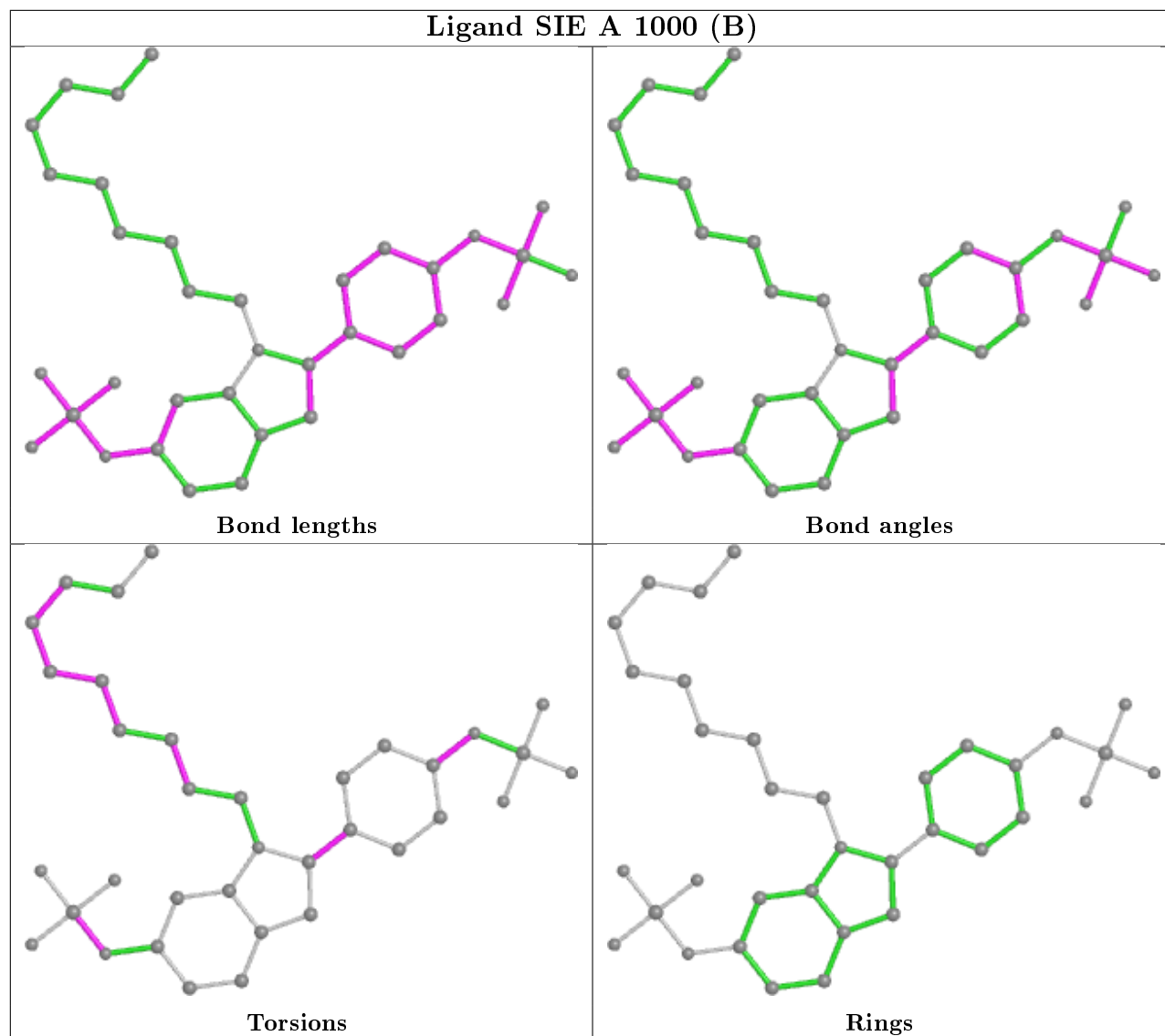
Mol	Chain	Res	Type	Atoms
2	A	1000[B]	SIE	NI1-CI2-CS1-CS2
2	A	1000[B]	SIE	NI1-CI2-CS1-CS6
2	A	1000[B]	SIE	CI6-O29-S27-N20
3	A	1101	XLS	O2-C2-C3-O3
2	A	1000[A]	SIE	CP2-CP1-NI1-CI8
3	A	1102	XLS	C2-C3-C4-O4
3	A	1102	XLS	O3-C3-C4-C5
3	A	1102	XLS	O3-C3-C4-O4
3	A	1102	XLS	C2-C3-C4-C5
3	A	1101	XLS	C1-C2-C3-O3
2	A	1000[A]	SIE	CP6-CP7-CP8-CP9
2	A	1000[B]	SIE	CP6-CP7-CP8-CP9
2	A	1000[A]	SIE	CP1-CP2-CP3-CP4
2	A	1000[B]	SIE	CP1-CP2-CP3-CP4
2	A	1000[A]	SIE	CS5-CS4-OS7-SS7
2	A	1000[A]	SIE	CP5-CP6-CP7-CP8
2	A	1000[B]	SIE	CI6-O29-S27-O28
2	A	1000[A]	SIE	CI6-O29-S27-O28
2	A	1000[A]	SIE	NI1-CI2-CS1-CS2
2	A	1000[A]	SIE	NI1-CI2-CS1-CS6
2	A	1000[A]	SIE	CP2-CP1-NI1-CI2
2	A	1000[B]	SIE	CP5-CP6-CP7-CP8
3	A	1101	XLS	C1-C2-C3-C4
3	A	1101	XLS	O2-C2-C3-C4
2	A	1000[B]	SIE	CI3-CI2-CS1-CS2
2	A	1000[A]	SIE	CI3-CI2-CS1-CS2
2	A	1000[A]	SIE	CI3-CI2-CS1-CS6
2	A	1000[B]	SIE	CI3-CI2-CS1-CS6
2	A	1000[A]	SIE	CI6-O29-S27-N20
2	A	1000[B]	SIE	CS3-CS4-OS7-SS7
2	A	1000[B]	SIE	CS5-CS4-OS7-SS7
2	A	1000[A]	SIE	CS3-CS4-OS7-SS7
2	A	1000[A]	SIE	CP3-CP4-CP5-CP6
2	A	1000[B]	SIE	CP3-CP4-CP5-CP6
2	A	1000[B]	SIE	CI6-O29-S27-O27
3	A	1100	XLS	C2-C3-C4-C5
2	A	1000[A]	SIE	CP4-CP5-CP6-CP7
2	A	1000[B]	SIE	CP4-CP5-CP6-CP7

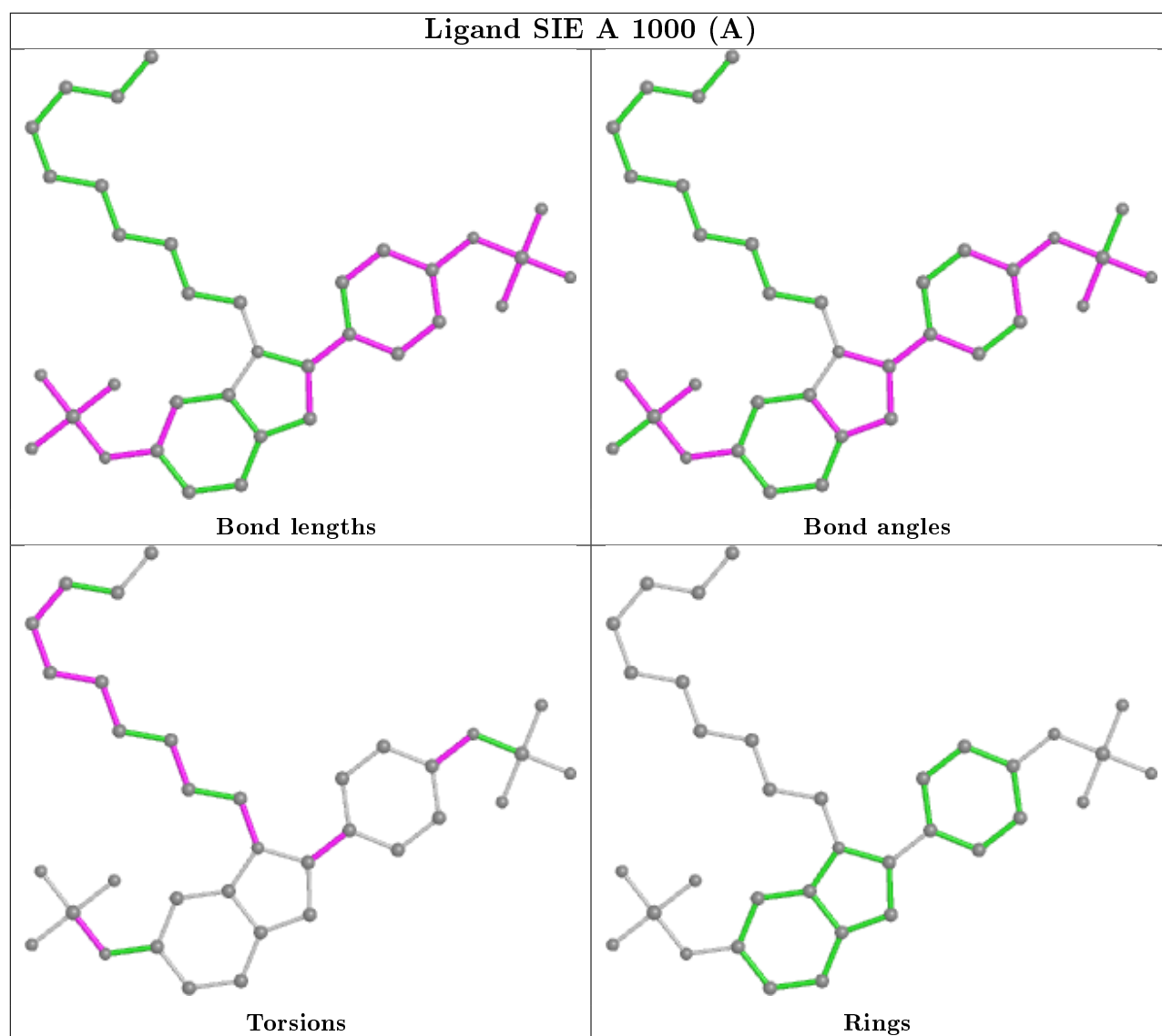
There are no ring outliers.

3 monomers are involved in 42 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1000[B]	SIE	20	0
2	A	1000[A]	SIE	21	0
4	A	1200	SO4	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 [i](#)

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

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	721/731 (98%)	-0.06	17 (2%) 59 57	12, 24, 46, 69	0

All (17) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	427	LYS	6.3
1	A	435	MET	4.9
1	A	340	ASP	4.4
1	A	171	LYS	4.0
1	A	223	ILE	2.7
1	A	174	TYR	2.6
1	A	375	ARG	2.6
1	A	170	VAL	2.5
1	A	383	LEU	2.4
1	A	890	LEU	2.3
1	A	775	VAL	2.2
1	A	704	SER	2.2
1	A	720	GLU	2.2
1	A	428	ASN	2.1
1	A	233	LYS	2.1
1	A	773	LYS	2.0
1	A	368	GLN	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 monosaccharides in this entry.

## 6.4 Ligands ⓘ

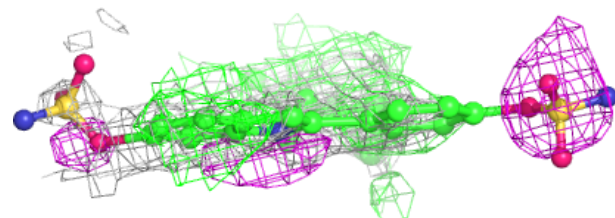
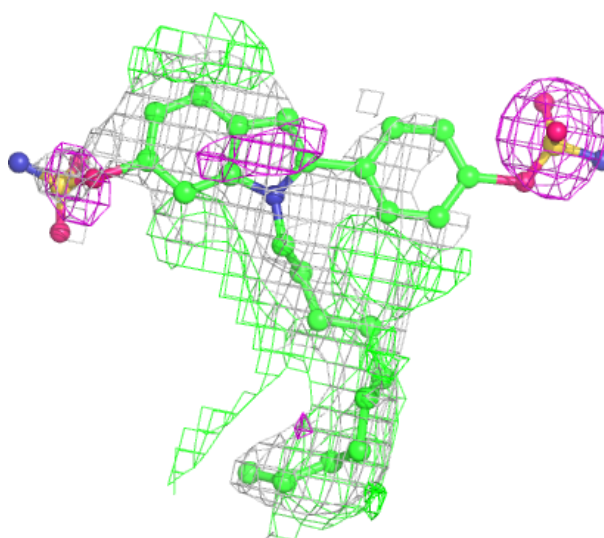
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	SIE	A	1000[B]	35/35	0.23	0.49	63,81,101,102	35
2	SIE	A	1000[A]	35/35	0.23	0.49	63,78,102,102	35
3	XLS	A	1102	10/10	0.80	0.32	76,78,78,80	0
4	SO4	A	1203	5/5	0.90	0.16	84,84,85,86	0
4	SO4	A	1204	5/5	0.94	0.17	53,54,55,56	0
4	SO4	A	1202	5/5	0.94	0.18	58,59,60,60	0
3	XLS	A	1100	10/10	0.94	0.16	38,40,43,44	0
3	XLS	A	1101	10/10	0.96	0.12	34,37,39,39	0
4	SO4	A	1200	5/5	0.98	0.09	50,50,52,52	0
4	SO4	A	1201	5/5	0.98	0.10	47,47,48,49	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 SIE A 1000 (B):**

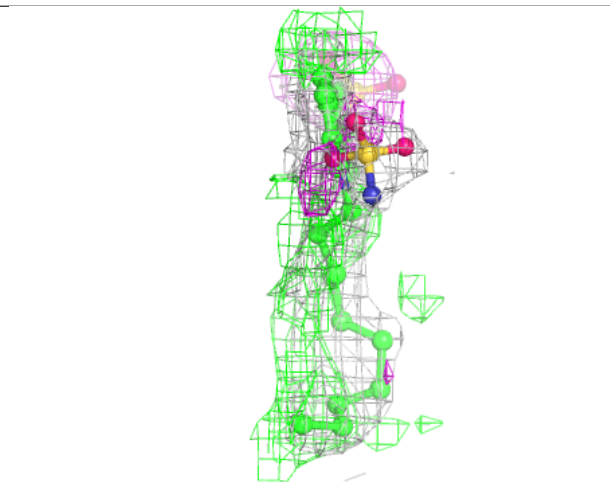
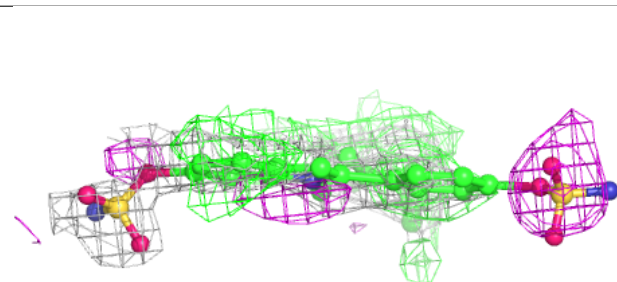
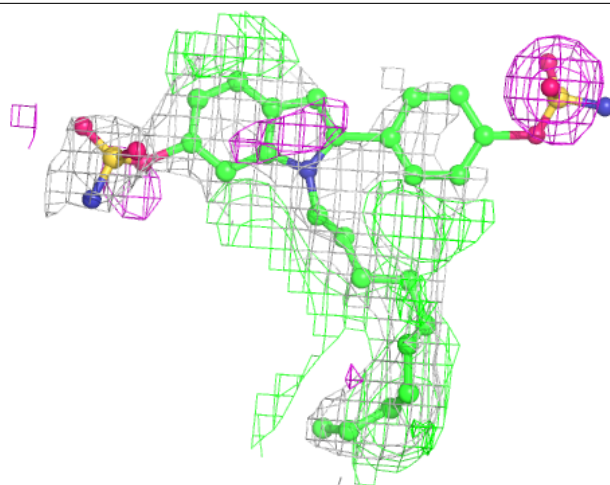
$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)





**Electron density around SIE A 1000 (A):**

$2mF_o-DF_c$  (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.