Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2022 – 12:59 PM EDT

PDB ID	:	3VZB
Title	:	Crystal structure of Sphingosine Kinase 1
Authors	:	Min, X.; Walker, N.P.; Wang, Z.
Deposited on	:	2012-10-10
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*
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:

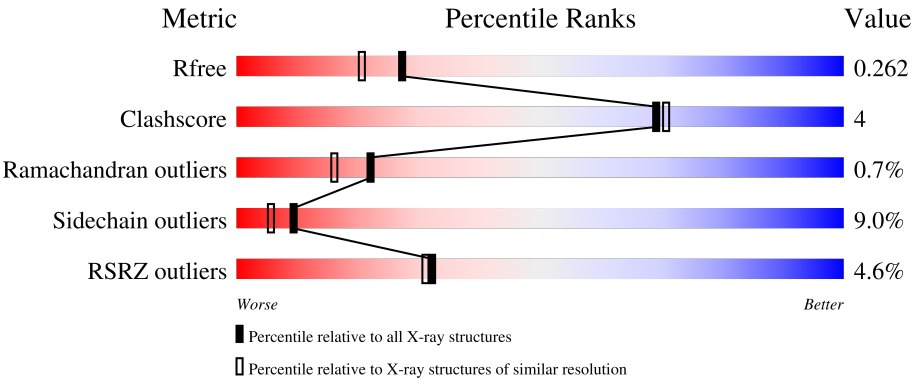
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.29
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.29

1 Overall quality at a glance (i)

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 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 <=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	360	2% 85% 13%
1	B	360	5% 77% 15% 6%
1	C	360	6% 83% 11%

2 Entry composition (i)

There are 5 unique types of molecules in this entry. The entry contains 8663 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.

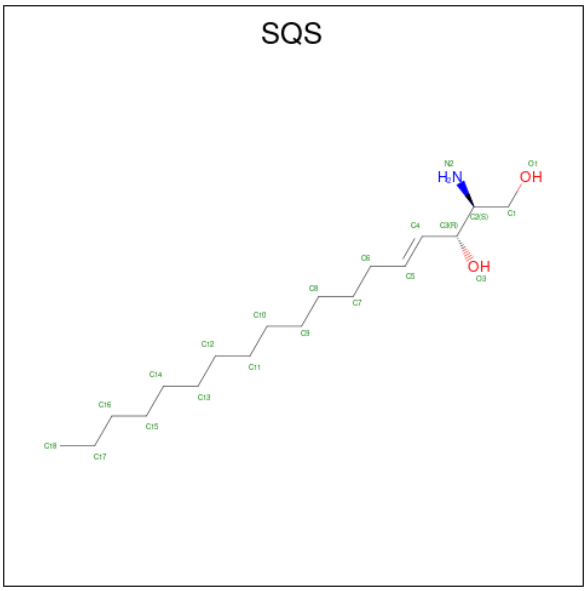
- Molecule 1 is a protein called Sphingosine kinase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	360	Total	C	N	O	S	0	1	0
			2803	1793	498	491	21			
1	B	339	Total	C	N	O	S	0	1	0
			2659	1705	468	466	20			
1	C	344	Total	C	N	O	S	0	1	0
			2700	1728	477	474	21			

There are 12 discrepancies between the modelled and reference sequences:

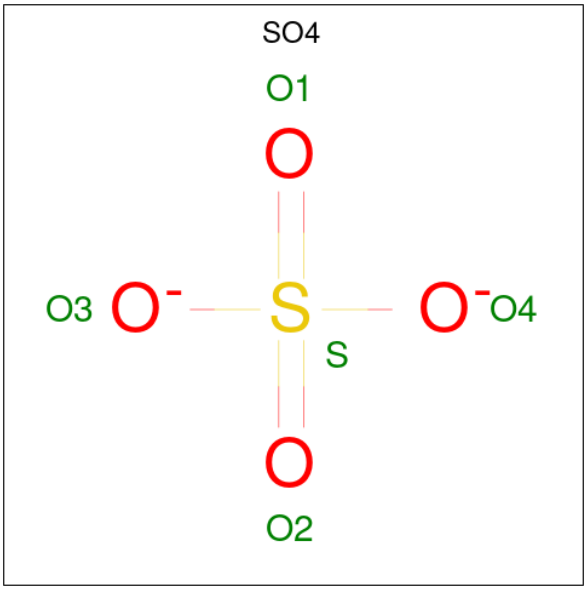
Chain	Residue	Modelled	Actual	Comment	Reference
A	5	ALA	-	expression tag	UNP Q9NYA1
A	6	MET	-	expression tag	UNP Q9NYA1
A	7	GLY	-	expression tag	UNP Q9NYA1
A	8	SER	-	expression tag	UNP Q9NYA1
B	5	ALA	-	expression tag	UNP Q9NYA1
B	6	MET	-	expression tag	UNP Q9NYA1
B	7	GLY	-	expression tag	UNP Q9NYA1
B	8	SER	-	expression tag	UNP Q9NYA1
C	5	ALA	-	expression tag	UNP Q9NYA1
C	6	MET	-	expression tag	UNP Q9NYA1
C	7	GLY	-	expression tag	UNP Q9NYA1
C	8	SER	-	expression tag	UNP Q9NYA1

- Molecule 2 is (2S,3R,4E)-2-aminooctadec-4-ene-1,3-diol (three-letter code: SQS) (formula: $C_{18}H_{37}NO_2$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			21	18	1	2		
2	B	1	Total	C	N	O	0	0
			21	18	1	2		

- Molecule 3 is SULFATE ION (three-letter code: SO4) (formula: O_4S).



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

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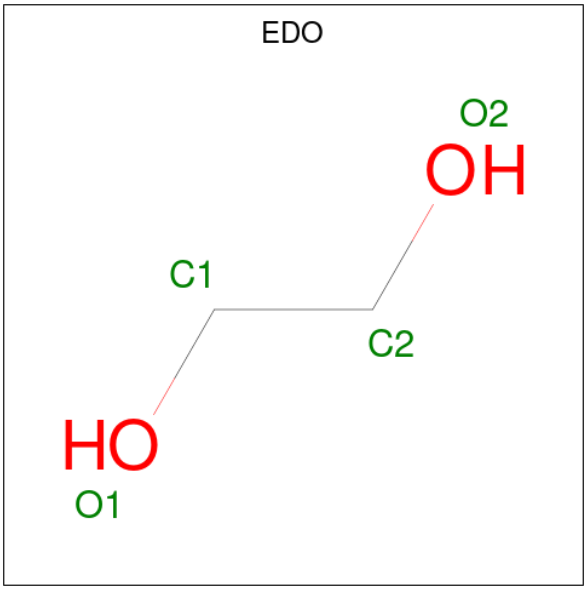
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	1	Total O S 5 4 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: $C_2H_6O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0

- Molecule 5 is water.

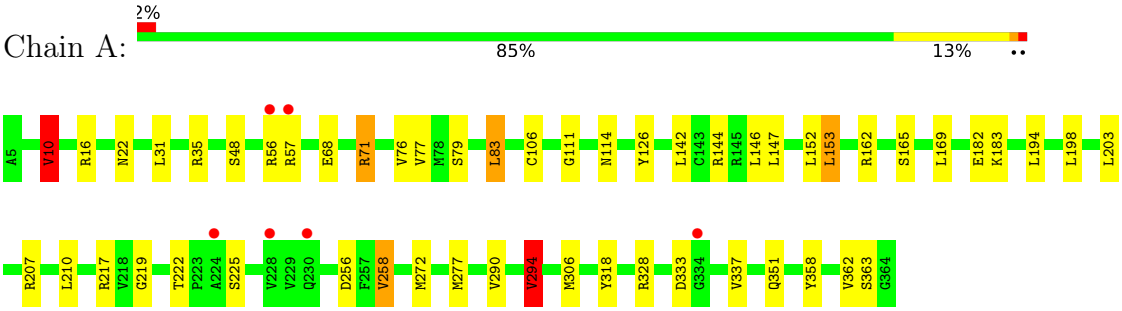
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	182	Total O 182 182	0	0
5	B	120	Total O 120 120	0	0
5	C	82	Total O 82 82	0	0

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.

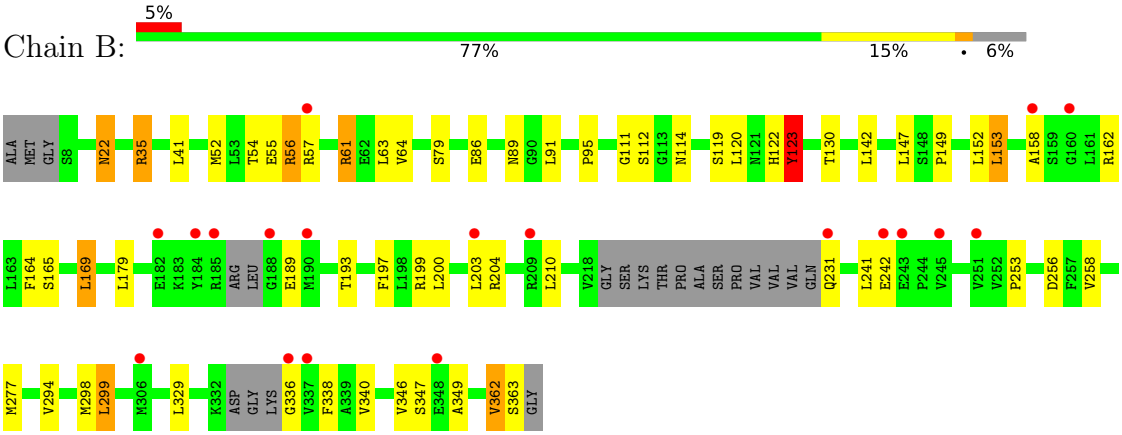
• Molecule 1: Sphingosine kinase 1

Chain A:



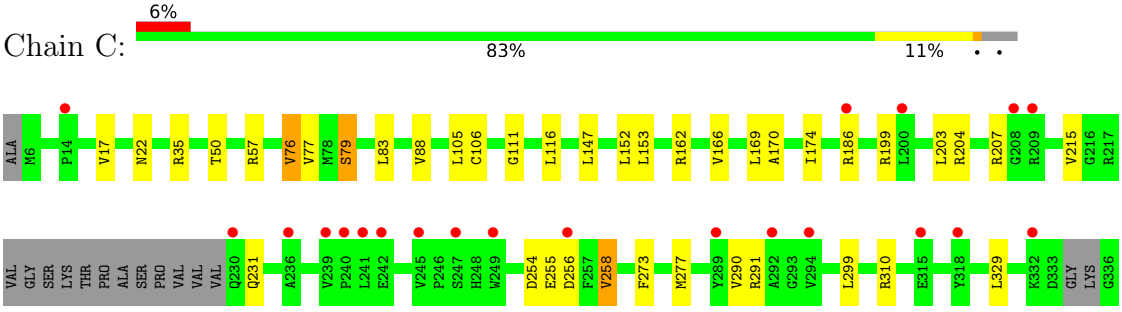
• Molecule 1: Sphingosine kinase 1

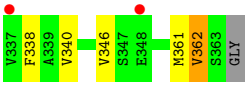
Chain B:



• Molecule 1: Sphingosine kinase 1

Chain C:




V337
F338
A339
V340
V346
S347
E348
M361
V362
S363
GLY

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α, β, γ	101.86Å 226.26Å 106.49Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	48.22 – 2.00 48.17 – 2.00	Depositor EDS
% Data completeness (in resolution range)	99.7 (48.22-2.00) 99.7 (48.17-2.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.02 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.213 , 0.262 0.216 , 0.262	Depositor DCC
R_{free} test set	4143 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	34.2	Xtriage
Anisotropy	0.026	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 43.3	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8663	wwPDB-VP
Average B, all atoms (Å^2)	39.0	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.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: SQS, EDO, SO4

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	0.46	0/2871	0.70	2/3896 (0.1%)
1	B	0.44	0/2722	0.69	3/3691 (0.1%)
1	C	0.43	0/2764	0.66	0/3747
All	All	0.44	0/8357	0.68	5/11334 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	294	VAL	CB-CA-C	-5.94	100.12	111.40
1	B	123	TYR	N-CA-CB	5.55	120.59	110.60
1	A	10	VAL	CB-CA-C	-5.44	101.06	111.40
1	B	35	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	B	35	ARG	NE-CZ-NH1	5.16	122.88	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	362	VAL	Peptide

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2803	0	2847	22	0
1	B	2659	0	2686	25	0
1	C	2700	0	2726	15	0
2	A	21	0	37	0	0
2	B	21	0	37	0	0
3	A	5	0	0	0	0
3	B	5	0	0	0	0
3	C	5	0	0	1	0
4	A	24	0	36	6	0
4	B	20	0	30	2	0
4	C	16	0	24	0	0
5	A	182	0	0	1	1
5	B	120	0	0	1	0
5	C	82	0	0	0	0
All	All	8663	0	8423	62	1

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 4.

All (62) 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:B:119:SER:O	1:B:122:HIS:O	1.61	1.17
1:B:111:GLY:O	1:B:114:ASN:ND2	2.10	0.85
1:A:362:VAL:HG22	4:A:403:EDO:H11	1.59	0.84
1:B:169:LEU:HD12	1:B:340:VAL:HG22	1.67	0.76
1:A:362:VAL:HG22	4:A:403:EDO:C1	2.19	0.73
1:B:89:ASN:HD21	1:B:164:PHE:H	1.37	0.71
1:B:336:GLY:N	1:B:347:SER:O	2.26	0.68
1:A:68:GLU:O	1:A:71:ARG:HG3	1.96	0.65
1:A:337:VAL:HG13	4:A:406:EDO:H12	1.80	0.64
1:C:207:ARG:HA	1:C:255:GLU:O	2.02	0.60
1:B:203:LEU:HD21	1:B:299:LEU:HD22	1.82	0.60
1:B:120:LEU:HD22	1:B:363:SER:HB3	1.84	0.59
1:C:258:VAL:HG22	1:C:290:VAL:HB	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:79:SER:HB3	1:C:83:LEU:HD12	1.86	0.57
1:B:142:LEU:HA	1:B:362:VAL:HG21	1.87	0.57
1:A:111:GLY:O	1:A:114:ASN:ND2	2.37	0.56
1:A:294:VAL:HG13	1:A:318:TYR:HB2	1.88	0.55
1:A:258:VAL:HG22	1:A:290:VAL:HB	1.88	0.55
1:A:126:TYR:OH	1:A:144:ARG:NH2	2.41	0.53
1:A:207:ARG:NH1	1:A:333:ASP:OD2	2.43	0.52
1:B:61:ARG:NH1	1:B:86[A]:GLU:OE2	2.42	0.52
1:B:52:MET:SD	1:B:63:LEU:HD13	2.50	0.52
1:B:122:HIS:O	1:B:123:TYR:CG	2.63	0.52
1:C:106:CYS:HB2	1:C:362:VAL:CG1	2.41	0.51
1:A:106:CYS:HB2	1:A:362:VAL:HG13	1.93	0.50
1:A:10:VAL:HG13	1:A:146:LEU:HD23	1.94	0.49
1:C:77:VAL:HG13	1:C:83:LEU:HB3	1.94	0.49
1:B:193:THR:HG22	1:B:197:PHE:CE1	2.46	0.49
1:C:76:VAL:HB	1:C:106:CYS:HB3	1.95	0.49
1:B:22:ASN:HD22	1:B:22:ASN:C	2.16	0.49
1:A:77:VAL:HG13	1:A:83:LEU:HD13	1.95	0.49
1:B:242:GLU:N	1:B:242:GLU:OE1	2.45	0.49
1:A:142:LEU:HA	1:A:362:VAL:HG21	1.94	0.48
1:B:329:LEU:HD23	1:B:338:PHE:HE2	1.78	0.48
1:C:77:VAL:CG1	1:C:83:LEU:HB3	2.44	0.48
1:B:54:THR:O	1:B:54:THR:HG23	2.14	0.47
1:C:79:SER:CB	1:C:83:LEU:HD12	2.45	0.47
1:A:328:ARG:HH21	1:A:351:GLN:HE22	1.62	0.46
1:B:153:LEU:HB3	1:B:165:SER:HB3	1.96	0.46
1:A:153:LEU:HB3	1:A:165:SER:HB3	1.98	0.46
1:B:64:VAL:HG11	1:B:91:LEU:HG	1.98	0.46
1:B:55:GLU:O	1:B:56:ARG:CB	2.64	0.45
1:B:114:ASN:HB2	4:B:407:EDO:O1	2.16	0.45
1:A:362:VAL:O	4:A:403:EDO:H12	2.16	0.45
1:B:95:PRO:HA	1:B:231:GLN:HE22	1.82	0.45
1:C:169:LEU:HD13	1:C:340:VAL:HG22	1.97	0.45
1:C:329:LEU:HD23	1:C:338:PHE:HE2	1.82	0.44
1:C:231:GLN:HA	1:C:231:GLN:OE1	2.18	0.44
1:A:363:SER:HB2	5:A:517:HOH:O	2.18	0.43
1:C:106:CYS:HB2	1:C:362:VAL:HG13	2.00	0.42
1:A:16:ARG:HA	1:A:48:SER:O	2.19	0.42
1:A:272:MET:HB3	1:A:306:MET:HE2	2.02	0.42
1:A:219:GLY:H	4:A:404:EDO:C1	2.33	0.42
1:A:222:THR:HG22	4:A:404:EDO:H22	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:88:VAL:HG21	1:C:166:VAL:HG11	2.01	0.42
1:B:112:SER:OG	1:B:189:GLU:HA	2.20	0.42
1:B:158:ALA:HB2	1:B:349:ALA:HB3	2.01	0.42
1:A:71:ARG:HG3	1:A:71:ARG:H	1.66	0.41
1:C:111:GLY:HA3	3:C:401:SO4:O4	2.20	0.41
1:C:170:ALA:HB1	1:C:174:ILE:HB	2.03	0.41
1:B:363:SER:HB2	5:B:508:HOH:O	2.21	0.40
1:B:149:PRO:O	4:B:406:EDO:H12	2.22	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:561:HOH:O	5:A:561:HOH:O[3_654]	1.92	0.28

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	359/360 (100%)	350 (98%)	7 (2%)	2 (1%)	25 19
1	B	332/360 (92%)	320 (96%)	8 (2%)	4 (1%)	13 7
1	C	339/360 (94%)	327 (96%)	11 (3%)	1 (0%)	41 37
All	All	1030/1080 (95%)	997 (97%)	26 (2%)	7 (1%)	22 16

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	56	ARG
1	B	123	TYR
1	B	79	SER
1	C	79	SER

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Mol	Chain	Res	Type
1	A	79	SER
1	A	57	ARG
1	B	253	PRO

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	300/299 (100%)	273 (91%)	27 (9%)	9 6
1	B	285/299 (95%)	260 (91%)	25 (9%)	10 6
1	C	289/299 (97%)	262 (91%)	27 (9%)	9 5
All	All	874/897 (97%)	795 (91%)	79 (9%)	9 6

All (79) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	VAL
1	A	22	ASN
1	A	31	LEU
1	A	35[A]	ARG
1	A	35[B]	ARG
1	A	56	ARG
1	A	71	ARG
1	A	76	VAL
1	A	83	LEU
1	A	147	LEU
1	A	152	LEU
1	A	153	LEU
1	A	162	ARG
1	A	169	LEU
1	A	182	GLU
1	A	183	LYS
1	A	194	LEU
1	A	198	LEU
1	A	203	LEU

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Mol	Chain	Res	Type
1	A	210	LEU
1	A	217	ARG
1	A	225	SER
1	A	256	ASP
1	A	258	VAL
1	A	277	MET
1	A	294	VAL
1	A	358	TYR
1	B	22	ASN
1	B	35	ARG
1	B	41	LEU
1	B	57	ARG
1	B	61	ARG
1	B	130	THR
1	B	147	LEU
1	B	152	LEU
1	B	153	LEU
1	B	162	ARG
1	B	169	LEU
1	B	179	LEU
1	B	199	ARG
1	B	200	LEU
1	B	204	ARG
1	B	210	LEU
1	B	241	LEU
1	B	256	ASP
1	B	258	VAL
1	B	277	MET
1	B	294	VAL
1	B	298	MET
1	B	299	LEU
1	B	346	VAL
1	B	362	VAL
1	C	17	VAL
1	C	22	ASN
1	C	35	ARG
1	C	50	THR
1	C	57	ARG
1	C	76	VAL
1	C	105	LEU
1	C	116	LEU
1	C	147	LEU

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Mol	Chain	Res	Type
1	C	152	LEU
1	C	153	LEU
1	C	162	ARG
1	C	186	ARG
1	C	199	ARG
1	C	203	LEU
1	C	204	ARG
1	C	215	VAL
1	C	254	ASP
1	C	256	ASP
1	C	258	VAL
1	C	273	PHE
1	C	277	MET
1	C	291	ARG
1	C	299	LEU
1	C	310	ARG
1	C	346	VAL
1	C	361	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	22	ASN
1	A	351	GLN
1	B	22	ASN
1	B	89	ASN
1	B	231	GLN
1	B	351	GLN
1	C	22	ASN
1	C	32	GLN
1	C	85	HIS
1	C	131	ASN
1	C	230	GLN
1	C	351	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)

20 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	EDO	A	404	-	3,3,3	0.40	0	2,2,2	0.13	0
3	SO4	B	402	-	4,4,4	0.28	0	6,6,6	0.31	0
4	EDO	A	407	-	3,3,3	0.38	0	2,2,2	0.71	0
4	EDO	B	404	-	3,3,3	0.48	0	2,2,2	0.18	0
4	EDO	A	405	-	3,3,3	0.41	0	2,2,2	0.35	0
4	EDO	A	408	-	3,3,3	0.48	0	2,2,2	0.23	0
4	EDO	C	405	-	3,3,3	0.50	0	2,2,2	0.27	0
4	EDO	B	405	-	3,3,3	0.53	0	2,2,2	0.26	0
4	EDO	A	403	-	3,3,3	0.25	0	2,2,2	0.76	0
4	EDO	C	404	-	3,3,3	0.39	0	2,2,2	0.55	0
4	EDO	C	403	-	3,3,3	0.45	0	2,2,2	0.21	0
4	EDO	C	402	-	3,3,3	0.51	0	2,2,2	0.16	0
4	EDO	B	403	-	3,3,3	0.51	0	2,2,2	0.28	0
2	SQS	A	401	-	19,20,20	0.49	0	18,21,21	0.96	1 (5%)
3	SO4	C	401	-	4,4,4	0.39	0	6,6,6	0.49	0
4	EDO	B	406	-	3,3,3	0.33	0	2,2,2	0.28	0
4	EDO	B	407	-	3,3,3	0.40	0	2,2,2	0.42	0
2	SQS	B	401	-	19,20,20	0.68	1 (5%)	18,21,21	0.78	1 (5%)
3	SO4	A	402	-	4,4,4	0.33	0	6,6,6	0.10	0
4	EDO	A	406	-	3,3,3	0.39	0	2,2,2	0.21	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
4	EDO	A	408	-	-	1/1/1/1	-
4	EDO	B	407	-	-	0/1/1/1	-
4	EDO	A	404	-	-	1/1/1/1	-
2	SQS	A	401	-	-	12/21/21/21	-
4	EDO	C	405	-	-	1/1/1/1	-
2	SQS	B	401	-	-	9/21/21/21	-
4	EDO	B	405	-	-	1/1/1/1	-
4	EDO	A	403	-	-	1/1/1/1	-
4	EDO	A	407	-	-	0/1/1/1	-
4	EDO	A	406	-	-	0/1/1/1	-
4	EDO	C	404	-	-	1/1/1/1	-
4	EDO	B	404	-	-	0/1/1/1	-
4	EDO	C	403	-	-	0/1/1/1	-
4	EDO	B	406	-	-	1/1/1/1	-
4	EDO	C	402	-	-	0/1/1/1	-
4	EDO	B	403	-	-	0/1/1/1	-
4	EDO	A	405	-	-	0/1/1/1	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	401	SQS	C3-C4	2.19	1.53	1.50

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	401	SQS	O3-C3-C2	3.03	112.13	107.31
2	B	401	SQS	O3-C3-C2	2.36	111.06	107.31

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	401	SQS	O3-C3-C4-C5
2	A	401	SQS	C2-C3-C4-C5
2	A	401	SQS	O1-C1-C2-C3
2	A	401	SQS	O1-C1-C2-N2
2	B	401	SQS	O3-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
2	B	401	SQS	C2-C3-C4-C5
2	B	401	SQS	C13-C14-C15-C16
2	A	401	SQS	C10-C11-C12-C13
2	A	401	SQS	C13-C14-C15-C16
2	A	401	SQS	C12-C13-C14-C15
4	A	403	EDO	O1-C1-C2-O2
4	A	404	EDO	O1-C1-C2-O2
4	A	408	EDO	O1-C1-C2-O2
4	B	406	EDO	O1-C1-C2-O2
4	C	404	EDO	O1-C1-C2-O2
2	B	401	SQS	C10-C11-C12-C13
2	A	401	SQS	C5-C6-C7-C8
2	B	401	SQS	C12-C13-C14-C15
2	A	401	SQS	C7-C8-C9-C10
2	A	401	SQS	C9-C10-C11-C12
2	B	401	SQS	C7-C8-C9-C10
4	C	405	EDO	O1-C1-C2-O2
2	B	401	SQS	C5-C6-C7-C8
2	A	401	SQS	C14-C15-C16-C17
2	B	401	SQS	C9-C10-C11-C12
4	B	405	EDO	O1-C1-C2-O2
2	A	401	SQS	C4-C5-C6-C7
2	B	401	SQS	C14-C15-C16-C17

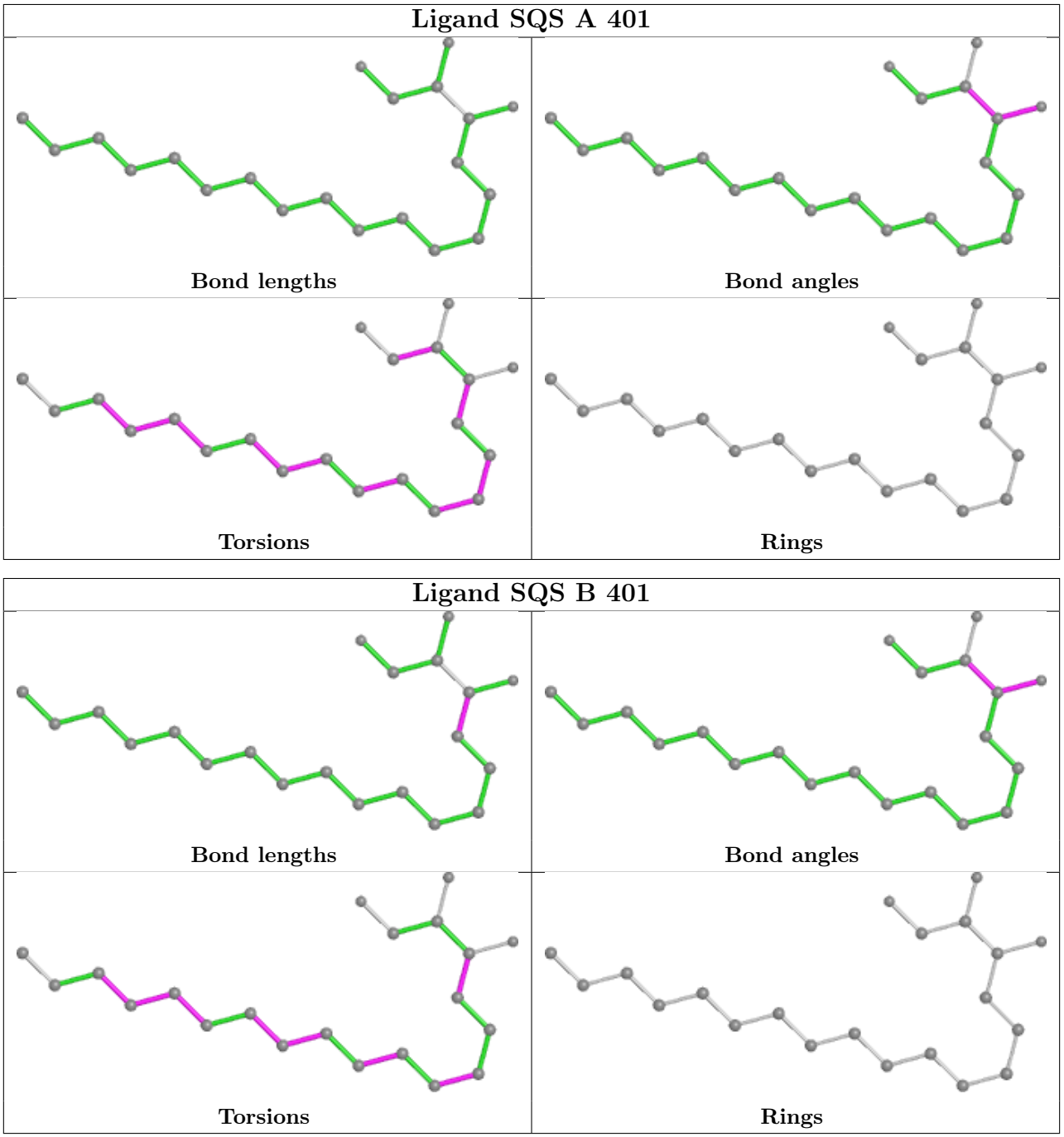
There are no ring outliers.

6 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	404	EDO	2	0
4	A	403	EDO	3	0
3	C	401	SO4	1	0
4	B	406	EDO	1	0
4	B	407	EDO	1	0
4	A	406	EDO	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 then 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^{th} 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	360/360 (100%)	-0.01	6 (1%)	70	68	21, 31, 54, 70	0
1	B	339/360 (94%)	0.51	19 (5%)	24	23	20, 35, 71, 96	0
1	C	344/360 (95%)	0.56	23 (6%)	17	17	29, 42, 61, 85	0
All	All	1043/1080 (96%)	0.35	48 (4%)	32	31	20, 37, 63, 96	0

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	348	GLU	5.5
1	C	208	GLY	4.8
1	B	182	GLU	4.8
1	B	231	GLN	4.1
1	A	224	ALA	3.6
1	B	188	GLY	3.6
1	C	249	TRP	3.5
1	B	57	ARG	3.4
1	C	247	SER	3.2
1	B	185	ARG	3.1
1	B	158	ALA	3.0
1	C	318	TYR	3.0
1	C	14	PRO	3.0
1	C	315	GLU	2.9
1	C	240	PRO	2.8
1	C	241	LEU	2.8
1	C	209	ARG	2.7
1	B	306	MET	2.7
1	C	245	VAL	2.5
1	A	228	VAL	2.5
1	C	200	LEU	2.5
1	B	243	GLU	2.5
1	B	203	LEU	2.4

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Mol	Chain	Res	Type	RSRZ
1	B	245	VAL	2.4
1	C	348	GLU	2.4
1	B	160	GLY	2.4
1	C	256	ASP	2.4
1	C	230	GLN	2.4
1	C	236	ALA	2.4
1	C	239	VAL	2.4
1	A	56	ARG	2.3
1	C	242	GLU	2.3
1	B	336	GLY	2.2
1	B	209	ARG	2.2
1	C	294	VAL	2.2
1	A	57	ARG	2.2
1	A	230	GLN	2.2
1	B	184	TYR	2.1
1	B	337	VAL	2.1
1	C	289	TYR	2.1
1	C	292	ALA	2.1
1	C	186	ARG	2.1
1	A	334	GLY	2.1
1	B	251	VAL	2.1
1	B	190	MET	2.0
1	B	242	GLU	2.0
1	C	332	LYS	2.0
1	C	337	VAL	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 (i)

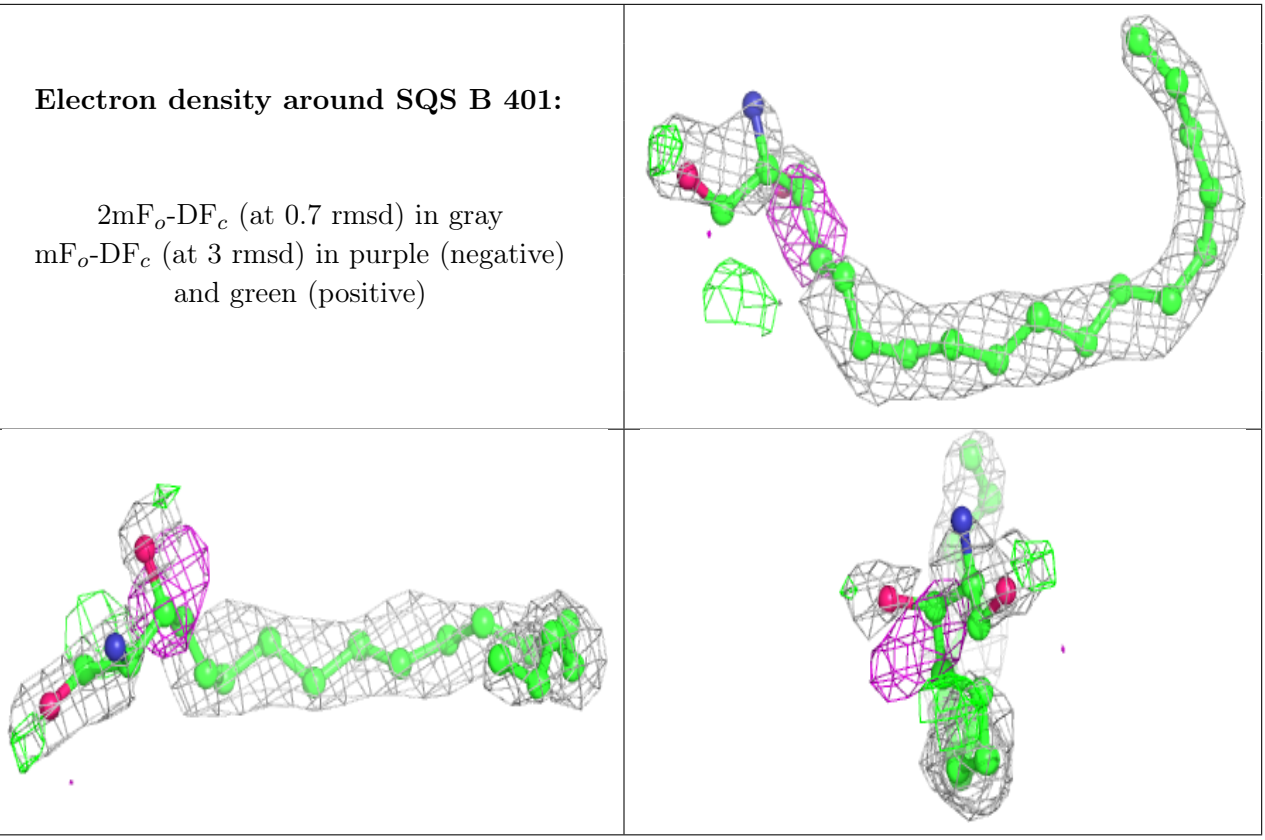
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SQS	B	401	21/21	0.60	0.38	56,62,71,73	0
4	EDO	C	402	4/4	0.73	0.28	48,51,53,58	0
4	EDO	C	403	4/4	0.74	0.25	51,55,55,56	0
4	EDO	C	405	4/4	0.75	0.18	49,50,50,52	0
4	EDO	B	403	4/4	0.81	0.22	40,44,46,50	0
2	SQS	A	401	21/21	0.83	0.18	47,51,76,82	0
4	EDO	A	408	4/4	0.85	0.15	50,51,51,51	0
4	EDO	B	405	4/4	0.87	0.17	51,52,52,52	0
4	EDO	B	407	4/4	0.89	0.27	55,55,55,56	0
4	EDO	A	403	4/4	0.89	0.32	36,44,47,49	0
4	EDO	B	404	4/4	0.90	0.28	59,60,61,61	0
4	EDO	C	404	4/4	0.90	0.13	42,43,43,44	0
4	EDO	A	407	4/4	0.90	0.16	38,39,40,41	0
4	EDO	B	406	4/4	0.91	0.20	42,45,46,49	0
4	EDO	A	406	4/4	0.91	0.20	35,38,39,39	0
3	SO4	B	402	5/5	0.92	0.14	60,61,64,71	0
4	EDO	A	405	4/4	0.92	0.14	43,43,45,46	0
4	EDO	A	404	4/4	0.93	0.34	45,48,50,52	0
3	SO4	A	402	5/5	0.94	0.12	70,74,74,76	0
3	SO4	C	401	5/5	0.97	0.12	47,48,49,50	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.

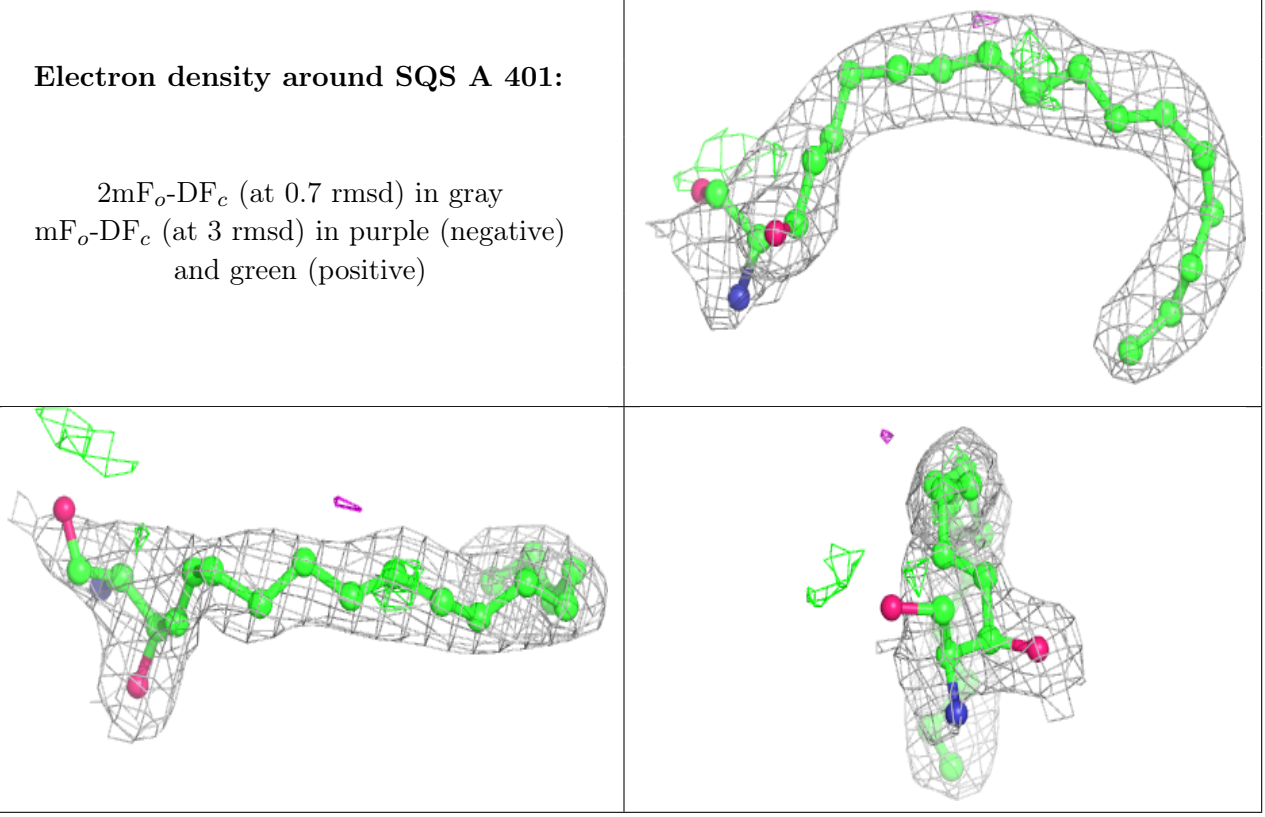
Electron density around SQS B 401:

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



Electron density around SQS A 401:

$2mF_o$-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.