



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:16 PM UTC

PDB ID : 1GM9 / pdb_00001gm9
Title : Crystal structures of penicillin acylase enzyme-substrate complexes: Structural insights into the catalytic mechanism
Authors : McVey, C.E.; Walsh, M.A.; Dodson, G.G.; Wilson, K.S.; Brannigan, J.A.
Deposited on : 2001-09-12
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

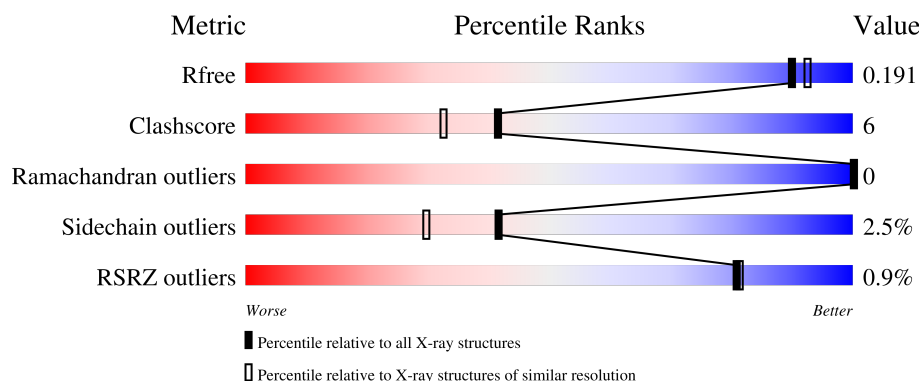
1 Overall quality at a glance

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	209	
2	B	557	

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
3	EDO	A	1210	-	-	X	-

2 Entry composition [i](#)

There are 6 unique types of molecules in this entry. The entry contains 6882 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.

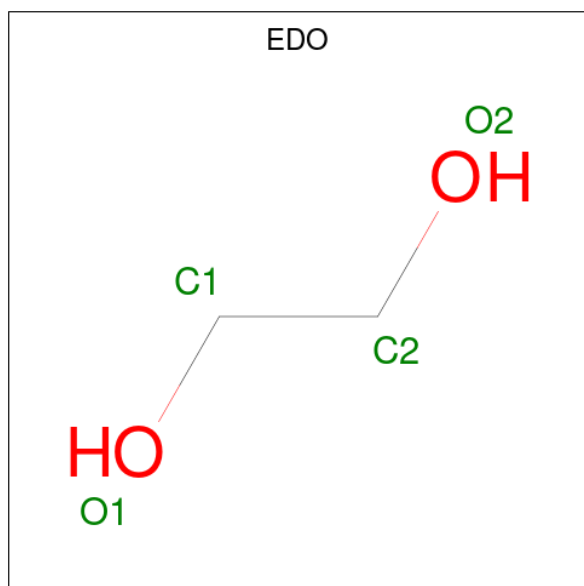
- Molecule 1 is a protein called PENICILLIN G ACYLASE ALPHA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	207	Total	C	N	O	S	8	2	0
			1678	1072	280	317	9			

- Molecule 2 is a protein called PENICILLIN G ACYLASE BETA SUBUNIT.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	557	Total	C	N	O	S	3	2	0
			4434	2815	772	837	10			

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

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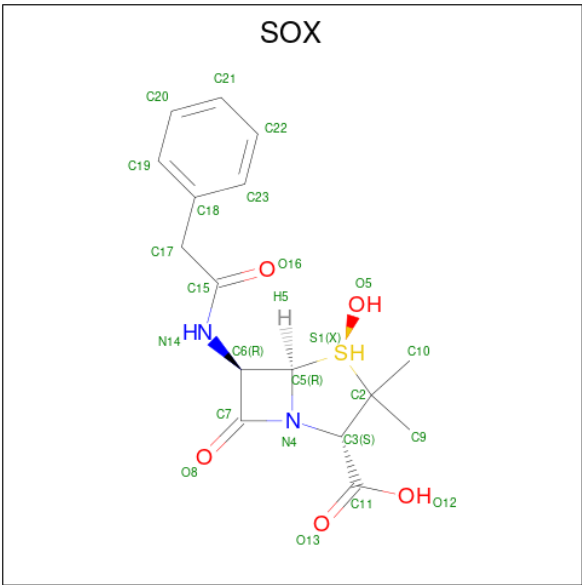
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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0
3	B	1	Total C O 4 2 2	0	0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

- Molecule 4 is CALCIUM ION (CCD ID: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	B	1	Total Ca 1 1	0	0

- Molecule 5 is N-[(2S,4S,6R)-2-(DIHYDROXYMETHYL)-4-HYDROXY-3,3-DIMETHYL-7-
OXO-4LAMBDA 4 -THIA-1-AZABICYCLO[3.2.0]HEPT-6-YL]-2-PHENYLAC ETAMIDE
(CCD ID: SOX) (formula: C₁₆H₂₀N₂O₅S).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	B	1	Total	C	N	O	S	0	0
			24	16	2	5	1		

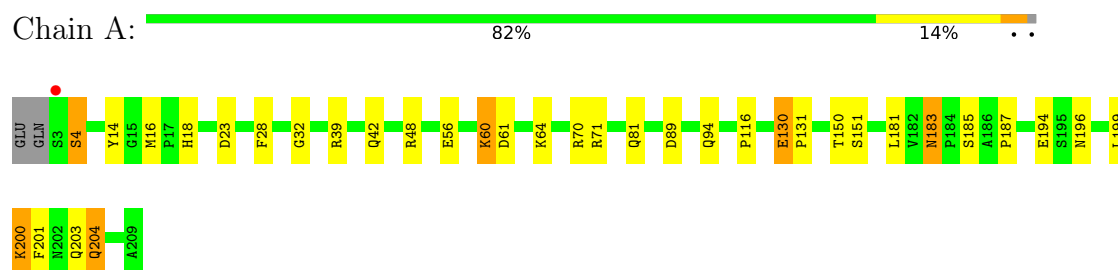
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	192	Total	O	3	3
			192	192		
6	B	509	Total	O	2	2
			509	509		

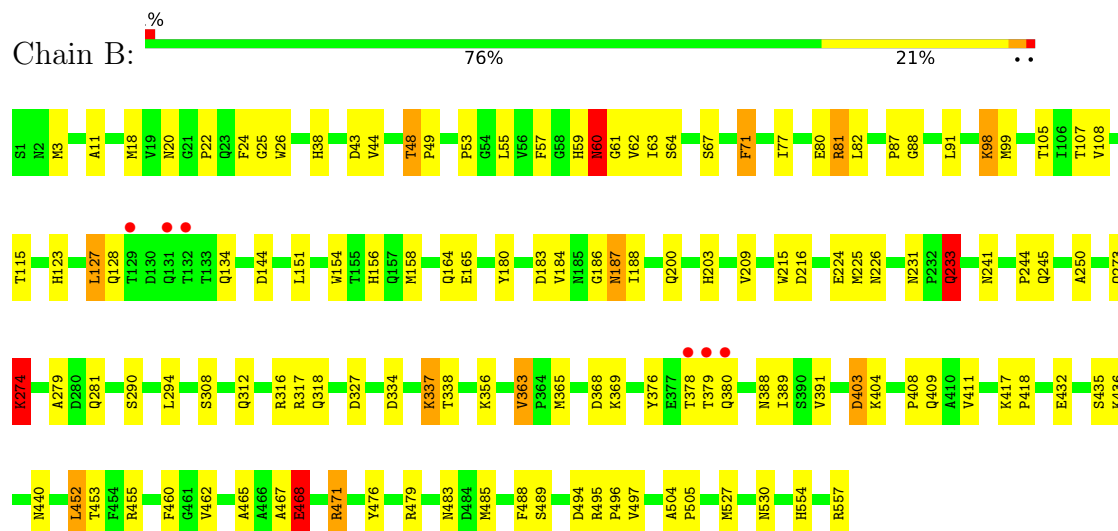
3 Residue-property plots [i](#)

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: PENICILLIN G ACYLASE ALPHA SUBUNIT



• Molecule 2: PENICILLIN G ACYLASE BETA SUBUNIT



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	51.20Å 131.70Å 64.00Å 90.00° 105.90° 90.00°	Depositor
Resolution (Å)	30.00 – 1.80 30.00 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.5 (30.00-1.80) 97.6 (30.00-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 1.76Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.153 , 0.190 0.155 , 0.191	Depositor DCC
R_{free} test set	2332 reflections (3.01%)	wwPDB-VP
Wilson B-factor (Å ²)	13.1	Xtriage
Anisotropy	0.143	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 50.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	6882	wwPDB-VP
Average B, all atoms (Å ²)	16.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.90% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, SME, CA, SOX

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	1.17	3/1711 (0.2%)	1.80	29/2319 (1.3%)
2	B	1.16	3/4560 (0.1%)	1.83	91/6218 (1.5%)
All	All	1.17	6/6271 (0.1%)	1.82	120/8537 (1.4%)

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	432	GLU	CG-CD	23.20	2.10	1.52
1	A	60	LYS	CD-CE	13.75	1.93	1.52
2	B	290	SER	CA-CB	6.85	1.64	1.53
1	A	204	GLN	CG-CD	6.12	1.67	1.52
1	A	200	LYS	CG-CD	-5.61	1.35	1.52
2	B	489	SER	CA-C	-5.54	1.48	1.53

All (120) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	337	LYS	CA-CB-CG	12.84	139.77	114.10
2	B	378	THR	CA-C-N	11.72	142.03	121.75
2	B	378	THR	C-N-CA	11.72	142.03	121.75
1	A	71	ARG	CD-NE-CZ	8.97	136.96	124.40
2	B	379	THR	O-C-N	-8.96	113.03	123.25
2	B	312	GLN	CB-CG-CD	8.70	127.39	112.60
2	B	409	GLN	OE1-CD-NE2	8.58	131.18	122.60
2	B	71	PHE	CA-CB-CG	-8.21	105.59	113.80
2	B	290	SER	CA-CB-OG	-8.19	94.71	111.10
2	B	432	GLU	CB-CG-CD	-8.16	98.72	112.60
2	B	468	GLU	CB-CG-CD	-7.97	99.06	112.60
2	B	455	ARG	NE-CZ-NH1	7.40	128.90	121.50
2	B	554	HIS	CA-CB-CG	-7.38	106.42	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	471	ARG	CD-NE-CZ	7.31	134.63	124.40
2	B	290	SER	CB-CA-C	-7.28	97.16	110.63
2	B	200	GLN	CA-C-O	7.14	129.12	121.55
2	B	455	ARG	NE-CZ-NH2	-7.12	112.79	119.20
1	A	187	PRO	O-C-N	-7.11	114.83	123.01
2	B	316	ARG	CA-C-O	7.06	128.03	120.55
2	B	460	PHE	CA-CB-CG	7.05	120.85	113.80
2	B	81	ARG	CD-NE-CZ	6.94	134.12	124.40
2	B	184	VAL	CA-C-O	-6.92	113.17	120.57
2	B	403	ASP	CA-CB-CG	-6.84	105.76	112.60
2	B	338	THR	CA-C-O	6.82	128.81	121.11
1	A	28	PHE	CA-CB-CG	-6.75	107.05	113.80
2	B	417	LYS	CA-C-N	6.73	126.69	119.76
2	B	417	LYS	C-N-CA	6.73	126.69	119.76
2	B	245	GLN	N-CA-CB	-6.65	100.66	111.24
1	A	48	ARG	NE-CZ-NH2	-6.64	113.22	119.20
1	A	70	ARG	NH1-CZ-NH2	6.63	127.92	119.30
1	A	130	GLU	CA-C-N	6.62	126.86	119.32
1	A	130	GLU	C-N-CA	6.62	126.86	119.32
1	A	60	LYS	N-CA-C	6.60	120.20	111.75
1	A	203	GLN	OE1-CD-NE2	6.52	129.12	122.60
1	A	116	PRO	CA-C-N	6.51	129.31	120.38
1	A	116	PRO	C-N-CA	6.51	129.31	120.38
2	B	338	THR	O-C-N	-6.49	114.75	123.19
2	B	327	ASP	CA-CB-CG	6.46	119.06	112.60
2	B	224	GLU	CB-CG-CD	6.35	123.40	112.60
2	B	164	GLN	CB-CG-CD	6.33	123.37	112.60
2	B	455	ARG	CD-NE-CZ	6.33	133.27	124.40
2	B	64	SER	N-CA-CB	6.33	122.56	111.55
2	B	186	GLY	O-C-N	6.30	129.50	122.50
2	B	489	SER	O-C-N	-6.26	118.65	121.53
2	B	318	GLN	OE1-CD-NE2	-6.18	116.42	122.60
2	B	233	GLN	CB-CG-CD	6.14	123.05	112.60
2	B	376	TYR	CA-C-N	6.14	129.47	120.82
2	B	376	TYR	C-N-CA	6.14	129.47	120.82
2	B	274	LYS	CA-CB-CG	6.07	126.24	114.10
1	A	116	PRO	O-C-N	-6.06	115.20	122.89
2	B	134	GLN	CB-CG-CD	6.05	122.88	112.60
2	B	144	ASP	CA-CB-CG	-6.01	106.59	112.60
1	A	71	ARG	NE-CZ-NH1	-6.00	115.50	121.50
1	A	23	ASP	O-C-N	5.95	129.94	123.10
2	B	316	ARG	O-C-N	-5.91	115.86	122.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	411	VAL	N-CA-CB	5.89	119.54	111.41
2	B	81	ARG	NE-CZ-NH2	5.82	124.44	119.20
1	A	204	GLN	CB-CG-CD	-5.76	102.80	112.60
2	B	312	GLN	OE1-CD-NE2	-5.76	116.84	122.60
2	B	418	PRO	N-CA-CB	5.75	108.43	103.31
2	B	164	GLN	O-C-N	-5.74	115.60	122.15
1	A	4	SER	CA-C-O	5.73	126.58	120.10
2	B	60	ASN	CA-CB-CG	5.72	118.32	112.60
1	A	204	GLN	CG-CD-NE2	5.71	124.97	116.40
1	A	204	GLN	CG-CD-OE1	-5.69	109.43	120.80
2	B	380	GLN	N-CA-CB	5.66	120.30	110.39
2	B	183	ASP	CA-CB-CG	5.64	118.24	112.60
1	A	60	LYS	CD-CE-NZ	5.63	129.92	111.90
2	B	184	VAL	O-C-N	5.61	127.54	121.87
2	B	11	ALA	O-C-N	5.57	129.62	123.16
2	B	530	ASN	OD1-CG-ND2	-5.55	117.05	122.60
1	A	201	PHE	CA-CB-CG	-5.54	108.26	113.80
2	B	363	VAL	CA-C-O	5.54	123.15	119.38
2	B	244	PRO	CB-CA-C	-5.50	104.31	112.55
2	B	48	THR	CA-C-O	5.48	125.08	119.76
2	B	557	ARG	NE-CZ-NH1	-5.48	116.02	121.50
2	B	273	GLN	CA-CB-CG	5.47	125.04	114.10
2	B	465	ALA	CA-C-O	-5.43	115.47	121.28
2	B	530	ASN	CB-CG-OD1	5.42	131.63	120.80
2	B	273	GLN	CB-CG-CD	-5.41	103.40	112.60
2	B	87	PRO	N-CA-CB	5.40	108.05	103.19
1	A	151	SER	N-CA-C	-5.39	104.48	111.71
2	B	250	ALA	O-C-N	5.39	129.29	122.65
2	B	467	ALA	O-C-N	-5.39	116.06	122.20
2	B	187	ASN	OD1-CG-ND2	5.37	127.97	122.60
2	B	462	VAL	CB-CA-C	-5.37	104.62	110.37
2	B	403	ASP	OD1-CG-OD2	5.36	135.75	122.90
1	A	116	PRO	CA-C-O	5.31	127.36	121.36
1	A	81	GLN	OE1-CD-NE2	5.31	127.91	122.60
2	B	200	GLN	OE1-CD-NE2	5.30	127.90	122.60
1	A	200	LYS	CB-CG-CD	5.30	123.48	111.30
2	B	53	PRO	CA-C-N	5.29	126.70	121.62
2	B	53	PRO	C-N-CA	5.29	126.70	121.62
2	B	356	LYS	CA-C-O	-5.29	114.95	120.55
1	A	64	LYS	O-C-N	5.28	127.72	122.12
2	B	530	ASN	O-C-N	-5.27	115.62	122.37
2	B	408	PRO	N-CA-CB	5.25	108.00	103.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	334	ASP	CA-CB-CG	5.24	117.84	112.60
2	B	215	TRP	CA-CB-CG	-5.24	103.65	113.60
1	A	94	GLN	CA-C-O	-5.23	114.88	120.42
2	B	356	LYS	O-C-N	5.21	127.65	122.12
2	B	128	GLN	O-C-N	5.21	129.00	123.42
2	B	279	ALA	O-C-N	-5.21	116.60	122.12
1	A	32	GLY	CA-C-O	5.21	126.11	120.75
2	B	391	VAL	CA-C-O	5.20	126.36	120.95
2	B	108	VAL	CA-C-O	-5.20	115.02	120.27
2	B	108	VAL	O-C-N	5.20	128.59	123.18
2	B	494	ASP	CA-CB-CG	-5.19	107.41	112.60
2	B	25	GLY	N-CA-C	-5.17	104.03	112.83
2	B	82	LEU	O-C-N	5.16	130.14	122.97
2	B	165	GLU	CG-CD-OE1	5.14	130.23	118.40
2	B	317	ARG	CA-CB-CG	-5.12	103.85	114.10
2	B	462	VAL	CA-C-O	5.11	122.85	119.38
1	A	196	ASN	CA-CB-CG	-5.08	107.52	112.60
2	B	380	GLN	N-CA-C	-5.07	106.93	113.01
2	B	203	HIS	CA-CB-CG	5.06	118.86	113.80
2	B	317	ARG	CD-NE-CZ	5.05	131.48	124.40
2	B	308	SER	CA-C-O	-5.05	114.17	119.97
2	B	127	LEU	CB-CA-C	-5.01	100.64	110.11
1	A	61	ASP	OD1-CG-OD2	5.01	134.93	122.90

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	1678	0	1627	15	0
2	B	4434	0	4260	69	0
3	A	4	0	6	6	0
3	B	40	0	59	5	0
4	B	1	0	0	0	0
5	B	24	0	18	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	A	192	0	0	1	0
6	B	509	0	0	5	0
All	All	6882	0	5970	78	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 6.

All (78) 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)
3:A:1210:EDO:H21	2:B:77:ILE:HD11	1.44	0.99
3:A:1210:EDO:H21	2:B:77:ILE:CD1	1.98	0.93
2:B:59:HIS:HD2	2:B:61:GLY:H	1.24	0.81
2:B:479:ARG:HH21	2:B:483:ASN:HD22	1.25	0.80
3:A:1210:EDO:C2	2:B:77:ILE:HD11	2.12	0.80
1:A:39:ARG:HH11	1:A:42:GLN:HE22	1.30	0.78
2:B:80:GLU:OE2	2:B:123:HIS:HD2	1.69	0.76
2:B:488:PHE:CE1	2:B:497:VAL:HG22	2.22	0.75
1:A:194:GLU:OE2	2:B:233:GLN:HG2	1.87	0.74
2:B:388:ASN:HD22	2:B:389:ILE:H	1.39	0.70
1:A:18:HIS:ND1	2:B:38:HIS:HE1	1.90	0.69
2:B:187:ASN:HA	2:B:231:ASN:HD21	1.59	0.67
2:B:452:LEU:HD12	2:B:453:THR:H	1.59	0.67
2:B:468:GLU:CD	2:B:468:GLU:H	2.06	0.64
2:B:71:PHE:CE2	5:B:1569:SOX:H5	2.33	0.64
2:B:123:HIS:HE1	2:B:216:ASP:OD1	1.81	0.64
2:B:26:TRP:CD2	2:B:452:LEU:HD11	2.33	0.63
2:B:38:HIS:HD2	2:B:43:ASP:OD1	1.82	0.63
2:B:452:LEU:HD12	2:B:453:THR:N	2.14	0.63
1:A:181[A]:LEU:HD22	3:B:1564:EDO:H12	1.81	0.61
2:B:81:ARG:HH21	2:B:91:LEU:HD22	1.66	0.60
2:B:60:ASN:ND2	2:B:63:ILE:H	2.02	0.58
1:A:183:ASN:C	1:A:183:ASN:HD22	2.11	0.58
2:B:88:GLY:O	2:B:98:LYS:HE3	2.04	0.58
1:A:199:LEU:HG	2:B:225:MET:HE1	1.85	0.58
2:B:44:VAL:HG11	2:B:158:MET:HB3	1.87	0.56
2:B:59:HIS:CD2	2:B:61:GLY:H	2.15	0.56
2:B:71:PHE:HE2	5:B:1569:SOX:H5	1.70	0.56
2:B:479:ARG:HH21	2:B:483:ASN:ND2	2.02	0.55
2:B:60:ASN:HD22	2:B:60:ASN:C	2.13	0.55
2:B:98:LYS:HD3	2:B:99:MET:O	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:105:THR:OG1	2:B:115:THR:HG22	2.07	0.55
1:A:199:LEU:CG	2:B:225:MET:HE1	2.37	0.55
2:B:226:ASN:O	3:B:1566:EDO:H22	2.07	0.54
2:B:60:ASN:HD21	2:B:63:ILE:H	1.55	0.54
2:B:71:PHE:HZ	5:B:1569:SOX:HS	1.56	0.53
3:B:1563:EDO:H22	6:B:2229:HOH:O	2.07	0.53
1:A:14:TYR:OH	2:B:527:MET:HE1	2.10	0.52
2:B:488:PHE:HE1	2:B:497:VAL:HG22	1.74	0.52
2:B:26:TRP:CE3	2:B:452:LEU:HD11	2.46	0.51
3:A:1210:EDO:O2	6:A:2192:HOH:O	2.00	0.50
1:A:183:ASN:HD22	1:A:185:SER:H	1.59	0.50
2:B:337:LYS:HG3	6:B:2307:HOH:O	2.11	0.50
2:B:60:ASN:HD22	2:B:62:VAL:H	1.60	0.49
2:B:369:LYS:HE2	6:B:2328:HOH:O	2.12	0.49
2:B:388:ASN:ND2	2:B:389:ILE:H	2.09	0.49
2:B:488:PHE:CD1	2:B:497:VAL:HG22	2.49	0.47
2:B:188:ILE:H	2:B:231:ASN:ND2	2.12	0.47
1:A:56:GLU:HG2	2:B:107:THR:HB	1.95	0.47
2:B:365:MET:HE3	6:B:2328:HOH:O	2.13	0.47
2:B:81:ARG:NH2	2:B:91:LEU:HD22	2.30	0.46
3:A:1210:EDO:H12	2:B:127:LEU:HD13	1.97	0.46
1:A:183:ASN:ND2	1:A:185:SER:H	2.14	0.45
2:B:48:THR:HB	2:B:55:LEU:HA	1.98	0.45
2:B:241:ASN:ND2	5:B:1569:SOX:H6	2.32	0.45
2:B:504:ALA:HA	2:B:505:PRO:C	2.42	0.45
2:B:48:THR:HA	2:B:49:PRO:HD3	1.88	0.44
2:B:225:MET:O	3:B:1566:EDO:H12	2.18	0.44
2:B:22:PRO:HB2	2:B:24:PHE:CE2	2.53	0.44
1:A:130:GLU:HB2	1:A:131:PRO:HD2	2.00	0.44
2:B:3:MET:HE3	2:B:180:TYR:HB2	2.01	0.43
2:B:452:LEU:HB2	2:B:476:TYR:HA	2.01	0.42
2:B:20:ASN:HD21	2:B:67:SER:H	1.67	0.42
2:B:98:LYS:HE2	2:B:99:MET:O	2.19	0.42
2:B:18:MET:O	2:B:485:MET:HA	2.19	0.42
2:B:495[A]:ARG:HA	2:B:496:PRO:HD3	1.81	0.42
2:B:274:LYS:HE3	2:B:281:GLN:HB3	2.02	0.42
2:B:363:VAL:O	2:B:368:ASP:HB3	2.20	0.41
2:B:80:GLU:OE2	2:B:123:HIS:CD2	2.61	0.41
2:B:151:LEU:HD23	2:B:151:LEU:C	2.46	0.41
1:A:14:TYR:CZ	2:B:527:MET:HE1	2.56	0.41
2:B:59:HIS:HE1	6:B:2480:HOH:O	2.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:THR:HG23	3:A:1210:EDO:H22	2.03	0.40
2:B:294:LEU:H	3:B:1559:EDO:C2	2.34	0.40
2:B:435:SER:HB2	2:B:440:ASN:HD22	1.86	0.40
1:A:89:ASP:OD1	2:B:156:HIS:HE1	2.05	0.40
2:B:22:PRO:HG3	2:B:57:PHE:CZ	2.56	0.40
2:B:471:ARG:HA	2:B:471:ARG:HD2	1.89	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	206/209 (99%)	202 (98%)	4 (2%)	0	100	100
2	B	557/557 (100%)	545 (98%)	12 (2%)	0	100	100
All	All	763/766 (100%)	747 (98%)	16 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	179/179 (100%)	174 (97%)	5 (3%)	38	26
2	B	462/460 (100%)	451 (98%)	11 (2%)	43	31

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	641/639 (100%)	625 (98%)	16 (2%)	42	30

All (16) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	4	SER
1	A	60	LYS
1	A	183	ASN
1	A	200	LYS
1	A	204	GLN
2	B	60	ASN
2	B	98	LYS
2	B	154	TRP
2	B	209	VAL
2	B	233	GLN
2	B	274	LYS
2	B	403	ASP
2	B	404	LYS
2	B	436	LYS
2	B	452	LEU
2	B	468	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (26) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	42	GLN
1	A	108	ASN
1	A	183	ASN
2	B	12	GLN
2	B	20	ASN
2	B	38	HIS
2	B	59	HIS
2	B	60	ASN
2	B	93	ASN
2	B	110	ASN
2	B	123	HIS
2	B	156	HIS
2	B	187	ASN
2	B	231	ASN
2	B	245	GLN
2	B	295	ASN

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Mol	Chain	Res	Type
2	B	318	GLN
2	B	388	ASN
2	B	409	GLN
2	B	420	GLN
2	B	440	ASN
2	B	464	GLN
2	B	472	HIS
2	B	473	GLN
2	B	483	ASN
2	B	550	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

1 non-standard protein/DNA/RNA residue is 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
1	SME	A	16	1	6,8,9	0.88	0	3,9,11	2.38	2 (66%)

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
1	SME	A	16	1	-	1/6/7/9	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	SME	OE-S-CG	3.32	114.59	105.89
1	A	16	SME	CE-S-CG	2.25	103.07	97.45

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	16	SME	CB-CG-S-CE

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 13 ligands modelled in this entry, 1 is monoatomic - leaving 12 for Mogul analysis.

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	$\# Z > 2$
5	SOX	B	1569	-	21,26,26	1.11	2 (9%)	28,40,40	3.74	7 (25%)
3	EDO	B	1566	-	3,3,3	0.73	0	2,2,2	1.88	1 (50%)
3	EDO	B	1567	-	3,3,3	0.52	0	2,2,2	0.27	0
3	EDO	B	1559	-	3,3,3	1.03	0	2,2,2	0.78	0
3	EDO	A	1210	-	3,3,3	0.70	0	2,2,2	1.25	0
3	EDO	B	1564	-	3,3,3	0.57	0	2,2,2	0.20	0
3	EDO	B	1562	-	3,3,3	0.44	0	2,2,2	0.41	0
3	EDO	B	1565	-	3,3,3	0.61	0	2,2,2	1.04	0
3	EDO	B	1560	-	3,3,3	0.54	0	2,2,2	0.07	0
3	EDO	B	1561	-	3,3,3	0.53	0	2,2,2	0.10	0
3	EDO	B	1563	-	3,3,3	0.72	0	2,2,2	0.72	0
3	EDO	B	1558	-	3,3,3	0.57	0	2,2,2	0.30	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
5	SOX	B	1569	-	-	0/12/48/48	0/3/3/3
3	EDO	B	1566	-	-	1/1/1/1	-
3	EDO	B	1567	-	-	0/1/1/1	-
3	EDO	B	1559	-	-	1/1/1/1	-
3	EDO	A	1210	-	-	1/1/1/1	-
3	EDO	B	1564	-	-	0/1/1/1	-
3	EDO	B	1562	-	-	0/1/1/1	-
3	EDO	B	1565	-	-	0/1/1/1	-
3	EDO	B	1560	-	-	0/1/1/1	-
3	EDO	B	1561	-	-	0/1/1/1	-
3	EDO	B	1563	-	-	0/1/1/1	-
3	EDO	B	1558	-	-	0/1/1/1	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	1569	SOX	O8-C7	-2.09	1.18	1.22
5	B	1569	SOX	C20-C19	2.06	1.42	1.38

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	B	1569	SOX	O8-C7-N4	14.46	151.69	131.75
5	B	1569	SOX	O8-C7-C6	-8.59	114.24	136.11
5	B	1569	SOX	C6-N14-C15	-4.95	112.03	121.80
5	B	1569	SOX	C7-C6-N14	-4.36	102.95	115.29
5	B	1569	SOX	C2-C3-N4	-4.29	102.24	105.89
5	B	1569	SOX	C3-N4-C7	4.16	137.93	126.38
5	B	1569	SOX	O12-C11-C3	-2.26	105.98	112.47
3	B	1566	EDO	O1-C1-C2	2.14	128.68	112.39

There are no chirality outliers.

All (3) torsion outliers are listed below:

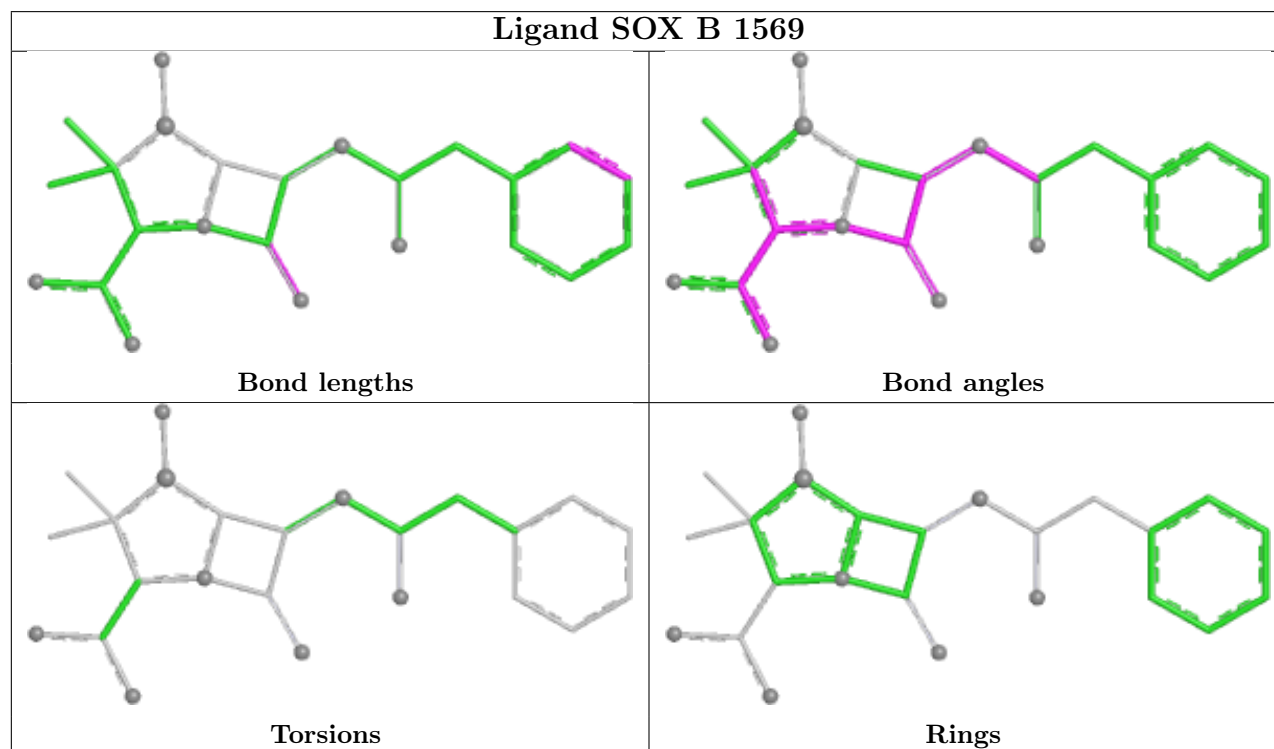
Mol	Chain	Res	Type	Atoms
3	B	1559	EDO	O1-C1-C2-O2
3	B	1566	EDO	O1-C1-C2-O2
3	A	1210	EDO	O1-C1-C2-O2

There are no ring outliers.

6 monomers are involved in 15 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	B	1569	SOX	4	0
3	B	1566	EDO	2	0
3	B	1559	EDO	1	0
3	A	1210	EDO	6	0
3	B	1564	EDO	1	0
3	B	1563	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 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, 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	206/209 (98%)	-0.59	1 (0%) 87 88	6, 14, 24, 47	5 (2%)
2	B	557/557 (100%)	-0.48	6 (1%) 78 78	5, 14, 30, 65	3 (0%)
All	All	763/766 (99%)	-0.51	7 (0%) 81 81	5, 14, 28, 65	8 (1%)

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	379	THR	3.9
2	B	132	THR	3.3
2	B	131	GLN	3.0
1	A	3	SER	2.4
2	B	380	GLN	2.3
2	B	129	THR	2.3
2	B	378	THR	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
1	SME	A	16	9/10	0.98	0.06	10,13,14,17	0

6.3 Carbohydrates [i](#)

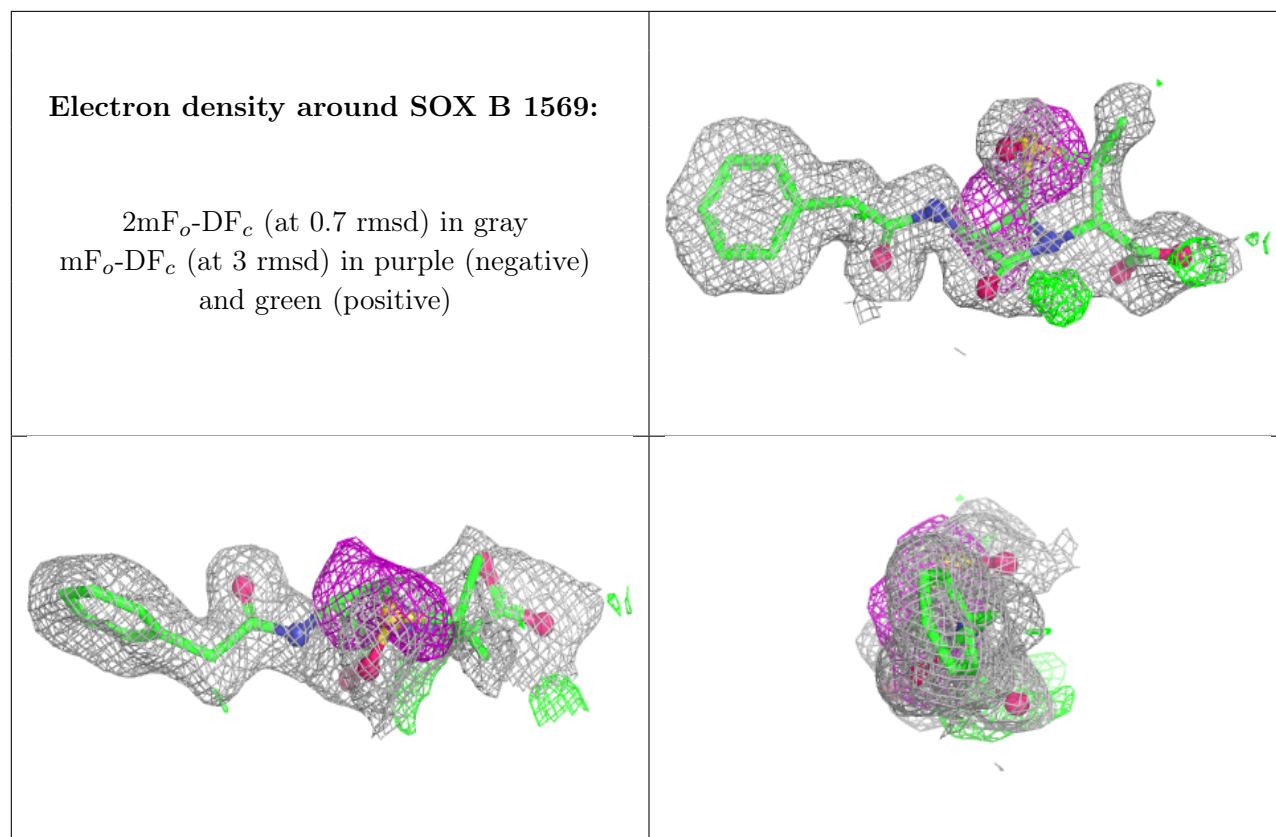
There are no oligosaccharides in this entry.

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, 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
5	SOX	B	1569	24/24	0.88	0.14	10,36,46,54	0
3	EDO	B	1567	4/4	0.92	0.10	31,31,33,42	0
3	EDO	B	1563	4/4	0.93	0.13	18,21,26,26	0
3	EDO	A	1210	4/4	0.93	0.10	29,31,34,35	0
3	EDO	B	1559	4/4	0.93	0.12	18,22,24,26	0
3	EDO	B	1566	4/4	0.96	0.09	19,22,28,30	0
3	EDO	B	1564	4/4	0.96	0.12	15,21,23,24	0
3	EDO	B	1565	4/4	0.96	0.12	20,24,26,28	0
3	EDO	B	1558	4/4	0.97	0.05	16,17,19,21	0
3	EDO	B	1560	4/4	0.97	0.07	15,17,21,26	0
3	EDO	B	1561	4/4	0.98	0.05	14,21,23,25	0
3	EDO	B	1562	4/4	0.98	0.05	12,14,15,17	0
4	CA	B	1568	1/1	1.00	0.01	10,10,10,10	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.