Full wwPDB X-ray Structure Validation Report (i)

Mar 23, 2024 – 10:29 PM EDT

PDB ID	:	1XKZ
Title	:	Crystal structure of the acylated beta-lactam sensor domain of Blar1 from S. aureus
Authors	:	Birck, C.; Cha, J.Y.; Cross, J.; Schulze-Briese, C.; Meroueh, S.O.; Schlegel, H.B.; Mobashery, S.; Samama, J.-P.
Deposited on	:	2004-09-30
Resolution	:	1.75 Å(reported)

The following versions of software and data (see references (i)) 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	:	2.36.1
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)	:	2.36.1

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 1.75 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.
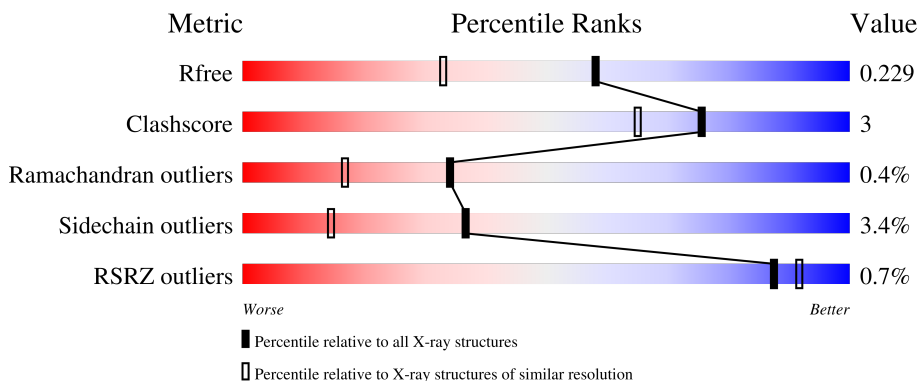
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	2340 (1.76-1.76)
Clashscore	141614	2466 (1.76-1.76)
Ramachandran outliers	138981	2437 (1.76-1.76)
Sidechain outliers	138945	2437 (1.76-1.76)
RSRZ outliers	127900	2298 (1.76-1.76)

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.

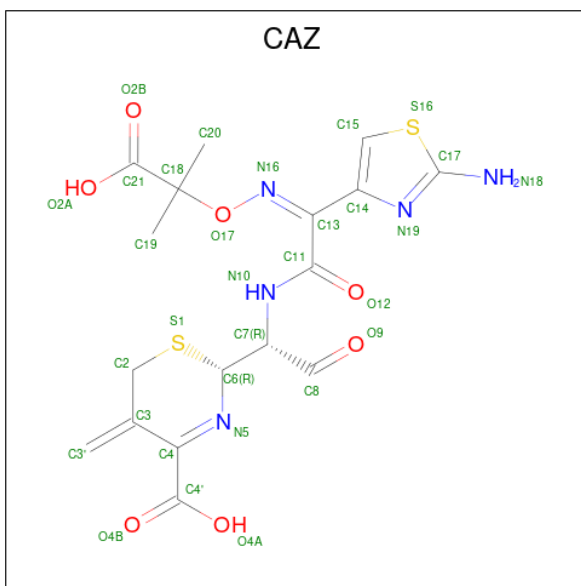| Mol	Chain	Length	Quality of chain
1	A	255	90% 5% · ·
1	B	255	90% 6% · ·
1	C	255	88% 7% · ·
1	D	255	86% 7% · ·

2 Entry composition ⓘ

There are 5 unique types of molecules in this entry. The entry contains 8056 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 Regulatory protein blaR1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	244	Total 1850	C 1188	N 310	O 343	S 9	0	0	0
1	B	247	Total 1917	C 1228	N 323	O 357	S 9	0	0	0
1	C	248	Total 1937	C 1236	N 327	O 365	S 9	0	0	0
1	D	244	Total 1927	C 1232	N 319	O 367	S 9	0	0	0

- Molecule 2 is ACYLATED CEFTAZIDIME (three-letter code: CAZ) (formula: $C_{17}H_{19}N_5O_7S_2$).

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 31	C 17	N 5	O 7	S 2	0	0
2	B	1	Total 31	C 17	N 5	O 7	S 2	0	0

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	S	0	0
			31	17	5	7	2		
2	D	1	Total	C	N	O	S	0	0
			31	17	5	7	2		

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

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

- Molecule 4 is 4-(2-HYDROXYETHYL)-1-PIPERAZINE ETHANESULFONIC ACID (three-letter code: EPE) (formula: $C_8H_{18}N_2O_4S$).
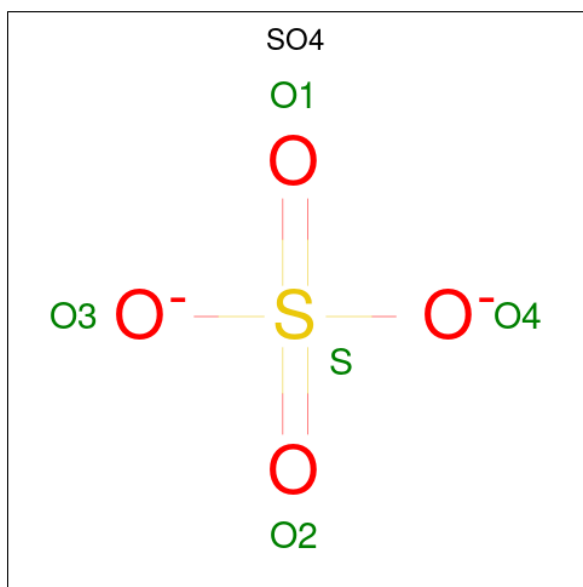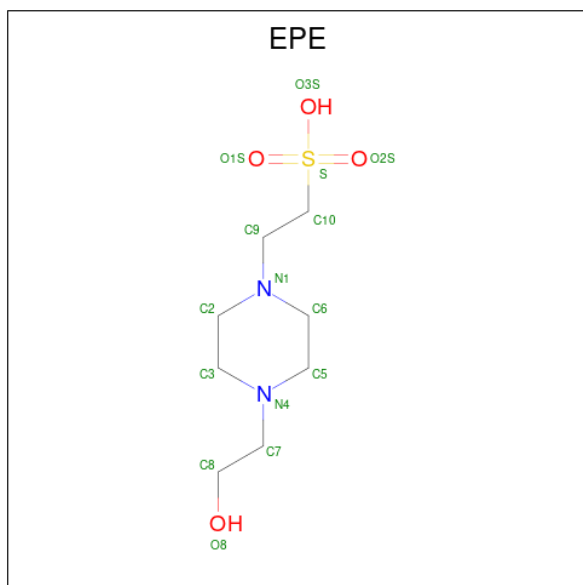
EPE

| Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	C	N	O	S		
4	B	1	15	8	2	4	1	0	0

• Molecule 5 is water.

| Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	26	Total 26	O 26	0	0
5	B	81	Total 81	O 81	0	0
5	C	91	Total 91	O 91	0	0
5	D	78	Total 78	O 78	0	0

3 Residue-property plots ⓘ

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.
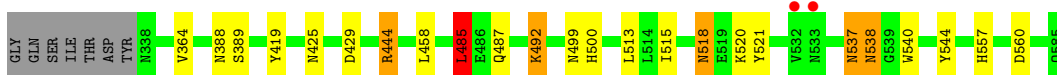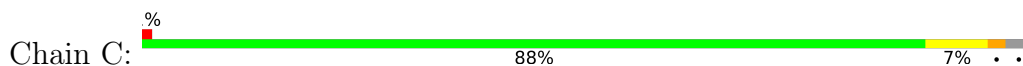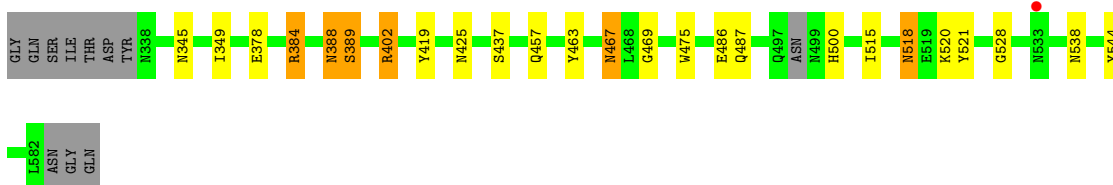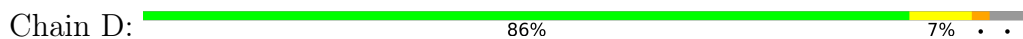
• Molecule 1: Regulatory protein blaR1
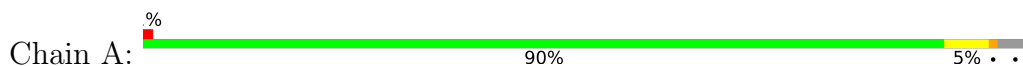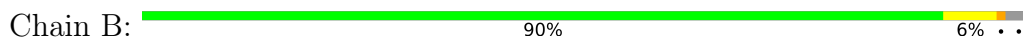
Chain A:

• Molecule 1: Regulatory protein blaR1

Chain B:

• Molecule 1: Regulatory protein blaR1

Chain C:

• Molecule 1: Regulatory protein blaR1

Chain D:

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	59.20Å 109.79Å 91.61Å 90.00° 106.13° 90.00°	Depositor
Resolution (Å)	69.00 – 1.75 68.66 – 1.75	Depositor EDS
% Data completeness (in resolution range)	97.9 (69.00-1.75) 97.9 (68.66-1.75)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.07	Depositor
$< I/\sigma(I) >$ [1]	3.69 (at 1.75Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.205 , 0.234 0.200 , 0.229	Depositor DCC
R_{free} test set	10262 reflections (9.27%)	wwPDB-VP
Wilson B-factor (Å^2)	18.6	Xtriage
Anisotropy	0.249	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 49.0	EDS
L-test for twinning[2]	$< |L| > = 0.49, < L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.021 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	8056	wwPDB-VP
Average B, all atoms (Å^2)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.20% of the height of the origin peak. No significant pseudotranslation is detected.*

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[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: CAZ, EPE, 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	0.96	0/1898	0.87	2/2579 (0.1%)
1	B	1.02	1/1968 (0.1%)	0.94	4/2673 (0.1%)
1	C	1.00	1/1986 (0.1%)	0.94	5/2690 (0.2%)
1	D	1.06	3/1976 (0.2%)	1.01	6/2677 (0.2%)
All	All	1.01	5/7828 (0.1%)	0.94	17/10619 (0.2%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	544	TYR	CD2-CE2	5.84	1.48	1.39
1	B	363	PHE	CE2-CZ	5.75	1.48	1.37
1	D	544	TYR	CD2-CE2	5.65	1.47	1.39
1	D	437	SER	CB-OG	5.41	1.49	1.42
1	D	463	TYR	CD1-CE1	5.20	1.47	1.39

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	384	ARG	NE-CZ-NH1	15.15	127.88	120.30
1	D	384	ARG	NE-CZ-NH2	-14.37	113.11	120.30
1	B	389	SER	O-C-N	-12.09	103.36	122.70
1	D	402	ARG	NE-CZ-NH2	-10.93	114.84	120.30
1	D	402	ARG	NE-CZ-NH1	8.17	124.38	120.30
1	B	389	SER	CA-C-N	8.05	134.91	117.20
1	C	444	ARG	NE-CZ-NH2	-6.33	117.13	120.30
1	B	485	LEU	CB-CG-CD2	6.20	121.53	111.00
1	B	540	TRP	CB-CA-C	-6.12	98.16	110.40
1	C	389	SER	O-C-N	-5.91	113.24	122.70
1	C	485	LEU	CB-CG-CD2	5.71	120.72	111.00
1	D	384	ARG	CD-NE-CZ	5.59	131.42	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	540	TRP	CB-CA-C	-5.54	99.33	110.40
1	D	389	SER	O-C-N	-5.46	113.96	122.70
1	C	540	TRP	CB-CA-C	-5.39	99.62	110.40
1	A	429	ASP	CB-CG-OD1	5.38	123.15	118.30
1	C	429	ASP	CB-CG-OD1	5.31	123.08	118.30

There are no chirality outliers.

There are no planarity outliers.

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	1850	0	1614	8	0
1	B	1917	0	1708	8	0
1	C	1937	0	1758	12	0
1	D	1927	0	1754	15	0
2	A	31	0	16	0	0
2	B	31	0	16	0	0
2	C	31	0	16	2	0
2	D	31	0	16	1	0
3	B	10	0	0	0	0
4	B	15	0	17	0	0
5	A	26	0	0	0	0
5	B	81	0	0	1	0
5	C	91	0	0	1	0
5	D	78	0	0	2	0
All	All	8056	0	6915	46	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 3.

All (46) 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:419:TYR:H	1:B:425:ASN:HD21	1.04	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:419:TYR:H	1:A:425:ASN:HD21	1.13	0.95
1:C:419:TYR:H	1:C:425:ASN:HD21	1.12	0.95
1:D:419:TYR:H	1:D:425:ASN:HD21	1.14	0.88
1:B:350:LEU:HD11	1:B:374:TYR:HB3	1.72	0.72
1:D:384:ARG:HD3	1:D:486:GLU:OE1	1.93	0.69
1:B:518:ASN:HD22	1:B:520:LYS:H	1.40	0.67
1:A:419:TYR:N	1:A:425:ASN:HD21	1.92	0.63
1:A:518:ASN:HD22	1:A:518:ASN:C	2.02	0.62
2:D:989:CAZ:H193	2:D:989:CAZ:HC22	1.83	0.60
1:B:419:TYR:N	1:B:425:ASN:HD21	1.89	0.60
1:D:518:ASN:ND2	1:D:521:TYR:H	2.00	0.59
1:C:538:ASN:ND2	1:C:557:HIS:NE2	2.50	0.59
1:D:518:ASN:C	1:D:518:ASN:HD22	2.07	0.58
1:D:518:ASN:ND2	1:D:520:LYS:H	2.02	0.58
1:C:419:TYR:N	1:C:425:ASN:HD21	1.94	0.57
1:B:457:GLN:HE22	1:B:500:HIS:HE1	1.54	0.56
1:C:518:ASN:ND2	1:C:520:LYS:H	2.06	0.53
1:D:515:ILE:HD13	5:D:62:HOH:O	2.09	0.53
2:C:989:CAZ:HC22	2:C:989:CAZ:H193	1.91	0.53
1:C:518:ASN:C	1:C:518:ASN:HD22	2.13	0.52
1:D:419:TYR:N	1:D:425:ASN:HD21	1.96	0.51
1:A:518:ASN:ND2	1:A:520:LYS:H	2.10	0.50
1:A:397:MET:HG2	1:A:509:LEU:HD22	1.94	0.50
1:C:419:TYR:H	1:C:425:ASN:ND2	1.95	0.50
1:D:388:ASN:HA	1:D:475:TRP:O	2.13	0.48
1:A:419:TYR:H	1:A:425:ASN:ND2	1.96	0.47
1:D:467:ASN:ND2	1:D:469:GLY:H	2.13	0.47
1:D:389:SER:HB2	1:D:528:GLY:HA2	1.97	0.46
1:C:364:VAL:HG11	1:C:485:LEU:HD23	1.97	0.46
1:D:457:GLN:OE1	1:D:500:HIS:HE1	2.00	0.45
1:A:516:LYS:HE3	1:A:521:TYR:OH	2.17	0.44
2:C:989:CAZ:H193	2:C:989:CAZ:C2	2.47	0.43
1:D:467:ASN:C	1:D:467:ASN:HD22	2.22	0.43
1:B:518:ASN:ND2	1:B:520:LYS:H	2.11	0.43
1:B:499:ASN:C	1:B:499:ASN:HD22	2.22	0.43
1:C:518:ASN:HD22	1:C:520:LYS:H	1.67	0.42
1:C:518:ASN:ND2	1:C:521:TYR:H	2.17	0.42
1:D:467:ASN:HD22	1:D:469:GLY:H	1.67	0.42
1:C:515:ILE:HD13	5:C:80:HOH:O	2.19	0.42
1:C:537:ASN:HD22	1:C:537:ASN:H	1.67	0.42
1:D:402:ARG:HD3	5:D:91:HOH:O	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:404:ILE:HD11	5:B:58:HOH:O	2.20	0.41
1:D:349:ILE:HD11	1:D:378:GLU:OE2	2.20	0.41
1:A:350:LEU:HD11	1:A:374:TYR:HB3	2.03	0.41
1:C:492:LYS:HB3	1:C:492:LYS:NZ	2.36	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	240/255 (94%)	230 (96%)	9 (4%)	1 (0%)	34	17
1	B	245/255 (96%)	237 (97%)	7 (3%)	1 (0%)	34	17
1	C	246/255 (96%)	238 (97%)	7 (3%)	1 (0%)	34	17
1	D	240/255 (94%)	233 (97%)	6 (2%)	1 (0%)	34	17
All	All	971/1020 (95%)	938 (97%)	29 (3%)	4 (0%)	34	17

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	388	ASN
1	D	388	ASN
1	B	388	ASN
1	C	388	ASN

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	170/232 (73%)	167 (98%)	3 (2%)	59	40
1	B	185/232 (80%)	180 (97%)	5 (3%)	44	22
1	C	192/232 (83%)	180 (94%)	12 (6%)	18	3
1	D	196/232 (84%)	191 (97%)	5 (3%)	46	23
All	All	743/928 (80%)	718 (97%)	25 (3%)	37	14

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	397	MET
1	A	487	GLN
1	A	518	ASN
1	B	437	SER
1	B	448	GLN
1	B	485	LEU
1	B	487	GLN
1	B	499	ASN
1	C	444	ARG
1	C	458	LEU
1	C	485	LEU
1	C	487	GLN
1	C	492	LYS
1	C	499	ASN
1	C	500	HIS
1	C	513	LEU
1	C	518	ASN
1	C	537	ASN
1	C	538	ASN
1	C	560	ASP
1	D	345	ASN
1	D	467	ASN
1	D	487	GLN
1	D	518	ASN
1	D	538	ASN

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	425	ASN
1	A	518	ASN
1	B	425	ASN
1	B	428	GLN
1	B	436	ASN
1	B	457	GLN
1	B	462	ASN
1	B	487	GLN
1	B	499	ASN
1	B	507	ASN
1	B	518	ASN
1	B	567	ASN
1	C	348	GLN
1	C	425	ASN
1	C	457	GLN
1	C	487	GLN
1	C	499	ASN
1	C	500	HIS
1	C	518	ASN
1	C	537	ASN
1	C	538	ASN
1	C	585	GLN
1	D	425	ASN
1	D	467	ASN
1	D	518	ASN
1	D	538	ASN

5.3.3   RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

5.5   Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

7 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	CAZ	C	989	1	24,32,32	2.24	10 (41%)	23,46,46	1.91	4 (17%)
4	EPE	B	2003	-	15,15,15	1.94	4 (26%)	18,20,20	1.33	4 (22%)
3	SO4	B	2002	-	4,4,4	0.51	0	6,6,6	0.34	0
3	SO4	B	2001	-	4,4,4	0.52	0	6,6,6	0.17	0
2	CAZ	D	989	1	24,32,32	2.29	7 (29%)	23,46,46	1.89	4 (17%)
2	CAZ	A	989	1	24,32,32	2.94	8 (33%)	23,46,46	2.11	6 (26%)
2	CAZ	B	989	1	24,32,32	2.58	8 (33%)	23,46,46	2.71	5 (21%)

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	CAZ	C	989	1	-	4/22/47/47	0/1/2/2
4	EPE	B	2003	-	-	0/9/19/19	0/1/1/1
2	CAZ	D	989	1	-	5/22/47/47	0/1/2/2
2	CAZ	A	989	1	-	4/22/47/47	0/1/2/2
2	CAZ	B	989	1	-	9/22/47/47	0/1/2/2

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	989	CAZ	C4-N5	9.04	1.49	1.28
2	B	989	CAZ	C4-N5	7.77	1.46	1.28
2	D	989	CAZ	C4-N5	7.31	1.45	1.28
2	C	989	CAZ	C4-N5	6.01	1.42	1.28
2	A	989	CAZ	C18-C21	5.33	1.59	1.53
2	A	989	CAZ	C7-N10	4.81	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	2003	EPE	C7-N4	4.65	1.58	1.47
2	D	989	CAZ	C4-C4'	4.35	1.57	1.48
2	A	989	CAZ	C13-N16	4.10	1.35	1.29
2	B	989	CAZ	C7-N10	4.03	1.52	1.46
2	B	989	CAZ	C13-N16	3.97	1.35	1.29
2	C	989	CAZ	C4-C4'	3.81	1.56	1.48
2	A	989	CAZ	C4-C4'	3.69	1.56	1.48
4	B	2003	EPE	C6-N1	3.67	1.57	1.46
2	B	989	CAZ	C2-S1	-3.58	1.74	1.82
2	A	989	CAZ	C2-S1	-3.39	1.74	1.82
2	C	989	CAZ	C2-S1	-3.35	1.74	1.82
2	C	989	CAZ	C13-C11	-3.30	1.44	1.50
2	B	989	CAZ	C4-C4'	3.28	1.55	1.48
2	B	989	CAZ	C13-C11	-3.20	1.44	1.50
2	D	989	CAZ	C13-C11	-3.19	1.44	1.50
2	D	989	CAZ	C2-S1	-3.16	1.75	1.82
2	B	989	CAZ	C15-S16	-3.05	1.65	1.70
2	C	989	CAZ	C7-N10	3.00	1.50	1.46
4	B	2003	EPE	C9-N1	2.65	1.53	1.47
4	B	2003	EPE	C5-N4	2.58	1.54	1.46
2	D	989	CAZ	O17-N16	2.44	1.48	1.42
2	D	989	CAZ	C7-N10	2.44	1.49	1.46
2	A	989	CAZ	O2B-C21	2.43	1.30	1.22
2	C	989	CAZ	O17-N16	2.39	1.47	1.42
2	A	989	CAZ	C13-C11	-2.23	1.46	1.50
2	C	989	CAZ	C20-C18	2.21	1.56	1.52
2	C	989	CAZ	C13-N16	2.16	1.32	1.29
2	B	989	CAZ	O2B-C21	2.16	1.29	1.22
2	C	989	CAZ	C4-C3	-2.12	1.39	1.46
2	C	989	CAZ	O2B-C21	2.05	1.28	1.22
2	D	989	CAZ	C17-N18	2.04	1.41	1.35

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	989	CAZ	C18-O17-N16	9.95	119.17	110.33
2	D	989	CAZ	C18-O17-N16	6.08	115.74	110.33
2	A	989	CAZ	C18-O17-N16	5.76	115.45	110.33
2	C	989	CAZ	C18-O17-N16	4.82	114.61	110.33
2	C	989	CAZ	C3-C2-S1	4.76	121.46	111.65
2	A	989	CAZ	O17-C18-C21	4.73	117.24	109.67
2	B	989	CAZ	O17-C18-C21	4.33	116.60	109.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	989	CAZ	C3-C2-S1	3.90	119.69	111.65
2	D	989	CAZ	C3-C2-S1	3.85	119.59	111.65
2	C	989	CAZ	C2-S1-C6	3.81	101.94	94.47
2	A	989	CAZ	C3-C2-S1	3.79	119.47	111.65
2	B	989	CAZ	C2-S1-C6	3.53	101.39	94.47
2	A	989	CAZ	C2-S1-C6	3.27	100.88	94.47
2	D	989	CAZ	O17-C18-C21	3.02	114.50	109.67
2	C	989	CAZ	O17-C18-C21	2.86	114.25	109.67
4	B	2003	EPE	C3-C2-N1	-2.72	105.06	110.64
4	B	2003	EPE	C9-N1-C6	-2.56	104.70	111.23
2	B	989	CAZ	C14-C15-S16	2.51	114.88	111.79
2	A	989	CAZ	C14-C15-S16	2.13	114.40	111.79
2	D	989	CAZ	C2-S1-C6	2.10	98.59	94.47
2	A	989	CAZ	C13-C11-N10	2.05	117.78	114.38
4	B	2003	EPE	O3S-S-C10	2.04	109.06	105.77
4	B	2003	EPE	C6-N1-C2	2.02	113.38	108.83

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	989	CAZ	C13-N16-O17-C18
2	B	989	CAZ	C19-C18-O17-N16
2	B	989	CAZ	C20-C18-O17-N16
2	B	989	CAZ	O17-C18-C21-O2A
2	B	989	CAZ	O17-C18-C21-O2B
2	A	989	CAZ	N5-C4-C4'-O4A
2	B	989	CAZ	N5-C4-C4'-O4A
2	C	989	CAZ	N5-C4-C4'-O4A
2	D	989	CAZ	N5-C4-C4'-O4A
2	A	989	CAZ	C3-C4-C4'-O4B
2	B	989	CAZ	C3-C4-C4'-O4B
2	C	989	CAZ	C3-C4-C4'-O4B
2	D	989	CAZ	C3-C4-C4'-O4B
2	C	989	CAZ	O12-C11-C13-N16
2	B	989	CAZ	N10-C11-C13-N16
2	C	989	CAZ	N10-C11-C13-N16
2	D	989	CAZ	N10-C11-C13-N16
2	A	989	CAZ	N10-C11-C13-N16
2	A	989	CAZ	O12-C11-C13-C14
2	D	989	CAZ	O12-C11-C13-C14
2	B	989	CAZ	O12-C11-C13-N16

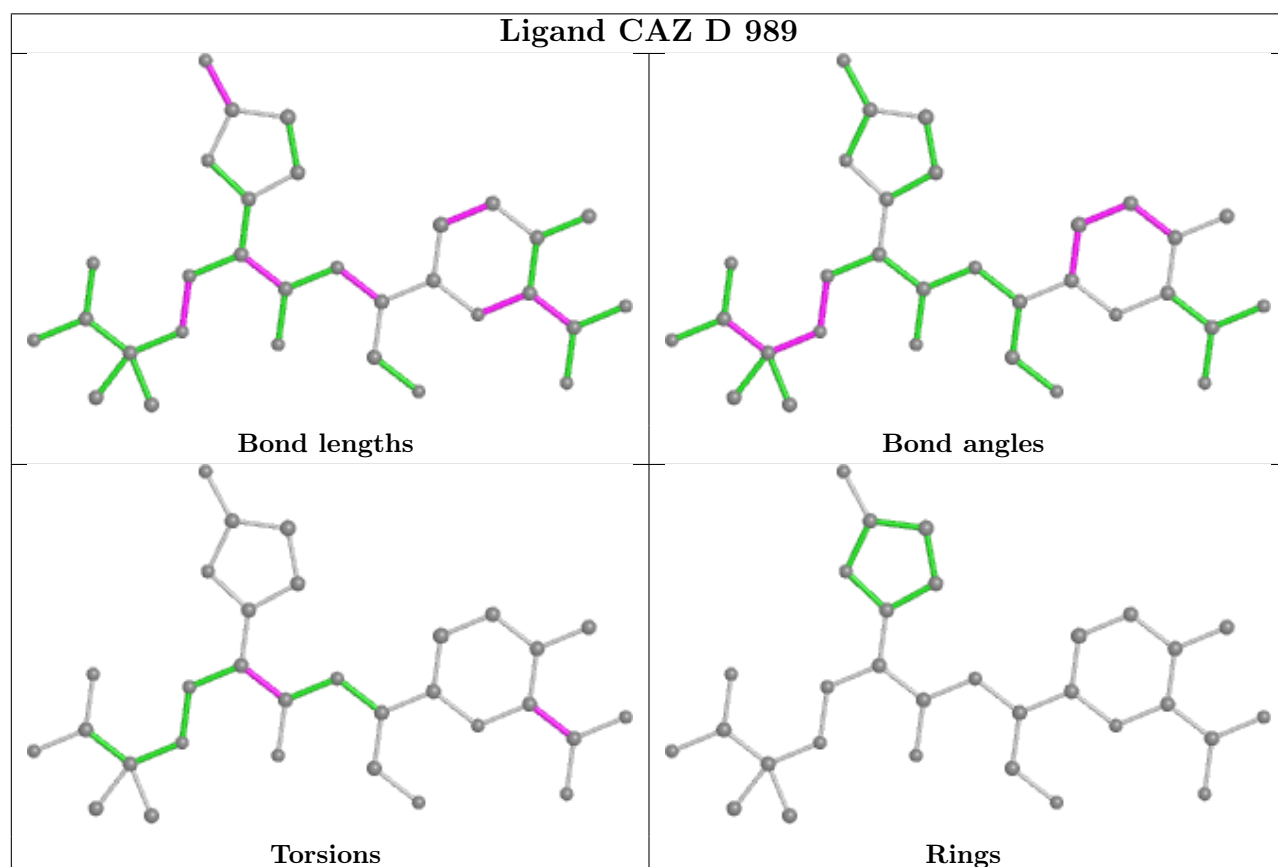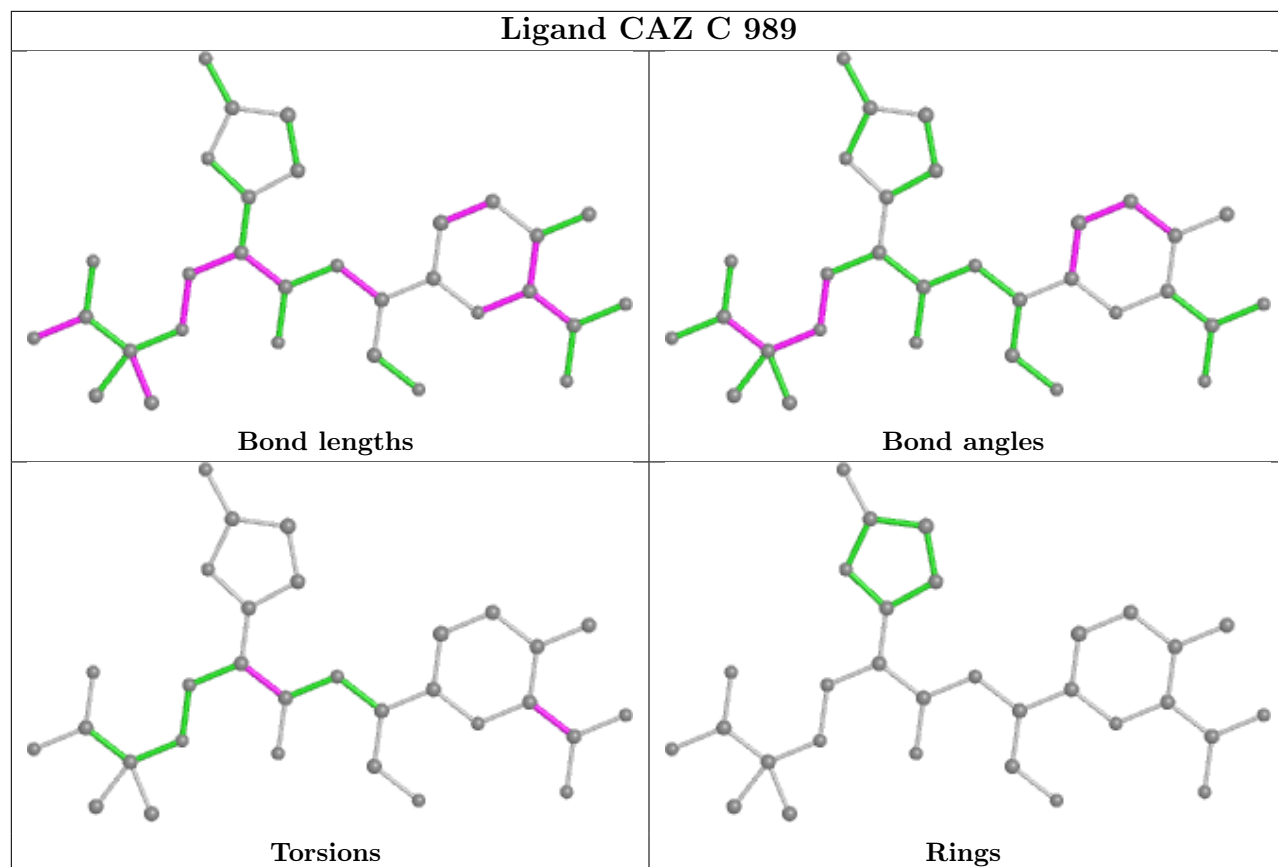*Continued on next page...*

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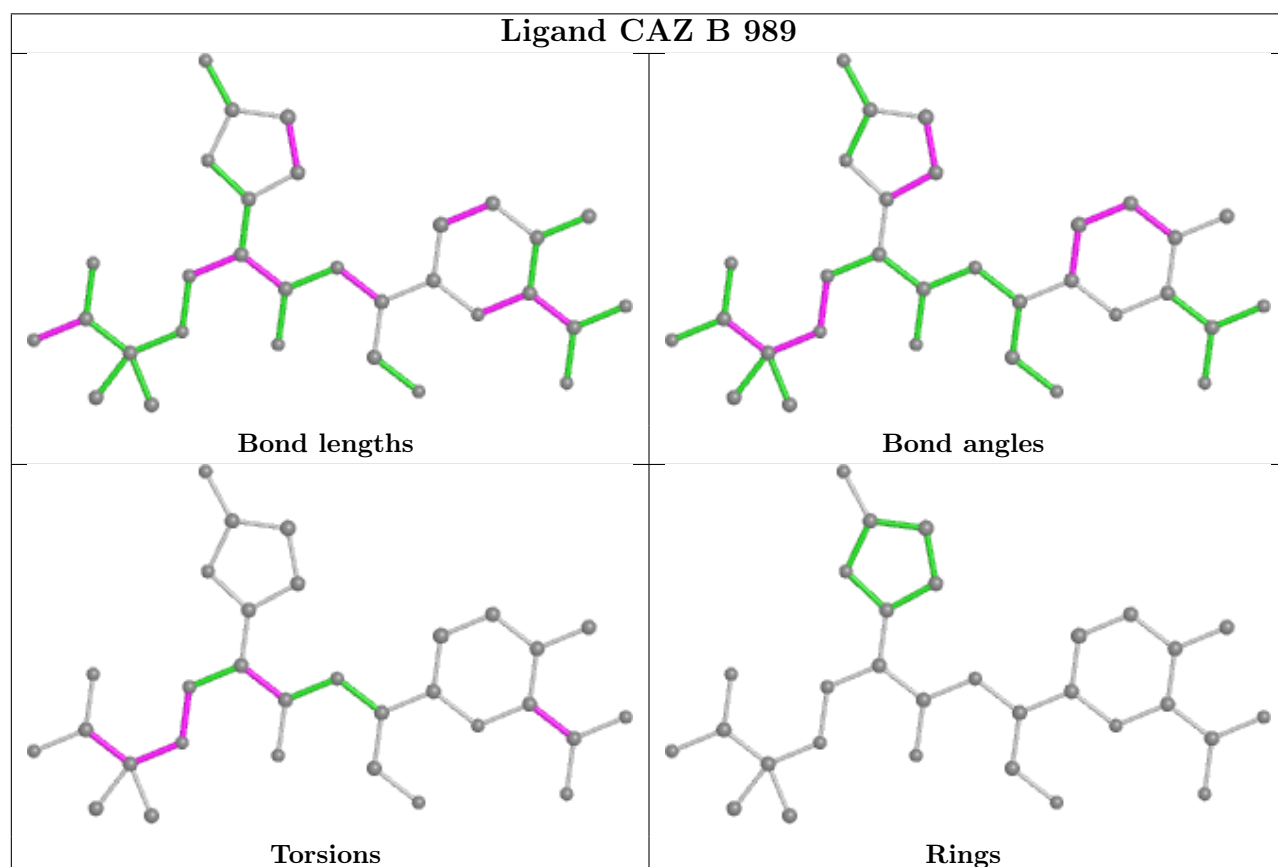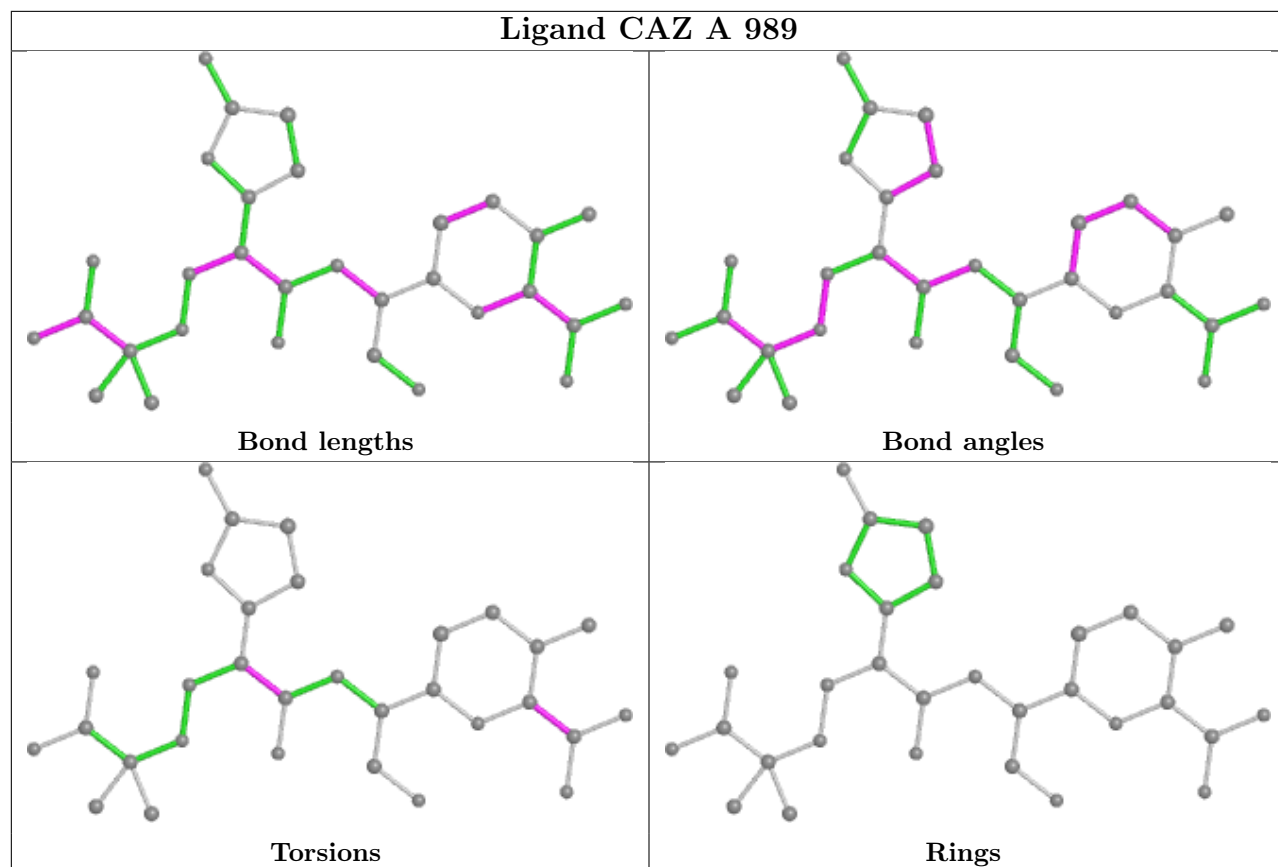| Mol	Chain	Res	Type	Atoms
2	D	989	CAZ	O12-C11-C13-N16

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	989	CAZ	2	0
2	D	989	CAZ	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.

Ligand CAZ C 989

Bond lengths

Bond angles

Torsions

Rings

Ligand CAZ D 989

Bond lengths

Bond angles

Torsions

Rings

Ligand CAZ A 989

Bond lengths

Bond angles

Torsions

Rings

Ligand CAZ B 989

Bond lengths

Bond angles

Torsions

Rings

5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	244/255 (95%)	0.10	3 (1%)	79	84	14, 27, 42, 48	0
1	B	247/255 (96%)	-0.36	1 (0%)	92	94	9, 18, 34, 40	0
1	C	248/255 (97%)	-0.30	2 (0%)	86	90	9, 17, 29, 40	0
1	D	244/255 (95%)	-0.32	1 (0%)	92	94	11, 19, 31, 40	0
All	All	983/1020 (96%)	-0.22	7 (0%)	87	92	9, 20, 37, 48	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	532	VAL	3.7
1	C	533	ASN	3.3
1	A	452	ASN	2.9
1	D	533	ASN	2.2
1	A	561	GLY	2.2
1	B	420	PRO	2.0
1	A	456	THR	2.0

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

There are no non-standard protein/DNA/RNA residues in this entry.
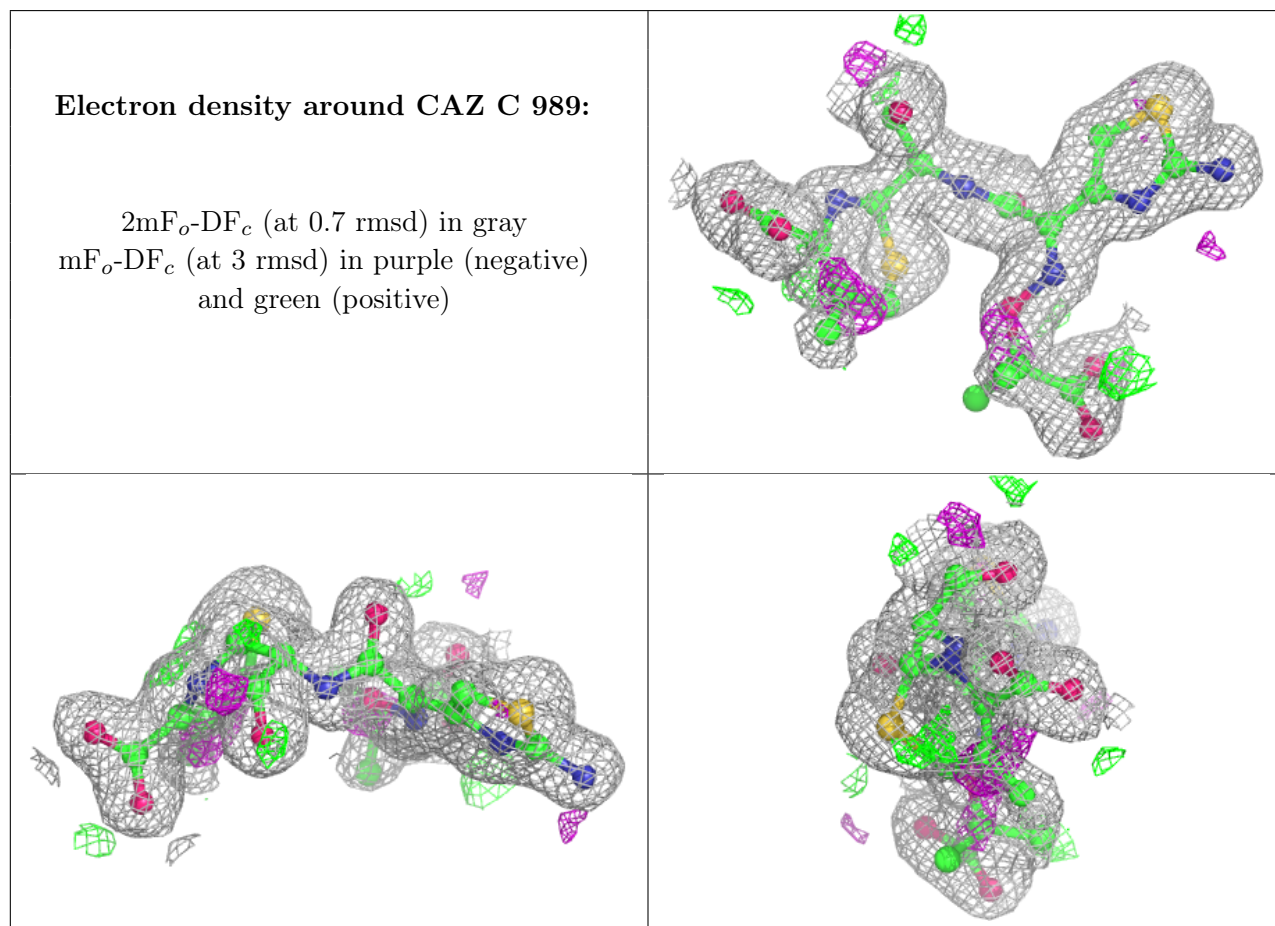
6.3 Carbohydrates ⓘ

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, 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
3	SO4	B	2001	5/5	0.89	0.19	48,50,50,50	0
2	CAZ	C	989	31/31	0.94	0.12	13,20,36,39	0
2	CAZ	A	989	31/31	0.94	0.11	15,25,39,40	0
2	CAZ	D	989	31/31	0.95	0.10	13,20,37,41	0
2	CAZ	B	989	31/31	0.95	0.10	14,22,39,40	0
3	SO4	B	2002	5/5	0.98	0.09	29,32,33,33	0
4	EPE	B	2003	15/15	0.98	0.08	19,20,25,25	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.
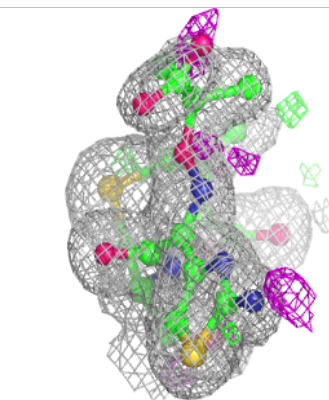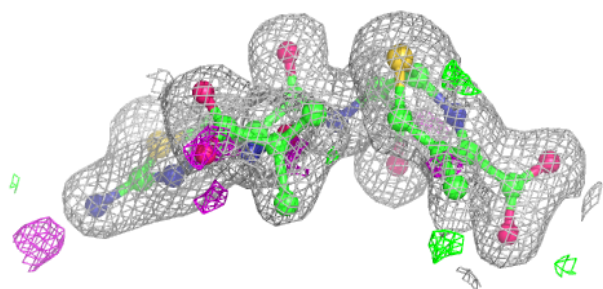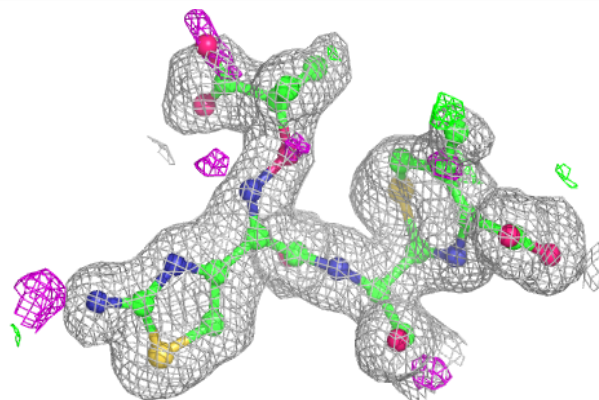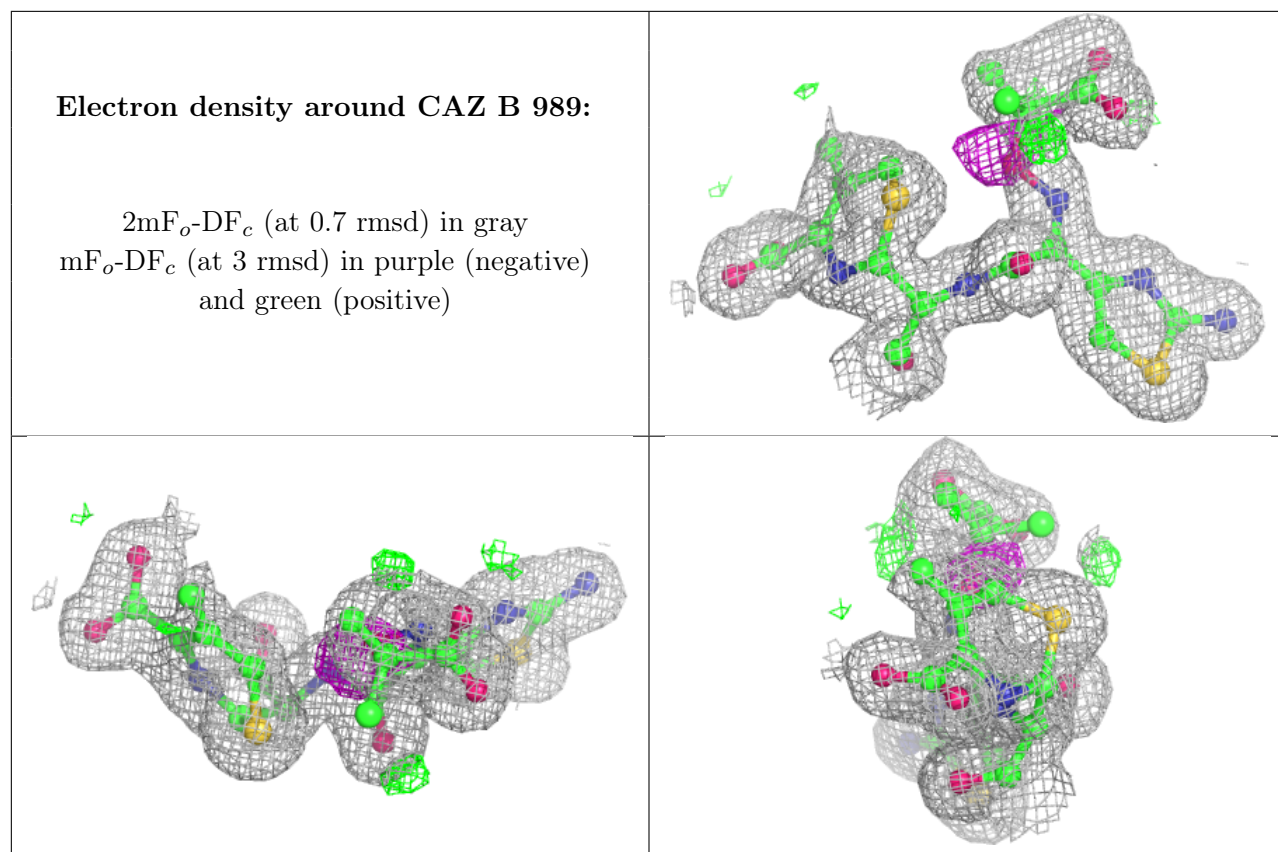

Electron density around CAZ C 989:

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

Electron density around CAZ A 989:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)
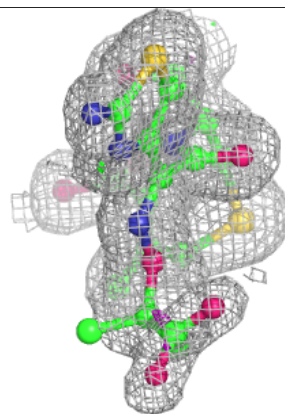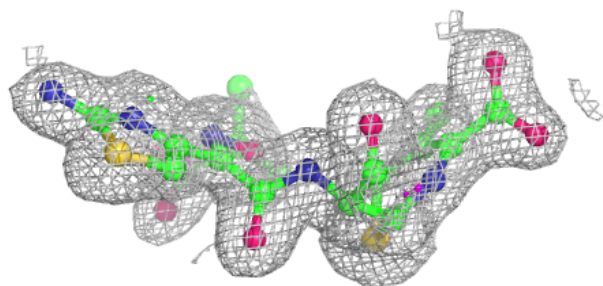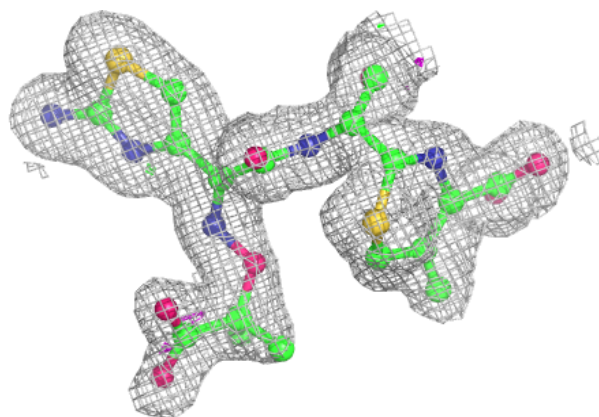
Electron density around CAZ D 989:

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

Electron density around CAZ B 989:

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

6.5 Other polymers ⓘ

There are no such residues in this entry.