Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2024 – 01:11 PM EST

PDB ID	:	4K39
Title	:	Native anSMEcpe with bound AdoMet and Cp18Cys peptide
Authors	:	Goldman, P.J.; Drennan, C.L.
Deposited on	:	2013-04-10
Resolution	:	1.78 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
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 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 1.78 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.
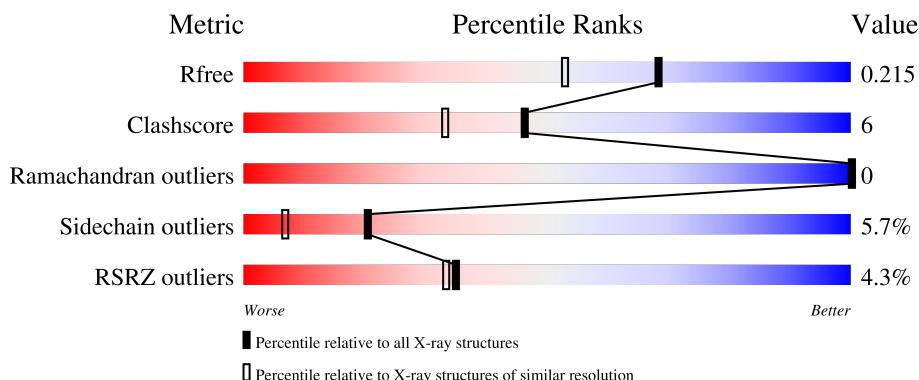
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	9185 (1.80-1.76)
Clashscore	141614	10184 (1.80-1.76)
Ramachandran outliers	138981	10051 (1.80-1.76)
Sidechain outliers	138945	10050 (1.80-1.76)
RSRZ outliers	127900	9032 (1.80-1.76)

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	370	3% / 85% / 11% / ··
1	B	370	4% / 85% / 10% / ··
2	C	18	22% / 22% / 22% / 11% / 44%
2	D	18	6% / 44% / 11% / 44%
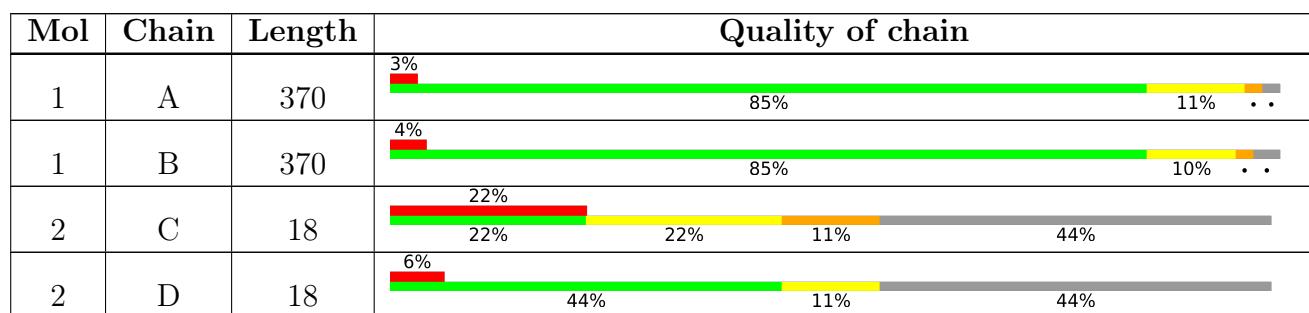
The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

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
5	GOL	A	506	-	-	-	X

2 Entry composition ⓘ

There are 7 unique types of molecules in this entry. The entry contains 6595 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 Anaerobic sulfatase-maturating enzyme.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	361	Total	C	N	O	S	0	1	0
			2940	1891	487	537	25			
1	B	359	Total	C	N	O	S	0	1	0
			2955	1898	491	541	25			

- Molecule 2 is a protein called Cp18Cys peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	10	Total	C	N	O	S	0	0	0
			68	42	13	12	1			
2	C	10	Total	C	N	O	S	0	1	0
			70	44	13	11	2			

- Molecule 3 is IRON/SULFUR CLUSTER (three-letter code: SF4) (formula: Fe_4S_4).
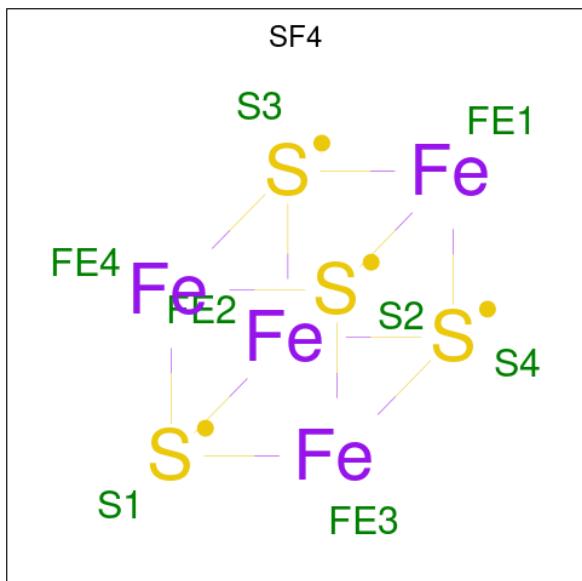
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 8	Fe 4	S 4	0	0
3	A	1	Total 8	Fe 4	S 4	0	0
3	A	1	Total 8	Fe 4	S 4	0	0
3	B	1	Total 8	Fe 4	S 4	0	0
3	B	1	Total 8	Fe 4	S 4	0	0
3	B	1	Total 8	Fe 4	S 4	0	0

- Molecule 4 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: $C_{15}H_{22}N_6O_5S$).
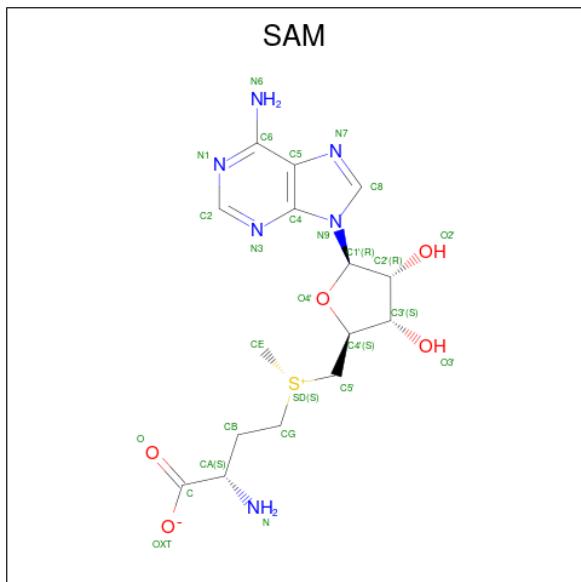
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total 27	C 15	N 6	O 5	S 1	0	0

- Molecule 5 is GLYCEROL (three-letter code: GOL) (formula: $C_3H_8O_3$).

GOL
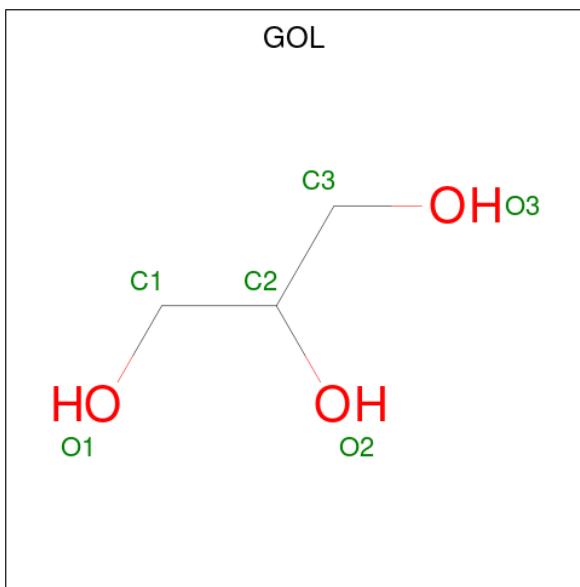
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total 6	C 3	O 3	0	0
5	A	1	Total 6	C 3	O 3	0	0
5	B	1	Total 6	C 3	O 3	0	0

- Molecule 6 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	B	1	Total 1	Cl 1	0	0

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	251	Total 251	O 251	0	0
7	B	210	Total 210	O 210	0	0
7	D	5	Total 5	O 5	0	0
7	C	2	Total 2	O 2	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: Anaerobic sulfatase-maturating enzyme
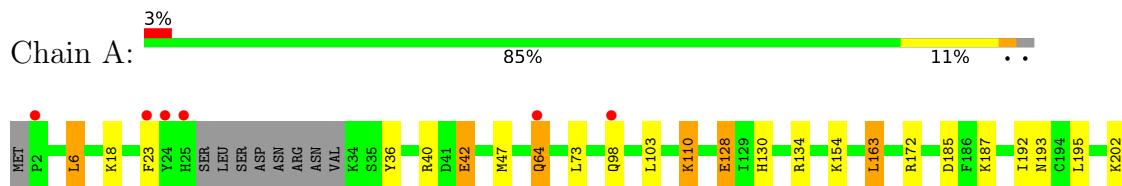
• Molecule 1: Anaerobic sulfatase-maturating enzyme
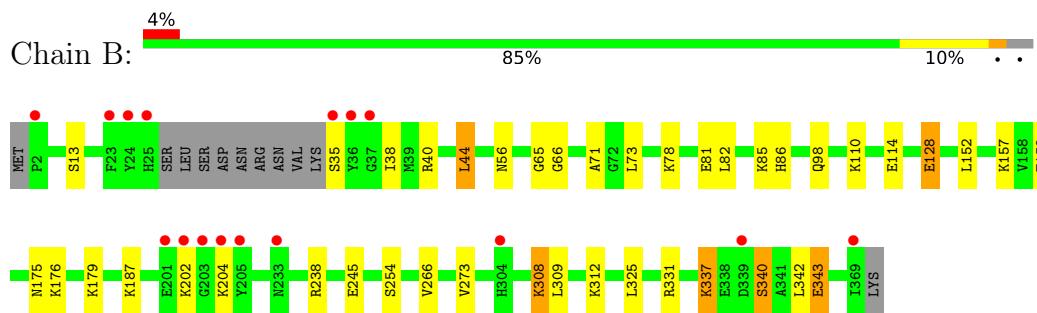
• Molecule 2: Cp18Cys peptide
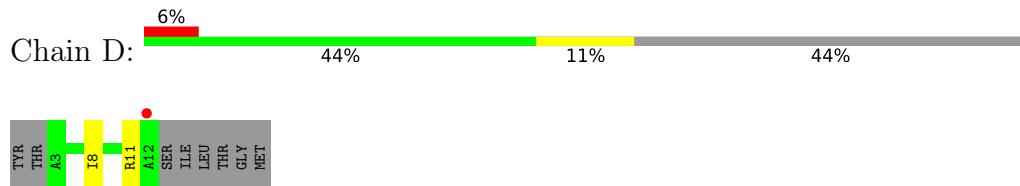
• Molecule 2: Cp18Cys peptide
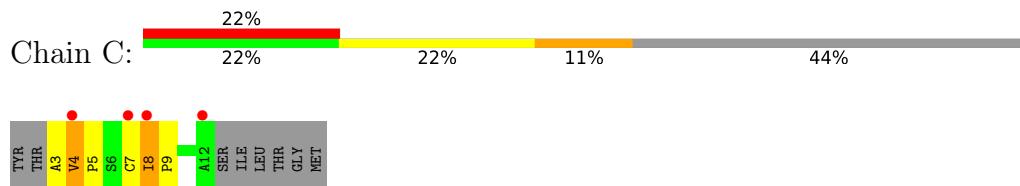
4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	44.03Å 91.92Å 91.00Å 90.00° 91.10° 90.00°	Depositor
Resolution (Å)	41.02 – 1.78 45.49 – 1.78	Depositor EDS
% Data completeness (in resolution range)	98.5 (41.02-1.78) 98.4 (45.49-1.78)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	1.30 (at 1.78Å)	Xtriage
Refinement program	PHENIX 1.8.2_1309	Depositor
R, R_{free}	0.180 , 0.215 0.180 , 0.215	Depositor DCC
R_{free} test set	3363 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å^2)	24.4	Xtriage
Anisotropy	0.550	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 43.2	EDS
L-test for twinning[2]	$<\lvert L \rvert> = 0.50$, $<L^2> = 0.33$	Xtriage
Estimated twinning fraction	0.009 for -h,-l,-k 0.000 for -h,l,k 0.031 for h,-k,-l	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	6595	wwPDB-VP
Average B, all atoms (Å^2)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 24.95 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.4758e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<\lvert L \rvert>$, $<L^2>$ 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: SF4, GOL, SAM, CL

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	0.61	0/3011	0.67	1/4048 (0.0%)
1	B	0.55	0/3023	0.62	0/4058
2	C	0.46	0/74	0.56	0/101
2	D	0.96	0/69	0.55	0/94
All	All	0.59	0/6177	0.64	1/8301 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	6	LEU	CA-CB-CG	5.27	127.42	115.30

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	2940	0	2844	42	0
1	B	2955	0	2885	30	0
2	C	70	0	73	8	0
2	D	68	0	71	1	0
3	A	24	0	0	1	0
3	B	24	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	A	27	0	22	4	0
5	A	12	0	16	1	0
5	B	6	0	8	0	0
6	B	1	0	0	0	0
7	A	251	0	0	5	0
7	B	210	0	0	6	0
7	C	2	0	0	1	0
7	D	5	0	0	0	0
All	All	6595	0	5919	76	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 (76) 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:343:GLU:HG3	7:B:771:HOH:O	1.56	1.05
1:B:337:LYS:CE	1:B:343:GLU:OE2	2.21	0.89
1:A:23:PHE:HA	7:A:769:HOH:O	1.78	0.83
3:A:503:SF4:S4	4:A:504:SAM:HE1	2.21	0.81
1:A:163:LEU:CD2	1:A:192:ILE:HD11	2.14	0.78
1:B:308:LYS:NZ	7:B:800:HOH:O	2.22	0.72
1:A:64:GLN:HG3	1:A:98:GLN:HB3	1.72	0.70
1:A:64:GLN:HE22	2:C:8:ILE:HB	1.58	0.68
1:B:337:LYS:HE3	1:B:343:GLU:OE2	1.94	0.67
1:B:13:SER:OG	1:B:35:SER:HB2	1.96	0.66
1:B:56:ASN:ND2	7:B:670:HOH:O	2.27	0.65
1:A:193:ASN:O	4:A:504:SAM:H2	1.97	0.65
1:B:175:ASN:HB2	1:B:179:LYS:NZ	2.13	0.64
1:A:64:GLN:OE1	1:A:98:GLN:HB2	2.03	0.59
1:A:110:LYS:HD2	7:A:698:HOH:O	2.01	0.59
1:B:238:ARG:NH1	1:B:245:GLU:OE1	2.33	0.58
1:B:337:LYS:NZ	1:B:343:GLU:OE2	2.37	0.58
1:A:185:ASP:OD1	1:A:187:LYS:HE3	2.04	0.57
1:B:159:GLU:OE1	2:D:11:ARG:NH2	2.35	0.57
1:A:312:LYS:HZ1	1:A:342:LEU:H	1.53	0.57
1:A:98:GLN:HG3	4:A:504:SAM:HB2	1.87	0.56
1:B:128:GLU:H	1:B:128:GLU:CD	2.09	0.54
1:A:306:PHE:HD2	1:A:307:ILE:HD13	1.73	0.54
1:A:47:MET:HG3	1:A:289:ILE:HD13	1.90	0.53
1:A:110:LYS:CD	7:A:698:HOH:O	2.57	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:38:ILE:HD12	1:B:71:ALA:HA	1.90	0.53
1:B:337:LYS:HE2	1:B:343:GLU:CD	2.30	0.52
1:A:312:LYS:HZ1	1:A:341:ALA:HB1	1.74	0.52
1:A:312:LYS:HZ1	1:A:342:LEU:N	2.08	0.52
1:A:163:LEU:HD23	1:A:192:ILE:HD11	1.90	0.52
1:A:172:ARG:O	5:A:505:GOL:H12	2.09	0.52
1:A:210:LYS:CB	1:A:210:LYS:NZ	2.73	0.52
1:A:210:LYS:HB2	1:A:210:LYS:HZ2	1.75	0.52
2:C:8:ILE:HD12	2:C:9:PRO:HD2	1.93	0.51
1:A:238:ARG:NH2	2:C:4:VAL:HG23	2.26	0.51
1:A:312:LYS:NZ	1:A:341:ALA:HB1	2.25	0.51
1:A:163:LEU:HD21	2:C:7[B]:CYS:HA	1.93	0.50
1:B:176:LYS:NZ	7:B:778:HOH:O	2.45	0.49
1:A:40:ARG:NH1	1:A:42:GLU:OE2	2.42	0.49
1:A:163:LEU:HD23	1:A:192:ILE:CD1	2.42	0.49
1:B:78:LYS:HD2	1:B:81:GLU:OE2	2.12	0.49
2:C:5:PRO:O	2:C:8:ILE:HG23	2.12	0.48
1:A:128:GLU:HB2	7:A:724:HOH:O	2.13	0.47
1:B:40:ARG:HG3	7:B:626:HOH:O	2.14	0.47
1:B:175:ASN:HB2	1:B:179:LYS:HZ1	1.78	0.47
1:A:36:TYR:HB2	1:A:269:SER:OG	2.15	0.47
1:A:163:LEU:HD21	1:A:192:ILE:HD11	1.96	0.46
1:A:308:LYS:HA	1:A:308:LYS:HD2	1.70	0.46
1:A:163:LEU:HD21	2:C:7[A]:CYS:HA	1.97	0.45
1:B:40:ARG:NH1	7:B:787:HOH:O	2.49	0.45
1:B:187:LYS:HA	1:B:187:LYS:HD2	1.86	0.45
1:B:337:LYS:CE	1:B:343:GLU:CD	2.83	0.44
1:B:110:LYS:HE3	1:B:114:GLU:OE2	2.19	0.43
1:B:85:LYS:HE2	1:B:86:HIS:CE1	2.54	0.43
1:B:202:LYS:HE2	1:B:202:LYS:HB2	1.79	0.43
1:A:163:LEU:CG	1:A:192:ILE:HD11	2.48	0.43
1:A:266:VAL:O	1:A:273:VAL:HA	2.20	0.42
1:A:64:GLN:OE1	1:A:98:GLN:CB	2.66	0.42
1:A:315:GLU:HA	1:A:318:LYS:HG3	2.01	0.42
1:B:337:LYS:HB2	1:B:340:SER:OG	2.20	0.42
1:B:44:LEU:HD13	1:B:82:LEU:HD12	2.01	0.42
1:A:163:LEU:HG	1:A:192:ILE:HD11	2.01	0.42
1:A:262:THR:HG23	7:A:800:HOH:O	2.19	0.41
1:B:110:LYS:HD2	1:B:110:LYS:HA	1.70	0.41
1:A:210:LYS:NZ	1:A:210:LYS:HB2	2.33	0.41
1:A:321:LYS:HE2	1:A:322:TRP:CZ2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:192:ILE:HG22	4:A:504:SAM:H2	2.02	0.41
2:C:3:ALA:N	7:C:102:HOH:O	2.53	0.41
1:A:130:HIS:CE1	1:A:134:ARG:HD3	2.55	0.41
1:A:238:ARG:HH22	2:C:4:VAL:HG23	1.84	0.41
1:B:266:VAL:O	1:B:273:VAL:HA	2.21	0.41
1:B:157:LYS:HE3	1:B:157:LYS:HB2	1.66	0.41
1:B:204:LYS:HG2	1:B:204:LYS:O	2.21	0.41
1:A:212:LYS:HD3	1:A:213:ASP:N	2.36	0.40
1:B:65:GLY:HA3	1:B:66:GLY:C	2.41	0.40
1:A:202:LYS:HD2	1:A:346:TYR:CE1	2.55	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	358/370 (97%)	352 (98%)	6 (2%)	0	100	100
1	B	356/370 (96%)	351 (99%)	5 (1%)	0	100	100
2	C	9/18 (50%)	9 (100%)	0	0	100	100
2	D	8/18 (44%)	8 (100%)	0	0	100	100
All	All	731/776 (94%)	720 (98%)	11 (2%)	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	321/339 (95%)	303 (94%)	18 (6%)	21	7
1	B	327/339 (96%)	310 (95%)	17 (5%)	23	8
2	C	8/15 (53%)	6 (75%)	2 (25%)	0	0
2	D	8/15 (53%)	7 (88%)	1 (12%)	4	1
All	All	664/708 (94%)	626 (94%)	38 (6%)	20	7

All (38) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	6	LEU
1	A	18	LYS
1	A	42	GLU
1	A	64	GLN
1	A	73	LEU
1	A	103	LEU
1	A	110	LYS
1	A	128	GLU
1	A	154	LYS
1	A	163	LEU
1	A	195	LEU
1	A	210	LYS
1	A	212	LYS
1	A	234	ARG
1	A	324	ARG
1	A	325	LEU
1	A	331	ARG
1	A	342	LEU
1	B	44	LEU
1	B	73	LEU
1	B	98	GLN
1	B	128	GLU
1	B	152	LEU
1	B	163	LEU
1	B	168	SER
1	B	254	SER
1	B	308	LYS
1	B	309	LEU
1	B	312	LYS
1	B	325	LEU

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Mol	Chain	Res	Type
1	B	331	ARG
1	B	337	LYS
1	B	340	SER
1	B	342	LEU
1	B	343	GLU
2	D	8	ILE
2	C	4	VAL
2	C	8	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 ⓘ

Of 11 ligands modelled in this entry, 1 is monoatomic - leaving 10 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	$\#|Z| > 2$
3	SF4	A	501	1	0,12,12	-	-	-		
5	GOL	A	505	-	5,5,5	0.33	0	5,5,5	0.51	0
3	SF4	B	503	1,7	0,12,12	-	-	-		

Mol	Type	Chain	Res	Link	Bond lengths				Bond angles		
					Counts	RMSZ	#|Z| > 2		Counts	RMSZ	#|Z| > 2
5	GOL	A	506	-	5,5,5	0.42	0		5,5,5	0.57	0
3	SF4	B	502	1	0,12,12	-	-		-		
5	GOL	B	505	-	5,5,5	0.57	0		5,5,5	1.03	0
3	SF4	B	501	1	0,12,12	-	-		-		
4	SAM	A	504	3	24,29,29	1.21	3 (12%)		23,42,42	1.38	3 (13%)
3	SF4	A	502	1	0,12,12	-	-		-		
3	SF4	A	503	4,1	0,12,12	-	-		-		

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
3	SF4	A	501	1	-	-	0/6/5/5
5	GOL	A	505	-	-	0/4/4/4	-
3	SF4	B	503	1,7	-	-	0/6/5/5
5	GOL	A	506	-	-	2/4/4/4	-
5	GOL	B	505	-	-	2/4/4/4	-
3	SF4	B	502	1	-	-	0/6/5/5
3	SF4	B	501	1	-	-	0/6/5/5
4	SAM	A	504	3	-	5/12/33/33	0/3/3/3
3	SF4	A	502	1	-	-	0/6/5/5
3	SF4	A	503	4,1	-	-	0/6/5/5

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	504	SAM	C5-C4	2.51	1.47	1.40
4	A	504	SAM	CE-SD	-2.42	1.63	1.78
4	A	504	SAM	OXT-C	-2.40	1.22	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	504	SAM	C4-C5-N7	-3.32	105.94	109.40
4	A	504	SAM	O4'-C1'-C2'	-2.64	103.07	106.93
4	A	504	SAM	N3-C2-N1	-2.38	124.96	128.68

There are no chirality outliers.

All (9) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	504	SAM	C3'-C4'-C5'-SD
5	A	506	GOL	C1-C2-C3-O3
5	B	505	GOL	C1-C2-C3-O3
5	B	505	GOL	O2-C2-C3-O3
4	A	504	SAM	C-CA-CB-CG
5	A	506	GOL	O2-C2-C3-O3
4	A	504	SAM	CB-CG-SD-CE
4	A	504	SAM	N-CA-CB-CG
4	A	504	SAM	O4'-C4'-C5'-SD

There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	505	GOL	1	0
4	A	504	SAM	4	0
3	A	503	SF4	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 SAM A 504

Bond lengths

Bond angles

Torsions

Rings
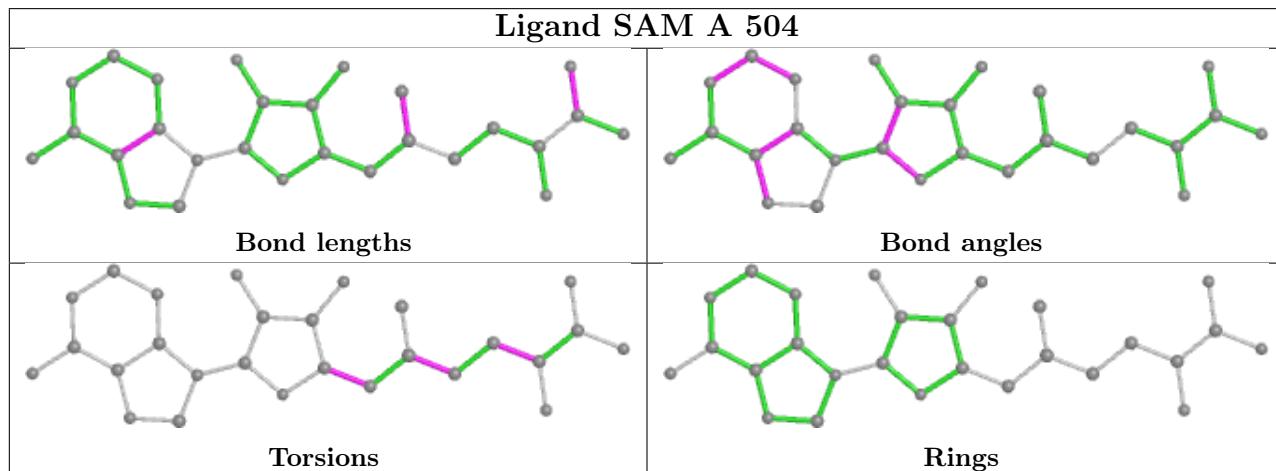
5.7 Other polymers ⓘ

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(Å^2)	Q<0.9
1	A	361/370 (97%)	0.20	11 (3%)	50	48	15, 23, 38, 53	0
1	B	359/370 (97%)	0.18	16 (4%)	33	31	16, 25, 45, 60	0
2	C	10/18 (55%)	2.73	4 (40%)	0	0	31, 37, 41, 46	0
2	D	10/18 (55%)	0.95	1 (10%)	7	6	24, 30, 36, 42	0
All	All	740/776 (95%)	0.23	32 (4%)	35	33	15, 24, 42, 60	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	12	ALA	9.3
1	A	369	ILE	6.8
1	A	24	TYR	6.1
2	C	8	ILE	5.6
1	B	36	TYR	4.5
1	B	204	LYS	4.3
1	B	35	SER	4.2
1	B	203	GLY	4.2
1	A	23	PHE	4.1
1	B	2	PRO	4.1
1	A	370	LYS	4.0
1	B	369	ILE	3.5
1	A	2	PRO	3.4
2	C	4	VAL	3.1
1	B	339	ASP	3.1
1	B	25	HIS	2.9
1	B	23	PHE	2.8
1	B	202	LYS	2.8
1	A	234	ARG	2.7
1	A	25	HIS	2.6
2	D	12	ALA	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	98	GLN	2.6
1	B	205	TYR	2.5
1	B	24	TYR	2.4
1	A	64	GLN	2.4
1	B	233	ASN	2.3
1	B	304	HIS	2.3
1	A	368	ASN	2.3
1	A	323	PHE	2.2
1	B	201	GLU	2.2
2	C	7[A]	CYS	2.1
1	B	37	GLY	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 ⓘ

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
5	GOL	B	505	6/6	0.68	0.29	43,49,50,52	0
5	GOL	A	506	6/6	0.73	0.54	29,38,43,46	0
4	SAM	A	504	27/27	0.83	0.18	18,25,28,29	27
5	GOL	A	505	6/6	0.86	0.20	24,28,31,39	0
3	SF4	A	503	8/8	0.96	0.09	18,25,27,28	0
3	SF4	A	502	8/8	0.98	0.07	22,23,25,25	0
3	SF4	B	503	8/8	0.98	0.09	19,30,32,35	0
3	SF4	B	502	8/8	0.99	0.09	19,21,21,23	0
3	SF4	A	501	8/8	0.99	0.10	18,18,21,23	0
3	SF4	B	501	8/8	0.99	0.10	19,20,22,23	0
6	CL	B	504	1/1	0.99	0.07	23,23,23,23	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 SAM A 504:

$2mF_o$-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.