



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:46 AM UTC

PDB ID : 6CHG / pdb_00006chg
Title : Crystal structure of the yeast COMPASS catalytic module
Authors : Hsu, P.L.; Li, H.; Zheng, N.
Deposited on : 2018-02-22
Resolution : 2.98 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

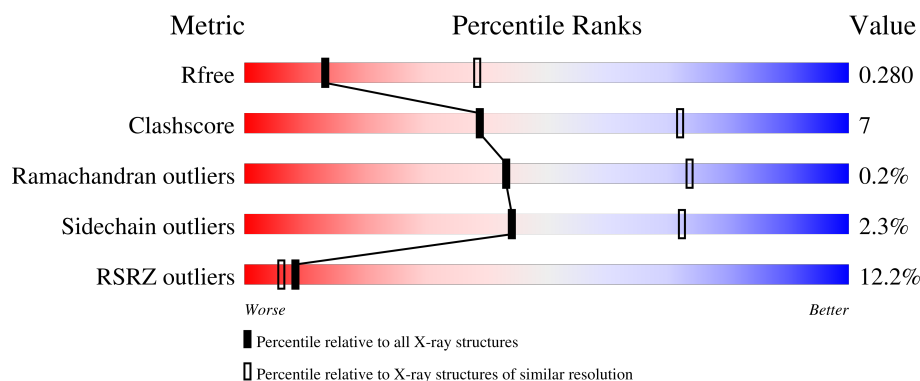
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.98 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.



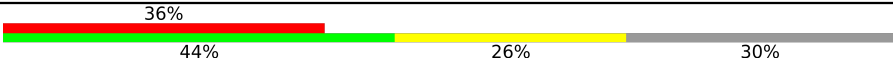
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	3580 (3.00-2.96)
Clashscore	190562	3904 (3.00-2.96)
Ramachandran outliers	187476	3761 (3.00-2.96)
Sidechain outliers	187428	3764 (3.00-2.96)
RSRZ outliers	180081	3579 (3.00-2.96)

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	312	7% 80% 17% ..
2	B	405	12% 77% 16% • 6%
3	C	153	11% 78% 16% 7%
4	D	439	9% 79% 13% • 7%
5	E	61	20% 59% 8% • 31%

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Mol	Chain	Length	Quality of chain
5	F	61	
6	J	4	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 21039 atoms, of which 10402 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 KLLA0E24487p.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	305	Total	C	H	N	O	S	0	0	0
			4730	1500	2361	395	455	19			

- Molecule 2 is a protein called KLLA0C10945p.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
2	B	382	Total	C	H	N	O	S	0	0	0
			6139	1985	3011	519	609	15			

- Molecule 3 is a protein called Histone-lysine N-methyltransferase, H3 lysine-4 specific.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
3	C	143	Total	C	H	N	O	S	0	0	0
			2297	722	1163	201	203	8			

- Molecule 4 is a protein called KLLA0A08800p.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
4	D	408	Total	C	H	N	O	S	0	0	0
			6400	2095	3127	539	622	17			

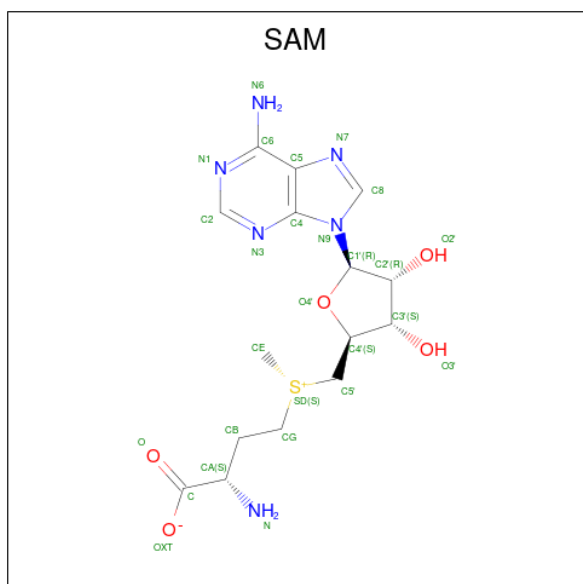
- Molecule 5 is a protein called KLLA0E03521p.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
5	E	42	Total	C	H	N	O	S	0	0	0
			697	216	355	63	62	1			
5	F	43	Total	C	H	N	O	S	0	0	0
			670	211	341	57	59	2			

- Molecule 6 is a protein called H3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
6	J	3	Total	C	H	N	O	S	0	0
			47	14	23	4	5	1		0

- Molecule 7 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
7	C	1	Total	C	H	N	O	S	0
			48	15	21	6	5	1	0

- Molecule 8 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	C	1	Total	Zn	0	0
			1	1		

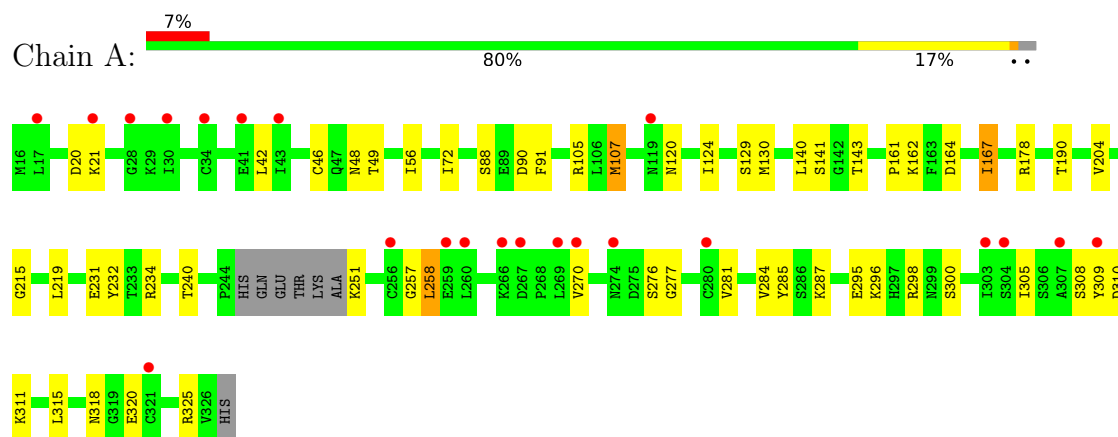
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	1	Total	O	0	0
			1	1		
9	B	3	Total	O	0	0
			3	3		
9	C	1	Total	O	0	0
			1	1		
9	D	5	Total	O	0	0
			5	5		

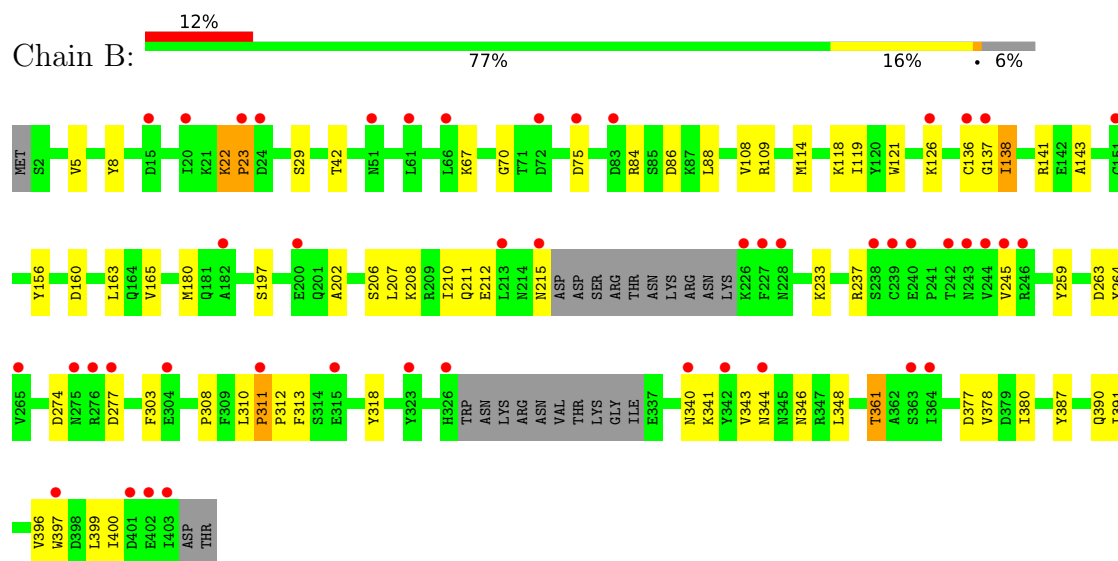
3 Residue-property plots [i](#)

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.

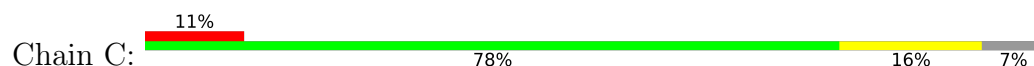
- Molecule 1: KLLA0E24487p

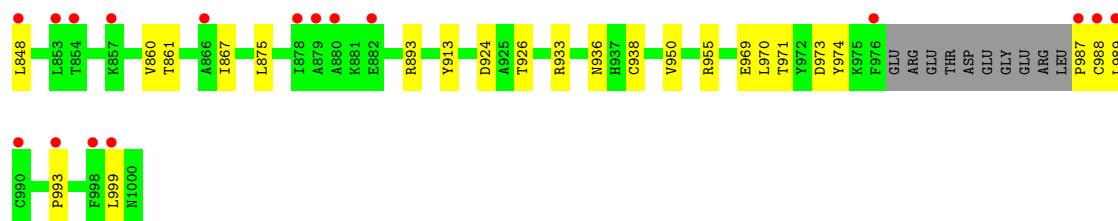


- Molecule 2: KLLA0C10945p

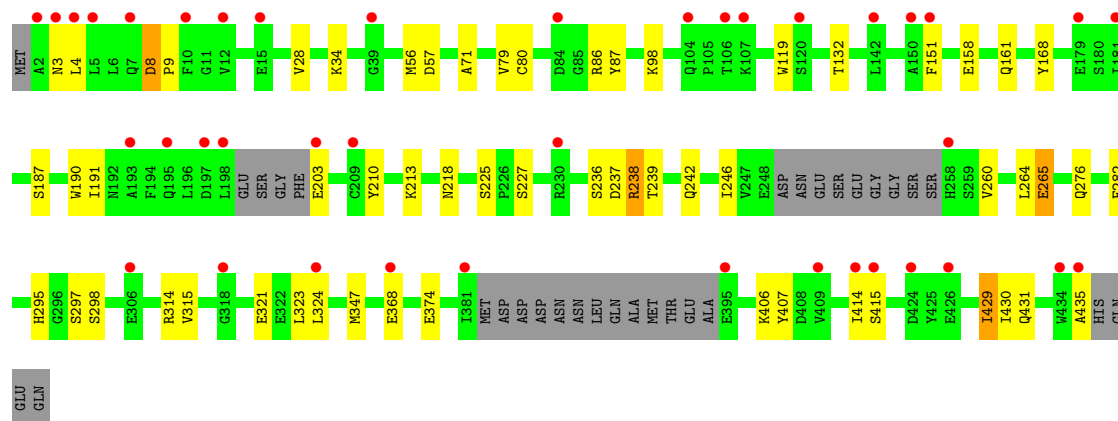
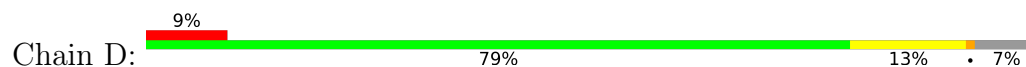


- Molecule 3: Histone-lysine N-methyltransferase, H3 lysine-4 specific

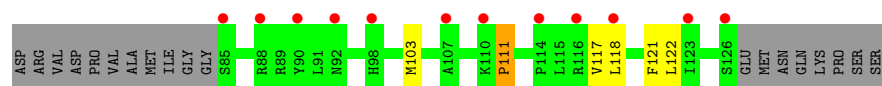




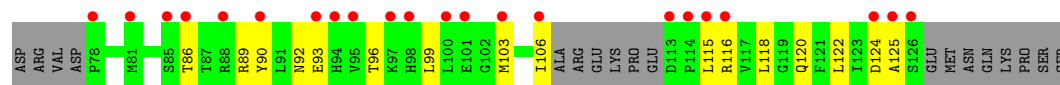
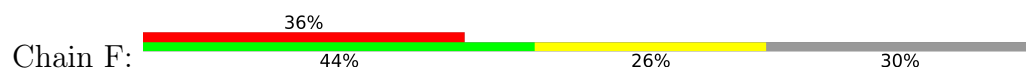
• Molecule 4: KLLA0A08800p



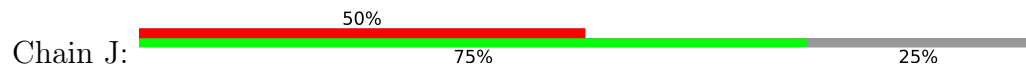
• Molecule 5: KLLA0E03521p



• Molecule 5: KLLA0E03521p



• Molecule 6: H3



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	163.84Å 138.32Å 136.13Å 90.00° 112.41° 90.00°	Depositor
Resolution (Å)	44.61 – 2.98 44.61 – 2.98	Depositor EDS
% Data completeness (in resolution range)	95.6 (44.61-2.98) 95.5 (44.61-2.98)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.43 (at 3.01Å)	Xtriage
Refinement program	PHENIX (1.10.1_2155: ???)	Depositor
R, R_{free}	0.228 , 0.271 0.233 , 0.280	Depositor DCC
R_{free} test set	2789 reflections (4.89%)	wwPDB-VP
Wilson B-factor (Å ²)	75.4	Xtriage
Anisotropy	0.481	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 34.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	21039	wwPDB-VP
Average B, all atoms (Å ²)	91.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.58% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: SAM, ZN

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	0.14	0/2414	0.47	2/3267 (0.1%)
2	B	0.15	0/3198	0.39	1/4323 (0.0%)
3	C	0.16	0/1154	0.44	1/1550 (0.1%)
4	D	0.14	0/3360	0.56	6/4577 (0.1%)
5	E	0.12	0/347	0.38	0/466
5	F	0.14	0/333	0.43	0/447
6	J	0.08	0/23	0.16	0/29
All	All	0.14	0/10829	0.47	10/14659 (0.1%)

There are no bond length outliers.

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	324	LEU	N-CA-C	17.95	137.35	114.56
4	D	324	LEU	CB-CA-C	-16.75	83.00	109.13
1	A	107	MET	N-CA-C	10.76	126.01	112.24
4	D	264	LEU	CB-CA-C	-8.22	98.18	110.67
4	D	238	ARG	N-CA-C	-8.12	93.15	108.17
4	D	264	LEU	N-CA-C	7.44	119.86	109.15
3	C	988	CYS	CB-CA-C	6.76	120.60	109.72
4	D	265	GLU	N-CA-C	6.64	119.81	111.24
2	B	23	PRO	N-CA-C	-6.21	99.67	112.47
1	A	276	SER	N-CA-C	-5.08	103.01	110.52

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	2369	2361	2380	33	0
2	B	3128	3011	3011	45	0
3	C	1134	1163	1163	20	0
4	D	3273	3127	3136	40	0
5	E	342	355	355	5	0
5	F	329	341	341	10	0
6	J	24	23	23	0	0
7	C	27	21	22	1	0
8	C	1	0	0	0	0
9	A	1	0	0	0	0
9	B	3	0	0	0	0
9	C	1	0	0	0	0
9	D	5	0	0	0	0
All	All	10637	10402	10431	144	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 7.

All (144) 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:C:987:PRO:O	3:C:999:LEU:N	2.11	0.83
4:D:238:ARG:O	4:D:239:THR:HG22	1.79	0.81
5:F:124:ASP:OD1	5:F:125:ALA:N	2.18	0.77
4:D:238:ARG:O	4:D:239:THR:CG2	2.33	0.76
1:A:88:SER:OG	1:A:90:ASP:OD1	2.04	0.75
4:D:236:SER:O	4:D:276:GLN:NE2	2.20	0.75
1:A:231:GLU:OE2	1:A:234:ARG:NH1	2.20	0.74
2:B:311:PRO:HB2	2:B:312:PRO:HD3	1.69	0.74
2:B:109:ARG:NH2	2:B:143:ALA:O	2.21	0.73
3:C:987:PRO:O	3:C:999:LEU:HB2	1.93	0.68
1:A:105:ARG:NH2	1:A:107:MET:SD	2.69	0.66
1:A:164:ASP:OD2	4:D:3:ASN:HB2	1.97	0.64
4:D:203:GLU:N	4:D:203:GLU:OE1	2.31	0.63
1:A:308:SER:O	1:A:309:TYR:C	2.42	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:314:ARG:NH1	4:D:315:VAL:O	2.33	0.61
2:B:70:GLY:O	5:F:89:ARG:NH1	2.34	0.60
3:C:973:ASP:OD1	3:C:974:TYR:N	2.35	0.59
1:A:120:ASN:ND2	1:A:162:LYS:O	2.37	0.58
4:D:242:GLN:NE2	4:D:265:GLU:OE2	2.38	0.57
2:B:387:TYR:O	2:B:391:ILE:HD12	2.05	0.56
4:D:238:ARG:C	4:D:239:THR:CG2	2.78	0.56
4:D:297:SER:O	4:D:298:SER:OG	2.19	0.56
2:B:311:PRO:CB	2:B:312:PRO:HD3	2.35	0.55
2:B:310:LEU:HB3	2:B:311:PRO:HD3	1.89	0.55
4:D:8:ASP:N	4:D:9:PRO:CD	2.70	0.54
3:C:936:ASN:ND2	3:C:969:GLU:OE2	2.40	0.54
3:C:987:PRO:HD2	3:C:999:LEU:HB3	1.90	0.54
3:C:987:PRO:HG2	3:C:999:LEU:HB2	1.89	0.54
2:B:387:TYR:O	2:B:390:GLN:N	2.41	0.54
3:C:893:ARG:HD3	4:D:374:GLU:OE2	2.09	0.53
4:D:86:ARG:NH1	4:D:87:TYR:OH	2.41	0.53
5:F:90:TYR:O	5:F:93:GLU:N	2.40	0.53
2:B:165:VAL:CG1	2:B:303:PHE:CZ	2.92	0.53
1:A:72:ILE:HA	1:A:88:SER:HA	1.89	0.53
3:C:933:ARG:O	7:C:1101:SAM:HE2	2.08	0.52
2:B:202:ALA:HB1	2:B:311:PRO:CG	2.39	0.52
4:D:238:ARG:C	4:D:239:THR:HG23	2.35	0.52
4:D:71:ALA:O	4:D:98:LYS:NZ	2.42	0.52
2:B:121:TRP:CZ2	2:B:138:ILE:HD11	2.45	0.52
2:B:264:TYR:CZ	2:B:348:LEU:HD21	2.46	0.51
3:C:867:ILE:HG23	3:C:989:LEU:O	2.09	0.51
2:B:344:ASN:OD1	2:B:346:ASN:N	2.43	0.50
5:E:103:MET:HE1	5:F:99:LEU:CD1	2.41	0.50
3:C:950:VAL:HG21	3:C:955:ARG:NH1	2.26	0.50
1:A:129:SER:OG	1:A:130:MET:N	2.45	0.50
1:A:124:ILE:HD11	4:D:57:ASP:HB3	1.94	0.50
3:C:860:VAL:HG11	3:C:970:LEU:HD11	1.95	0.49
2:B:5:VAL:HG11	2:B:67:LYS:HB2	1.94	0.49
2:B:88:LEU:CD2	2:B:108:VAL:HB	2.43	0.48
4:D:210:TYR:HB2	4:D:260:VAL:HG11	1.96	0.48
1:A:20:ASP:OD1	1:A:325:ARG:NH1	2.47	0.48
4:D:56:MET:HE1	4:D:347:MET:SD	2.54	0.47
2:B:22:LYS:N	2:B:23:PRO:CD	2.77	0.47
3:C:987:PRO:O	3:C:999:LEU:CA	2.62	0.47
4:D:158:GLU:HB3	4:D:161:GLN:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:311:PRO:CB	2:B:312:PRO:CD	2.93	0.47
1:A:300:SER:OG	1:A:318:ASN:OD1	2.32	0.47
2:B:308:PRO:O	2:B:313:PHE:HB3	2.15	0.46
3:C:893:ARG:CD	4:D:374:GLU:OE2	2.63	0.46
5:E:111:PRO:HG3	5:E:117:VAL:HG21	1.97	0.46
2:B:121:TRP:CH2	2:B:138:ILE:HD11	2.50	0.46
2:B:206:SER:O	2:B:210:ILE:HG23	2.15	0.46
2:B:377:ASP:OD2	2:B:378:VAL:N	2.49	0.46
2:B:207:LEU:O	2:B:210:ILE:HG12	2.15	0.46
2:B:311:PRO:HB2	2:B:312:PRO:CD	2.44	0.46
1:A:215:GLY:O	1:A:232:TYR:OH	2.28	0.46
1:A:257:GLY:O	1:A:305:ILE:HD13	2.16	0.46
1:A:308:SER:O	1:A:310:ASP:N	2.48	0.46
4:D:8:ASP:N	4:D:8:ASP:OD2	2.45	0.46
3:C:987:PRO:O	3:C:999:LEU:CB	2.62	0.46
4:D:414:ILE:O	4:D:415:SER:HB2	2.14	0.46
4:D:237:ASP:O	4:D:239:THR:N	2.48	0.46
3:C:924:ASP:OD1	3:C:926:THR:HG23	2.16	0.46
5:F:92:ASN:HA	5:F:96:THR:OG1	2.15	0.46
1:A:257:GLY:C	1:A:305:ILE:HD13	2.41	0.46
2:B:233:LYS:NZ	2:B:237:ARG:HD2	2.30	0.46
2:B:274:ASP:OD2	2:B:277:ASP:OD2	2.34	0.45
2:B:318:TYR:CG	2:B:341:LYS:HG2	2.52	0.45
2:B:396:VAL:O	2:B:400:ILE:HD12	2.16	0.45
1:A:161:PRO:HG2	1:A:164:ASP:O	2.16	0.45
2:B:245:VAL:HB	2:B:343:VAL:HG21	1.99	0.45
1:A:48:ASN:O	1:A:49:THR:HG22	2.16	0.45
1:A:46:CYS:HB2	1:A:72:ILE:HD11	1.99	0.45
4:D:246:ILE:O	4:D:260:VAL:HA	2.17	0.45
2:B:118:LYS:HB2	2:B:380:ILE:HG22	1.99	0.44
3:C:913:TYR:HD1	3:C:926:THR:HG22	1.82	0.44
1:A:219:LEU:CD2	1:A:258:LEU:HD21	2.47	0.44
3:C:861:THR:HG22	3:C:875:LEU:HD21	1.99	0.44
5:E:122:LEU:CD2	5:F:118:LEU:HD12	2.47	0.44
1:A:56:ILE:HD12	1:A:311:LYS:HE3	1.99	0.44
1:A:270:VAL:CG2	1:A:284:VAL:HG12	2.47	0.44
1:A:204:VAL:HG23	1:A:204:VAL:O	2.17	0.44
1:A:240:THR:O	1:A:287:LYS:NZ	2.48	0.44
1:A:141:SER:OG	1:A:143:THR:HG22	2.18	0.43
2:B:126:LYS:HB2	2:B:361:THR:OG1	2.18	0.43
2:B:141:ARG:HG2	2:B:263:ASP:OD1	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:429:ILE:HD12	4:D:430:ILE:N	2.34	0.43
1:A:270:VAL:HG23	1:A:284:VAL:HG12	1.99	0.43
1:A:295:GLU:OE2	1:A:298:ARG:NH2	2.52	0.43
4:D:168:TYR:O	4:D:187:SER:N	2.52	0.43
5:F:90:TYR:C	5:F:90:TYR:CD1	2.96	0.43
2:B:156:TYR:HB3	2:B:303:PHE:CE2	2.54	0.43
3:C:926:THR:O	3:C:933:ARG:NH2	2.52	0.43
2:B:160:ASP:HA	2:B:180:MET:HE3	2.00	0.43
2:B:208:LYS:O	2:B:212:GLU:HB2	2.19	0.43
2:B:42:THR:OG1	2:B:84:ARG:NH2	2.52	0.42
4:D:238:ARG:HG2	4:D:276:GLN:HG2	1.99	0.42
4:D:295:HIS:ND1	4:D:295:HIS:O	2.53	0.42
1:A:178:ARG:HH11	1:A:190:THR:HG21	1.84	0.42
1:A:284:VAL:HG23	1:A:285:TYR:CD1	2.55	0.42
1:A:277:GLY:O	1:A:296:LYS:O	2.37	0.42
4:D:406:LYS:NZ	4:D:407:TYR:CZ	2.87	0.42
4:D:431:GLN:HA	4:D:435:ALA:HA	2.02	0.42
2:B:137:GLY:O	2:B:138:ILE:HD12	2.20	0.41
2:B:211:GLN:O	2:B:215:ASN:N	2.53	0.41
2:B:311:PRO:HG2	2:B:312:PRO:CD	2.50	0.41
3:C:913:TYR:CD1	3:C:926:THR:HA	2.55	0.41
4:D:225:SER:O	4:D:227:SER:N	2.53	0.41
2:B:114:MET:HE1	2:B:121:TRP:CZ3	2.55	0.41
1:A:20:ASP:OD2	1:A:21:LYS:HG3	2.20	0.41
2:B:75:ASP:OD2	2:B:75:ASP:C	2.61	0.41
2:B:311:PRO:CG	2:B:312:PRO:CD	2.98	0.41
4:D:34:LYS:HB3	4:D:79:VAL:HG23	2.02	0.41
4:D:321:GLU:O	4:D:323:LEU:CD1	2.68	0.41
5:F:103:MET:O	5:F:106:ILE:N	2.54	0.41
2:B:396:VAL:HG13	2:B:397:TRP:N	2.36	0.41
5:E:118:LEU:O	5:E:121:PHE:N	2.54	0.41
2:B:86:ASP:OD1	2:B:86:ASP:N	2.52	0.41
5:F:115:LEU:HD12	5:F:116:ARG:N	2.36	0.41
1:A:318:ASN:O	1:A:320:GLU:N	2.54	0.41
4:D:8:ASP:N	4:D:9:PRO:HD3	2.36	0.41
4:D:119:TRP:HB2	4:D:132:THR:OG1	2.21	0.41
5:E:118:LEU:HB2	5:F:122:LEU:HD21	2.03	0.41
2:B:8:TYR:CE1	2:B:67:LYS:HB3	2.57	0.40
4:D:187:SER:O	4:D:218:ASN:ND2	2.41	0.40
2:B:114:MET:HE3	2:B:119:ILE:HB	2.03	0.40
3:C:938:CYS:HB3	3:C:971:THR:CG2	2.51	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:3:ASN:O	4:D:4:LEU:C	2.61	0.40
4:D:238:ARG:O	4:D:239:THR:HG23	2.18	0.40
1:A:91:PHE:N	1:A:91:PHE:CD1	2.89	0.40
2:B:211:GLN:HG3	2:B:233:LYS:HE2	2.04	0.40
4:D:190:TRP:NE1	4:D:213:LYS:HD2	2.36	0.40
1:A:167:ILE:HG23	4:D:4:LEU:HD23	2.03	0.40
4:D:368:GLU:HA	4:D:368:GLU:OE2	2.22	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	301/312 (96%)	277 (92%)	24 (8%)	0	100	100
2	B	376/405 (93%)	358 (95%)	17 (4%)	1 (0%)	36	67
3	C	139/153 (91%)	127 (91%)	11 (8%)	1 (1%)	18	50
4	D	400/439 (91%)	368 (92%)	32 (8%)	0	100	100
5	E	40/61 (66%)	37 (92%)	2 (5%)	1 (2%)	4	21
5	F	39/61 (64%)	35 (90%)	4 (10%)	0	100	100
6	J	1/4 (25%)	1 (100%)	0	0	100	100
All	All	1296/1435 (90%)	1203 (93%)	90 (7%)	3 (0%)	43	73

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	311	PRO
5	E	111	PRO
3	C	993	PRO

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	276/283 (98%)	269 (98%)	7 (2%)	42	71
2	B	352/375 (94%)	342 (97%)	10 (3%)	38	69
3	C	122/131 (93%)	121 (99%)	1 (1%)	73	86
4	D	360/387 (93%)	353 (98%)	7 (2%)	50	75
5	E	38/54 (70%)	38 (100%)	0	100	100
5	F	36/54 (67%)	34 (94%)	2 (6%)	19	50
6	J	3/4 (75%)	3 (100%)	0	100	100
All	All	1187/1288 (92%)	1160 (98%)	27 (2%)	44	72

All (27) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	42	LEU
1	A	140	LEU
1	A	167	ILE
1	A	251	LYS
1	A	258	LEU
1	A	281	VAL
1	A	315	LEU
2	B	22	LYS
2	B	29	SER
2	B	136	CYS
2	B	138	ILE
2	B	163	LEU
2	B	197	SER
2	B	259	TYR
2	B	340	ASN
2	B	361	THR
2	B	399	LEU
3	C	848	LEU
4	D	8	ASP
4	D	28	VAL

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Mol	Chain	Res	Type
4	D	80	CYS
4	D	151	PHE
4	D	191	ILE
4	D	282	PHE
4	D	429	ILE
5	F	86	THR
5	F	120	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (7) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	ASN
2	B	60	ASN
2	B	127	ASN
2	B	133	HIS
2	B	256	GLN
4	D	122	HIS
5	F	120	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 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	$\# Z > 2$
7	SAM	C	1101	-	27,29,29	1.12	4 (14%)	34,42,42	2.04	8 (23%)

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
7	SAM	C	1101	-	-	5/17/33/33	0/3/3/3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	C	1101	SAM	C2-N3	2.75	1.38	1.33
7	C	1101	SAM	C2-N1	2.58	1.38	1.33
7	C	1101	SAM	C5-N7	-2.22	1.35	1.39
7	C	1101	SAM	OXT-C	-2.18	1.23	1.30

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	1101	SAM	N3-C2-N1	-5.39	120.42	128.58
7	C	1101	SAM	C5-C4-N3	-4.88	119.99	126.72
7	C	1101	SAM	N9-C8-N7	-3.61	108.81	113.94
7	C	1101	SAM	N3-C4-N9	3.61	133.31	127.17
7	C	1101	SAM	C2-N3-C4	3.43	120.21	111.83
7	C	1101	SAM	C5-N7-C8	3.22	108.51	103.45
7	C	1101	SAM	OXT-C-O	-2.72	117.91	124.08
7	C	1101	SAM	C6-C5-C4	2.18	120.16	117.18

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	1101	SAM	CA-CB-CG-SD
7	C	1101	SAM	CB-CG-SD-CE
7	C	1101	SAM	O-C-CA-CB

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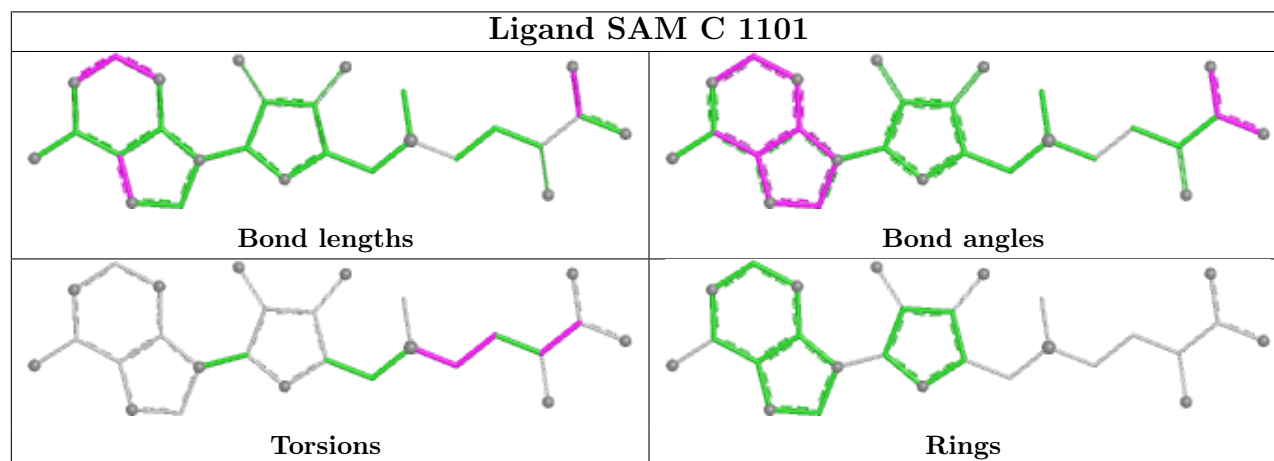
Mol	Chain	Res	Type	Atoms
7	C	1101	SAM	CB-CG-SD-C5'
7	C	1101	SAM	OXT-C-CA-CB

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	C	1101	SAM	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

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	305/312 (97%)	0.75	22 (7%) 21 13	52, 84, 121, 138	0
2	B	382/405 (94%)	0.93	47 (12%) 8 6	55, 87, 130, 164	0
3	C	143/153 (93%)	0.91	17 (11%) 9 6	59, 85, 169, 187	0
4	D	408/439 (92%)	0.78	40 (9%) 13 8	51, 84, 122, 156	0
5	E	42/61 (68%)	1.68	12 (28%) 1 1	107, 136, 156, 162	0
5	F	43/61 (70%)	2.22	22 (51%) 0 0	90, 128, 155, 159	0
6	J	3/4 (75%)	1.87	2 (66%) 0 0	83, 83, 108, 109	1 (33%)
All	All	1326/1435 (92%)	0.91	162 (12%) 8 6	51, 87, 140, 187	1 (0%)

All (162) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	309	TYR	8.5
4	D	434	TRP	6.1
3	C	989	LEU	5.6
3	C	853	LEU	5.4
2	B	304	GLU	5.4
4	D	197	ASP	5.0
5	F	126	SER	4.9
5	F	93	GLU	4.9
2	B	243	ASN	4.7
5	E	126	SER	4.5
5	F	116	ARG	4.4
4	D	2	ALA	4.3
4	D	209	CYS	4.1
2	B	340	ASN	4.1
3	C	848	LEU	4.0
2	B	315	GLU	4.0
2	B	227	PHE	4.0

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Mol	Chain	Res	Type	RSRZ
4	D	435	ALA	3.9
4	D	10	PHE	3.9
2	B	72	ASP	3.9
2	B	213	LEU	3.9
2	B	240	GLU	3.9
3	C	999	LEU	3.9
3	C	976	PHE	3.8
5	F	113	ASP	3.7
2	B	364	ILE	3.7
5	F	103	MET	3.7
5	F	85	SER	3.7
2	B	226	LYS	3.6
1	A	34	CYS	3.6
2	B	136	CYS	3.5
5	F	97	LYS	3.5
3	C	880	ALA	3.5
2	B	276	ARG	3.5
5	F	81	MET	3.5
4	D	179	GLU	3.5
5	F	101	GLU	3.5
5	F	98	HIS	3.5
5	F	114	PRO	3.4
3	C	988	CYS	3.4
2	B	20	ILE	3.4
2	B	326	HIS	3.3
4	D	324	LEU	3.3
3	C	854	THR	3.3
2	B	23	PRO	3.3
3	C	993	PRO	3.2
5	F	94	HIS	3.2
3	C	990	CYS	3.2
3	C	882	GLU	3.2
2	B	238	SER	3.2
5	E	92	ASN	3.2
3	C	987	PRO	3.2
4	D	381	ILE	3.1
2	B	182	ALA	3.1
5	F	115	LEU	3.1
4	D	4	LEU	3.0
4	D	258	HIS	3.0
5	F	95	VAL	3.0
5	E	118	LEU	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	21	LYS	3.0
2	B	403	ILE	3.0
2	B	277	ASP	3.0
4	D	5	LEU	3.0
5	E	114	PRO	3.0
2	B	61	LEU	2.9
1	A	30	ILE	2.9
2	B	402	GLU	2.9
4	D	395	GLU	2.9
4	D	3	ASN	2.9
1	A	307	ALA	2.9
2	B	151	CYS	2.9
2	B	215	ASN	2.8
4	D	426	GLU	2.8
2	B	239	CYS	2.8
4	D	107	LYS	2.8
2	B	51	ASN	2.8
1	A	259	GLU	2.8
2	B	397	TRP	2.8
3	C	998	PHE	2.8
2	B	66	LEU	2.8
5	E	98	HIS	2.8
2	B	242	THR	2.8
1	A	280	CYS	2.7
1	A	119	ASN	2.7
5	F	88	ARG	2.7
4	D	198	LEU	2.7
1	A	266	LYS	2.6
2	B	246	ARG	2.6
5	F	90	TYR	2.6
4	D	84	ASP	2.6
2	B	311	PRO	2.6
5	F	106	ILE	2.6
4	D	230	ARG	2.5
4	D	106	THR	2.5
3	C	879	ALA	2.5
1	A	28	GLY	2.5
2	B	244	VAL	2.5
1	A	41	GLU	2.5
1	A	304	SER	2.5
2	B	137	GLY	2.5
2	B	83	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
2	B	200	GLU	2.4
2	B	228	ASN	2.4
4	D	414	ILE	2.4
5	E	123	ILE	2.4
5	F	78	PRO	2.4
2	B	245	VAL	2.4
6	J	3	THR	2.4
3	C	866	ALA	2.4
2	B	24	ASP	2.3
5	F	86	THR	2.3
4	D	368	GLU	2.3
6	J	4	MET	2.3
4	D	120	SER	2.3
4	D	142	LEU	2.3
5	E	90	TYR	2.3
2	B	75	ASP	2.3
1	A	43	ILE	2.3
4	D	39	GLY	2.3
4	D	318	GLY	2.3
4	D	193	ALA	2.3
1	A	303	ILE	2.3
2	B	342	TYR	2.3
1	A	270	VAL	2.3
4	D	12	VAL	2.3
1	A	260	LEU	2.2
2	B	126	LYS	2.2
2	B	15	ASP	2.2
4	D	424	ASP	2.2
5	E	107	ALA	2.2
2	B	363	SER	2.2
5	E	110	LYS	2.2
5	F	125	ALA	2.2
5	F	124	ASP	2.2
1	A	269	LEU	2.1
4	D	203	GLU	2.1
4	D	104	GLN	2.1
2	B	344	ASN	2.1
4	D	7	GLN	2.1
1	A	274	ASN	2.1
1	A	267	ASP	2.1
5	F	100	LEU	2.1
4	D	151	PHE	2.1

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Mol	Chain	Res	Type	RSRZ
4	D	150	ALA	2.1
4	D	195	GLN	2.1
2	B	401	ASP	2.1
4	D	15	GLU	2.1
5	E	85	SER	2.0
2	B	265	VAL	2.0
1	A	17	LEU	2.0
2	B	275	ASN	2.0
4	D	306	GLU	2.0
3	C	857	LYS	2.0
4	D	409	VAL	2.0
4	D	415	SER	2.0
1	A	256	CYS	2.0
1	A	321	CYS	2.0
5	E	88	ARG	2.0
5	E	116	ARG	2.0
3	C	878	ILE	2.0
4	D	181	ILE	2.0
2	B	323	TYR	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 oligosaccharides 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.

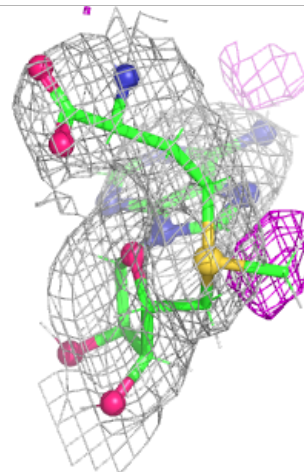
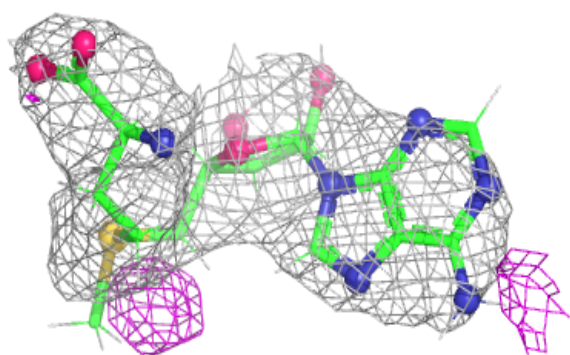
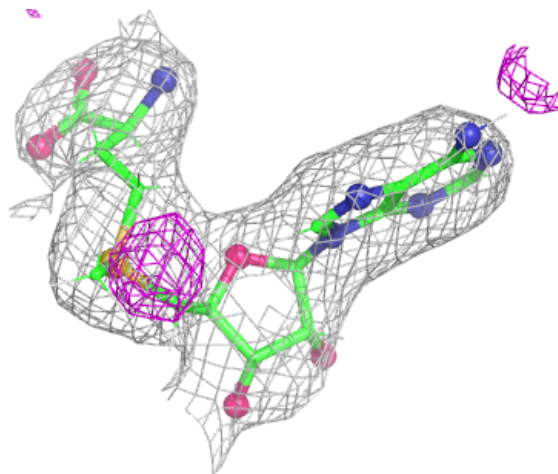
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
8	ZN	C	1102	1/1	0.78	0.12	115,115,115,115	1
7	SAM	C	1101	27/27	0.92	0.13	66,98,132,139	0

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 C 1101:

$2mF_o-DF_c$ (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.