



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 09:02 PM UTC

PDB ID : 5X6Y / pdb_00005x6y
Title : Crystal structure of Rice Dwarf Virus P5 in complex with S-adenosylmethionine
Authors : Nakamichi, Y.; Higashiura, A.; Nakagawa, A.
Deposited on : 2017-02-23
Resolution : 2.10 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

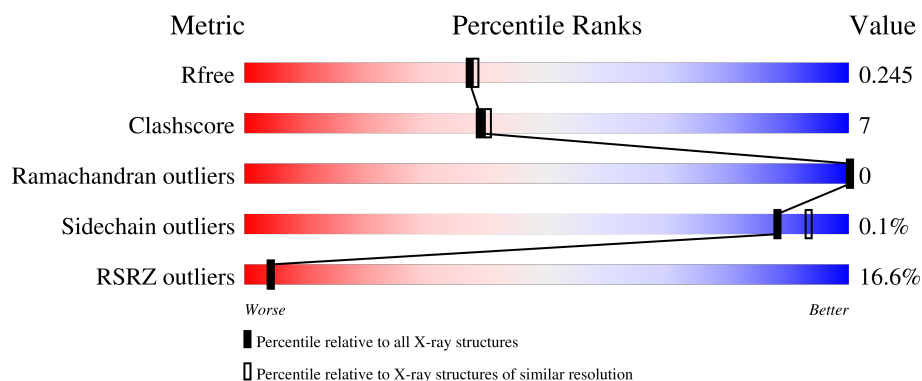
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	804	9% 85% 11% .
1	B	804	16% 73% 13% 14%
1	C	804	8% 85% 11% .
1	D	804	28% 69% 20% 11%

2 Entry composition [i](#)

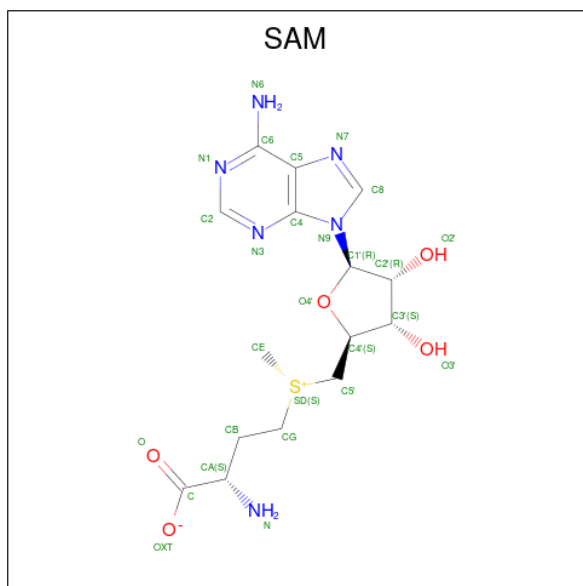
There are 5 unique types of molecules in this entry. The entry contains 24230 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 mRNA capping enzyme P5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	779	Total	C	N	O	S	0	2	0
			6208	3999	1028	1144	37			
1	B	694	Total	C	N	O	S	0	1	0
			5487	3538	914	1001	34			
1	C	774	Total	C	N	O	S	0	2	0
			6163	3973	1020	1133	37			
1	D	713	Total	C	N	O	S	0	0	0
			5640	3636	933	1034	37			

- Molecule 2 is S-ADENOSYLMETHIONINE (CCD ID: SAM) (formula: $C_{15}H_{22}N_6O_5S$).



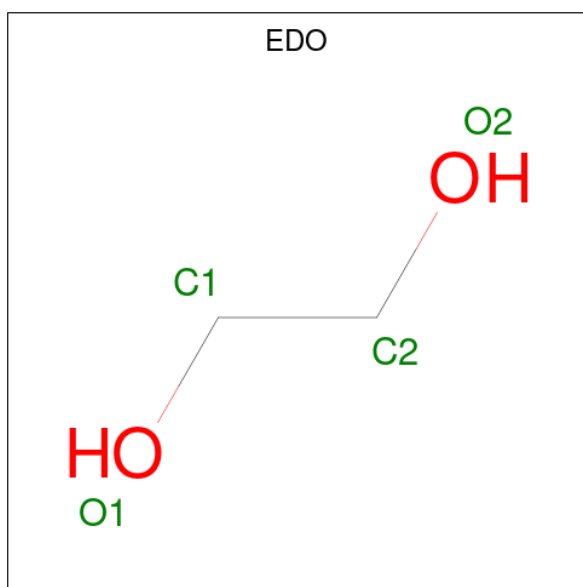
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
2	A	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	B	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
2	C	1	Total	C	N	O	S	0	0
			27	15	6	5	1		
2	C	1	Total	C	N	O	S	0	0
			27	15	6	5	1		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: $C_2H_6O_2$).



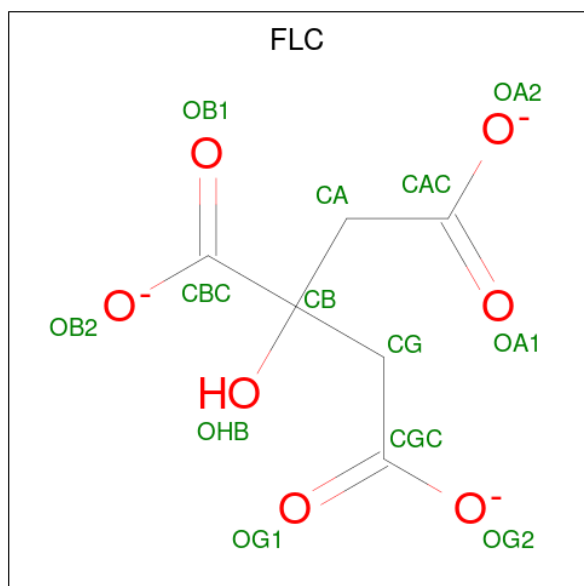
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	D	1	Total	C	O	0	0
			4	2	2		

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

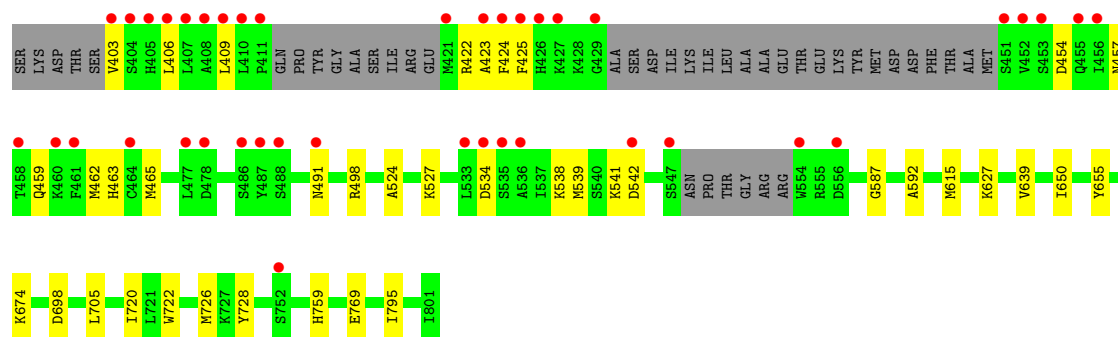
- Molecule 4 is CITRATE ANION (CCD ID: FLC) (formula: $C_6H_5O_7$).



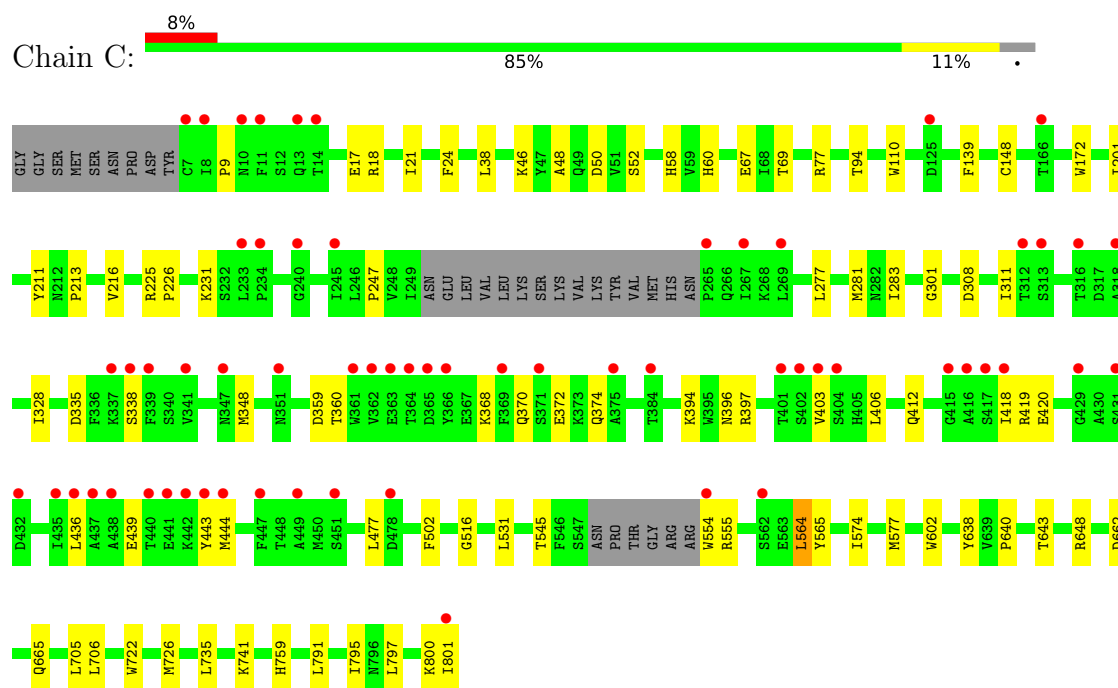
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			13	6	7		
4	B	1	Total	C	O	0	0
			13	6	7		
4	D	1	Total	C	O	0	0
			13	6	7		

- Molecule 5 is water.

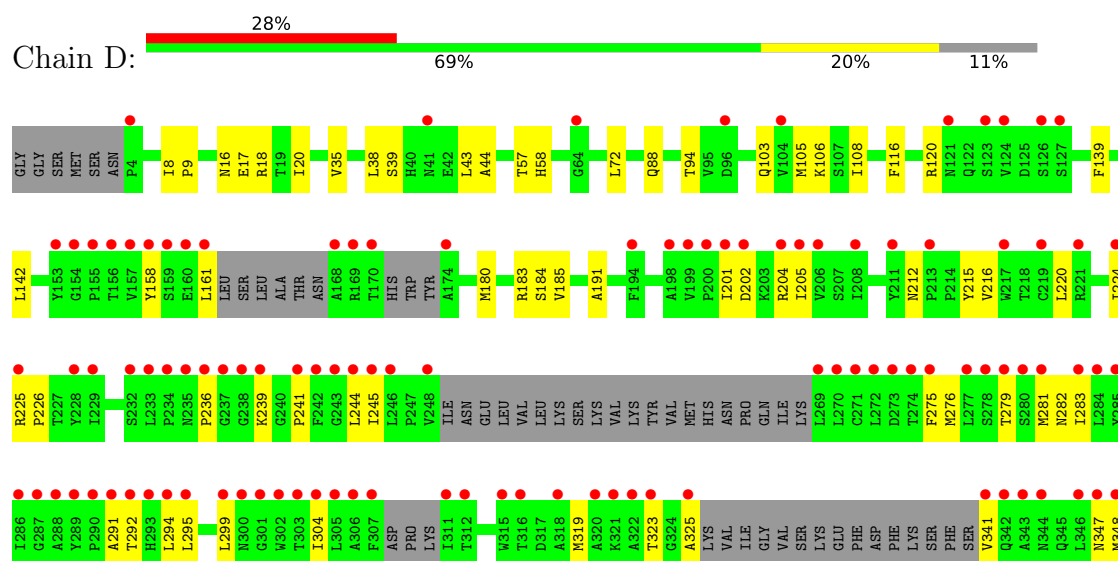
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	181	Total	O	0	0
			181	181		
5	B	110	Total	O	0	0
			110	110		
5	C	165	Total	O	0	0
			165	165		
5	D	66	Total	O	0	0
			66	66		

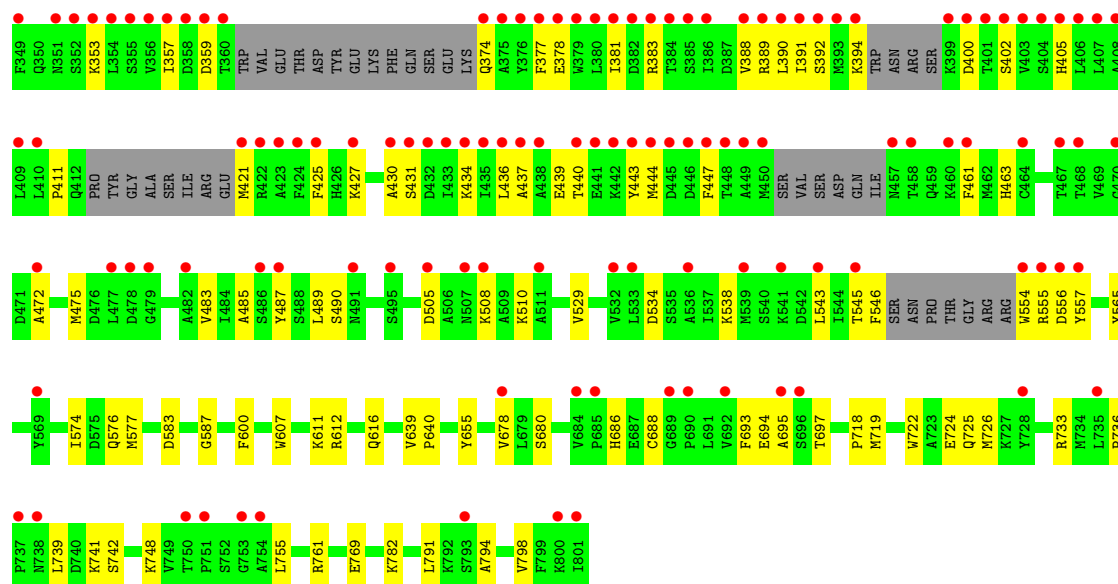


• Molecule 1: mRNA capping enzyme P5



• Molecule 1: mRNA capping enzyme P5





4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	60.18Å 122.78Å 129.26Å 73.80° 87.14° 86.08°	Depositor
Resolution (Å)	38.23 – 2.10 38.23 – 2.10	Depositor EDS
% Data completeness (in resolution range)	91.5 (38.23-2.10) 91.5 (38.23-2.10)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.66 (at 2.10Å)	Xtriage
Refinement program	PHENIX (dev_2614: ???)	Depositor
R, R_{free}	0.202 , 0.245 0.202 , 0.245	Depositor DCC
R_{free} test set	9513 reflections (4.60%)	wwPDB-VP
Wilson B-factor (Å ²)	24.5	Xtriage
Anisotropy	0.130	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 48.4	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	0.93	EDS
Total number of atoms	24230	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: FLC, EDO, SAM

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	0.42	0/6359	0.58	1/8630 (0.0%)
1	B	0.34	0/5611	0.53	0/7608
1	C	0.37	0/6311	0.53	0/8562
1	D	0.29	0/5765	0.48	0/7812
All	All	0.36	0/24046	0.53	1/32612 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	419	ARG	NE-CZ-NH2	5.39	124.05	119.20

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	6208	0	6195	71	0
1	B	5487	0	5526	78	0
1	C	6163	0	6172	62	0
1	D	5640	0	5653	123	0
2	A	54	0	44	3	0
2	B	27	0	22	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	54	0	44	3	0
3	A	12	0	18	0	0
3	B	12	0	18	2	0
3	C	4	0	6	0	0
3	D	8	0	12	0	0
4	A	13	0	5	2	0
4	B	13	0	5	1	0
4	D	13	0	5	1	0
5	A	181	0	0	0	0
5	B	110	0	0	2	0
5	C	165	0	0	2	0
5	D	66	0	0	0	0
All	All	24230	0	23725	324	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 (324) 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:D:205:ILE:CD1	1:D:225:ARG:HH11	1.08	1.64
1:D:205:ILE:HD11	1:D:225:ARG:NH1	1.12	1.38
1:D:205:ILE:CD1	1:D:225:ARG:NH1	1.82	1.07
1:C:705:LEU:HD21	1:C:791:LEU:HD21	1.54	0.89
1:A:417:SER:HA	1:A:448:THR:HG22	1.55	0.89
1:B:39:SER:OG	1:B:120:ARG:O	1.90	0.89
1:D:205:ILE:HD12	1:D:225:ARG:NH1	1.87	0.88
1:D:205:ILE:CD1	1:D:225:ARG:CZ	2.52	0.87
1:D:405:HIS:H	1:D:431:SER:HA	1.40	0.87
1:D:741:LYS:NZ	1:D:742:SER:OG	2.08	0.87
1:B:49:GLN:HB3	1:B:53:MET:HE2	1.59	0.82
1:C:545:THR:HG22	1:C:555:ARG:HG2	1.63	0.81
1:D:202:ASP:HA	1:D:281:MET:HE3	1.59	0.81
1:C:418:ILE:HG22	1:C:420:GLU:H	1.48	0.79
1:B:303:THR:HG22	1:B:326:LYS:HB2	1.69	0.75
1:D:359:ASP:HA	1:D:394:LYS:HD3	1.66	0.74
1:A:9:PRO:HB3	1:A:639:VAL:HG22	1.69	0.74
1:D:291:ALA:HB1	1:D:294:LEU:HD12	1.70	0.74
1:B:217:TRP:HD1	1:B:270:LEU:HD21	1.53	0.73
1:D:475:MET:HE1	1:D:483:VAL:HG21	1.72	0.72
1:D:35:VAL:HG11	1:D:105:MET:HE2	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:241:PRO:HD3	1:D:430:ALA:HB2	1.72	0.72
1:D:472:ALA:O	1:D:475:MET:HG2	1.89	0.71
1:A:18:ARG:HG3	1:B:18:ARG:HH11	1.56	0.71
1:A:797:LEU:HA	1:A:800:LYS:HG2	1.73	0.70
1:D:741:LYS:HD2	1:D:742:SER:N	2.06	0.70
1:D:545:THR:HG23	1:D:555:ARG:HG2	1.75	0.69
1:A:239:LYS:O	1:A:245:ILE:HG22	1.94	0.68
1:A:615:MET:HE2	1:A:615:MET:HA	1.76	0.68
1:B:103:GLN:H	3:B:902:EDO:H12	1.58	0.68
1:B:130:VAL:O	1:B:134:GLU:HG3	1.95	0.67
1:C:201:ILE:HG21	1:C:301:GLY:HA3	1.76	0.66
1:D:741:LYS:HD2	1:D:741:LYS:C	2.20	0.66
1:D:205:ILE:CD1	1:D:225:ARG:NE	2.58	0.66
1:D:205:ILE:CD1	1:D:225:ARG:HE	2.09	0.65
1:B:239:LYS:HG3	1:B:245:ILE:CG2	2.27	0.64
1:A:472:ALA:HB1	1:A:475:MET:HE2	1.80	0.63
1:B:615:MET:HE3	1:B:728:TYR:HE2	1.64	0.63
1:C:359:ASP:OD1	2:C:902:SAM:N	2.32	0.63
1:B:282:ASN:OD1	1:B:303:THR:OG1	2.16	0.62
1:A:615:MET:HE3	1:A:728:TYR:CE2	2.34	0.62
1:B:524:ALA:HA	1:B:539:MET:HE1	1.81	0.62
1:D:205:ILE:HD12	1:D:225:ARG:CZ	2.24	0.62
1:C:360:THR:O	1:C:394:LYS:NZ	2.33	0.61
1:C:403:VAL:HG21	1:C:406:LEU:HD22	1.81	0.61
1:D:574:ILE:HA	1:D:577:MET:HE2	1.82	0.61
1:D:205:ILE:HD11	1:D:225:ARG:CZ	2.12	0.61
1:A:533:LEU:HD12	1:A:535:SER:OG	2.01	0.60
1:A:460:LYS:HE3	1:A:464:CYS:HB3	1.83	0.60
1:A:239:LYS:C	1:A:245:ILE:HG22	2.27	0.60
1:D:680:SER:HA	1:D:695:ALA:HB2	1.83	0.60
1:C:308:ASP:HB3	1:C:311:ILE:HG13	1.84	0.60
1:D:39:SER:OG	1:D:120:ARG:O	2.13	0.60
1:D:607:TRP:HZ3	1:D:611:LYS:HD2	1.66	0.60
1:C:705:LEU:HD11	1:C:795:ILE:HG13	1.83	0.60
1:C:735:LEU:HD11	1:C:741:LYS:HD3	1.84	0.59
1:D:534:ASP:HB3	1:D:538:LYS:HZ2	1.67	0.59
1:A:532:VAL:HG11	1:A:537:ILE:HB	1.85	0.59
1:A:615:MET:HE3	1:A:728:TYR:HE2	1.67	0.59
1:A:277:LEU:HD23	1:A:283:ILE:HG13	1.85	0.58
1:A:447:PHE:HA	1:A:450:MET:SD	2.43	0.58
1:B:242:PHE:HB3	1:B:244:LEU:HD12	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:9:PRO:HB3	1:B:639:VAL:HG22	1.85	0.58
1:D:678:VAL:HG21	1:D:694:GLU:O	2.04	0.58
1:C:77:ARG:HG3	5:C:1062:HOH:O	2.04	0.57
1:D:505:ASP:HA	1:D:508:LYS:HE2	1.86	0.57
1:B:392:SER:HA	1:B:423:ALA:O	2.04	0.57
1:B:615:MET:HE3	1:B:728:TYR:CE2	2.39	0.57
1:B:347:ASN:HB2	1:B:350:GLN:CD	2.29	0.57
1:A:634:ARG:NH2	1:B:140:ALA:O	2.38	0.56
1:A:736:PRO:HG2	1:A:739:LEU:HD12	1.86	0.56
1:A:396:ASN:ND2	1:A:419:ARG:HG3	2.19	0.56
1:D:391:ILE:HB	1:D:425:PHE:HB2	1.88	0.56
1:D:275:PHE:CE1	1:D:276:MET:HE2	2.41	0.56
1:D:411:PRO:HB2	1:D:447:PHE:CD1	2.40	0.56
1:C:419:ARG:HA	1:C:444:MET:HG2	1.87	0.56
1:D:741:LYS:HZ2	1:D:742:SER:HG	1.48	0.56
1:A:8:ILE:HA	1:A:9:PRO:C	2.31	0.55
1:A:308:ASP:HB3	1:A:311:ILE:HG12	1.88	0.55
1:A:359:ASP:OD2	2:A:902:SAM:N	2.39	0.55
1:C:231:LYS:HE2	2:C:901:SAM:C6	2.37	0.55
1:C:277:LEU:HD23	1:C:283:ILE:HG13	1.87	0.55
1:D:239:LYS:HB3	1:D:245:ILE:HB	1.89	0.55
1:D:341:VAL:HG11	1:D:383:ARG:HH21	1.71	0.55
1:D:353:LYS:HD3	1:D:389:ARG:HD2	1.89	0.55
1:A:635:ASN:HD22	1:B:141:PRO:HG3	1.72	0.55
1:B:615:MET:HA	1:B:615:MET:HE2	1.89	0.55
1:B:48:ALA:CB	1:B:59:VAL:HG11	2.37	0.54
1:A:657:ARG:CZ	1:A:663:PRO:HG3	2.36	0.54
1:D:678:VAL:HG11	1:D:693:PHE:HB3	1.89	0.54
1:A:110:TRP:CD1	1:A:148:CYS:HA	2.43	0.54
1:D:35:VAL:CG1	1:D:105:MET:HE2	2.38	0.54
1:D:275:PHE:HE1	1:D:276:MET:HE2	1.71	0.54
1:A:533:LEU:O	1:A:534:ASP:HB3	2.08	0.54
1:B:239:LYS:HG3	1:B:245:ILE:HG22	1.90	0.54
1:B:403:VAL:HG21	1:B:406:LEU:HD22	1.90	0.54
1:D:686:HIS:HD2	1:D:688:CYS:H	1.54	0.54
1:C:640:PRO:HG2	1:D:161:LEU:HD22	1.90	0.53
1:B:356:VAL:HG22	1:B:391:ILE:HG12	1.91	0.53
1:D:276:MET:HE3	1:D:392:SER:HB2	1.89	0.53
1:D:719:MET:HE3	1:D:791:LEU:HD13	1.90	0.53
1:B:330:VAL:HG23	1:B:332:LYS:H	1.73	0.53
1:B:49:GLN:HB3	1:B:53:MET:CE	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:277:LEU:HD23	1:B:283:ILE:HG13	1.90	0.53
1:A:164:LEU:HD11	1:B:650:ILE:CG1	2.39	0.53
1:D:400:ASP:OD1	1:D:400:ASP:N	2.42	0.53
1:B:409:LEU:HD12	1:B:423:ALA:HA	1.90	0.52
1:D:103:GLN:OE1	1:D:583:ASP:HA	2.09	0.52
1:D:185:VAL:HG12	1:D:577:MET:HE3	1.91	0.52
1:D:205:ILE:HD13	1:D:225:ARG:HE	1.71	0.52
1:D:236:PRO:HB3	1:D:461:PHE:CE1	2.44	0.52
1:A:615:MET:HE1	1:A:729:MET:SD	2.49	0.52
1:B:498:ARG:HG2	1:B:498:ARG:HH11	1.74	0.52
1:D:678:VAL:HG22	1:D:697:THR:O	2.09	0.52
1:A:53:MET:HE3	1:B:74:ARG:HA	1.91	0.52
1:D:688:CYS:O	1:D:761:ARG:NH2	2.42	0.52
1:C:574:ILE:HD13	1:C:577:MET:HE3	1.92	0.52
1:A:447:PHE:CZ	1:A:455:GLN:HB2	2.46	0.51
1:A:31:SER:O	1:A:147:LYS:HE3	2.10	0.51
1:B:184:SER:OG	1:B:587:GLY:HA3	2.09	0.51
1:C:565:TYR:CZ	1:C:797:LEU:HD11	2.46	0.51
1:B:454:ASP:HA	1:B:457:ASN:ND2	2.25	0.51
1:B:328:ILE:HD13	1:B:348:MET:HE1	1.91	0.51
1:C:370:GLN:HE21	1:C:397:ARG:HD3	1.76	0.51
1:C:545:THR:HA	1:C:554:TRP:O	2.10	0.51
1:A:741:LYS:HD2	1:A:742:SER:N	2.25	0.51
1:A:759:HIS:HE2	4:A:906:FLC:CGC	2.19	0.51
1:C:800:LYS:O	1:C:801:ILE:HG13	2.11	0.51
1:A:759:HIS:NE2	4:A:906:FLC:OG2	2.29	0.51
1:C:67:GLU:OE1	1:C:69[A]:THR:HB	2.11	0.51
1:D:381:ILE:HD12	1:D:388:VAL:HG12	1.93	0.50
1:D:347:ASN:OD1	1:D:348:MET:N	2.44	0.50
1:C:58:HIS:CE1	1:D:58:HIS:CE1	3.00	0.50
1:A:477:LEU:HD13	1:A:506:ALA:HA	1.94	0.50
1:B:118:GLU:OE2	1:B:120:ARG:HB2	2.12	0.50
1:D:9:PRO:HB3	1:D:639:VAL:HG22	1.92	0.50
1:D:283:ILE:HG23	1:D:304:ILE:HG23	1.93	0.50
1:B:48:ALA:HB1	1:B:59:VAL:HG11	1.94	0.50
1:C:18:ARG:NH2	1:D:18:ARG:HG2	2.27	0.50
1:A:10:ASN:O	1:A:14:THR:OG1	2.26	0.50
1:B:391:ILE:O	1:B:424:PHE:HA	2.11	0.50
1:C:638:TYR:HD1	1:D:142:LEU:HD21	1.76	0.50
1:D:212:ASN:HB3	1:D:215:TYR:HD2	1.77	0.50
1:B:705:LEU:HD11	1:B:795:ILE:HD13	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:412:GLN:NE2	1:C:420:GLU:HB3	2.27	0.49
1:D:323:THR:HG22	1:D:325:ALA:H	1.78	0.49
1:D:611:LYS:HE2	1:D:612:ARG:NH2	2.27	0.49
1:D:722:TRP:CZ2	1:D:726:MET:HE3	2.48	0.49
1:A:741:LYS:HD2	1:A:741:LYS:C	2.38	0.49
1:C:24:PHE:CG	1:C:531:LEU:HD22	2.48	0.49
1:C:67:GLU:OE1	1:C:69[B]:THR:OG1	2.27	0.49
1:D:276:MET:O	1:D:279:THR:HG22	2.13	0.48
1:C:412:GLN:HE21	1:C:420:GLU:HB3	1.78	0.48
1:D:357:ILE:HA	1:D:392:SER:HB3	1.96	0.48
1:D:733:ARG:O	1:D:755:LEU:N	2.42	0.48
1:D:487:TYR:HE1	1:D:600:PHE:CD2	2.31	0.48
1:A:417:SER:CA	1:A:448:THR:HG22	2.36	0.48
1:B:212:ASN:OD1	1:B:214:PRO:HD2	2.13	0.48
1:C:139:PHE:HA	1:D:640:PRO:HB3	1.96	0.48
1:A:527:LYS:NZ	1:A:527:LYS:HB3	2.29	0.48
1:D:191:ALA:HA	1:D:224:ILE:HD11	1.96	0.48
1:D:616:GLN:HB2	1:D:725:GLN:CD	2.39	0.48
1:B:316:THR:HG23	1:B:327:VAL:HG13	1.96	0.48
1:A:687:GLU:OE2	1:A:800:LYS:NZ	2.33	0.48
1:A:172:TRP:HZ2	1:A:592:ALA:HB2	1.79	0.47
1:D:201:ILE:HD12	1:D:204:ARG:HD2	1.96	0.47
1:A:533:LEU:O	1:A:533:LEU:HD13	2.14	0.47
1:A:245:ILE:HD12	1:A:409:LEU:HB3	1.95	0.47
1:D:434:LYS:HB3	1:D:434:LYS:HE3	1.52	0.47
1:B:211:TYR:OH	1:B:463:HIS:ND1	2.30	0.47
1:C:705:LEU:CD2	1:C:791:LEU:HD21	2.37	0.47
1:D:38:LEU:O	1:D:94:THR:HA	2.15	0.47
1:A:216:VAL:HA	1:A:226:PRO:HG3	1.97	0.47
1:A:239:LYS:HB2	1:A:245:ILE:CG2	2.45	0.47
1:D:216:VAL:HG21	1:D:463:HIS:NE2	2.30	0.47
1:A:245:ILE:CD1	1:A:409:LEU:HB3	2.45	0.47
1:A:640:PRO:HG3	1:B:142:LEU:HD12	1.97	0.46
1:D:184:SER:OG	1:D:587:GLY:HA3	2.15	0.46
1:B:351:ASN:OD1	1:B:351:ASN:N	2.47	0.46
1:B:459:GLN:HA	1:B:462:MET:HE3	1.97	0.46
1:B:272:LEU:HD22	1:B:422:ARG:HD3	1.96	0.46
1:C:368:LYS:O	1:C:372:GLU:HG3	2.15	0.46
1:C:726:MET:HE1	1:C:759:HIS:HD2	1.80	0.46
1:D:794:ALA:O	1:D:798:VAL:HG23	2.15	0.46
1:A:164:LEU:HD11	1:B:650:ILE:HG12	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:57:THR:HG21	1:D:88:GLN:OE1	2.16	0.46
1:D:283:ILE:O	1:D:304:ILE:HA	2.16	0.46
1:D:374:GLN:NE2	1:D:378:GLU:OE2	2.46	0.46
1:D:485:ALA:HB1	1:D:489:LEU:HD13	1.98	0.46
1:B:655:TYR:CE1	1:B:769:GLU:HB3	2.50	0.46
1:D:16:ASN:HA	1:D:782:LYS:HE2	1.97	0.46
1:D:17:GLU:OE1	1:D:782:LYS:HE3	2.15	0.46
1:A:247:PRO:O	1:A:443:TYR:OH	2.28	0.46
1:C:225:ARG:NE	1:C:281:MET:SD	2.89	0.46
1:D:411:PRO:HG3	1:D:443:TYR:HE2	1.80	0.46
1:A:164:LEU:HD13	1:A:164:LEU:HA	1.60	0.46
1:D:543:LEU:HD12	1:D:557:TYR:CE1	2.51	0.46
1:B:38:LEU:O	1:B:94:THR:HA	2.15	0.46
1:C:516:GLY:HA3	1:C:602:TRP:CZ3	2.50	0.46
1:A:184:SER:OG	1:A:587:GLY:HA3	2.16	0.46
1:A:527:LYS:HE3	1:A:538:LYS:HA	1.96	0.46
1:B:173:TYR:HA	3:B:903:EDO:H21	1.97	0.45
1:D:447:PHE:HD2	1:D:447:PHE:O	1.98	0.45
1:B:347:ASN:HD22	1:B:350:GLN:NE2	2.15	0.45
1:D:436:LEU:HD22	1:D:439:GLU:HG3	1.98	0.45
1:B:217:TRP:CD1	1:B:270:LEU:HD21	2.42	0.45
1:B:462:MET:HA	1:B:465:MET:HE3	1.98	0.45
1:C:648:ARG:HD2	1:C:706:LEU:CD1	2.47	0.45
1:D:220:LEU:HD13	1:D:220:LEU:HA	1.76	0.45
1:D:72:LEU:HD22	1:D:108:ILE:HD13	1.99	0.45
1:D:205:ILE:HD12	1:D:225:ARG:NE	2.30	0.45
1:B:8:ILE:HA	1:B:9:PRO:C	2.42	0.45
1:C:46:LYS:NZ	1:C:50:ASP:OD2	2.50	0.45
1:D:282:ASN:HB2	1:D:353:LYS:O	2.17	0.45
1:D:299:LEU:HD12	1:D:323:THR:HG23	1.97	0.45
1:D:381:ILE:HG13	1:D:427:LYS:HG2	1.99	0.45
1:D:276:MET:CE	1:D:392:SER:HB2	2.47	0.45
1:A:643:THR:HG23	1:B:168:ALA:HB1	1.99	0.44
1:D:8:ILE:HA	1:D:9:PRO:C	2.41	0.44
1:D:106:LYS:HB2	1:D:116:PHE:CE2	2.51	0.44
1:A:655:TYR:CE1	1:A:769:GLU:HB3	2.53	0.44
1:C:370:GLN:HB2	1:C:397:ARG:HD3	1.99	0.44
1:D:546:PHE:HB2	1:D:554:TRP:CE2	2.52	0.44
2:A:901:SAM:H4'	2:A:901:SAM:HE3	1.72	0.44
1:B:110:TRP:CD1	1:B:148:CYS:HA	2.53	0.44
1:C:17:GLU:O	1:C:21:ILE:HG12	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:564:LEU:HD13	1:C:564:LEU:HA	1.78	0.44
1:D:475:MET:HE1	1:D:483:VAL:CG2	2.44	0.44
1:B:491:ASN:HD22	2:B:901:SAM:HE1	1.83	0.44
2:C:902:SAM:HG2	2:C:902:SAM:H4'	1.76	0.44
1:D:748:LYS:HD3	1:D:748:LYS:HA	1.78	0.43
1:C:216:VAL:HA	1:C:226:PRO:HG3	1.99	0.43
1:D:180:MET:HE2	1:D:183:ARG:HH21	1.83	0.43
1:D:565:TYR:OH	1:D:724:GLU:OE2	2.33	0.43
4:D:903:FLC:OA1	4:D:903:FLC:OHB	2.33	0.43
1:B:541:LYS:HB3	1:B:542:ASP:H	1.67	0.43
1:C:791:LEU:C	1:C:791:LEU:HD23	2.44	0.43
1:D:490:SER:OG	1:D:556:ASP:OD1	2.34	0.43
1:D:510:LYS:HA	1:D:607:TRP:CD1	2.53	0.43
1:A:172:TRP:CZ2	1:A:592:ALA:HB2	2.54	0.43
1:A:498:ARG:HG2	1:A:498:ARG:HH11	1.83	0.43
1:B:527:LYS:HD3	1:B:539:MET:HE2	2.01	0.43
1:D:576:GLN:OE1	1:D:718:PRO:HB3	2.19	0.43
1:A:379:TRP:CZ2	1:A:383:ARG:HD2	2.54	0.43
1:C:60:HIS:NE2	5:C:1002:HOH:O	2.35	0.43
1:D:292:THR:O	1:D:295:LEU:HD23	2.18	0.43
1:D:299:LEU:HB2	1:D:323:THR:HG23	2.00	0.43
1:D:447:PHE:C	1:D:447:PHE:CD2	2.97	0.43
1:A:311:ILE:HD12	1:A:315:TRP:CE3	2.53	0.43
1:D:239:LYS:CB	1:D:245:ILE:HB	2.48	0.43
1:C:335:ASP:CG	1:C:338:SER:HB2	2.44	0.43
1:A:486:SER:C	1:A:488:SER:H	2.27	0.42
1:B:216:VAL:HA	1:B:226:PRO:HG3	2.01	0.42
1:B:722:TRP:CZ2	1:B:726:MET:HE3	2.53	0.42
2:A:902:SAM:HG2	2:A:902:SAM:H4'	1.98	0.42
1:C:38:LEU:O	1:C:94:THR:HA	2.19	0.42
1:D:205:ILE:HD11	1:D:225:ARG:HH11	0.27	0.42
1:C:9:PRO:HG3	1:C:643:THR:HG21	2.00	0.42
1:A:87:MET:HE2	1:A:87:MET:HB3	1.96	0.42
1:C:247:PRO:O	1:C:443:TYR:OH	2.30	0.42
1:C:662:ASP:HB3	1:C:665:GLN:HG3	2.00	0.42
1:B:43:LEU:HD12	1:B:43:LEU:HA	1.77	0.42
1:B:87:MET:HE2	1:B:87:MET:HB3	1.94	0.42
1:B:220:LEU:HD13	1:B:220:LEU:HA	1.89	0.42
1:C:370:GLN:HE22	1:C:396:ASN:H	1.68	0.42
1:B:320:ALA:HB2	1:B:327:VAL:HG12	2.01	0.42
1:A:307:PHE:CE2	1:A:330:VAL:HG11	2.55	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:674:LYS:HD3	1:A:698:ASP:CG	2.45	0.42
1:B:347:ASN:HB2	1:B:350:GLN:CG	2.49	0.42
1:B:201:ILE:HG21	1:B:301:GLY:HA3	2.02	0.42
1:A:289:TYR:HA	1:A:290:PRO:HA	1.82	0.42
1:B:406:LEU:HD13	1:B:425:PHE:CE1	2.55	0.42
1:C:110:TRP:CD1	1:C:148:CYS:HA	2.55	0.42
1:C:554:TRP:CD2	1:C:555:ARG:HG3	2.55	0.42
1:A:762:GLU:O	1:A:766:LEU:HB2	2.20	0.41
1:C:48:ALA:O	1:C:52:SER:HB3	2.20	0.41
1:C:211:TYR:CZ	1:C:213:PRO:HG3	2.55	0.41
1:B:274:THR:HG22	1:B:297:LEU:HD11	2.02	0.41
1:C:360:THR:C	1:C:394:LYS:HZ1	2.29	0.41
1:C:374:GLN:NE2	1:C:403:VAL:HG12	2.35	0.41
1:C:705:LEU:C	1:C:705:LEU:HD23	2.45	0.41
1:D:20:ILE:HG21	1:D:529:VAL:HG11	2.02	0.41
1:D:319:MET:O	1:D:323:THR:HB	2.20	0.41
1:D:736:PRO:HG2	1:D:739:LEU:HD12	2.01	0.41
1:C:436:LEU:HB2	1:C:439:GLU:HG3	2.03	0.41
1:D:543:LEU:HD11	1:D:555:ARG:NH2	2.36	0.41
1:A:38:LEU:O	1:A:94:THR:HA	2.20	0.41
1:B:524:ALA:CA	1:B:539:MET:HE1	2.49	0.41
1:B:720:ILE:HD13	1:B:720:ILE:HA	1.87	0.41
1:A:419:ARG:HG2	1:A:420:GLU:N	2.36	0.41
1:B:534:ASP:OD1	1:B:538:LYS:HG2	2.21	0.41
1:C:477:LEU:HD21	1:C:502:PHE:CE1	2.55	0.41
1:A:531:LEU:HD21	1:A:595:THR:HG21	2.02	0.41
1:B:627:LYS:HG3	5:B:1033:HOH:O	2.19	0.41
1:B:674:LYS:NZ	1:B:698:ASP:OD2	2.46	0.41
1:C:797:LEU:HD22	1:C:800:LYS:HD3	2.03	0.41
1:B:347:ASN:HB2	1:B:350:GLN:HG2	2.03	0.41
1:D:377:PHE:HB3	1:D:391:ILE:HD12	2.03	0.41
1:D:437:ALA:HA	1:D:440:THR:HG23	2.03	0.41
1:A:211:TYR:CZ	1:A:213:PRO:HG3	2.56	0.41
1:A:245:ILE:O	1:A:245:ILE:HG23	2.20	0.41
1:A:766:LEU:HD23	1:A:766:LEU:HA	1.72	0.41
1:B:172:TRP:HZ2	1:B:592:ALA:HB2	1.86	0.41
1:C:172:TRP:CG	1:D:8:ILE:HG23	2.55	0.41
1:C:554:TRP:CE2	1:C:555:ARG:HG3	2.56	0.41
1:D:43:LEU:HD12	1:D:43:LEU:HA	1.88	0.41
1:D:421:MET:HG3	1:D:444:MET:SD	2.60	0.41
1:D:655:TYR:CE1	1:D:769:GLU:HB3	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:755:LEU:HD12	1:D:755:LEU:HA	1.86	0.41
1:D:236:PRO:HG2	1:D:244:LEU:HD12	2.03	0.41
1:D:402:SER:HA	1:D:434:LYS:HA	2.03	0.41
1:B:147:LYS:HE3	5:B:1064:HOH:O	2.21	0.40
1:D:447:PHE:HD2	1:D:447:PHE:C	2.29	0.40
1:B:311:ILE:HG21	1:B:329:GLY:HA3	2.03	0.40
1:B:356:VAL:CG2	1:B:391:ILE:HG23	2.51	0.40
1:A:523:LEU:O	1:A:527:LYS:HG3	2.22	0.40
1:B:759:HIS:NE2	4:B:905:FLC:OA2	2.54	0.40
1:C:722:TRP:CZ2	1:C:726:MET:HE2	2.57	0.40
1:D:139:PHE:CZ	1:D:158:TYR:HB3	2.57	0.40
1:D:216:VAL:HA	1:D:226:PRO:HG3	2.04	0.40
1:C:328:ILE:HD13	1:C:348:MET:HE1	2.03	0.40
1:D:353:LYS:CD	1:D:389:ARG:HD2	2.49	0.40
1:A:574:ILE:HA	1:A:577:MET:HE3	2.04	0.40
1:D:38:LEU:HD21	1:D:44:ALA:HB2	2.04	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	775/804 (96%)	752 (97%)	23 (3%)	0	100	100
1	B	677/804 (84%)	658 (97%)	19 (3%)	0	100	100
1	C	770/804 (96%)	750 (97%)	20 (3%)	0	100	100
1	D	691/804 (86%)	670 (97%)	21 (3%)	0	100	100
All	All	2913/3216 (91%)	2830 (97%)	83 (3%)	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	691/711 (97%)	691 (100%)	0	100	100
1	B	615/711 (86%)	615 (100%)	0	100	100
1	C	686/711 (96%)	685 (100%)	1 (0%)	88	93
1	D	627/711 (88%)	626 (100%)	1 (0%)	87	93
All	All	2619/2844 (92%)	2617 (100%)	2 (0%)	88	93

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	564	LEU
1	D	390	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	121	ASN
1	A	264	ASN
1	A	457	ASN
1	A	593	ASN
1	A	665	GLN
1	B	13	GLN
1	B	88	GLN
1	B	350	GLN
1	B	597	ASN
1	B	665	GLN
1	B	756	GLN
1	B	781	ASN
1	C	88	GLN
1	C	195	ASN
1	C	370	GLN
1	C	459	GLN
1	C	491	ASN

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Mol	Chain	Res	Type
1	C	597	ASN
1	C	616	GLN
1	C	665	GLN
1	C	781	ASN
1	D	41	ASN
1	D	586	ASN
1	D	738	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 oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

17 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	SAM	A	902	-	27,29,29	1.11	4 (14%)	34,42,42	2.11	9 (26%)
3	EDO	B	904	-	3,3,3	0.43	0	2,2,2	0.61	0
4	FLC	D	903	-	12,12,12	1.10	0	17,17,17	1.30	1 (5%)
4	FLC	A	906	-	12,12,12	1.55	1 (8%)	17,17,17	1.74	6 (35%)
2	SAM	C	901	-	27,29,29	1.10	4 (14%)	34,42,42	2.01	11 (32%)
2	SAM	A	901	-	27,29,29	1.19	4 (14%)	34,42,42	1.90	8 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	EDO	A	904	-	3,3,3	0.56	0	2,2,2	0.45	0
3	EDO	B	902	-	3,3,3	0.55	0	2,2,2	0.26	0
3	EDO	A	903	-	3,3,3	0.60	0	2,2,2	0.26	0
3	EDO	B	903	-	3,3,3	0.48	0	2,2,2	0.21	0
3	EDO	C	903	-	3,3,3	0.35	0	2,2,2	0.37	0
2	SAM	C	902	-	27,29,29	1.08	4 (14%)	34,42,42	2.11	9 (26%)
3	EDO	D	901	-	3,3,3	0.43	0	2,2,2	0.35	0
4	FLC	B	905	-	12,12,12	1.39	1 (8%)	17,17,17	1.68	3 (17%)
3	EDO	D	902	-	3,3,3	0.48	0	2,2,2	0.29	0
2	SAM	B	901	-	27,29,29	1.10	4 (14%)	34,42,42	2.03	9 (26%)
3	EDO	A	905	-	3,3,3	0.60	0	2,2,2	0.53	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
2	SAM	A	902	-	-	4/17/33/33	0/3/3/3
3	EDO	B	904	-	-	0/1/1/1	-
4	FLC	D	903	-	-	1/16/16/16	-
4	FLC	A	906	-	-	7/16/16/16	-
2	SAM	C	901	-	-	6/17/33/33	0/3/3/3
2	SAM	A	901	-	-	8/17/33/33	0/3/3/3
3	EDO	A	904	-	-	1/1/1/1	-
3	EDO	B	902	-	-	0/1/1/1	-
3	EDO	A	903	-	-	0/1/1/1	-
3	EDO	B	903	-	-	1/1/1/1	-
3	EDO	C	903	-	-	0/1/1/1	-
2	SAM	C	902	-	-	4/17/33/33	0/3/3/3
3	EDO	D	901	-	-	0/1/1/1	-
4	FLC	B	905	-	-	7/16/16/16	-
3	EDO	D	902	-	-	1/1/1/1	-
2	SAM	B	901	-	-	3/17/33/33	0/3/3/3
3	EDO	A	905	-	-	0/1/1/1	-

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	901	SAM	C2-N1	3.27	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	901	SAM	C2-N3	2.75	1.38	1.33
2	A	901	SAM	C2-N3	2.67	1.38	1.33
2	C	902	SAM	C2-N3	2.59	1.38	1.33
2	B	901	SAM	C2-N1	2.58	1.38	1.33
2	A	902	SAM	C2-N3	2.57	1.38	1.33
2	C	901	SAM	C2-N1	2.54	1.38	1.33
2	A	902	SAM	C8-N7	2.53	1.36	1.31
2	C	901	SAM	C2-N3	2.53	1.38	1.33
2	A	901	SAM	C8-N7	2.50	1.36	1.31
2	C	902	SAM	C2-N1	2.47	1.38	1.33
4	A	906	FLC	CB-CBC	2.46	1.56	1.53
2	A	902	SAM	C2-N1	2.33	1.38	1.33
2	C	902	SAM	C8-N7	2.32	1.36	1.31
2	B	901	SAM	C8-N7	2.28	1.36	1.31
2	C	901	SAM	C8-N7	2.24	1.36	1.31
2	C	902	SAM	OXT-C	-2.16	1.23	1.30
4	B	905	FLC	CA-CB	-2.15	1.51	1.54
2	A	902	SAM	OXT-C	-2.15	1.23	1.30
2	B	901	SAM	OXT-C	-2.13	1.23	1.30
2	A	901	SAM	OXT-C	-2.03	1.24	1.30
2	C	901	SAM	OXT-C	-2.02	1.24	1.30

All (56) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	902	SAM	N3-C2-N1	-6.23	119.16	128.58
2	A	902	SAM	N3-C2-N1	-6.05	119.42	128.58
2	C	901	SAM	N3-C2-N1	-5.59	120.12	128.58
2	B	901	SAM	N3-C2-N1	-5.47	120.30	128.58
2	A	901	SAM	N3-C2-N1	-5.41	120.40	128.58
2	C	902	SAM	N9-C8-N7	-4.46	107.61	113.94
2	A	902	SAM	C5-C4-N3	-4.40	120.66	126.72
2	B	901	SAM	N9-C8-N7	-4.34	107.77	113.94
2	C	901	SAM	N9-C8-N7	-4.34	107.78	113.94
2	C	902	SAM	C5-C4-N3	-4.31	120.78	126.72
2	B	901	SAM	C5-C4-N3	-4.10	121.07	126.72
2	A	902	SAM	N9-C8-N7	-4.05	108.19	113.94
2	A	901	SAM	N9-C8-N7	-4.04	108.21	113.94
2	C	901	SAM	C5-C4-N3	-4.01	121.19	126.72
2	C	902	SAM	C5-N7-C8	3.88	109.56	103.45
4	B	905	FLC	CB-CA-CAC	-3.75	103.66	113.92
2	C	902	SAM	C2-N3-C4	3.69	120.84	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	902	SAM	C2-N3-C4	3.62	120.67	111.83
2	B	901	SAM	C5-N7-C8	3.60	109.11	103.45
2	A	902	SAM	C5-N7-C8	3.58	109.08	103.45
2	C	901	SAM	C5-N7-C8	3.56	109.05	103.45
4	B	905	FLC	OB2-CBC-CB	3.44	119.75	113.14
2	A	901	SAM	C5-C4-N3	-3.44	121.97	126.72
2	B	901	SAM	C2-N3-C4	3.33	119.97	111.83
4	A	906	FLC	CB-CG-CGC	-3.32	104.83	113.92
2	A	901	SAM	OXT-C-O	-3.28	116.64	124.08
2	C	901	SAM	C2-N3-C4	3.28	119.83	111.83
2	A	902	SAM	OXT-C-O	-3.23	116.74	124.08
2	C	902	SAM	C4-C5-N7	-3.11	107.02	110.58
4	A	906	FLC	OB2-CBC-CB	3.08	119.05	113.14
2	A	901	SAM	C5-N7-C8	3.03	108.21	103.45
4	D	903	FLC	OB2-CBC-CB	3.01	118.92	113.14
2	A	901	SAM	C2-N3-C4	2.98	119.12	111.83
2	A	902	SAM	C4-C5-N7	-2.86	107.31	110.58
2	A	901	SAM	C4-N9-C8	2.80	108.68	105.74
2	B	901	SAM	C4-C5-N7	-2.72	107.47	110.58
2	B	901	SAM	OXT-C-O	-2.71	117.92	124.08
2	C	901	SAM	O4'-C1'-N9	2.70	113.28	108.09
2	C	902	SAM	N3-C4-N9	2.68	131.73	127.17
2	B	901	SAM	N3-C4-N9	2.66	131.70	127.17
2	C	901	SAM	N3-C4-N9	2.57	131.54	127.17
2	B	901	SAM	C4-N9-C8	2.55	108.41	105.74
2	C	901	SAM	C4-C5-N7	-2.55	107.67	110.58
2	A	901	SAM	N3-C4-N9	2.54	131.49	127.17
2	C	901	SAM	OXT-C-O	-2.54	118.33	124.08
2	A	902	SAM	N3-C4-N9	2.49	131.41	127.17
2	C	902	SAM	C4-N9-C8	2.46	108.33	105.74
4	A	906	FLC	OHB-CB-CBC	2.38	112.34	108.96
2	C	901	SAM	C4-N9-C8	2.38	108.24	105.74
2	C	902	SAM	OXT-C-O	-2.35	118.75	124.08
4	A	906	FLC	OA2-CAC-CA	2.29	121.59	114.35
4	B	905	FLC	OG2-CGC-CG	2.06	120.88	114.35
2	A	902	SAM	C2'-C3'-C4'	2.05	106.57	102.61
4	A	906	FLC	OB2-CBC-OB1	-2.04	117.34	123.86
4	A	906	FLC	OA2-CAC-OA1	-2.02	118.13	123.33
2	C	901	SAM	CG-SD-C5'	2.01	108.34	103.43

There are no chirality outliers.

All (43) torsion outliers are listed below:

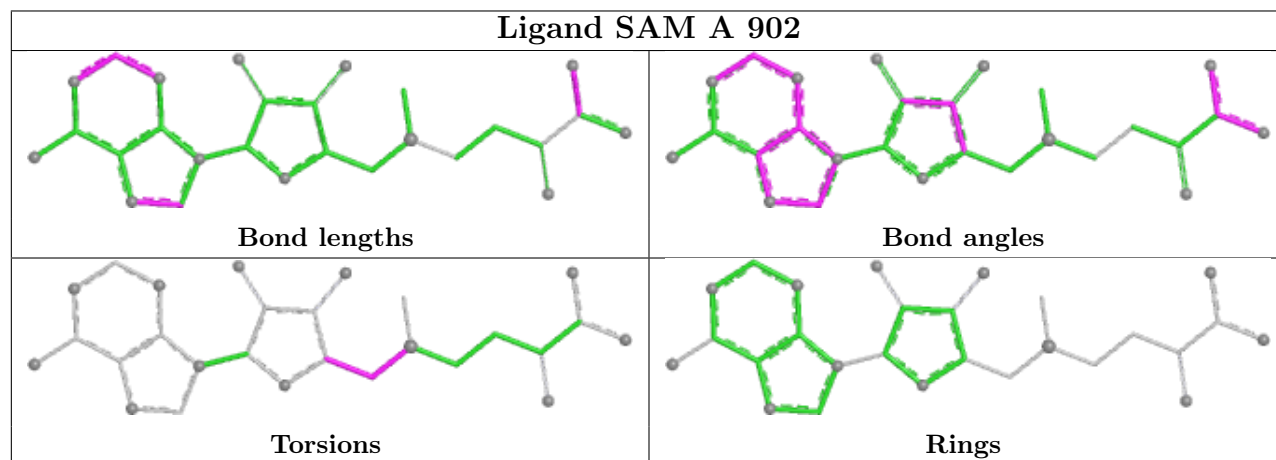
Mol	Chain	Res	Type	Atoms
2	A	901	SAM	N-CA-CB-CG
2	A	901	SAM	C-CA-CB-CG
2	A	901	SAM	CB-CG-SD-C5'
2	A	901	SAM	C4'-C5'-SD-CE
2	A	901	SAM	O4'-C4'-C5'-SD
2	A	901	SAM	C3'-C4'-C5'-SD
2	A	902	SAM	C4'-C5'-SD-CE
2	A	902	SAM	O4'-C4'-C5'-SD
2	A	902	SAM	C3'-C4'-C5'-SD
2	B	901	SAM	CA-CB-CG-SD
2	C	901	SAM	N-CA-CB-CG
2	C	901	SAM	C-CA-CB-CG
2	C	901	SAM	CA-CB-CG-SD
2	C	901	SAM	C4'-C5'-SD-CE
2	C	901	SAM	O4'-C4'-C5'-SD
2	C	901	SAM	C3'-C4'-C5'-SD
2	C	902	SAM	C4'-C5'-SD-CE
2	C	902	SAM	O4'-C4'-C5'-SD
2	C	902	SAM	C3'-C4'-C5'-SD
4	A	906	FLC	CAC-CA-CB-CBC
4	A	906	FLC	CAC-CA-CB-CG
4	A	906	FLC	CAC-CA-CB-OHB
4	A	906	FLC	CG-CB-CBC-OB1
4	A	906	FLC	CG-CB-CBC-OB2
4	A	906	FLC	OHB-CB-CBC-OB1
4	A	906	FLC	OHB-CB-CBC-OB2
4	B	905	FLC	CA-CB-CBC-OB1
4	B	905	FLC	CA-CB-CBC-OB2
4	B	905	FLC	OHB-CB-CBC-OB1
4	B	905	FLC	OHB-CB-CBC-OB2
4	B	905	FLC	CA-CB-CG-CGC
4	B	905	FLC	CBC-CB-CG-CGC
4	B	905	FLC	OHB-CB-CG-CGC
2	A	901	SAM	CB-CG-SD-CE
3	A	904	EDO	O1-C1-C2-O2
2	B	901	SAM	O-C-CA-CB
2	A	902	SAM	C4'-C5'-SD-CG
2	C	902	SAM	C4'-C5'-SD-CG
2	B	901	SAM	OXT-C-CA-CB
3	D	902	EDO	O1-C1-C2-O2
4	D	903	FLC	CAC-CA-CB-CG
3	B	903	EDO	O1-C1-C2-O2
2	A	901	SAM	OXT-C-CA-N

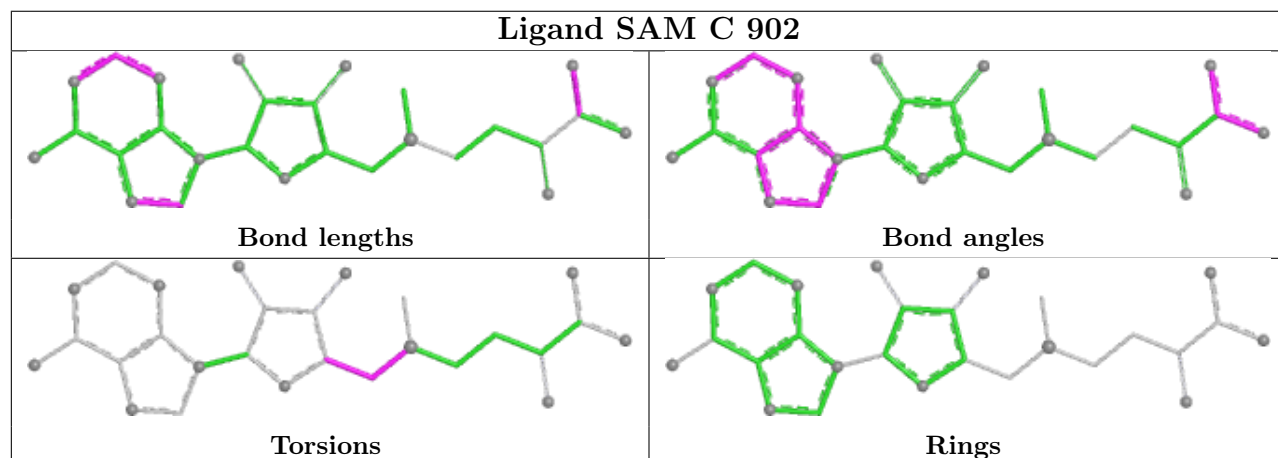
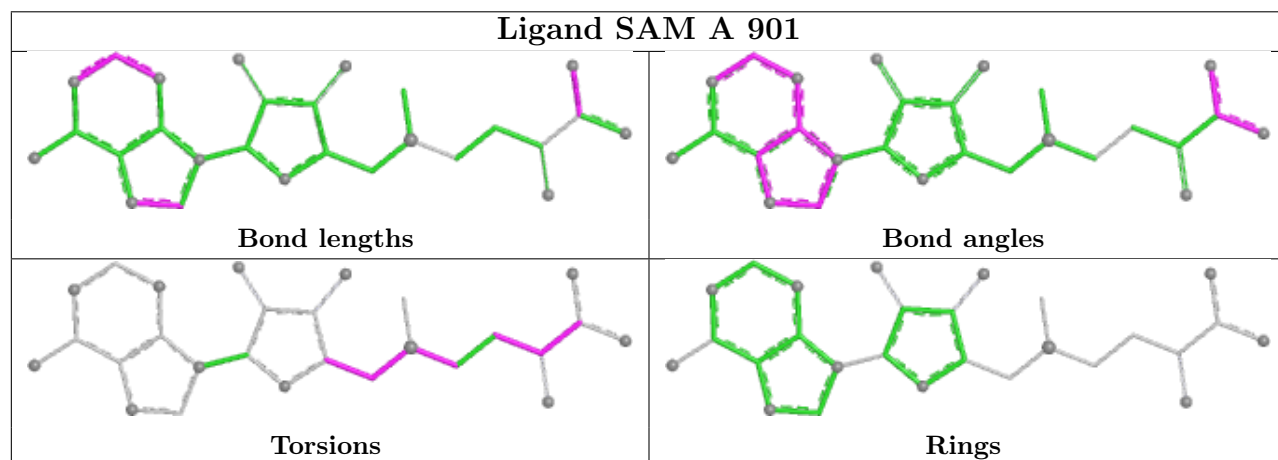
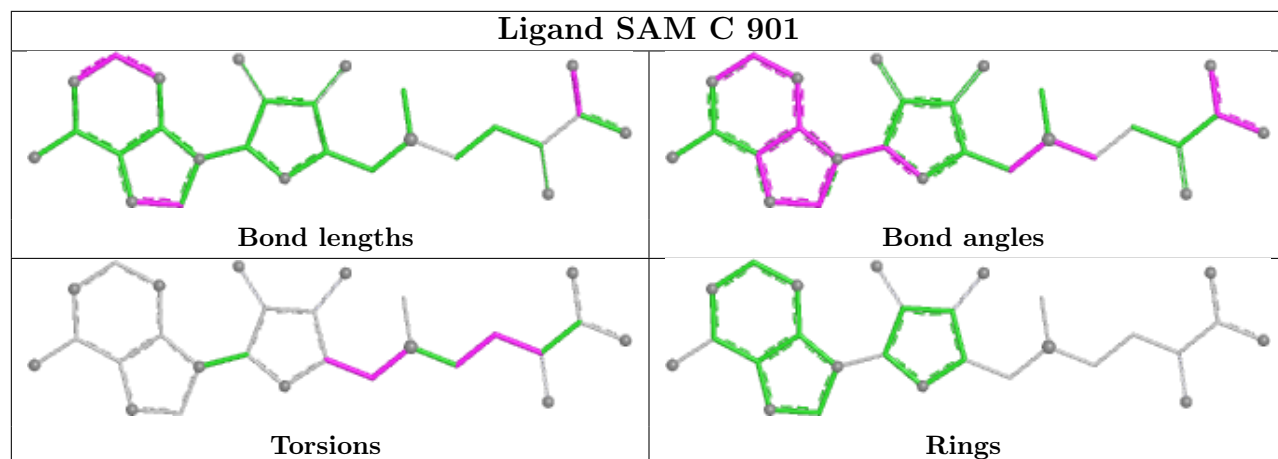
There are no ring outliers.

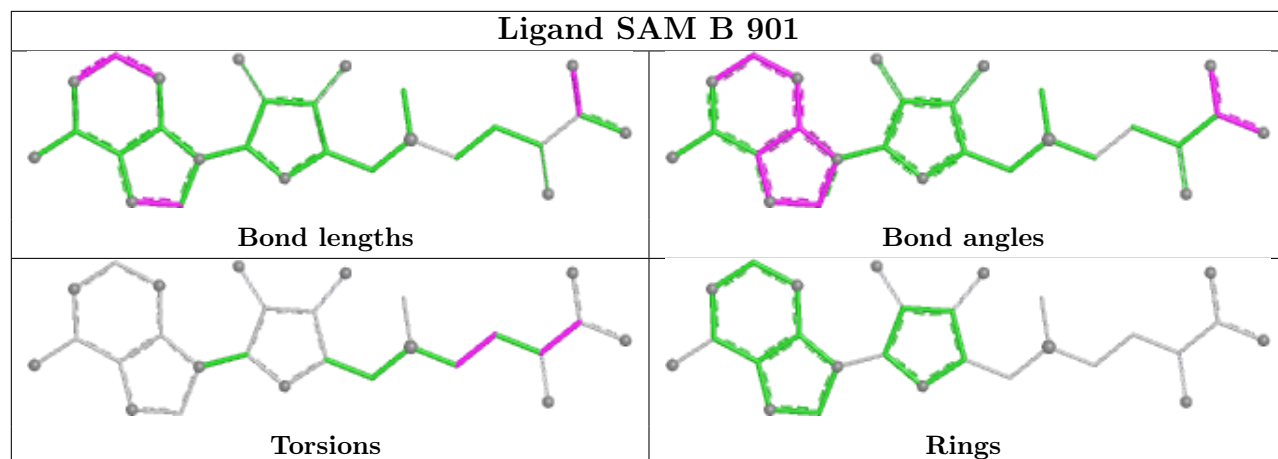
10 monomers are involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	902	SAM	2	0
4	D	903	FLC	1	0
4	A	906	FLC	2	0
2	C	901	SAM	1	0
2	A	901	SAM	1	0
3	B	902	EDO	1	0
3	B	903	EDO	1	0
2	C	902	SAM	2	0
4	B	905	FLC	1	0
2	B	901	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	779/804 (96%)	0.33	74 (9%) 14 14	9, 23, 67, 83	2 (0%)
1	B	694/804 (86%)	0.70	125 (18%) 3 3	12, 30, 83, 94	1 (0%)
1	C	774/804 (96%)	0.30	62 (8%) 18 19	10, 27, 60, 83	2 (0%)
1	D	713/804 (88%)	1.47	229 (32%) 1 1	16, 44, 87, 106	0
All	All	2960/3216 (92%)	0.69	490 (16%) 4 4	9, 31, 79, 106	5 (0%)

All (490) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	380	LEU	9.4
1	B	408	ALA	7.0
1	D	157	VAL	6.9
1	B	307	PHE	6.6
1	D	311	ILE	6.5
1	D	554	TRP	6.5
1	D	269	LEU	6.4
1	D	408	ALA	6.2
1	D	295	LEU	6.2
1	B	234	PRO	6.2
1	D	375	ALA	6.1
1	D	433	ILE	6.1
1	B	356	VAL	6.0
1	B	328	ILE	6.0
1	A	533	LEU	5.9
1	A	418	ILE	5.9
1	D	379	TRP	5.8
1	B	407	LEU	5.8
1	B	403	VAL	5.7
1	B	452	VAL	5.6
1	B	4	PRO	5.6

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Mol	Chain	Res	Type	RSRZ
1	A	535	SER	5.5
1	D	403	VAL	5.4
1	A	438	ALA	5.4
1	A	416	ALA	5.3
1	B	451	SER	5.3
1	D	341	VAL	5.2
1	B	554	TRP	5.0
1	D	248	VAL	5.0
1	D	443	TYR	5.0
1	D	359	ASP	4.9
1	D	354	LEU	4.9
1	D	277	LEU	4.9
1	B	308	ASP	4.9
1	A	451	SER	4.9
1	D	315	TRP	4.8
1	B	269	LEU	4.8
1	D	307	PHE	4.7
1	C	554	TRP	4.7
1	B	290	PRO	4.7
1	D	377	PHE	4.6
1	D	356	VAL	4.6
1	D	343	ALA	4.6
1	A	536	ALA	4.6
1	D	270	LEU	4.6
1	D	407	LEU	4.6
1	D	293	HIS	4.6
1	A	437	ALA	4.6
1	D	450	MET	4.5
1	A	362	VAL	4.5
1	B	309	PRO	4.5
1	B	284	LEU	4.5
1	D	432	ASP	4.5
1	D	401	THR	4.4
1	D	388	VAL	4.4
1	D	158	TYR	4.4
1	A	448	THR	4.4
1	D	156	THR	4.4
1	C	362	VAL	4.4
1	A	366	TYR	4.4
1	D	292	THR	4.4
1	D	384	THR	4.4
1	D	423	ALA	4.4

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Mol	Chain	Res	Type	RSRZ
1	D	347	ASN	4.3
1	A	5	ASP	4.3
1	B	429	GLY	4.3
1	B	458	THR	4.3
1	D	404	SER	4.3
1	B	248	VAL	4.3
1	B	409	LEU	4.3
1	D	390	LEU	4.3
1	B	381	ILE	4.3
1	C	8	ILE	4.3
1	C	234	PRO	4.3
1	B	354	LEU	4.3
1	A	4	PRO	4.3
1	D	234	PRO	4.3
1	D	322	ALA	4.2
1	D	201	ILE	4.2
1	D	155	PRO	4.2
1	D	801	ILE	4.2
1	D	291	ALA	4.2
1	D	325	ALA	4.2
1	D	438	ALA	4.2
1	D	487	TYR	4.1
1	D	458	THR	4.1
1	D	344	ASN	4.1
1	B	487	TYR	4.1
1	D	440	THR	4.1
1	D	381	ILE	4.0
1	B	406	LEU	4.0
1	D	243	GLY	4.0
1	B	357	ILE	4.0
1	D	304	ILE	4.0
1	D	434	LYS	4.0
1	D	289	TYR	3.9
1	D	495	SER	3.9
1	C	7	CYS	3.9
1	A	235	ASN	3.9
1	D	170	THR	3.9
1	D	302	TRP	3.9
1	D	378	GLU	3.9
1	B	421	MET	3.9
1	D	306	ALA	3.9
1	D	449	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	389	ARG	3.9
1	D	123	SER	3.8
1	B	291	ALA	3.8
1	D	533	LEU	3.8
1	B	166	THR	3.8
1	C	801	ILE	3.8
1	D	357	ILE	3.8
1	D	431	SER	3.8
1	D	405	HIS	3.8
1	D	424	PHE	3.8
1	A	404	SER	3.8
1	D	557	TYR	3.8
1	C	10	ASN	3.8
1	B	346	LEU	3.8
1	D	200	PRO	3.8
1	B	425	PHE	3.8
1	D	382	ASP	3.7
1	D	219	CYS	3.7
1	D	409	LEU	3.7
1	D	385	SER	3.7
1	B	311	ILE	3.7
1	D	392	SER	3.7
1	A	538	LYS	3.7
1	B	533	LEU	3.6
1	D	376	TYR	3.7
1	B	245	ILE	3.6
1	B	306	ALA	3.6
1	D	437	ALA	3.6
1	A	361	TRP	3.6
1	D	351	ASN	3.6
1	D	199	VAL	3.6
1	B	316	THR	3.6
1	D	442	LYS	3.6
1	A	450	MET	3.5
1	D	246	LEU	3.5
1	D	406	LEU	3.5
1	D	355	SER	3.5
1	A	245	ILE	3.5
1	A	447	PHE	3.5
1	D	275	PHE	3.5
1	B	325	ALA	3.5
1	B	410	LEU	3.5

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Mol	Chain	Res	Type	RSRZ
1	D	383	ARG	3.5
1	D	239	LYS	3.5
1	C	316	THR	3.5
1	B	270	LEU	3.4
1	B	305	LEU	3.4
1	C	431	SER	3.4
1	D	464	CYS	3.4
1	B	330	VAL	3.4
1	A	449	ALA	3.4
1	D	318	ALA	3.4
1	B	275	PHE	3.4
1	D	457	ASN	3.4
1	A	452	VAL	3.4
1	D	360	THR	3.4
1	A	417	SER	3.4
1	C	451	SER	3.4
1	B	423	ALA	3.4
1	B	312	THR	3.4
1	D	320	ALA	3.4
1	D	444	MET	3.3
1	C	14	THR	3.3
1	C	432	ASP	3.3
1	C	403	VAL	3.3
1	D	213	PRO	3.3
1	D	198	ALA	3.3
1	D	272	LEU	3.3
1	A	534	ASP	3.3
1	B	352	SER	3.3
1	D	352	SER	3.3
1	B	237	GLY	3.3
1	D	285	TYR	3.3
1	B	456	ILE	3.3
1	A	554	TRP	3.3
1	D	323	THR	3.3
1	B	331	SER	3.3
1	A	6	TYR	3.3
1	B	392	SER	3.2
1	C	441	GLU	3.2
1	D	751	PRO	3.2
1	D	244	LEU	3.2
1	C	371	SER	3.2
1	D	312	THR	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	237	GLY	3.2
1	A	444	MET	3.2
1	B	388	VAL	3.2
1	C	318	ALA	3.2
1	C	436	LEU	3.2
1	D	273	ASP	3.2
1	B	238	GLY	3.2
1	B	303	THR	3.2
1	C	401	THR	3.2
1	D	283	ILE	3.1
1	D	305	LEU	3.1
1	A	487	TYR	3.1
1	D	204	ARG	3.1
1	A	532	VAL	3.1
1	A	439	GLU	3.1
1	B	391	ILE	3.1
1	D	245	ILE	3.1
1	A	371	SER	3.1
1	B	235	ASN	3.1
1	D	737	PRO	3.1
1	A	801	ILE	3.1
1	C	435	ILE	3.1
1	D	393	MET	3.1
1	B	384	THR	3.1
1	D	316	THR	3.1
1	B	236	PRO	3.1
1	D	290	PRO	3.1
1	B	317	ASP	3.1
1	D	427	LYS	3.1
1	A	436	LEU	3.1
1	C	402	SER	3.1
1	A	454	ASP	3.0
1	C	444	MET	3.0
1	C	404	SER	3.0
1	D	386	ILE	3.0
1	D	217	TRP	3.0
1	B	411	PRO	3.0
1	C	265	PRO	3.0
1	B	427	LYS	3.0
1	B	246	LEU	3.0
1	D	233	LEU	3.0
1	B	243	GLY	3.0

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Mol	Chain	Res	Type	RSRZ
1	B	351	ASN	3.0
1	D	301	GLY	3.0
1	D	545	THR	3.0
1	D	477	LEU	3.0
1	A	309	PRO	3.0
1	B	461	PHE	3.0
1	A	540	SER	2.9
1	B	322	ALA	2.9
1	D	174	ALA	2.9
1	D	430	ALA	2.9
1	D	441	GLU	2.9
1	D	300	ASN	2.9
1	B	201	ILE	2.9
1	A	401	THR	2.9
1	A	398	SER	2.9
1	A	246	LEU	2.9
1	D	299	LEU	2.9
1	D	543	LEU	2.9
1	C	440	THR	2.9
1	B	333	GLU	2.9
1	C	363	GLU	2.9
1	D	486	SER	2.9
1	B	329	GLY	2.9
1	B	542	ASP	2.9
1	C	366	TYR	2.9
1	A	238	GLY	2.8
1	A	415	GLY	2.8
1	C	437	ALA	2.8
1	C	438	ALA	2.8
1	B	244	LEU	2.8
1	D	410	LEU	2.8
1	D	532	VAL	2.8
1	A	547	SER	2.8
1	B	453	SER	2.8
1	B	383	ARG	2.8
1	B	405	HIS	2.8
1	D	281	MET	2.8
1	A	363	GLU	2.8
1	C	269	LEU	2.8
1	D	467	THR	2.8
1	C	361	TRP	2.8
1	D	491	ASN	2.8

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Mol	Chain	Res	Type	RSRZ
1	D	738	ASN	2.8
1	A	455	GLN	2.8
1	A	445	ASP	2.8
1	D	445	ASP	2.8
1	D	425	PHE	2.8
1	D	241	PRO	2.8
1	D	678	VAL	2.8
1	C	418	ILE	2.8
1	D	224	ILE	2.8
1	D	402	SER	2.7
1	D	754	ALA	2.7
1	D	436	LEU	2.7
1	C	364	THR	2.7
1	A	265	PRO	2.7
1	B	464	CYS	2.7
1	C	338	SER	2.7
1	D	421	MET	2.7
1	D	399	LYS	2.7
1	D	225	ARG	2.7
1	A	458	THR	2.7
1	D	279	THR	2.7
1	B	121	ASN	2.7
1	B	293	HIS	2.7
1	D	692	VAL	2.7
1	D	287	GLY	2.7
1	D	511	ALA	2.7
1	A	443	TYR	2.7
1	D	121	ASN	2.7
1	D	153	TYR	2.7
1	A	433	ILE	2.7
1	C	429	GLY	2.7
1	D	470	GLY	2.7
1	B	318	ALA	2.6
1	D	168	ALA	2.6
1	D	472	ALA	2.6
1	B	387	ASP	2.6
1	A	434	LYS	2.6
1	D	389	ARG	2.6
1	D	479	GLY	2.6
1	B	426	HIS	2.6
1	D	242	PHE	2.6
1	B	488	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	D	800	LYS	2.6
1	D	208	ILE	2.6
1	B	271	CYS	2.6
1	D	695	ALA	2.6
1	B	460	LYS	2.6
1	D	394	LYS	2.6
1	A	365	ASP	2.6
1	B	358	ASP	2.6
1	A	403	VAL	2.6
1	B	386	ILE	2.6
1	C	13	GLN	2.6
1	D	154	GLY	2.6
1	B	348	MET	2.6
1	C	337	LYS	2.6
1	A	400	ASP	2.6
1	C	125	ASP	2.6
1	B	232	SER	2.6
1	B	283	ILE	2.5
1	D	271	CYS	2.5
1	A	18	ARG	2.5
1	C	384	THR	2.5
1	D	96	ASP	2.5
1	D	556	ASP	2.5
1	B	350	GLN	2.5
1	C	11	PHE	2.5
1	D	447	PHE	2.5
1	A	249	ILE	2.5
1	D	689	GLY	2.5
1	C	369	PHE	2.5
1	B	310	LYS	2.5
1	D	286	ILE	2.5
1	D	41	ASN	2.5
1	D	507	ASN	2.5
1	A	440	THR	2.5
1	B	424	PHE	2.5
1	C	447	PHE	2.5
1	D	238	GLY	2.5
1	D	391	ILE	2.5
1	D	448	THR	2.4
1	B	320	ALA	2.4
1	C	416	ALA	2.4
1	C	449	ALA	2.4

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Mol	Chain	Res	Type	RSRZ
1	D	346	LEU	2.4
1	A	336	PHE	2.4
1	B	382	ASP	2.4
1	D	229	ILE	2.4
1	D	446	ASP	2.4
1	B	547	SER	2.4
1	D	211	TYR	2.4
1	D	348	MET	2.4
1	B	272	LEU	2.4
1	D	284	LEU	2.4
1	B	534	ASP	2.4
1	A	330	VAL	2.4
1	C	245	ILE	2.4
1	D	104	VAL	2.4
1	B	315	TRP	2.4
1	A	750	THR	2.4
1	D	274	THR	2.4
1	D	303	THR	2.4
1	C	351	ASN	2.4
1	C	339	PHE	2.4
1	D	205	ILE	2.4
1	D	508	LYS	2.4
1	B	247	PRO	2.4
1	D	236	PRO	2.4
1	B	536	ALA	2.3
1	D	505	ASP	2.3
1	B	231	LYS	2.3
1	D	159	SER	2.3
1	D	278	SER	2.3
1	C	166	THR	2.3
1	D	342	GLN	2.3
1	D	735	LEU	2.3
1	B	5	ASP	2.3
1	B	239	LYS	2.3
1	D	461	PHE	2.3
1	C	562	SER	2.3
1	D	468	THR	2.3
1	D	288	ALA	2.3
1	B	477	LEU	2.3
1	C	415	GLY	2.3
1	D	169	ARG	2.3
1	D	400	ASP	2.3

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Mol	Chain	Res	Type	RSRZ
1	C	417	SER	2.3
1	A	537	ILE	2.3
1	D	374	GLN	2.3
1	C	341	VAL	2.3
1	A	384	THR	2.3
1	D	4	PRO	2.3
1	B	240	GLY	2.3
1	B	332	LYS	2.3
1	D	753	GLY	2.3
1	B	390	LEU	2.3
1	C	233	LEU	2.3
1	B	385	SER	2.2
1	D	194	PHE	2.2
1	D	435	ILE	2.2
1	D	685	PRO	2.2
1	D	536	ALA	2.2
1	D	380	LEU	2.2
1	D	160	GLU	2.2
1	A	13	GLN	2.2
1	A	379	TRP	2.2
1	B	404	SER	2.2
1	C	313	SER	2.2
1	D	126	SER	2.2
1	D	793	SER	2.2
1	D	349	PHE	2.2
1	A	396	ASN	2.2
1	B	304	ILE	2.2
1	D	690	PRO	2.2
1	C	478	ASP	2.2
1	D	478	ASP	2.2
1	B	165	ALA	2.2
1	D	127	SER	2.2
1	A	264	ASN	2.2
1	D	294	LEU	2.2
1	D	728	TYR	2.2
1	A	442	LYS	2.2
1	D	235	ASN	2.2
1	B	241	PRO	2.1
1	B	292	THR	2.2
1	D	684	VAL	2.1
1	B	210	GLY	2.1
1	D	232	SER	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	696	SER	2.1
1	D	353	LYS	2.1
1	D	202	ASP	2.1
1	D	358	ASP	2.1
1	C	312	THR	2.1
1	D	750	THR	2.1
1	A	370	GLN	2.1
1	A	263	HIS	2.1
1	C	240	GLY	2.1
1	D	124	VAL	2.1
1	D	221	ARG	2.1
1	A	239	LYS	2.1
1	D	460	LYS	2.1
1	B	313	SER	2.1
1	B	355	SER	2.1
1	B	535	SER	2.1
1	D	539	MET	2.1
1	D	228	TYR	2.1
1	D	64	GLY	2.1
1	D	422	ARG	2.1
1	D	280	SER	2.1
1	B	491	ASN	2.1
1	A	446	ASP	2.1
1	B	478	ASP	2.1
1	B	455	GLN	2.1
1	C	443	TYR	2.1
1	A	240	GLY	2.1
1	B	327	VAL	2.1
1	A	441	GLU	2.0
1	B	752	SER	2.1
1	D	161	LEU	2.0
1	C	347	ASN	2.0
1	B	556	ASP	2.0
1	C	365	ASP	2.0
1	C	442	LYS	2.0
1	D	321	LYS	2.0
1	A	267	ILE	2.0
1	B	205	ILE	2.0
1	C	267	ILE	2.0
1	B	157	VAL	2.0
1	D	206	VAL	2.0
1	B	486	SER	2.0

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Mol	Chain	Res	Type	RSRZ
1	C	375	ALA	2.0
1	D	482	ALA	2.0
1	B	167	ASN	2.0
1	D	555	ARG	2.0
1	A	368	LYS	2.0
1	D	541	LYS	2.0
1	D	569	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.

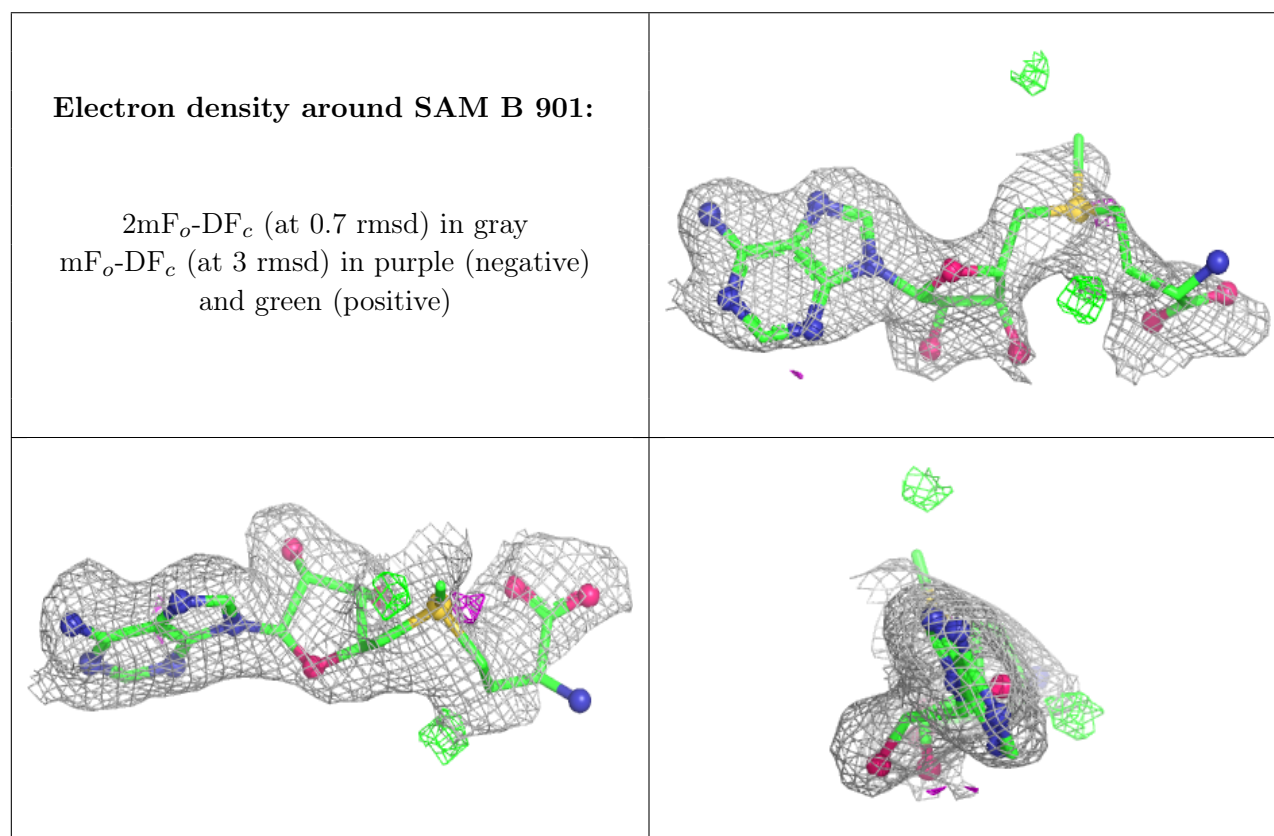
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	SAM	B	901	27/27	0.80	0.14	44,59,83,92	0
2	SAM	A	901	27/27	0.83	0.14	31,43,80,84	0
2	SAM	A	902	27/27	0.88	0.12	36,50,54,57	0
4	FLC	B	905	13/13	0.88	0.11	26,30,35,45	0
3	EDO	B	902	4/4	0.89	0.14	20,27,32,38	0
3	EDO	D	901	4/4	0.89	0.12	25,25,26,29	0
2	SAM	C	902	27/27	0.89	0.12	39,49,55,57	0
3	EDO	A	903	4/4	0.90	0.11	24,25,26,27	0
3	EDO	B	903	4/4	0.90	0.13	33,38,39,44	0
3	EDO	A	904	4/4	0.92	0.10	24,26,28,34	0
3	EDO	B	904	4/4	0.92	0.09	18,19,20,30	0
3	EDO	A	905	4/4	0.92	0.09	25,26,27,32	0
2	SAM	C	901	27/27	0.92	0.10	28,34,62,69	0
4	FLC	A	906	13/13	0.93	0.08	22,24,35,41	0
4	FLC	D	903	13/13	0.93	0.07	25,32,36,36	0
3	EDO	D	902	4/4	0.95	0.11	26,30,36,38	0

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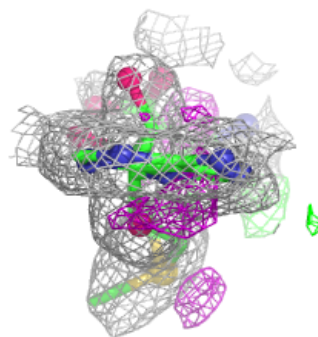
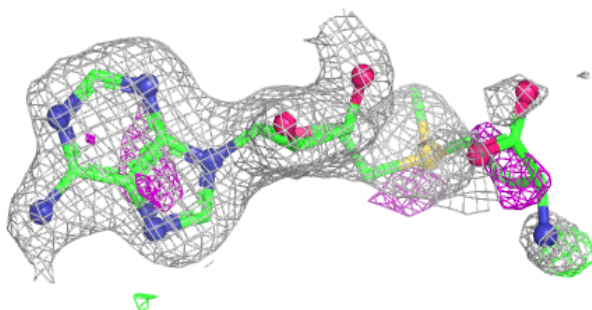
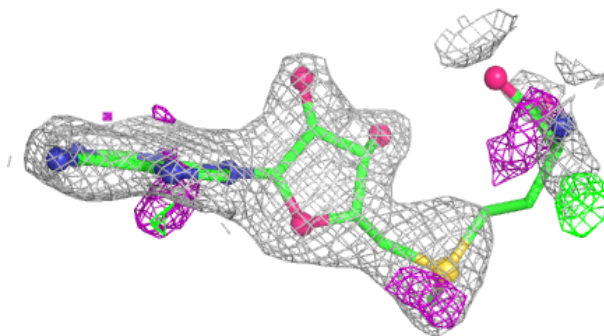
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	EDO	C	903	4/4	0.96	0.07	19,23,25,27	0

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.

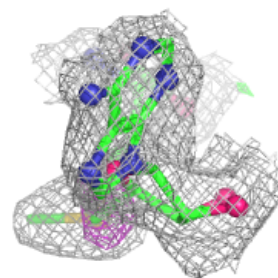
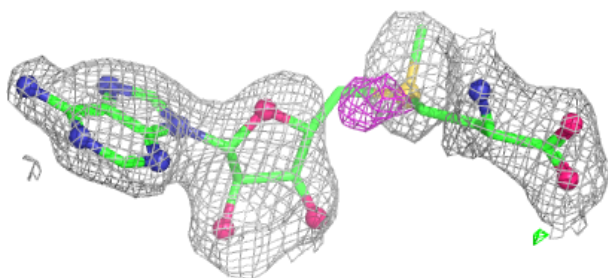
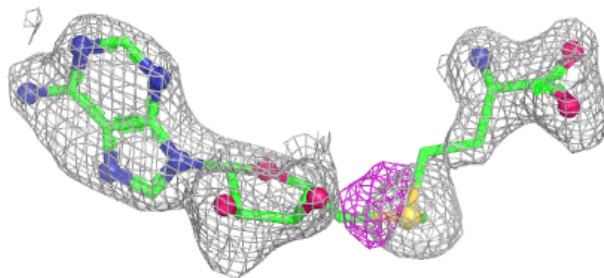


Electron density around SAM A 901:

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

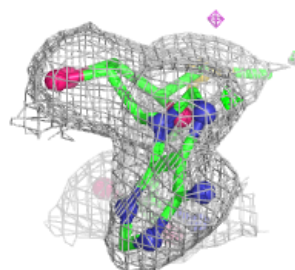
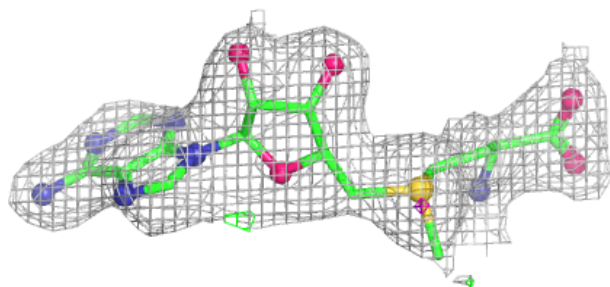
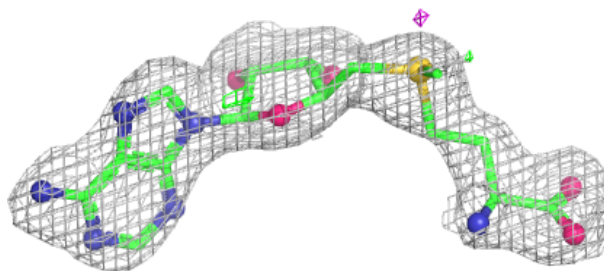
**Electron density around SAM A 902:**

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

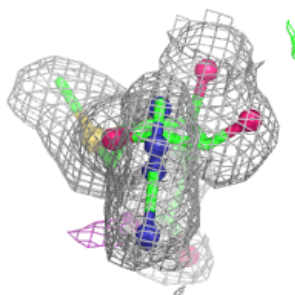
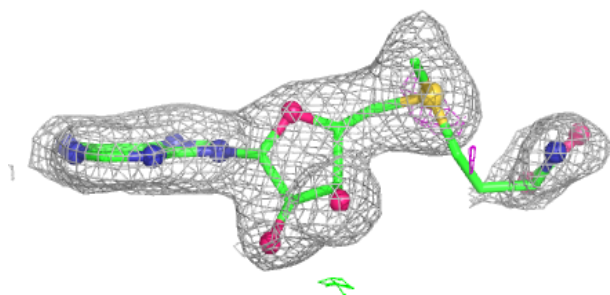
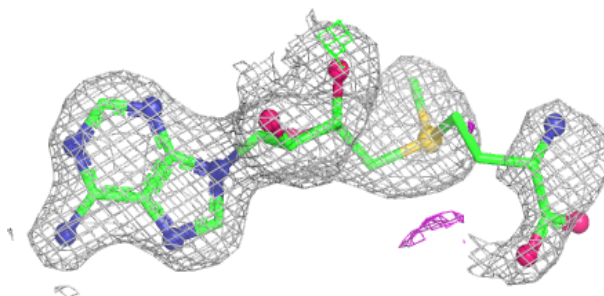


Electron density around SAM C 902:

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

**Electron density around SAM C 901:**

$2mF_o-DF_c$ (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.