



Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 02:49 am BST

PDB ID : 1KIA
Title : Crystal structure of glycine N-methyltransferase complexed with S-adenosylmethionine and acetate
Authors : Takusagawa, F.; Huang, Y.
Deposited on : 2001-12-02
Resolution : 2.80 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

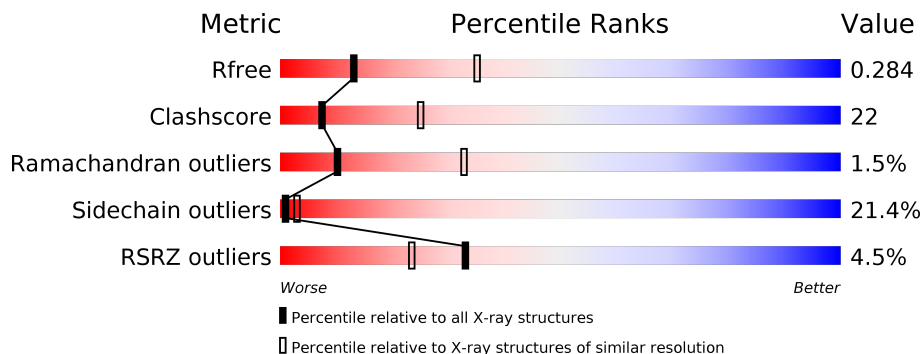
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on 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	292	 4% 52% 32% 11% 6%
1	B	292	 4% 50% 33% 11% 6%
1	C	292	 5% 52% 32% 10% 6%
1	D	292	 4% 50% 33% 11% 6%

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	ACT	D	3294	-	-	X	-

2 Entry composition [i](#)

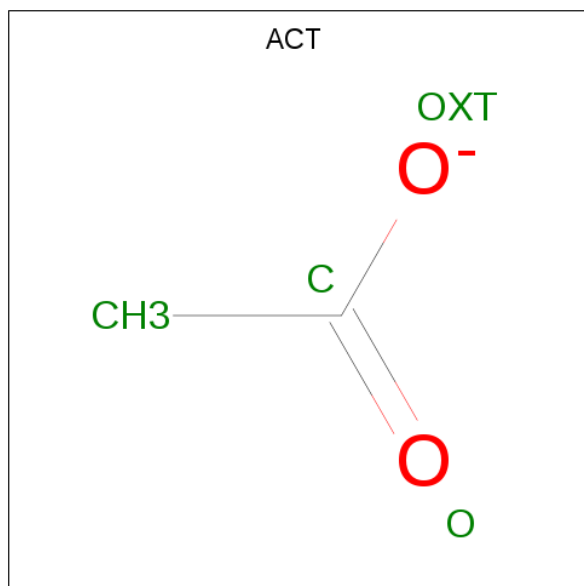
There are 4 unique types of molecules in this entry. The entry contains 8999 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Glycine N-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	275	Total 2160	C 1373	N 376	O 400	S 11	0	0	0
1	B	275	Total 2160	C 1373	N 376	O 400	S 11	0	0	0
1	C	275	Total 2160	C 1373	N 376	O 400	S 11	0	0	0
1	D	275	Total 2160	C 1373	N 376	O 400	S 11	0	0	0

- Molecule 2 is ACETATE ION (three-letter code: ACT) (formula: C₂H₃O₂).



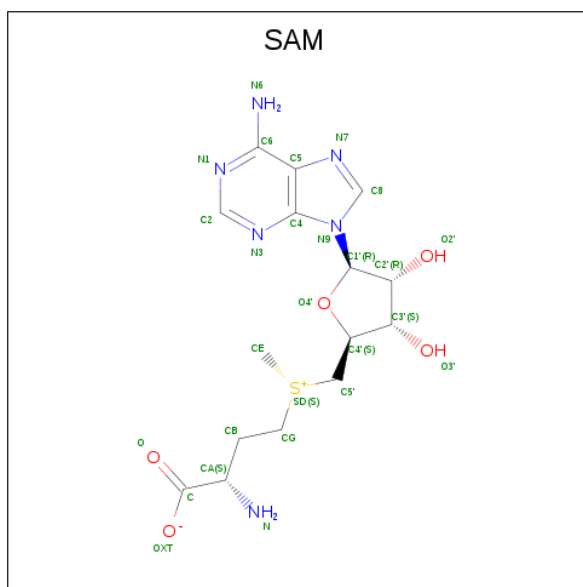
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
			Total	C	O		
2	A	1	Total 4	C 2	O 2	0	0
2	B	1	Total 4	C 2	O 2	0	0

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

- Molecule 3 is S-ADENOSYLMETHIONINE (three-letter code: SAM) (formula: C₁₅H₂₂N₆O₅S).



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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	65	Total O 65 65	0	0
4	B	59	Total O 59 59	0	0
4	C	53	Total O 53 53	0	0

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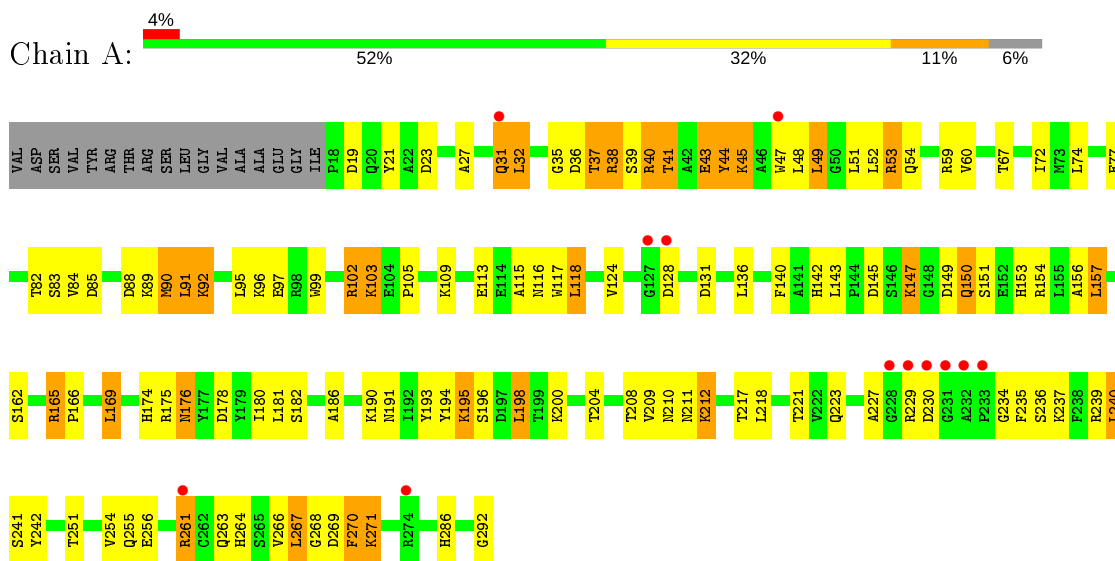
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	D	58	Total	O	0	0
			58	58		

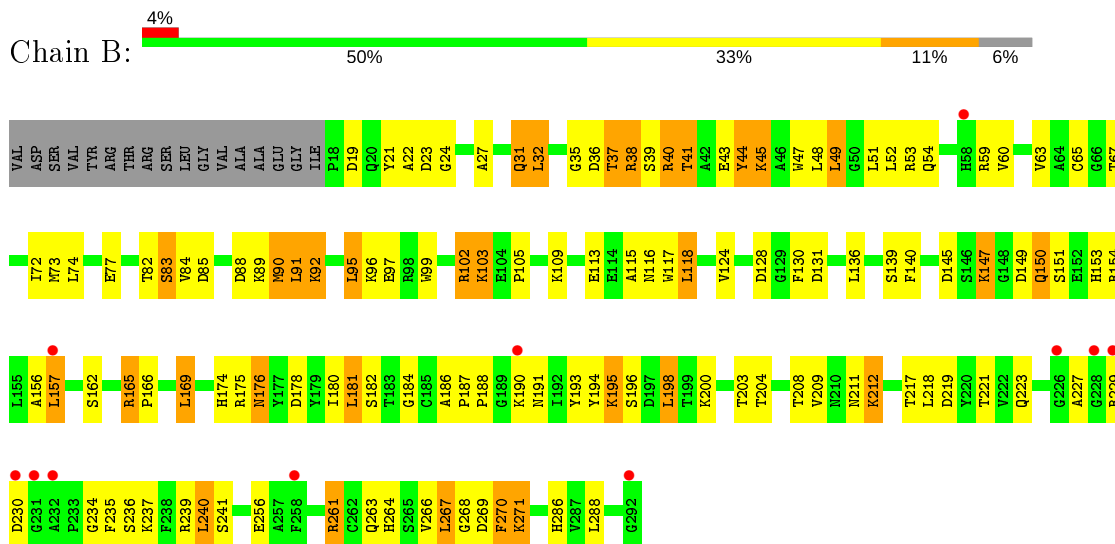
3 Residue-property plots i

These plots are drawn for all protein, RNA and DNA 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: Glycine N-methyltransferase

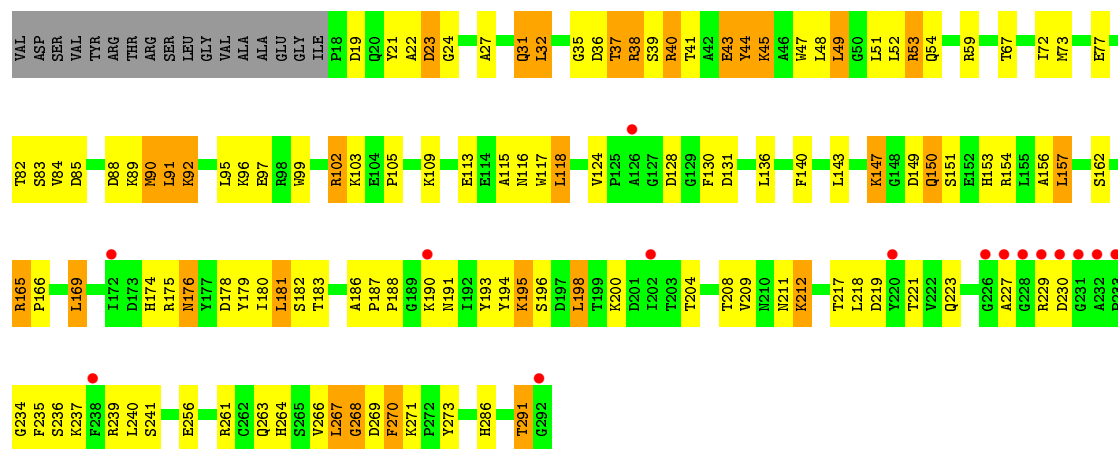


- Molecule 1: Glycine N-methyltransferase

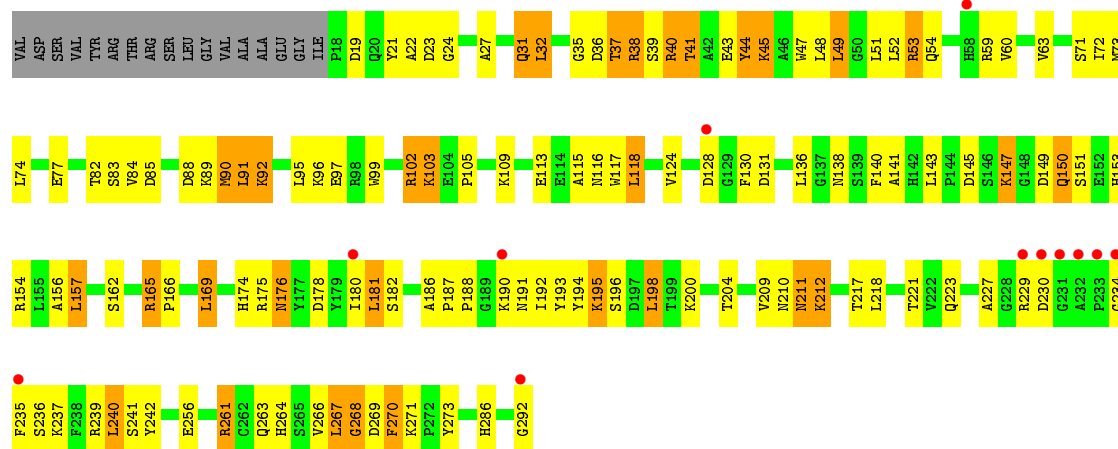


- Molecule 1: Glycine N-methyltransferase





• Molecule 1: Glycine N-methyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.95Å 117.01Å 137.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	8.00 – 2.80 89.19 – 2.80	Depositor EDS
% Data completeness (in resolution range)	(Not available) (8.00-2.80) 99.4 (89.19-2.80)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.79 (at 2.82Å)	Xtrriage
Refinement program	X-PLOR 3.851	Depositor
R, R_{free}	0.216 , 0.286 0.230 , 0.284	Depositor DCC
R_{free} test set	3693 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å ²)	37.5	Xtrriage
Anisotropy	0.346	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 70.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.87	EDS
Total number of atoms	8999	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.89% 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: SAM, ACT

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	0.33	0/2215	0.58	0/3002
1	B	0.33	0/2215	0.57	0/3002
1	C	0.32	0/2215	0.57	0/3002
1	D	0.34	0/2215	0.58	0/3002
All	All	0.33	0/8860	0.58	0/12008

There are no bond length outliers.

There are no bond angle outliers.

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	2160	0	2114	98	0
1	B	2160	0	2114	99	1
1	C	2160	0	2114	86	0
1	D	2160	0	2114	103	1
2	A	4	0	3	0	0
2	B	4	0	3	0	0
2	C	4	0	3	0	0
2	D	4	0	3	2	0
3	A	27	0	22	2	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	27	0	22	3	0
3	C	27	0	22	1	0
3	D	27	0	22	1	0
4	A	65	0	0	1	0
4	B	59	0	0	2	0
4	C	53	0	0	0	0
4	D	58	0	0	0	0
All	All	8999	0	8556	384	1

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 22.

All (384) 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:27:ALA:HA	1:D:90:MET:HE3	1.53	0.90
1:A:150:GLN:HG2	1:A:153:HIS:ND1	1.88	0.89
1:B:150:GLN:HG2	1:B:153:HIS:ND1	1.91	0.86
1:C:150:GLN:HG2	1:C:153:HIS:ND1	1.91	0.86
1:A:36:ASP:HA	1:A:38:ARG:HH21	1.41	0.85
1:C:36:ASP:HA	1:C:38:ARG:HH21	1.41	0.84
1:D:150:GLN:HG2	1:D:153:HIS:ND1	1.93	0.83
1:A:27:ALA:HA	1:A:90:MET:HE3	1.60	0.83
1:B:27:ALA:HA	1:B:90:MET:HE3	1.60	0.83
1:D:191:ASN:HD22	1:D:194:TYR:H	1.29	0.80
1:A:191:ASN:HD22	1:A:194:TYR:H	1.29	0.80
1:B:36:ASP:HA	1:B:38:ARG:HH21	1.46	0.79
1:D:227:ALA:HB3	1:D:234:GLY:HA3	1.65	0.78
1:A:227:ALA:CB	1:A:234:GLY:HA3	2.14	0.77
1:D:227:ALA:CB	1:D:234:GLY:HA3	2.14	0.76
1:D:36:ASP:HA	1:D:38:ARG:HH21	1.48	0.76
1:A:227:ALA:HB3	1:A:234:GLY:HA3	1.66	0.76
1:C:227:ALA:HB3	1:C:234:GLY:HA3	1.67	0.76
1:B:227:ALA:HB3	1:B:234:GLY:HA3	1.67	0.76
1:C:227:ALA:CB	1:C:234:GLY:HA3	2.16	0.76
1:C:191:ASN:HD22	1:C:194:TYR:H	1.33	0.76
1:A:217:THR:HG21	1:A:239:ARG:HE	1.52	0.74
1:B:191:ASN:HD22	1:B:194:TYR:H	1.34	0.74
1:A:269:ASP:O	1:A:270:PHE:HB2	1.88	0.74
1:B:227:ALA:CB	1:B:234:GLY:HA3	2.18	0.73
1:C:31:GLN:H	1:C:31:GLN:NE2	1.87	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:198:LEU:HG	1:C:223:GLN:O	1.89	0.72
1:B:269:ASP:O	1:B:270:PHE:HB2	1.90	0.71
1:D:217:THR:HG21	1:D:239:ARG:HE	1.54	0.71
1:D:31:GLN:H	1:D:31:GLN:NE2	1.89	0.70
1:B:217:THR:HG21	1:B:239:ARG:HE	1.56	0.70
1:C:31:GLN:HE21	1:C:31:GLN:H	1.37	0.69
1:D:31:GLN:H	1:D:31:GLN:HE21	1.39	0.69
1:C:217:THR:HG21	1:C:239:ARG:HE	1.57	0.69
1:D:269:ASP:O	1:D:270:PHE:HB2	1.91	0.68
1:B:198:LEU:HG	1:B:223:GLN:O	1.94	0.68
1:A:36:ASP:HB3	1:A:39:SER:HB3	1.76	0.67
1:A:84:VAL:HA	1:A:113:GLU:O	1.94	0.67
1:B:31:GLN:HE21	1:B:31:GLN:H	1.42	0.67
1:A:31:GLN:H	1:A:31:GLN:NE2	1.93	0.67
1:A:31:GLN:H	1:A:31:GLN:HE21	1.41	0.67
1:C:269:ASP:O	1:C:270:PHE:HB2	1.94	0.67
1:A:198:LEU:HG	1:A:223:GLN:O	1.95	0.66
1:B:31:GLN:NE2	1:B:31:GLN:H	1.93	0.66
1:D:32:LEU:HG	1:D:198:LEU:HD23	1.76	0.66
1:D:138:ASN:HD22	2:D:3294:ACT:CH3	2.08	0.66
1:C:67:THR:HG23	1:C:90:MET:HE1	1.78	0.65
1:C:27:ALA:HA	1:C:90:MET:HE3	1.77	0.65
1:D:227:ALA:HB3	1:D:234:GLY:CA	2.27	0.64
1:B:84:VAL:HA	1:B:113:GLU:O	1.98	0.64
1:D:198:LEU:HG	1:D:223:GLN:O	1.96	0.64
1:A:227:ALA:HB3	1:A:234:GLY:CA	2.28	0.63
1:D:36:ASP:HB3	1:D:39:SER:HB3	1.80	0.62
1:C:32:LEU:HG	1:C:198:LEU:HD23	1.81	0.62
1:B:227:ALA:HB3	1:B:234:GLY:CA	2.29	0.62
1:D:49:LEU:HG	1:D:53:ARG:NH2	2.15	0.62
1:C:227:ALA:HB3	1:C:234:GLY:CA	2.29	0.62
1:D:191:ASN:HB3	1:D:194:TYR:O	1.99	0.62
1:B:36:ASP:HB3	1:B:39:SER:HB3	1.82	0.61
1:C:84:VAL:HB	1:C:115:ALA:HB3	1.82	0.61
1:C:209:VAL:HB	1:C:212:LYS:HZ3	1.65	0.61
1:C:36:ASP:HB3	1:C:39:SER:HB3	1.82	0.61
1:C:84:VAL:HA	1:C:113:GLU:O	2.00	0.60
1:B:174:HIS:CE1	1:B:286:HIS:HE2	2.20	0.60
1:D:209:VAL:HB	1:D:212:LYS:NZ	2.17	0.60
1:D:84:VAL:HA	1:D:113:GLU:O	2.00	0.60
1:C:209:VAL:HB	1:C:212:LYS:NZ	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:51:LEU:HD11	1:D:169:LEU:HD21	1.85	0.58
1:B:32:LEU:HG	1:B:198:LEU:HD23	1.85	0.58
1:D:138:ASN:HD22	2:D:3294:ACT:H2	1.67	0.58
1:A:166:PRO:HB3	1:A:292:GLY:HA2	1.85	0.58
1:A:67:THR:HG23	1:A:90:MET:HE1	1.86	0.57
1:B:99:TRP:O	1:B:102:ARG:HB3	2.05	0.57
1:B:184:GLY:HA3	1:D:211:ASN:ND2	2.19	0.57
1:B:131:ASP:HA	1:B:165:ARG:HD3	1.86	0.57
1:B:35:GLY:CA	1:B:196:SER:HB2	2.35	0.57
1:B:200:LYS:HG3	1:B:235:PHE:HE2	1.70	0.57
1:C:85:ASP:HB3	1:C:91:LEU:HD22	1.86	0.57
1:D:174:HIS:CE1	1:D:286:HIS:HE2	2.22	0.57
1:A:27:ALA:HA	1:A:90:MET:CE	2.34	0.56
1:D:72:ILE:HD11	1:D:97:GLU:HG2	1.86	0.56
1:A:174:HIS:CE1	1:A:286:HIS:HE2	2.23	0.56
1:A:84:VAL:HB	1:A:115:ALA:HB3	1.86	0.56
1:C:131:ASP:HA	1:C:165:ARG:HD3	1.87	0.56
1:C:99:TRP:O	1:C:102:ARG:HB3	2.05	0.56
1:D:49:LEU:HD21	1:D:77:GLU:HG3	1.86	0.56
1:A:191:ASN:HB3	1:A:194:TYR:O	2.06	0.56
1:A:32:LEU:HG	1:A:198:LEU:HD23	1.87	0.56
1:A:48:LEU:O	1:A:52:LEU:HG	2.06	0.56
1:B:139:SER:OG	3:B:1293:SAM:H5'2	2.05	0.55
1:B:176:ASN:HD21	1:B:178:ASP:HB2	1.71	0.55
1:C:44:TYR:HB3	1:C:270:PHE:CD1	2.40	0.55
1:B:51:LEU:HD11	1:B:169:LEU:HD21	1.87	0.55
1:B:85:ASP:HB3	1:B:91:LEU:HD22	1.88	0.55
1:C:174:HIS:CE1	1:C:286:HIS:HE2	2.25	0.55
1:C:49:LEU:HD21	1:C:77:GLU:HG3	1.88	0.55
1:C:191:ASN:HB3	1:C:194:TYR:O	2.06	0.55
1:D:72:ILE:CD1	1:D:97:GLU:HG2	2.37	0.55
1:C:200:LYS:HG3	1:C:235:PHE:HE2	1.72	0.54
1:C:72:ILE:CD1	1:C:97:GLU:HG2	2.37	0.54
1:B:40:ARG:HA	1:B:195:LYS:CE	2.38	0.54
1:D:40:ARG:HA	1:D:195:LYS:CE	2.37	0.54
1:A:227:ALA:HB1	1:A:234:GLY:HA3	1.89	0.54
1:C:51:LEU:HD11	1:C:169:LEU:HD21	1.89	0.54
1:B:84:VAL:HB	1:B:115:ALA:HB3	1.90	0.54
1:B:191:ASN:HB3	1:B:194:TYR:O	2.07	0.54
1:B:174:HIS:HD2	1:B:175:ARG:O	1.90	0.53
1:B:72:ILE:HD11	1:B:97:GLU:HG2	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:72:ILE:HD11	1:C:97:GLU:HG2	1.90	0.53
1:D:99:TRP:O	1:D:102:ARG:HB3	2.08	0.53
1:C:35:GLY:CA	1:C:196:SER:HB2	2.39	0.53
1:D:131:ASP:HA	1:D:165:ARG:HD3	1.91	0.53
1:D:200:LYS:HG3	1:D:235:PHE:HE2	1.74	0.53
1:B:174:HIS:HE1	1:B:286:HIS:HE2	1.55	0.53
1:B:47:TRP:CZ2	1:B:267:LEU:HD11	2.44	0.53
1:D:85:ASP:HB3	1:D:91:LEU:HD22	1.90	0.53
1:A:72:ILE:HD11	1:A:97:GLU:HG2	1.91	0.53
1:B:72:ILE:CD1	1:B:97:GLU:HG2	2.39	0.53
1:D:47:TRP:CZ2	1:D:267:LEU:HD11	2.44	0.53
1:A:154:ARG:HG2	1:A:256:GLU:OE2	2.08	0.52
1:D:35:GLY:CA	1:D:196:SER:HB2	2.39	0.52
1:B:44:TYR:HB3	1:B:270:PHE:CD1	2.43	0.52
1:D:84:VAL:HB	1:D:115:ALA:HB3	1.91	0.52
1:B:40:ARG:HA	1:B:195:LYS:HE3	1.90	0.52
1:D:40:ARG:HA	1:D:195:LYS:HE3	1.92	0.52
1:C:153:HIS:O	1:C:157:LEU:HB2	2.10	0.52
1:A:35:GLY:CA	1:A:196:SER:HB2	2.39	0.52
1:A:44:TYR:HB3	1:A:270:PHE:CD1	2.45	0.52
1:A:37:THR:HG23	1:A:38:ARG:CZ	2.39	0.52
1:C:221:THR:HG23	1:C:237:LYS:HE2	1.92	0.52
1:A:221:THR:HG23	1:A:237:LYS:HE2	1.90	0.51
1:C:227:ALA:HB1	1:C:234:GLY:HA3	1.92	0.51
1:D:19:ASP:C	1:D:21:TYR:H	2.13	0.51
1:B:153:HIS:O	1:B:157:LEU:HB2	2.10	0.51
1:B:49:LEU:HD21	1:B:77:GLU:HG3	1.92	0.51
1:C:154:ARG:HG2	1:C:256:GLU:OE2	2.10	0.51
1:A:140:PHE:CE1	1:A:157:LEU:HD13	2.44	0.51
1:D:153:HIS:O	1:D:157:LEU:HB2	2.09	0.51
1:D:37:THR:HG23	1:D:38:ARG:CZ	2.40	0.51
1:A:131:ASP:HA	1:A:165:ARG:HD3	1.92	0.51
1:A:51:LEU:HD11	1:A:169:LEU:HD21	1.92	0.51
1:A:72:ILE:CD1	1:A:97:GLU:HG2	2.39	0.51
1:C:191:ASN:O	1:C:195:LYS:HG2	2.11	0.51
1:C:174:HIS:HD2	1:C:175:ARG:O	1.94	0.51
1:D:180:ILE:HG12	1:D:186:ALA:HA	1.93	0.51
1:D:49:LEU:O	1:D:53:ARG:HG2	2.11	0.51
1:B:67:THR:HG23	1:B:90:MET:HE1	1.93	0.51
1:D:154:ARG:HG2	1:D:256:GLU:OE2	2.11	0.51
1:C:180:ILE:HG12	1:C:186:ALA:HA	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:116:ASN:HA	3:A:293:SAM:N1	2.26	0.50
1:B:116:ASN:HA	3:B:1293:SAM:N1	2.26	0.50
1:C:47:TRP:CZ2	1:C:267:LEU:HD11	2.46	0.50
1:D:264:HIS:HE1	1:D:286:HIS:ND1	2.09	0.50
1:A:264:HIS:HE1	1:A:286:HIS:ND1	2.09	0.50
1:D:48:LEU:O	1:D:52:LEU:HG	2.11	0.50
1:C:165:ARG:HG2	1:C:166:PRO:O	2.12	0.50
1:C:140:PHE:CE1	1:C:157:LEU:HD13	2.46	0.50
1:A:165:ARG:HG2	1:A:166:PRO:O	2.12	0.50
1:B:19:ASP:C	1:B:21:TYR:H	2.14	0.50
1:D:227:ALA:HB1	1:D:234:GLY:HA3	1.90	0.50
1:A:19:ASP:C	1:A:21:TYR:H	2.14	0.50
1:A:47:TRP:CZ2	1:A:267:LEU:HD11	2.46	0.50
1:D:191:ASN:O	1:D:195:LYS:HG2	2.12	0.50
1:C:40:ARG:HA	1:C:195:LYS:HE3	1.94	0.50
1:A:200:LYS:HG3	1:A:235:PHE:HE2	1.76	0.50
1:D:140:PHE:CE1	1:D:157:LEU:HD13	2.46	0.50
1:A:49:LEU:HD21	1:A:77:GLU:HG3	1.92	0.49
1:B:88:ASP:O	1:B:92:LYS:HB3	2.11	0.49
1:C:40:ARG:HA	1:C:195:LYS:CE	2.42	0.49
1:B:27:ALA:HA	1:B:90:MET:CE	2.37	0.49
1:B:37:THR:HG23	1:B:38:ARG:NH2	2.27	0.49
1:B:84:VAL:HG11	1:B:124:VAL:HG21	1.93	0.49
1:B:180:ILE:HG12	1:B:186:ALA:HA	1.94	0.49
1:B:200:LYS:HG3	1:B:235:PHE:CE2	2.47	0.49
1:A:153:HIS:O	1:A:157:LEU:HB2	2.13	0.49
1:D:174:HIS:HD2	1:D:175:ARG:O	1.95	0.49
1:C:19:ASP:C	1:C:21:TYR:H	2.14	0.49
1:B:37:THR:HG23	1:B:38:ARG:CZ	2.43	0.49
1:C:37:THR:HG23	1:C:38:ARG:CZ	2.43	0.49
1:C:48:LEU:O	1:C:52:LEU:HG	2.13	0.49
1:B:191:ASN:O	1:B:195:LYS:HG2	2.13	0.49
1:A:208:THR:HG23	1:A:212:LYS:C	2.33	0.49
1:A:99:TRP:O	1:A:102:ARG:HB3	2.12	0.49
1:B:48:LEU:O	1:B:52:LEU:HG	2.13	0.48
1:A:209:VAL:HB	1:A:212:LYS:NZ	2.27	0.48
1:D:196:SER:OG	1:D:198:LEU:HB2	2.13	0.48
1:C:21:TYR:CE1	3:C:2293:SAM:H3'	2.48	0.48
1:B:264:HIS:HE1	1:B:286:HIS:ND1	2.11	0.48
1:B:60:VAL:HG11	1:B:74:LEU:CD1	2.44	0.48
1:C:84:VAL:HG11	1:C:124:VAL:HG21	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:40:ARG:HA	1:A:195:LYS:CE	2.44	0.48
1:C:200:LYS:HG3	1:C:235:PHE:CE2	2.49	0.48
1:C:264:HIS:HE1	1:C:286:HIS:ND1	2.12	0.47
1:D:117:TRP:CZ3	1:D:140:PHE:HA	2.49	0.47
1:D:174:HIS:HE1	1:D:286:HIS:HE2	1.60	0.47
1:B:49:LEU:HG	1:B:53:ARG:NH2	2.29	0.47
1:B:130:PHE:O	1:B:165:ARG:HB3	2.14	0.47
1:B:39:SER:O	1:B:195:LYS:HE3	2.14	0.47
1:D:165:ARG:HG2	1:D:166:PRO:O	2.14	0.47
1:A:176:ASN:HD21	1:A:178:ASP:HB2	1.80	0.47
1:B:227:ALA:HB1	1:B:234:GLY:HA3	1.95	0.47
1:B:165:ARG:HG2	1:B:166:PRO:O	2.14	0.47
1:D:37:THR:HG23	1:D:38:ARG:NH2	2.29	0.47
1:B:204:THR:HA	1:B:218:LEU:HD23	1.97	0.47
1:D:105:PRO:O	1:D:109:LYS:HE3	2.14	0.47
1:D:200:LYS:HG3	1:D:235:PHE:CE2	2.50	0.47
1:A:39:SER:O	1:A:195:LYS:HE3	2.13	0.47
1:D:147:LYS:HE2	1:D:147:LYS:O	2.15	0.47
1:C:27:ALA:HA	1:C:90:MET:CE	2.44	0.47
1:B:154:ARG:HG2	1:B:256:GLU:OE2	2.15	0.47
1:C:291:THR:OG1	1:C:291:THR:O	2.32	0.47
1:C:37:THR:HG23	1:C:38:ARG:NH2	2.30	0.47
1:D:209:VAL:HB	1:D:212:LYS:HZ2	1.79	0.47
1:B:209:VAL:HB	1:B:212:LYS:NZ	2.30	0.47
1:C:40:ARG:HD2	1:C:193:TYR:O	2.15	0.47
1:D:84:VAL:HG11	1:D:124:VAL:HG21	1.97	0.47
1:A:174:HIS:HD2	1:A:175:ARG:O	1.98	0.46
1:A:204:THR:HA	1:A:218:LEU:HD23	1.97	0.46
1:D:44:TYR:HB3	1:D:270:PHE:CD1	2.50	0.46
1:B:203:THR:HA	1:D:210:ASN:HD21	1.81	0.46
1:B:221:THR:HG23	1:B:237:LYS:HE2	1.97	0.46
1:C:176:ASN:HD21	1:C:178:ASP:HB2	1.79	0.46
1:B:147:LYS:O	1:B:147:LYS:HE2	2.15	0.46
1:B:40:ARG:HD2	1:B:193:TYR:O	2.16	0.46
1:A:196:SER:OG	1:A:198:LEU:HB2	2.15	0.46
1:A:140:PHE:CZ	1:A:157:LEU:HD13	2.50	0.46
1:C:84:VAL:HG11	1:C:124:VAL:CG2	2.45	0.46
1:A:85:ASP:HB3	1:A:91:LEU:HD22	1.96	0.46
1:D:40:ARG:CG	1:D:41:THR:N	2.79	0.46
1:B:219:ASP:OD1	1:B:239:ARG:HB2	2.16	0.45
1:B:103:LYS:HD3	1:B:103:LYS:HA	1.72	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:27:ALA:HA	1:D:90:MET:CE	2.36	0.45
1:A:84:VAL:HG11	1:A:124:VAL:HG21	1.99	0.45
1:B:105:PRO:O	1:B:109:LYS:HE3	2.16	0.45
1:C:130:PHE:O	1:C:165:ARG:HB3	2.17	0.45
1:A:37:THR:HG23	1:A:38:ARG:NH2	2.31	0.45
1:B:35:GLY:HA3	1:B:196:SER:HB2	1.98	0.45
1:C:208:THR:HG23	1:C:212:LYS:C	2.36	0.45
1:D:221:THR:HG23	1:D:237:LYS:HE2	1.98	0.45
1:D:239:ARG:O	1:D:240:LEU:HD13	2.15	0.45
1:D:39:SER:O	1:D:195:LYS:HE3	2.15	0.45
1:D:45:LYS:O	1:D:49:LEU:HB2	2.16	0.45
1:A:147:LYS:HE2	1:A:147:LYS:O	2.17	0.45
1:B:84:VAL:HG11	1:B:124:VAL:CG2	2.46	0.45
1:C:88:ASP:O	1:C:92:LYS:HB3	2.17	0.45
1:D:261:ARG:NH2	1:D:292:GLY:O	2.49	0.45
1:A:180:ILE:HG12	1:A:186:ALA:HA	1.98	0.45
1:B:117:TRP:CZ3	1:B:140:PHE:HA	2.51	0.45
1:C:117:TRP:CZ3	1:C:140:PHE:HA	2.52	0.45
1:A:60:VAL:HG11	1:A:74:LEU:CD1	2.47	0.45
1:C:147:LYS:HE2	1:C:147:LYS:O	2.17	0.45
1:D:268:GLY:N	1:D:273:TYR:HB2	2.32	0.45
1:A:191:ASN:HD22	1:A:194:TYR:N	2.06	0.45
1:B:140:PHE:CE1	1:B:157:LEU:HD13	2.52	0.44
1:B:63:VAL:HA	1:B:84:VAL:CG2	2.48	0.44
1:D:19:ASP:HB3	1:D:22:ALA:HB2	1.98	0.44
1:D:84:VAL:HG11	1:D:124:VAL:CG2	2.47	0.44
1:A:105:PRO:O	1:A:109:LYS:HE3	2.17	0.44
1:A:176:ASN:HD22	1:A:176:ASN:C	2.19	0.44
1:B:198:LEU:HD12	1:B:198:LEU:HA	1.84	0.44
1:A:200:LYS:HG3	1:A:235:PHE:CE2	2.52	0.44
1:B:261:ARG:HE	1:B:261:ARG:HA	1.83	0.44
1:C:49:LEU:HG	1:C:53:ARG:NH2	2.32	0.44
1:A:210:ASN:HD22	1:A:210:ASN:HA	1.62	0.44
1:A:36:ASP:CG	1:A:38:ARG:HE	2.20	0.44
1:A:88:ASP:O	1:A:92:LYS:HB3	2.18	0.44
1:B:239:ARG:O	1:B:240:LEU:HD13	2.18	0.44
1:D:176:ASN:HD21	1:D:178:ASP:HB2	1.83	0.44
1:B:264:HIS:ND1	1:B:288:LEU:HD21	2.33	0.44
1:C:176:ASN:C	1:C:176:ASN:HD22	2.20	0.44
1:D:49:LEU:O	1:D:53:ARG:CG	2.65	0.44
1:D:88:ASP:O	1:D:92:LYS:HB3	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:181:LEU:HA	1:C:181:LEU:HD12	1.83	0.43
1:D:261:ARG:NE	1:D:261:ARG:HA	2.32	0.43
1:A:239:ARG:O	1:A:240:LEU:HD13	2.17	0.43
1:B:149:ASP:C	1:B:151:SER:H	2.22	0.43
1:B:261:ARG:HA	1:B:261:ARG:NE	2.33	0.43
1:D:116:ASN:OD1	1:D:118:LEU:HB2	2.18	0.43
1:A:40:ARG:HA	1:A:195:LYS:HE3	2.00	0.43
1:A:254:VAL:HG13	1:A:255:GLN:N	2.34	0.43
1:A:40:ARG:CG	1:A:41:THR:N	2.82	0.43
1:A:43:GLU:O	1:A:45:LYS:N	2.52	0.43
1:B:118:LEU:HD13	1:B:156:ALA:HB2	2.01	0.43
1:B:176:ASN:C	1:B:176:ASN:HD22	2.21	0.43
1:D:176:ASN:HD22	1:D:176:ASN:C	2.21	0.43
1:A:149:ASP:C	1:A:151:SER:H	2.21	0.43
1:A:84:VAL:HG11	1:A:124:VAL:CG2	2.48	0.43
1:B:91:LEU:HA	1:B:91:LEU:HD12	1.86	0.43
1:A:116:ASN:OD1	1:A:118:LEU:HB2	2.18	0.43
1:B:267:LEU:HB3	1:B:271:LYS:O	2.18	0.43
1:C:150:GLN:O	1:C:153:HIS:HB2	2.19	0.43
1:C:35:GLY:HA3	1:C:196:SER:HB2	1.99	0.43
1:D:60:VAL:HG11	1:D:74:LEU:CD1	2.48	0.43
1:A:117:TRP:CZ3	1:A:140:PHE:HA	2.54	0.43
1:A:143:LEU:HA	1:A:143:LEU:HD12	1.86	0.43
1:A:150:GLN:O	1:A:153:HIS:HB2	2.19	0.43
1:A:198:LEU:HD12	1:A:198:LEU:HA	1.83	0.43
1:B:187:PRO:HA	1:B:188:PRO:HD3	1.93	0.43
1:D:40:ARG:HG3	1:D:41:THR:N	2.32	0.43
1:A:40:ARG:HD2	1:A:193:TYR:O	2.18	0.43
1:C:149:ASP:C	1:C:151:SER:H	2.21	0.43
1:C:198:LEU:HD12	1:C:198:LEU:HA	1.83	0.43
1:C:268:GLY:N	1:C:273:TYR:HB2	2.34	0.43
1:A:49:LEU:HG	1:A:53:ARG:NH2	2.34	0.42
1:D:103:LYS:HD3	1:D:103:LYS:HA	1.73	0.42
1:D:264:HIS:CE1	1:D:286:HIS:ND1	2.87	0.42
1:D:21:TYR:CE1	3:D:3293:SAM:H3'	2.54	0.42
1:D:91:LEU:HA	1:D:91:LEU:HD12	1.86	0.42
1:D:209:VAL:HB	1:D:212:LYS:HZ3	1.83	0.42
1:A:261:ARG:NE	1:A:261:ARG:HA	2.34	0.42
1:B:24:GLY:CA	1:B:89:LYS:HD2	2.50	0.42
1:D:181:LEU:HA	1:D:181:LEU:HD12	1.89	0.42
1:D:32:LEU:CG	1:D:198:LEU:HD23	2.47	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:261:ARG:HE	1:D:261:ARG:HA	1.85	0.42
1:D:63:VAL:HA	1:D:84:VAL:CG2	2.50	0.42
1:A:21:TYR:CE1	3:A:293:SAM:H3'	2.55	0.42
1:B:40:ARG:CG	1:B:41:THR:N	2.81	0.42
1:B:95:LEU:HB3	4:B:5030:HOH:O	2.20	0.42
1:B:139:SER:CB	3:B:1293:SAM:H5'2	2.50	0.42
1:D:198:LEU:HA	1:D:198:LEU:HD12	1.80	0.42
1:C:187:PRO:HA	1:C:188:PRO:HD3	1.92	0.42
1:D:204:THR:HA	1:D:218:LEU:HD23	2.02	0.42
1:B:145:ASP:OD2	1:B:145:ASP:O	2.38	0.42
1:A:131:ASP:CG	1:A:165:ARG:HH21	2.22	0.42
1:B:65:CYS:HB2	1:B:83:SER:HB3	2.01	0.42
1:A:174:HIS:HE1	1:A:286:HIS:HE2	1.66	0.42
1:B:19:ASP:HB3	1:B:22:ALA:HB2	2.02	0.42
1:C:179:TYR:CE2	1:C:183:THR:HG21	2.55	0.41
1:C:196:SER:OG	1:C:198:LEU:HB2	2.20	0.41
1:D:149:ASP:C	1:D:151:SER:H	2.23	0.41
1:A:103:LYS:HA	1:A:103:LYS:HD3	1.71	0.41
1:B:191:ASN:ND2	1:B:193:TYR:H	2.17	0.41
1:C:116:ASN:OD1	1:C:118:LEU:HB2	2.21	0.41
1:B:187:PRO:HB2	4:B:5120:HOH:O	2.19	0.41
1:C:45:LYS:O	1:C:49:LEU:HB2	2.20	0.41
1:D:118:LEU:HD13	1:D:156:ALA:HB2	2.03	0.41
1:D:35:GLY:HA3	1:D:196:SER:HB2	2.02	0.41
1:A:145:ASP:OD2	1:A:145:ASP:O	2.38	0.41
1:D:140:PHE:CZ	1:D:157:LEU:HD13	2.56	0.41
1:A:118:LEU:HD13	1:A:156:ALA:HB2	2.02	0.41
1:B:45:LYS:O	1:B:49:LEU:HB2	2.20	0.41
1:C:19:ASP:HB3	1:C:22:ALA:HB2	2.03	0.41
1:C:43:GLU:O	1:C:45:LYS:N	2.53	0.41
1:D:210:ASN:HD22	1:D:210:ASN:HA	1.63	0.41
1:A:35:GLY:HA3	1:A:196:SER:HB2	2.01	0.41
1:B:181:LEU:HA	1:B:181:LEU:HD12	1.83	0.41
1:C:36:ASP:CG	1:C:38:ARG:HE	2.23	0.41
1:D:141:ALA:HB1	1:D:242:TYR:HB3	2.01	0.41
1:A:142:HIS:CE1	1:A:242:TYR:HE1	2.38	0.41
1:A:157:LEU:HD12	1:A:157:LEU:HA	1.94	0.41
1:A:209:VAL:HB	1:A:212:LYS:HZ3	1.86	0.41
1:B:208:THR:HG23	1:B:212:LYS:C	2.41	0.41
1:D:130:PHE:O	1:D:165:ARG:HB3	2.21	0.41
1:C:143:LEU:HA	1:C:143:LEU:HD12	1.82	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:204:THR:HA	1:C:218:LEU:HD23	2.03	0.41
1:D:145:ASP:OD2	1:D:145:ASP:O	2.39	0.41
1:C:140:PHE:CZ	1:C:157:LEU:HD13	2.55	0.41
1:C:24:GLY:CA	1:C:89:LYS:HD2	2.51	0.41
1:D:36:ASP:CG	1:D:38:ARG:HE	2.24	0.41
1:D:24:GLY:CA	1:D:89:LYS:HD2	2.51	0.41
1:A:191:ASN:O	1:A:195:LYS:HG2	2.21	0.41
1:B:36:ASP:CG	1:B:38:ARG:HE	2.24	0.41
1:A:251:THR:O	1:A:255:GLN:HG3	2.21	0.41
1:C:219:ASP:OD1	1:C:239:ARG:HB2	2.21	0.41
1:C:23:ASP:OD1	1:C:24:GLY:N	2.54	0.41
1:D:187:PRO:HA	1:D:188:PRO:HD3	1.92	0.41
1:D:192:ILE:HG13	1:D:193:TYR:N	2.35	0.41
1:C:118:LEU:HD13	1:C:156:ALA:HB2	2.02	0.40
1:D:191:ASN:HD22	1:D:194:TYR:N	2.07	0.40
1:A:267:LEU:HB3	1:A:271:LYS:O	2.21	0.40
1:A:37:THR:H	1:A:38:ARG:NH2	2.19	0.40
1:C:105:PRO:O	1:C:109:LYS:HE3	2.22	0.40
1:D:143:LEU:HA	1:D:143:LEU:HD12	1.88	0.40
1:A:176:ASN:ND2	1:A:176:ASN:C	2.75	0.40
1:C:39:SER:O	1:C:195:LYS:HE3	2.20	0.40
1:A:49:LEU:HD12	1:A:49:LEU:HA	1.83	0.40
1:B:150:GLN:O	1:B:153:HIS:HB2	2.21	0.40
1:B:196:SER:OG	1:B:198:LEU:HB2	2.22	0.40
1:A:264:HIS:CE1	1:A:286:HIS:ND1	2.88	0.40
1:A:45:LYS:O	1:A:49:LEU:HB2	2.21	0.40
1:A:89:LYS:NZ	4:A:5159:HOH:O	2.54	0.40
1:B:118:LEU:HA	1:B:118:LEU:HD12	1.93	0.40
1:B:264:HIS:CE1	1:B:286:HIS:ND1	2.89	0.40
1:D:131:ASP:CG	1:D:165:ARG:HH21	2.25	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:227:ALA:N	1:D:53:ARG:NE[2_675]	2.12	0.08

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	273/292 (94%)	252 (92%)	17 (6%)	4 (2%)	10	33
1	B	273/292 (94%)	254 (93%)	15 (6%)	4 (2%)	10	33
1	C	273/292 (94%)	253 (93%)	16 (6%)	4 (2%)	10	33
1	D	273/292 (94%)	252 (92%)	17 (6%)	4 (2%)	10	33
All	All	1092/1168 (94%)	1011 (93%)	65 (6%)	16 (2%)	10	33

All (16) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	44	TYR
1	B	44	TYR
1	C	44	TYR
1	D	44	TYR
1	A	268	GLY
1	D	268	GLY
1	A	270	PHE
1	B	268	GLY
1	B	270	PHE
1	C	150	GLN
1	C	268	GLY
1	A	150	GLN
1	B	150	GLN
1	C	270	PHE
1	D	150	GLN
1	D	270	PHE

5.3.2 Protein sidechains [i](#)

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	229/242 (95%)	181 (79%)	48 (21%)	1	3
1	B	229/242 (95%)	181 (79%)	48 (21%)	1	3
1	C	229/242 (95%)	179 (78%)	50 (22%)	1	3
1	D	229/242 (95%)	179 (78%)	50 (22%)	1	3
All	All	916/968 (95%)	720 (79%)	196 (21%)	1	3

All (196) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ASP
1	A	31	GLN
1	A	32	LEU
1	A	37	THR
1	A	38	ARG
1	A	40	ARG
1	A	41	THR
1	A	43	GLU
1	A	45	LYS
1	A	49	LEU
1	A	53	ARG
1	A	54	GLN
1	A	59	ARG
1	A	82	THR
1	A	83	SER
1	A	90	MET
1	A	91	LEU
1	A	92	LYS
1	A	95	LEU
1	A	96	LYS
1	A	102	ARG
1	A	103	LYS
1	A	118	LEU
1	A	128	ASP
1	A	136	LEU
1	A	147	LYS
1	A	157	LEU
1	A	162	SER
1	A	165	ARG
1	A	169	LEU

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Mol	Chain	Res	Type
1	A	176	ASN
1	A	181	LEU
1	A	182	SER
1	A	190	LYS
1	A	195	LYS
1	A	198	LEU
1	A	211	ASN
1	A	212	LYS
1	A	229	ARG
1	A	230	ASP
1	A	236	SER
1	A	240	LEU
1	A	241	SER
1	A	261	ARG
1	A	263	GLN
1	A	266	VAL
1	A	267	LEU
1	A	271	LYS
1	B	23	ASP
1	B	31	GLN
1	B	32	LEU
1	B	37	THR
1	B	38	ARG
1	B	40	ARG
1	B	41	THR
1	B	43	GLU
1	B	45	LYS
1	B	49	LEU
1	B	54	GLN
1	B	59	ARG
1	B	73	MET
1	B	82	THR
1	B	83	SER
1	B	90	MET
1	B	91	LEU
1	B	92	LYS
1	B	95	LEU
1	B	96	LYS
1	B	102	ARG
1	B	103	LYS
1	B	118	LEU
1	B	128	ASP

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Mol	Chain	Res	Type
1	B	136	LEU
1	B	147	LYS
1	B	157	LEU
1	B	162	SER
1	B	165	ARG
1	B	169	LEU
1	B	176	ASN
1	B	181	LEU
1	B	182	SER
1	B	190	LYS
1	B	195	LYS
1	B	198	LEU
1	B	211	ASN
1	B	212	LYS
1	B	229	ARG
1	B	230	ASP
1	B	236	SER
1	B	240	LEU
1	B	241	SER
1	B	261	ARG
1	B	263	GLN
1	B	266	VAL
1	B	267	LEU
1	B	271	LYS
1	C	23	ASP
1	C	31	GLN
1	C	32	LEU
1	C	37	THR
1	C	38	ARG
1	C	40	ARG
1	C	41	THR
1	C	43	GLU
1	C	45	LYS
1	C	49	LEU
1	C	53	ARG
1	C	54	GLN
1	C	59	ARG
1	C	73	MET
1	C	82	THR
1	C	83	SER
1	C	90	MET
1	C	91	LEU

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Mol	Chain	Res	Type
1	C	92	LYS
1	C	95	LEU
1	C	96	LYS
1	C	102	ARG
1	C	103	LYS
1	C	118	LEU
1	C	128	ASP
1	C	136	LEU
1	C	147	LYS
1	C	157	LEU
1	C	162	SER
1	C	165	ARG
1	C	169	LEU
1	C	176	ASN
1	C	181	LEU
1	C	182	SER
1	C	190	LYS
1	C	195	LYS
1	C	198	LEU
1	C	211	ASN
1	C	212	LYS
1	C	229	ARG
1	C	230	ASP
1	C	236	SER
1	C	240	LEU
1	C	241	SER
1	C	261	ARG
1	C	263	GLN
1	C	266	VAL
1	C	267	LEU
1	C	271	LYS
1	C	291	THR
1	D	23	ASP
1	D	31	GLN
1	D	32	LEU
1	D	37	THR
1	D	38	ARG
1	D	40	ARG
1	D	41	THR
1	D	43	GLU
1	D	45	LYS
1	D	49	LEU

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Mol	Chain	Res	Type
1	D	53	ARG
1	D	54	GLN
1	D	59	ARG
1	D	71	SER
1	D	73	MET
1	D	82	THR
1	D	83	SER
1	D	90	MET
1	D	91	LEU
1	D	92	LYS
1	D	95	LEU
1	D	96	LYS
1	D	102	ARG
1	D	103	LYS
1	D	118	LEU
1	D	128	ASP
1	D	136	LEU
1	D	147	LYS
1	D	157	LEU
1	D	162	SER
1	D	165	ARG
1	D	169	LEU
1	D	176	ASN
1	D	181	LEU
1	D	182	SER
1	D	190	LYS
1	D	195	LYS
1	D	198	LEU
1	D	211	ASN
1	D	212	LYS
1	D	229	ARG
1	D	230	ASP
1	D	236	SER
1	D	240	LEU
1	D	241	SER
1	D	261	ARG
1	D	263	GLN
1	D	266	VAL
1	D	267	LEU
1	D	271	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (34) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	31	GLN
1	A	159	ASN
1	A	174	HIS
1	A	176	ASN
1	A	191	ASN
1	A	210	ASN
1	A	211	ASN
1	A	264	HIS
1	B	31	GLN
1	B	159	ASN
1	B	174	HIS
1	B	176	ASN
1	B	191	ASN
1	B	210	ASN
1	B	211	ASN
1	B	264	HIS
1	C	31	GLN
1	C	159	ASN
1	C	174	HIS
1	C	176	ASN
1	C	191	ASN
1	C	210	ASN
1	C	211	ASN
1	C	264	HIS
1	D	31	GLN
1	D	138	ASN
1	D	159	ASN
1	D	174	HIS
1	D	176	ASN
1	D	191	ASN
1	D	210	ASN
1	D	211	ASN
1	D	263	GLN
1	D	264	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates i

There are no carbohydrates in this entry.

5.6 Ligand geometry i

8 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	ACT	D	3294	-	1,3,3	0.28	0	0,3,3	0.00	-
3	SAM	A	293	-	21,29,29	0.94	1 (4%)	18,42,42	1.26	2 (11%)
3	SAM	C	2293	-	21,29,29	1.06	3 (14%)	18,42,42	1.21	1 (5%)
2	ACT	C	2294	-	1,3,3	1.50	0	0,3,3	0.00	-
3	SAM	B	1293	-	21,29,29	1.01	1 (4%)	18,42,42	1.21	1 (5%)
2	ACT	B	1294	-	1,3,3	0.25	0	0,3,3	0.00	-
3	SAM	D	3293	-	21,29,29	1.02	1 (4%)	18,42,42	1.25	3 (16%)
2	ACT	A	294	-	1,3,3	0.51	0	0,3,3	0.00	-

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	SAM	C	2293	-	-	2/8/33/33	0/3/3/3
3	SAM	A	293	-	-	2/8/33/33	0/3/3/3
3	SAM	B	1293	-	-	2/8/33/33	0/3/3/3
3	SAM	D	3293	-	-	2/8/33/33	0/3/3/3

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	2293	SAM	C2-N3	2.40	1.36	1.32
3	D	3293	SAM	C2-N3	2.37	1.35	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1293	SAM	C2-N3	2.32	1.35	1.32
3	C	2293	SAM	C4-N3	2.21	1.38	1.35
3	A	293	SAM	C2-N3	2.20	1.35	1.32
3	C	2293	SAM	C8-N7	-2.06	1.31	1.34

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	3293	SAM	O2'-C2'-C3'	2.97	121.44	111.82
3	C	2293	SAM	O2'-C2'-C3'	2.88	121.14	111.82
3	A	293	SAM	O2'-C2'-C3'	2.84	121.02	111.82
3	B	1293	SAM	O2'-C2'-C3'	2.75	120.73	111.82
3	A	293	SAM	O3'-C3'-C4'	-2.23	104.61	111.05
3	D	3293	SAM	C2'-C3'-C4'	2.01	106.55	102.64
3	D	3293	SAM	O3'-C3'-C4'	-2.00	105.26	111.05

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	293	SAM	N-CA-CB-CG
3	A	293	SAM	C-CA-CB-CG
3	C	2293	SAM	N-CA-CB-CG
3	C	2293	SAM	C-CA-CB-CG
3	B	1293	SAM	N-CA-CB-CG
3	B	1293	SAM	C-CA-CB-CG
3	D	3293	SAM	N-CA-CB-CG
3	D	3293	SAM	C-CA-CB-CG

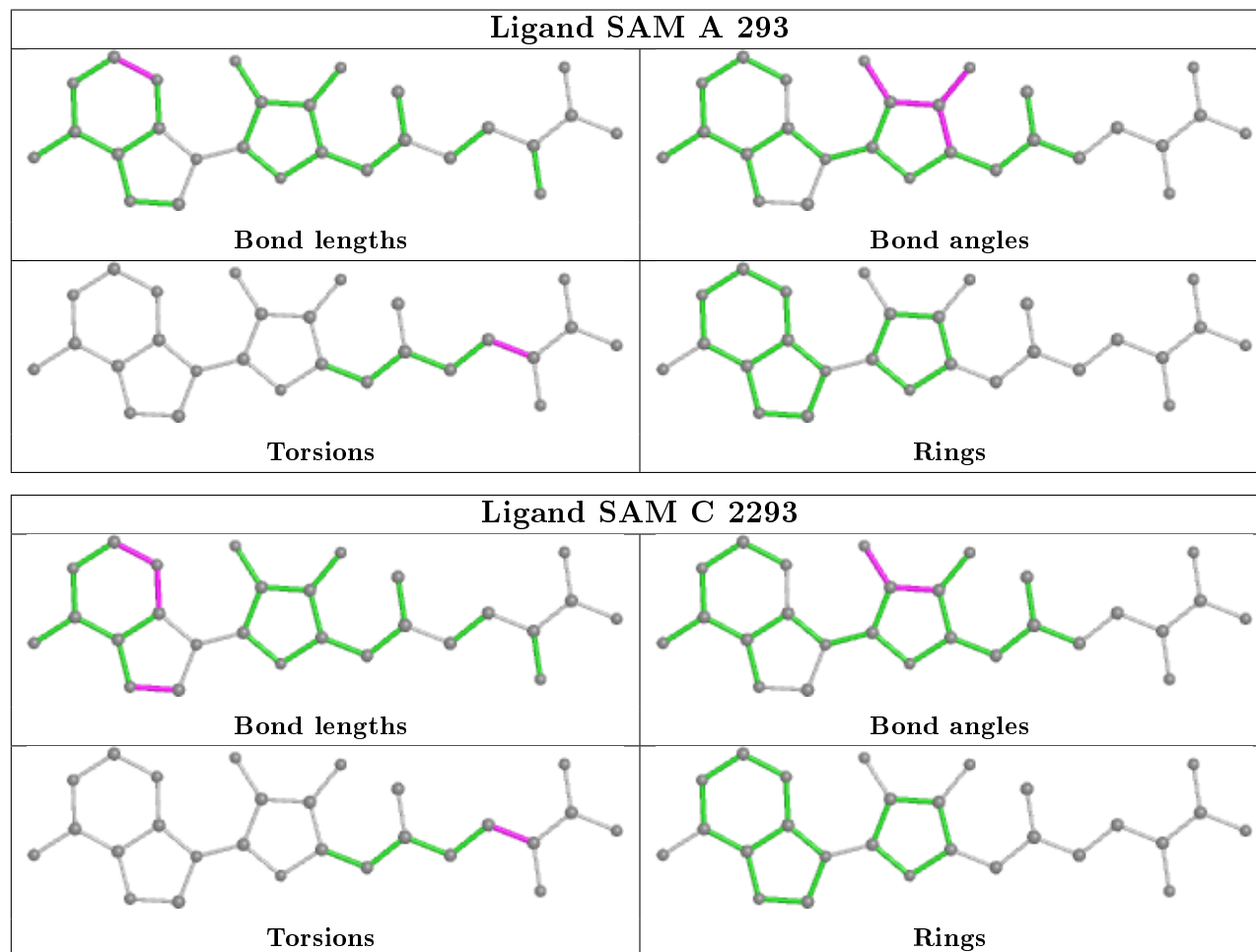
There are no ring outliers.

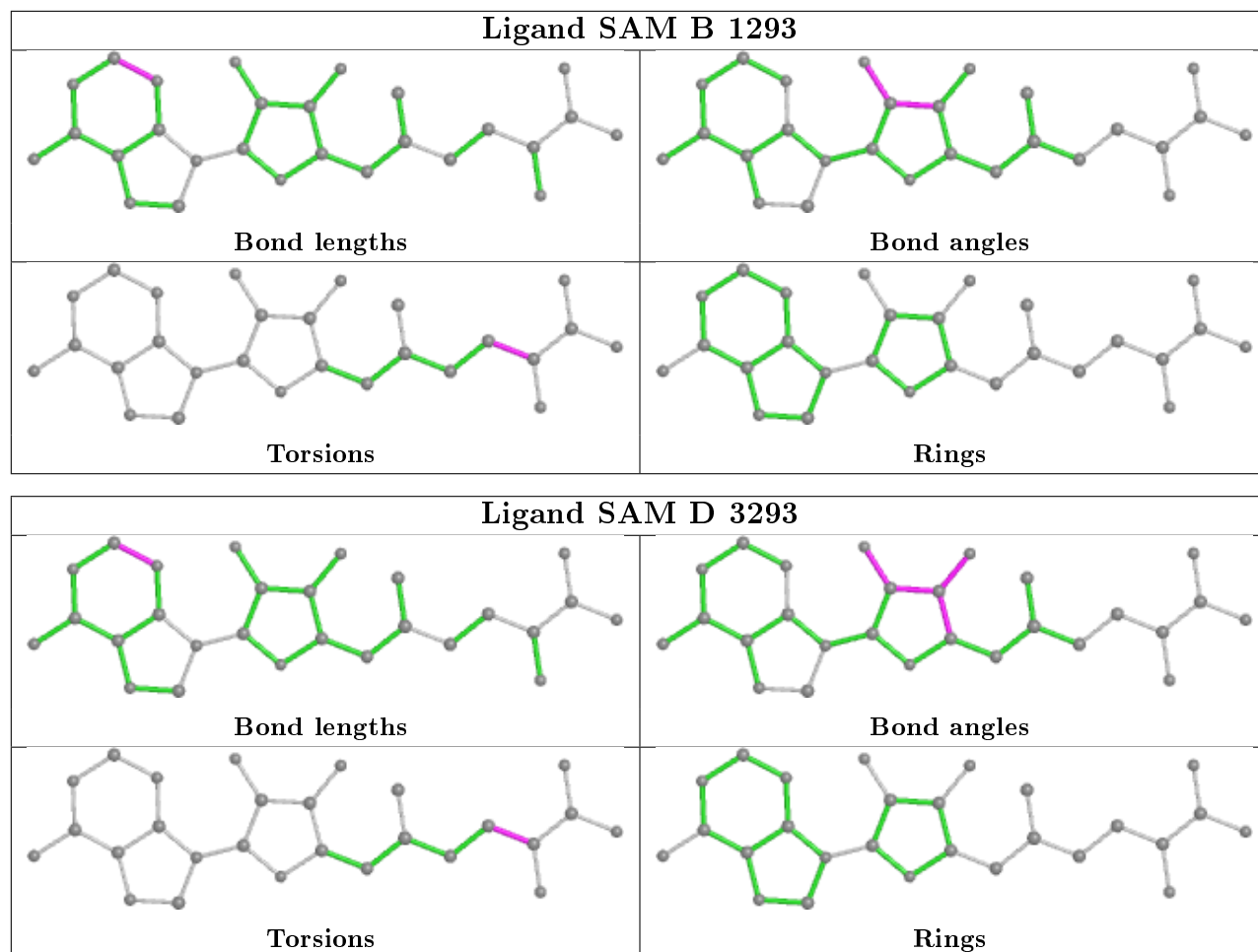
5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	3294	ACT	2	0
3	A	293	SAM	2	0
3	C	2293	SAM	1	0
3	B	1293	SAM	3	0
3	D	3293	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	275/292 (94%)	0.27	12 (4%) 34 24	4, 19, 55, 97	0
1	B	275/292 (94%)	0.12	11 (4%) 38 28	7, 22, 56, 97	0
1	C	275/292 (94%)	0.29	15 (5%) 25 16	6, 24, 60, 97	0
1	D	275/292 (94%)	0.06	12 (4%) 34 24	3, 16, 52, 99	0
All	All	1100/1168 (94%)	0.18	50 (4%) 33 23	3, 21, 57, 99	0

All (50) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	231	GLY	20.0
1	A	231	GLY	19.2
1	A	230	ASP	13.5
1	C	230	ASP	9.6
1	A	232	ALA	9.6
1	A	233	PRO	7.4
1	A	47	TRP	7.3
1	B	230	ASP	7.1
1	C	229	ARG	6.8
1	A	229	ARG	6.5
1	B	228	GLY	5.9
1	C	232	ALA	5.9
1	C	233	PRO	5.2
1	C	228	GLY	5.1
1	C	126	ALA	4.7
1	D	230	ASP	4.2
1	C	226	GLY	4.0
1	B	231	GLY	3.9
1	A	128	ASP	3.8
1	B	292	GLY	3.8
1	D	190	LYS	3.8

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Mol	Chain	Res	Type	RSRZ
1	D	292	GLY	3.8
1	C	292	GLY	3.7
1	A	274	ARG	3.6
1	D	180	ILE	3.5
1	C	202	ILE	3.4
1	B	157	LEU	3.4
1	A	127	GLY	3.3
1	B	190	LYS	3.2
1	D	229	ARG	3.1
1	D	234	GLY	3.1
1	C	190	LYS	3.0
1	D	232	ALA	3.0
1	B	226	GLY	3.0
1	B	229	ARG	2.9
1	D	231	GLY	2.9
1	D	235	PHE	2.8
1	B	58	HIS	2.7
1	A	261	ARG	2.7
1	B	232	ALA	2.7
1	C	220	TYR	2.6
1	A	228	GLY	2.6
1	D	58	HIS	2.6
1	C	238	PHE	2.5
1	A	31	GLN	2.3
1	C	227	ALA	2.3
1	D	128	ASP	2.2
1	B	258	PHE	2.1
1	C	172	ILE	2.1
1	D	233	PRO	2.1

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](#)

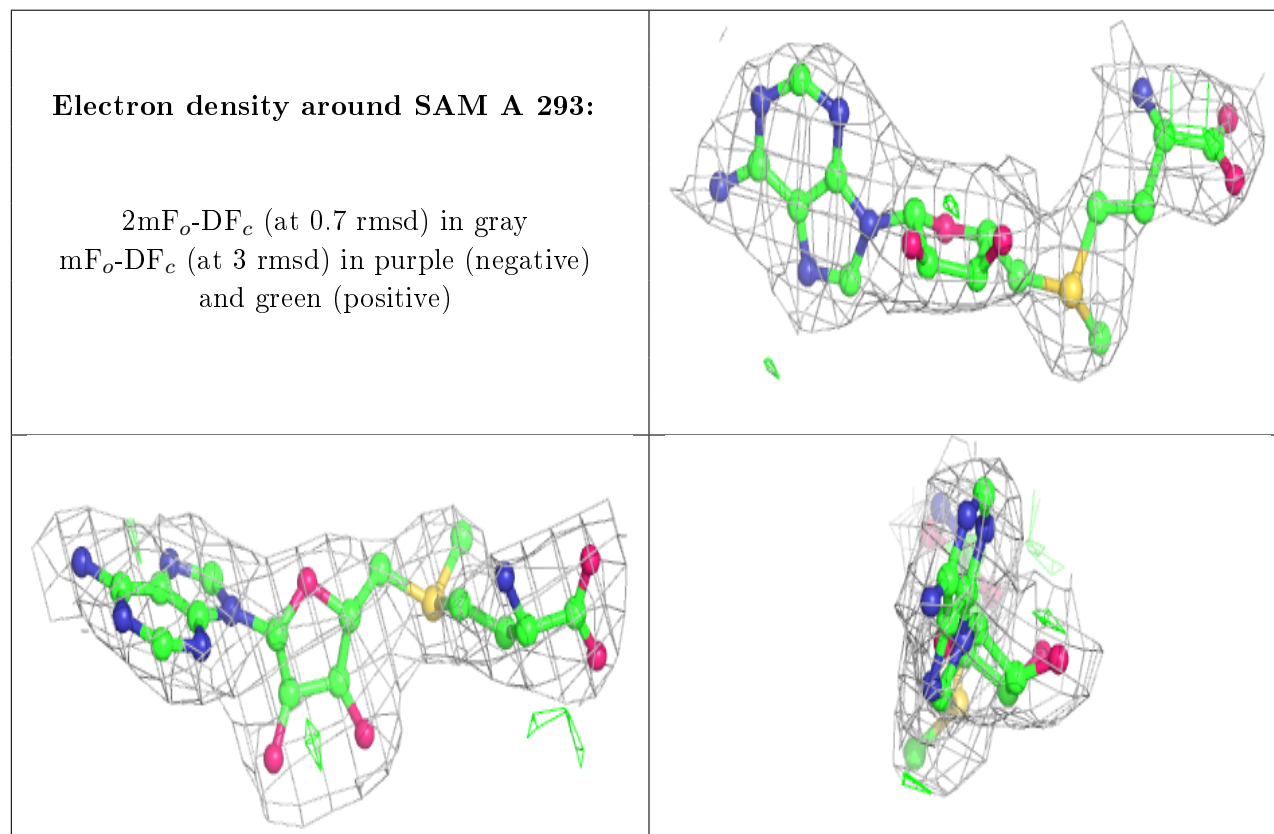
There are no carbohydrates in this entry.

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.

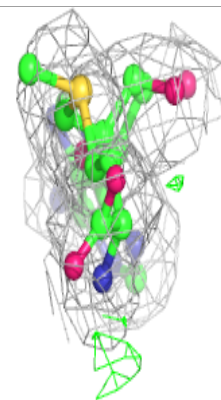
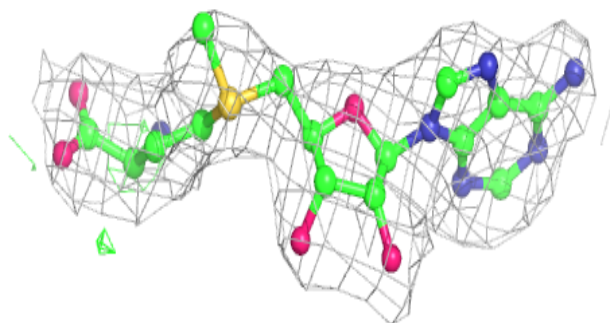
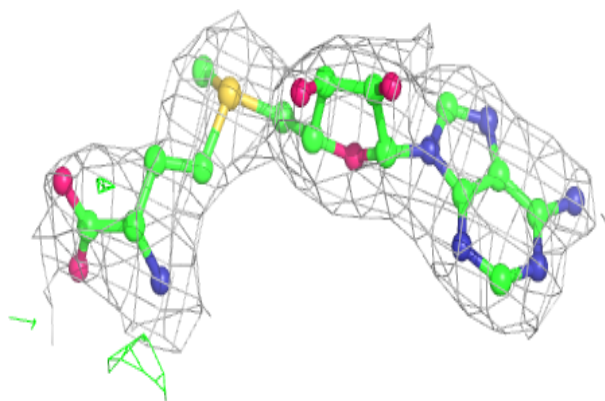
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	ACT	D	3294	4/4	0.91	0.29	2,8,10,11	0
3	SAM	A	293	27/27	0.94	0.19	2,17,25,26	0
3	SAM	C	2293	27/27	0.94	0.17	15,25,36,41	0
3	SAM	B	1293	27/27	0.94	0.22	10,23,37,40	0
3	SAM	D	3293	27/27	0.94	0.21	2,24,35,35	0
2	ACT	C	2294	4/4	0.95	0.35	2,9,17,19	0
2	ACT	B	1294	4/4	0.96	0.24	14,20,23,28	0
2	ACT	A	294	4/4	0.96	0.16	29,30,30,31	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.

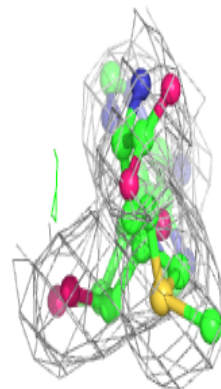
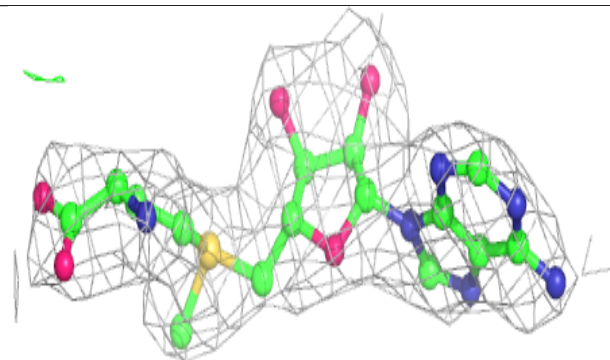
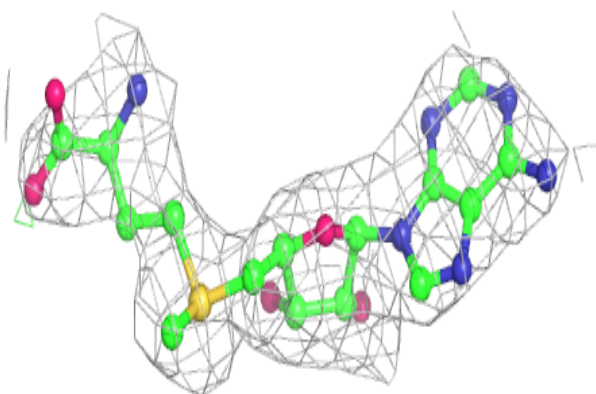


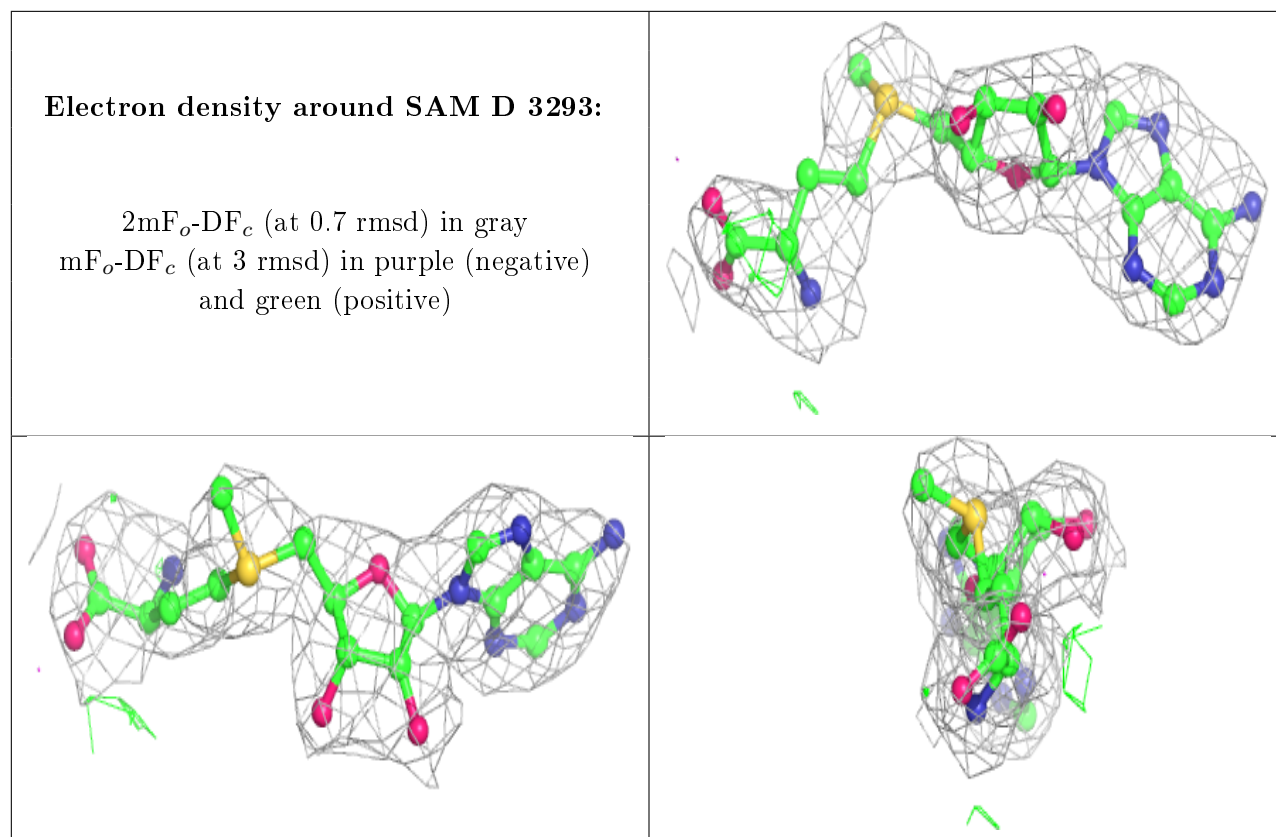
Electron density around SAM C 2293:

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

**Electron density around SAM B 1293:**

$2mF_o-DF_c$ (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.