Full wwPDB X-ray Structure Validation Report (i)

Sep 3, 2023 – 12:10 PM EDT

PDB ID	:	3ROD
Title	:	Methyltransferase
Authors	:	Peng, Y.; Yee, V.C.
Deposited on	:	2011-04-25
Resolution	:	2.72 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 (i) 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 (i)) were used in the production of this report:

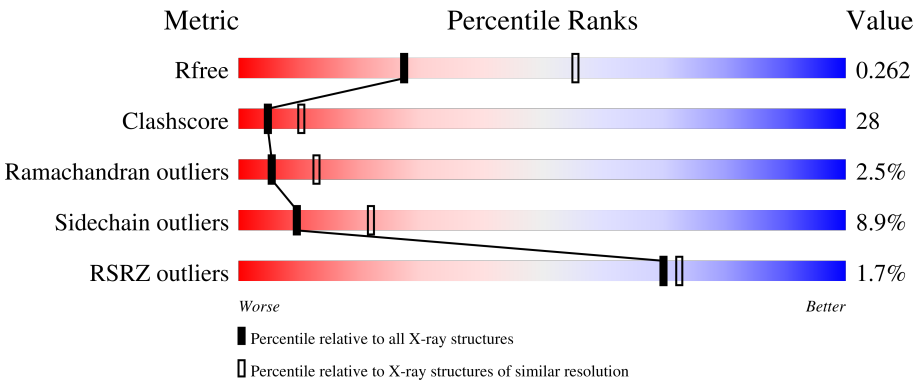
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.72 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	3359 (2.74-2.70)
Clashscore	141614	3686 (2.74-2.70)
Ramachandran outliers	138981	3622 (2.74-2.70)
Sidechain outliers	138945	3623 (2.74-2.70)
RSRZ outliers	127900	3276 (2.74-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	283	% 45% 44% • 8%
1	B	283	% 58% 28% 5% 8%
1	C	283	2% 43% 41% 7% • 8%
1	D	283	2% 47% 37% 7% 9%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 8272 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 Nicotinamide N-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	259	2023	1299	329	384	11	0	0	0
1	B	259	2023	1299	329	384	11	0	0	0
1	C	259	2023	1299	329	384	11	0	0	0
1	D	257	2013	1294	327	381	11	0	0	0

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-18	MET	-	expression tag	UNP P40261
A	-17	GLY	-	expression tag	UNP P40261
A	-16	SER	-	expression tag	UNP P40261
A	-15	SER	-	expression tag	UNP P40261
A	-14	HIS	-	expression tag	UNP P40261
A	-13	HIS	-	expression tag	UNP P40261
A	-12	HIS	-	expression tag	UNP P40261
A	-11	HIS	-	expression tag	UNP P40261
A	-10	HIS	-	expression tag	UNP P40261
A	-9	HIS	-	expression tag	UNP P40261
A	-8	SER	-	expression tag	UNP P40261
A	-7	SER	-	expression tag	UNP P40261
A	-6	GLY	-	expression tag	UNP P40261
A	-5	LEU	-	expression tag	UNP P40261
A	-4	VAL	-	expression tag	UNP P40261
A	-3	PRO	-	expression tag	UNP P40261
A	-2	ARG	-	expression tag	UNP P40261
A	-1	GLY	-	expression tag	UNP P40261
A	0	SER	-	expression tag	UNP P40261
A	100	ALA	LYS	engineered mutation	UNP P40261
A	101	ALA	GLU	engineered mutation	UNP P40261

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Chain	Residue	Modelled	Actual	Comment	Reference
A	103	ALA	GLU	engineered mutation	UNP P40261
B	-18	MET	-	expression tag	UNP P40261
B	-17	GLY	-	expression tag	UNP P40261
B	-16	SER	-	expression tag	UNP P40261
B	-15	SER	-	expression tag	UNP P40261
B	-14	HIS	-	expression tag	UNP P40261
B	-13	HIS	-	expression tag	UNP P40261
B	-12	HIS	-	expression tag	UNP P40261
B	-11	HIS	-	expression tag	UNP P40261
B	-10	HIS	-	expression tag	UNP P40261
B	-9	HIS	-	expression tag	UNP P40261
B	-8	SER	-	expression tag	UNP P40261
B	-7	SER	-	expression tag	UNP P40261
B	-6	GLY	-	expression tag	UNP P40261
B	-5	LEU	-	expression tag	UNP P40261
B	-4	VAL	-	expression tag	UNP P40261
B	-3	PRO	-	expression tag	UNP P40261
B	-2	ARG	-	expression tag	UNP P40261
B	-1	GLY	-	expression tag	UNP P40261
B	0	SER	-	expression tag	UNP P40261
B	100	ALA	LYS	engineered mutation	UNP P40261
B	101	ALA	GLU	engineered mutation	UNP P40261
B	103	ALA	GLU	engineered mutation	UNP P40261
C	-18	MET	-	expression tag	UNP P40261
C	-17	GLY	-	expression tag	UNP P40261
C	-16	SER	-	expression tag	UNP P40261
C	-15	SER	-	expression tag	UNP P40261
C	-14	HIS	-	expression tag	UNP P40261
C	-13	HIS	-	expression tag	UNP P40261
C	-12	HIS	-	expression tag	UNP P40261
C	-11	HIS	-	expression tag	UNP P40261
C	-10	HIS	-	expression tag	UNP P40261
C	-9	HIS	-	expression tag	UNP P40261
C	-8	SER	-	expression tag	UNP P40261
C	-7	SER	-	expression tag	UNP P40261
C	-6	GLY	-	expression tag	UNP P40261
C	-5	LEU	-	expression tag	UNP P40261
C	-4	VAL	-	expression tag	UNP P40261
C	-3	PRO	-	expression tag	UNP P40261
C	-2	ARG	-	expression tag	UNP P40261
C	-1	GLY	-	expression tag	UNP P40261
C	0	SER	-	expression tag	UNP P40261

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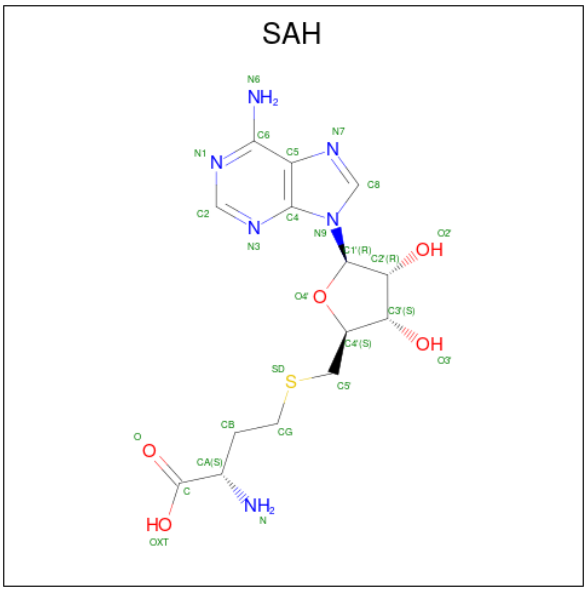
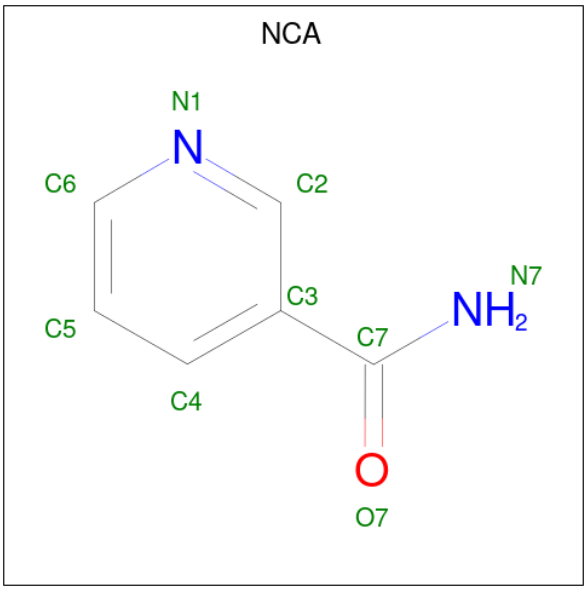
Chain	Residue	Modelled	Actual	Comment	Reference
C	100	ALA	LYS	engineered mutation	UNP P40261
C	101	ALA	GLU	engineered mutation	UNP P40261
C	103	ALA	GLU	engineered mutation	UNP P40261
D	-18	MET	-	expression tag	UNP P40261
D	-17	GLY	-	expression tag	UNP P40261
D	-16	SER	-	expression tag	UNP P40261
D	-15	SER	-	expression tag	UNP P40261
D	-14	HIS	-	expression tag	UNP P40261
D	-13	HIS	-	expression tag	UNP P40261
D	-12	HIS	-	expression tag	UNP P40261
D	-11	HIS	-	expression tag	UNP P40261
D	-10	HIS	-	expression tag	UNP P40261
D	-9	HIS	-	expression tag	UNP P40261
D	-8	SER	-	expression tag	UNP P40261
D	-7	SER	-	expression tag	UNP P40261
D	-6	GLY	-	expression tag	UNP P40261
D	-5	LEU	-	expression tag	UNP P40261
D	-4	VAL	-	expression tag	UNP P40261
D	-3	PRO	-	expression tag	UNP P40261
D	-2	ARG	-	expression tag	UNP P40261
D	-1	GLY	-	expression tag	UNP P40261
D	0	SER	-	expression tag	UNP P40261
D	100	ALA	LYS	engineered mutation	UNP P40261
D	101	ALA	GLU	engineered mutation	UNP P40261
D	103	ALA	GLU	engineered mutation	UNP P40261

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	B	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	C	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 3 is NICOTINAMIDE (three-letter code: NCA) (formula: $C_6H_6N_2O$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
3	A	1	9	6	2	1	0	0
3	B	1	9	6	2	1	0	0
3	C	1	9	6	2	1	0	0
3	D	1	9	6	2	1	0	0

- Molecule 4 is water.

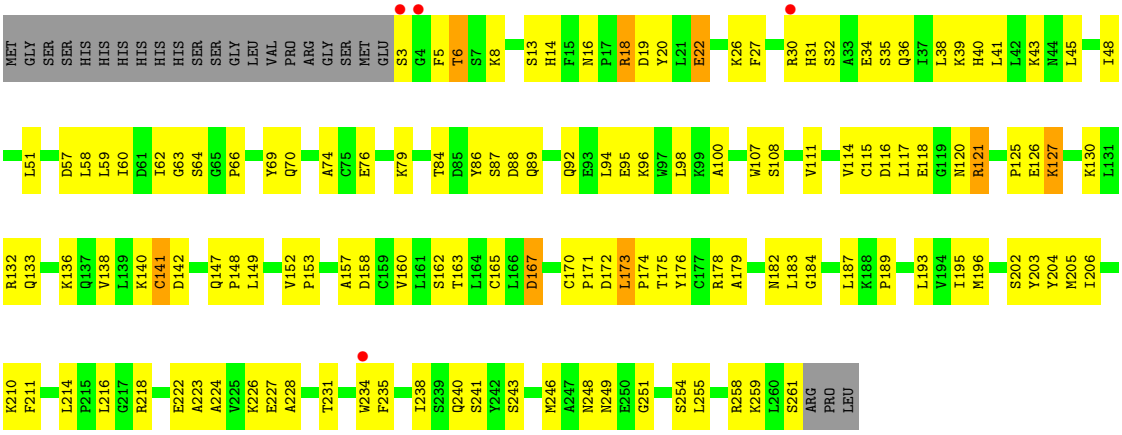
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	A	18	18	18	0	0
4	B	13	13	13	0	0
4	C	16	16	16	0	0
4	D	3	3	3	0	0

3 Residue-property plots (i)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

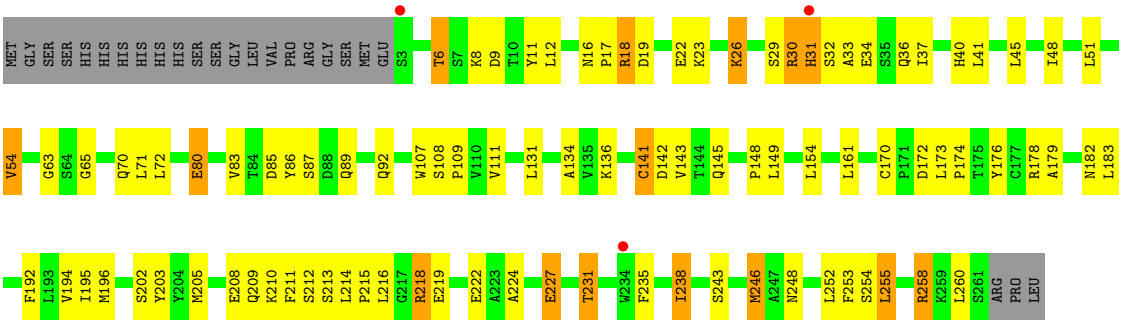
• Molecule 1: Nicotinamide N-methyltransferase

Chain A:



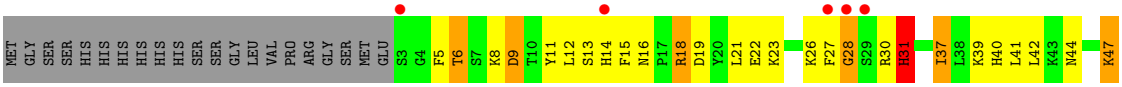
• Molecule 1: Nicotinamide N-methyltransferase

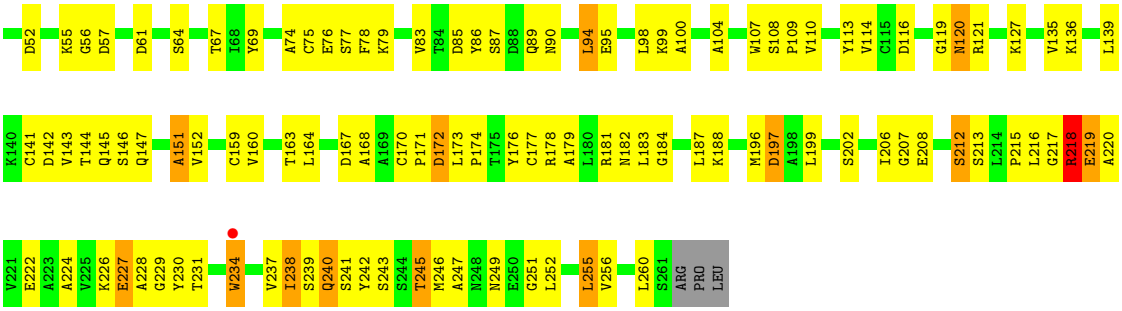
Chain B:



• Molecule 1: Nicotinamide N-methyltransferase

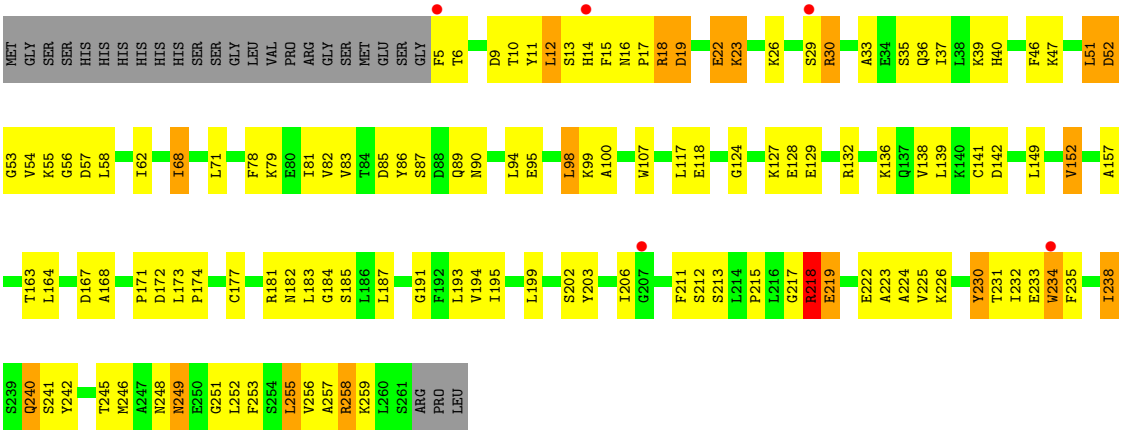
Chain C:





- Molecule 1: Nicotinamide N-methyltransferase

Chain D:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α, β, γ	60.66Å 61.79Å 74.34Å 106.57° 103.98° 104.14°	Depositor
Resolution (Å)	39.67 – 2.72 39.67 – 2.72	Depositor EDS
% Data completeness (in resolution range)	98.0 (39.67-2.72) 98.1 (39.67-2.72)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$< I/\sigma(I) >$ [1]	2.20 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.205 , 0.264 0.206 , 0.262	Depositor DCC
R_{free} test set	1272 reflections (5.10%)	wwPDB-VP
Wilson B-factor (Å^2)	41.6	Xtriage
Anisotropy	0.099	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 45.0	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.000 for -k,-h,-l	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	8272	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 7.52% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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

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	0.85	0/2067	0.81	0/2799
1	B	0.82	0/2067	0.81	0/2799
1	C	0.79	1/2067 (0.0%)	0.83	0/2799
1	D	0.77	0/2057	0.78	0/2786
All	All	0.81	1/8258 (0.0%)	0.81	0/11183

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	47	LYS	CD-CE	5.70	1.65	1.51

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	2023	0	2029	101	0
1	B	2023	0	2029	90	0
1	C	2023	0	2029	133	0
1	D	2013	0	2021	138	0
2	A	26	0	19	2	0
2	B	26	0	19	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	26	0	19	2	0
2	D	26	0	19	2	0
3	A	9	0	6	1	0
3	B	9	0	6	0	0
3	C	9	0	6	1	0
3	D	9	0	6	2	0
4	A	18	0	0	0	0
4	B	13	0	0	0	0
4	C	16	0	0	0	0
4	D	3	0	0	0	0
All	All	8272	0	8208	455	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 28.

All (455) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:205:MET:SD	1:B:210:LYS:HE2	1.96	1.05
1:A:196:MET:HG2	1:A:254:SER:HB2	1.40	1.03
1:C:47:LYS:HD2	1:C:234:TRP:CH2	1.94	1.02
1:B:45:LEU:HD21	1:B:196:MET:HE2	1.43	0.99
1:C:41:LEU:HD22	1:C:196:MET:HE3	1.46	0.97
1:C:199:LEU:HD22	1:C:217:GLY:HA2	1.43	0.97
1:D:36:GLN:HE22	1:D:39:LYS:HD2	1.32	0.95
1:C:47:LYS:HD2	1:C:234:TRP:CZ3	2.02	0.95
1:A:94:LEU:O	1:A:98:LEU:HD13	1.66	0.95
1:D:47:LYS:HG2	1:D:234:TRP:HH2	1.30	0.93
1:D:172:ASP:OD1	1:D:174:PRO:HD2	1.73	0.87
1:A:121:ARG:NH1	1:A:121:ARG:HB3	1.88	0.87
1:D:57:ASP:HA	1:D:79:LYS:HE2	1.57	0.87
1:D:12:LEU:HD12	1:D:12:LEU:H	1.38	0.87
1:C:47:LYS:HG3	1:D:47:LYS:HD3	1.55	0.87
1:A:202:SER:HB3	1:A:248:ASN:HD21	1.40	0.85
1:D:182:ASN:O	1:D:185:SER:HB3	1.76	0.84
1:D:9:ASP:HA	1:D:12:LEU:HD13	1.60	0.82
1:A:121:ARG:HH21	1:C:30:ARG:HB3	1.44	0.82
1:D:226:LYS:HA	1:D:230:TYR:O	1.79	0.81
1:C:27:PHE:CG	1:C:28:GLY:N	2.49	0.81
1:D:230:TYR:HB3	1:D:258:ARG:O	1.82	0.80
1:A:121:ARG:HB3	1:A:121:ARG:HH11	1.45	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:47:LYS:HG2	1:D:234:TRP:CH2	2.17	0.79
1:D:206:ILE:HG22	1:D:206:ILE:O	1.82	0.79
1:C:41:LEU:HD22	1:C:196:MET:CE	2.13	0.79
1:D:62:ILE:HD12	1:D:141:CYS:SG	2.22	0.79
1:C:23:LYS:HD2	1:C:207:GLY:HA2	1.64	0.78
1:C:47:LYS:CG	1:D:47:LYS:HD3	2.13	0.78
1:C:40:HIS:NE2	1:C:238:ILE:HG21	1.99	0.78
1:B:214:LEU:HD23	1:B:216:LEU:HD11	1.65	0.77
1:A:18:ARG:H	1:A:18:ARG:CD	1.98	0.77
1:A:45:LEU:HD21	1:A:196:MET:CE	2.15	0.77
1:D:187:LEU:HD22	1:D:191:GLY:HA3	1.67	0.77
1:D:13:SER:HB3	1:D:14:HIS:CE1	2.19	0.76
1:C:219:GLU:H	1:C:219:GLU:CD	1.88	0.76
1:D:225:VAL:HG21	1:D:255:LEU:HD21	1.68	0.76
1:D:238:ILE:HD13	1:D:238:ILE:H	1.51	0.76
1:D:5:PHE:N	1:D:212:SER:HG	1.84	0.75
1:B:18:ARG:CD	1:B:18:ARG:H	1.99	0.75
1:D:233:GLU:HB2	1:D:256:VAL:O	1.86	0.74
1:C:47:LYS:HD2	1:C:234:TRP:HH2	1.49	0.74
1:D:255:LEU:HD12	1:D:256:VAL:N	2.02	0.74
1:D:164:LEU:O	3:D:302:NCA:N7	2.20	0.74
1:A:205:MET:SD	1:A:210:LYS:HB2	2.27	0.74
1:C:27:PHE:CD2	1:C:28:GLY:N	2.54	0.74
1:D:18:ARG:O	1:D:22:GLU:HB2	1.86	0.74
1:B:45:LEU:HD21	1:B:196:MET:CE	2.17	0.74
1:C:242:TYR:O	1:C:243:SER:C	2.25	0.72
1:B:194:VAL:O	1:B:195:ILE:HD13	1.90	0.71
1:D:18:ARG:HB2	1:D:18:ARG:HH21	1.56	0.71
1:D:193:LEU:HD11	1:D:195:ILE:HD11	1.73	0.71
1:C:18:ARG:O	1:C:22:GLU:HB2	1.92	0.70
1:D:219:GLU:CD	1:D:219:GLU:H	1.94	0.69
1:D:251:GLY:C	1:D:252:LEU:HD12	2.13	0.69
1:A:45:LEU:HD21	1:A:196:MET:HE2	1.75	0.69
1:A:214:LEU:HD23	1:A:216:LEU:HD11	1.75	0.69
1:A:235:PHE:CE1	1:A:255:LEU:HD23	2.29	0.68
1:D:238:ILE:HD11	1:D:252:LEU:HB2	1.74	0.68
1:A:218:ARG:HD3	1:B:218:ARG:NH2	2.09	0.68
1:D:36:GLN:NE2	1:D:39:LYS:HD2	2.07	0.68
1:D:234:TRP:HB3	1:D:256:VAL:HB	1.74	0.67
1:B:89:GLN:HA	1:B:92:GLN:HG3	1.76	0.67
1:C:240:GLN:O	1:C:251:GLY:HA2	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:149:LEU:O	1:D:152:VAL:HG22	1.93	0.67
1:A:36:GLN:OE1	1:A:39:LYS:NZ	2.27	0.67
1:B:16:ASN:OD1	1:B:18:ARG:HD3	1.94	0.67
1:D:12:LEU:HD12	1:D:12:LEU:N	2.09	0.67
1:C:160:VAL:HG23	1:C:187:LEU:HG	1.77	0.67
1:B:108:SER:N	1:B:109:PRO:CD	2.58	0.66
1:B:37:ILE:HD13	1:B:252:LEU:HD11	1.77	0.66
1:C:42:LEU:HD13	1:C:113:TYR:HD2	1.60	0.66
1:B:71:LEU:HD11	1:B:83:VAL:CG1	2.25	0.66
1:B:218:ARG:HG2	1:B:235:PHE:CE2	2.31	0.66
1:A:173:LEU:HB3	1:A:174:PRO:HD3	1.78	0.65
1:D:230:TYR:HD1	1:D:258:ARG:O	1.79	0.65
1:C:234:TRP:CD1	1:C:234:TRP:C	2.69	0.65
1:C:61:ASP:OD2	1:C:64:SER:HB3	1.97	0.65
1:C:5:PHE:HD1	1:C:171:PRO:HB3	1.62	0.64
1:B:9:ASP:HA	1:B:12:LEU:HB2	1.79	0.64
1:D:118:GLU:OE1	1:D:127:LYS:NZ	2.25	0.64
1:D:33:ALA:O	1:D:37:ILE:HG13	1.97	0.64
1:C:41:LEU:CD2	1:C:196:MET:HE3	2.27	0.64
1:B:238:ILE:HD13	1:B:238:ILE:O	1.98	0.64
1:D:163:THR:O	2:D:301:SAH:N	2.31	0.63
1:D:94:LEU:HD22	1:D:98:LEU:HD22	1.80	0.63
1:D:234:TRP:CD1	1:D:234:TRP:C	2.70	0.63
1:A:121:ARG:H	1:A:121:ARG:HD2	1.64	0.63
1:D:10:THR:HA	1:D:13:SER:HB2	1.81	0.63
1:D:26:LYS:HB2	1:D:30:ARG:NH2	2.14	0.63
1:C:170:CYS:SG	1:C:176:TYR:HA	2.40	0.62
1:A:107:TRP:O	1:A:111:VAL:HG23	2.00	0.61
1:A:27:PHE:HD2	1:A:38:LEU:HD23	1.66	0.61
1:C:163:THR:O	2:C:301:SAH:N	2.34	0.61
1:D:85:ASP:O	1:D:141:CYS:N	2.33	0.61
1:A:27:PHE:CD2	1:A:38:LEU:HD23	2.36	0.61
1:A:223:ALA:O	1:A:227:GLU:HG2	2.00	0.61
1:B:71:LEU:HD11	1:B:83:VAL:HG11	1.82	0.61
1:C:224:ALA:HA	1:C:227:GLU:HB2	1.80	0.61
1:D:37:ILE:O	1:D:40:HIS:N	2.33	0.61
1:A:45:LEU:HD21	1:A:196:MET:HE1	1.81	0.61
1:C:172:ASP:OD2	1:C:174:PRO:HD2	2.01	0.61
1:D:36:GLN:NE2	1:D:36:GLN:HA	2.15	0.60
1:A:63:GLY:O	2:A:301:SAH:N	2.34	0.60
1:D:167:ASP:O	1:D:213:SER:HA	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:230:TYR:CD1	1:D:258:ARG:O	2.54	0.60
1:B:8:LYS:HB2	1:B:86:TYR:CE2	2.37	0.60
1:C:37:ILE:CD1	1:C:240:GLN:HG3	2.31	0.60
1:C:99:LYS:O	1:C:100:ALA:HB3	2.02	0.60
1:C:255:LEU:C	1:C:255:LEU:HD12	2.21	0.60
1:B:255:LEU:HD23	1:B:255:LEU:O	2.02	0.59
1:D:240:GLN:O	1:D:251:GLY:HA2	2.01	0.59
1:A:40:HIS:CD2	1:A:238:ILE:HG21	2.36	0.59
1:B:248:ASN:O	1:B:248:ASN:CG	2.40	0.59
1:D:258:ARG:NH1	1:D:258:ARG:HG2	2.17	0.59
1:D:12:LEU:HD11	1:D:86:TYR:CE2	2.37	0.59
1:C:15:PHE:HD2	1:C:90:ASN:HD21	1.49	0.59
1:D:6:THR:H	1:D:212:SER:HB3	1.66	0.59
1:C:56:GLY:O	1:C:78:PHE:HA	2.03	0.59
1:A:167:ASP:OD1	1:A:216:LEU:HD12	2.03	0.59
1:C:94:LEU:O	1:C:98:LEU:HD22	2.02	0.59
1:B:143:VAL:HG12	1:B:183:LEU:HD21	1.84	0.58
1:B:179:ALA:O	1:B:183:LEU:HG	2.03	0.58
1:D:139:LEU:HD12	1:D:149:LEU:HD13	1.83	0.58
1:C:40:HIS:CD2	1:C:238:ILE:HG21	2.38	0.58
1:A:171:PRO:HD2	1:A:175:THR:HG21	1.85	0.58
1:B:30:ARG:HD3	1:B:31:HIS:N	2.18	0.58
1:C:164:LEU:HD23	1:C:197:ASP:HA	1.85	0.58
1:B:30:ARG:O	1:B:32:SER:N	2.37	0.58
1:A:206:ILE:HD12	1:A:211:PHE:CE2	2.38	0.58
1:C:184:GLY:CA	1:C:230:TYR:OH	2.51	0.58
1:B:141:CYS:SG	1:B:142:ASP:N	2.76	0.58
1:B:80:GLU:HB3	1:B:136:LYS:HG3	1.86	0.57
1:A:40:HIS:NE2	1:A:238:ILE:HG21	2.19	0.57
1:D:258:ARG:HG2	1:D:258:ARG:HH11	1.70	0.57
1:B:202:SER:HA	1:B:213:SER:O	2.04	0.57
1:D:11:TYR:OH	1:D:168:ALA:HB1	2.04	0.57
1:C:243:SER:C	1:C:245:THR:H	2.07	0.57
1:A:238:ILE:O	1:A:238:ILE:HG13	2.04	0.57
1:C:170:CYS:HB3	1:C:176:TYR:HB2	1.86	0.57
1:D:19:ASP:O	1:D:23:LYS:HB2	2.05	0.57
1:C:41:LEU:HD21	1:C:252:LEU:HD23	1.85	0.57
1:C:255:LEU:HD12	1:C:256:VAL:N	2.19	0.57
1:D:12:LEU:HD11	1:D:86:TYR:HE2	1.70	0.56
1:C:37:ILE:HD11	1:C:240:GLN:HG3	1.87	0.56
1:D:53:GLY:O	1:D:55:LYS:HG3	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:161:LEU:CD1	1:B:194:VAL:HB	2.35	0.56
1:A:170:CYS:SG	1:A:176:TYR:HA	2.45	0.56
1:B:194:VAL:C	1:B:195:ILE:HD13	2.26	0.56
1:A:60:ILE:HD13	1:A:157:ALA:HB2	1.88	0.56
1:C:16:ASN:OD1	1:C:18:ARG:HD3	2.06	0.56
1:D:89:GLN:OE1	1:D:89:GLN:N	2.35	0.56
1:A:238:ILE:HD12	1:A:240:GLN:HB3	1.88	0.55
1:C:18:ARG:HH21	1:C:18:ARG:HB2	1.71	0.55
1:D:234:TRP:CD1	1:D:235:PHE:N	2.74	0.55
1:B:214:LEU:HD21	1:B:216:LEU:HD21	1.88	0.55
1:B:161:LEU:HD13	1:B:194:VAL:HB	1.88	0.55
1:C:47:LYS:HD2	1:C:234:TRP:HZ3	1.65	0.55
1:D:213:SER:O	1:D:215:PRO:HD3	2.07	0.55
1:B:218:ARG:HG3	1:B:218:ARG:HH11	1.71	0.55
1:B:30:ARG:HD3	1:B:31:HIS:H	1.72	0.55
1:B:196:MET:HG2	1:B:254:SER:HB2	1.89	0.55
1:C:5:PHE:CD1	1:C:171:PRO:HB3	2.41	0.55
1:B:218:ARG:NE	1:B:222:GLU:OE2	2.40	0.55
1:D:219:GLU:OE1	1:D:219:GLU:N	2.38	0.55
1:B:18:ARG:H	1:B:18:ARG:HD2	1.70	0.55
1:C:13:SER:HB2	1:C:14:HIS:ND1	2.22	0.55
1:C:23:LYS:HZ3	1:C:246:MET:CG	2.19	0.55
1:C:47:LYS:HG3	1:D:47:LYS:CD	2.33	0.55
1:D:5:PHE:N	1:D:171:PRO:HB3	2.22	0.55
1:D:47:LYS:HE2	1:D:52:ASP:OD2	2.07	0.54
1:A:240:GLN:O	1:A:251:GLY:HA2	2.07	0.54
1:B:80:GLU:HB3	1:B:136:LYS:CG	2.38	0.54
1:C:207:GLY:O	1:C:208:GLU:HG2	2.08	0.54
1:D:16:ASN:OD1	1:D:18:ARG:HD3	2.08	0.54
1:B:208:GLU:O	1:B:208:GLU:HG3	2.07	0.54
1:C:42:LEU:HD13	1:C:113:TYR:CD2	2.39	0.54
1:C:173:LEU:N	1:C:174:PRO:HD3	2.23	0.54
1:A:64:SER:O	2:A:301:SAH:HA	2.08	0.53
1:C:31:HIS:CE1	1:C:39:LYS:NZ	2.76	0.53
1:C:142:ASP:HA	2:C:301:SAH:N1	2.22	0.53
1:A:76:GLU:OE2	1:A:130:LYS:HD3	2.09	0.53
1:C:173:LEU:N	1:C:174:PRO:CD	2.71	0.53
1:B:107:TRP:O	1:B:111:VAL:HG23	2.08	0.53
1:A:115:CYS:O	1:A:120:ASN:HA	2.08	0.53
1:C:47:LYS:CD	1:C:234:TRP:HH2	2.21	0.53
1:C:215:PRO:O	1:C:216:LEU:HD23	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:15:PHE:CE1	1:C:206:ILE:HD11	2.44	0.53
1:D:157:ALA:O	1:D:187:LEU:HD23	2.08	0.53
1:B:231:THR:HG22	1:B:260:LEU:CD2	2.38	0.53
1:C:234:TRP:C	1:C:234:TRP:HD1	2.12	0.53
1:A:18:ARG:H	1:A:18:ARG:HD2	1.71	0.52
1:A:22:GLU:O	1:A:26:LYS:HD3	2.09	0.52
1:A:203:TYR:C	1:A:203:TYR:CD1	2.82	0.52
1:C:216:LEU:HD22	1:C:220:ALA:HB1	1.91	0.52
1:D:193:LEU:CD1	1:D:195:ILE:HD11	2.39	0.52
1:D:193:LEU:HD22	1:D:230:TYR:CE1	2.44	0.52
1:C:179:ALA:HA	1:C:182:ASN:HB2	1.90	0.52
1:D:202:SER:HA	1:D:213:SER:O	2.08	0.52
1:A:196:MET:HG2	1:A:254:SER:CB	2.25	0.52
1:B:148:PRO:O	1:B:149:LEU:HD23	2.09	0.52
1:D:206:ILE:O	1:D:206:ILE:CG2	2.55	0.52
1:D:6:THR:H	1:D:212:SER:CB	2.22	0.52
1:D:12:LEU:H	1:D:12:LEU:CD1	2.15	0.52
1:D:62:ILE:HG13	1:D:183:LEU:CD2	2.40	0.52
1:C:61:ASP:OD2	1:C:64:SER:CB	2.57	0.52
1:D:11:TYR:O	1:D:15:PHE:HB3	2.10	0.52
1:B:22:GLU:O	1:B:26:LYS:HG2	2.10	0.52
1:A:66:PRO:C	1:A:94:LEU:HD21	2.31	0.52
1:D:17:PRO:HG3	1:D:90:ASN:OD1	2.10	0.52
1:B:149:LEU:HD12	1:B:154:LEU:HD12	1.93	0.51
1:B:203:TYR:CD1	1:B:203:TYR:C	2.84	0.51
1:D:127:LYS:O	1:D:127:LYS:HG3	2.10	0.51
1:A:63:GLY:HA3	1:A:165:CYS:SG	2.49	0.51
1:B:203:TYR:CE2	1:B:248:ASN:HB3	2.46	0.51
1:A:8:LYS:NZ	1:A:142:ASP:OD2	2.41	0.51
1:C:170:CYS:CB	1:C:176:TYR:HB2	2.40	0.51
1:A:16:ASN:OD1	1:A:18:ARG:HD3	2.10	0.51
1:B:218:ARG:HG3	1:B:218:ARG:NH1	2.25	0.51
1:A:8:LYS:HB3	1:A:86:TYR:CE2	2.46	0.51
1:C:145:GLN:HA	1:C:145:GLN:OE1	2.10	0.51
1:D:195:ILE:HD13	1:D:195:ILE:N	2.25	0.51
1:C:69:TYR:HB3	1:C:107:TRP:CZ3	2.45	0.51
1:C:242:TYR:O	1:C:243:SER:O	2.28	0.51
1:C:119:GLY:O	1:C:121:ARG:N	2.44	0.51
1:C:246:MET:O	1:C:247:ALA:HB2	2.12	0.51
1:A:41:LEU:O	1:A:45:LEU:HG	2.11	0.50
1:B:33:ALA:O	1:B:37:ILE:HG13	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:13:SER:HG	1:A:14:HIS:HD1	1.53	0.50
1:A:39:LYS:O	1:A:43:LYS:HG3	2.12	0.50
1:B:41:LEU:O	1:B:45:LEU:HG	2.10	0.50
1:C:234:TRP:HB3	1:C:256:VAL:HB	1.94	0.50
1:A:172:ASP:OD1	1:A:174:PRO:HD2	2.11	0.50
1:C:9:ASP:HA	1:C:12:LEU:HD12	1.93	0.50
1:B:205:MET:SD	1:B:210:LYS:CE	2.86	0.50
1:C:57:ASP:HA	1:C:79:LYS:HG2	1.93	0.50
1:D:194:VAL:C	1:D:195:ILE:HD13	2.32	0.50
1:A:62:ILE:HG13	1:A:183:LEU:HD22	1.94	0.50
1:D:68:ILE:HD11	1:D:107:TRP:CG	2.47	0.50
1:D:187:LEU:O	1:D:259:LYS:NZ	2.44	0.50
1:A:222:GLU:O	1:A:226:LYS:HG3	2.12	0.49
1:C:168:ALA:HB2	3:C:302:NCA:N7	2.27	0.49
1:D:149:LEU:O	1:D:152:VAL:CG2	2.59	0.49
1:B:255:LEU:HD23	1:B:255:LEU:C	2.33	0.49
1:C:206:ILE:O	1:C:208:GLU:N	2.45	0.49
1:A:58:LEU:HD21	1:A:60:ILE:HD11	1.95	0.49
1:A:241:SER:HA	1:A:249:ASN:HD21	1.77	0.49
1:D:68:ILE:HD11	1:D:107:TRP:CD2	2.47	0.49
1:D:129:GLU:OE1	1:D:129:GLU:HA	2.11	0.49
1:A:48:ILE:HG12	1:A:234:TRP:HZ2	1.77	0.49
1:A:95:GLU:OE2	1:A:138:VAL:HG21	2.12	0.49
1:D:37:ILE:HD12	1:D:242:TYR:CE1	2.46	0.49
1:A:114:VAL:O	1:A:118:GLU:HG3	2.13	0.49
1:D:95:GLU:HA	1:D:98:LEU:HB2	1.94	0.49
1:C:23:LYS:HD3	1:C:207:GLY:H	1.78	0.49
1:C:238:ILE:HG12	1:C:238:ILE:O	2.13	0.49
1:D:99:LYS:O	1:D:100:ALA:C	2.50	0.49
1:C:113:TYR:O	1:C:116:ASP:HB2	2.13	0.48
1:C:151:ALA:O	1:C:152:VAL:C	2.51	0.48
1:D:203:TYR:HA	1:D:211:PHE:O	2.13	0.48
1:B:71:LEU:HB3	1:B:131:LEU:HD11	1.95	0.48
1:B:173:LEU:HD12	1:B:173:LEU:HA	1.63	0.48
1:B:231:THR:HG22	1:B:260:LEU:HD23	1.93	0.48
1:C:21:LEU:CD2	1:C:67:THR:HG22	2.43	0.48
1:A:173:LEU:O	1:A:176:TYR:HB3	2.14	0.48
1:C:219:GLU:CD	1:C:219:GLU:N	2.61	0.48
1:A:5:PHE:O	1:A:6:THR:C	2.51	0.48
1:A:116:ASP:O	1:A:117:LEU:C	2.52	0.48
1:C:127:LYS:O	1:C:127:LYS:HG3	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:234:TRP:C	1:D:234:TRP:HD1	2.14	0.48
1:A:224:ALA:O	1:A:228:ALA:HB2	2.14	0.48
1:B:253:PHE:CD1	1:B:253:PHE:C	2.86	0.48
1:C:237:VAL:O	1:C:238:ILE:CG2	2.62	0.48
1:A:76:GLU:CG	1:A:127:LYS:HZ1	2.27	0.48
1:C:85:ASP:N	1:C:141:CYS:HB2	2.29	0.48
1:D:171:PRO:O	1:D:172:ASP:HB3	2.14	0.48
1:C:242:TYR:C	1:C:243:SER:O	2.53	0.47
1:B:31:HIS:ND1	1:B:36:GLN:NE2	2.62	0.47
1:C:27:PHE:HZ	1:C:113:TYR:CD1	2.32	0.47
1:C:173:LEU:O	1:C:177:CYS:HB2	2.14	0.47
1:D:248:ASN:OD1	1:D:248:ASN:C	2.52	0.47
1:A:178:ARG:HH21	1:A:178:ARG:HG3	1.79	0.47
1:B:40:HIS:NE2	1:B:238:ILE:HG21	2.29	0.47
1:D:238:ILE:HD13	1:D:238:ILE:N	2.23	0.47
1:A:160:VAL:HG23	1:A:187:LEU:HG	1.95	0.47
1:D:255:LEU:HD12	1:D:255:LEU:C	2.34	0.47
1:A:35:SER:O	1:A:39:LYS:HG3	2.14	0.47
1:A:176:TYR:O	1:A:179:ALA:HB3	2.14	0.47
1:C:234:TRP:O	1:C:255:LEU:HA	2.15	0.47
1:A:100:ALA:HB2	1:A:132:ARG:CZ	2.45	0.47
1:B:72:LEU:HD23	1:B:131:LEU:HD22	1.97	0.47
1:B:196:MET:HG2	1:B:254:SER:CB	2.45	0.47
1:C:239:SER:O	1:C:240:GLN:C	2.54	0.47
1:D:40:HIS:CE1	1:D:238:ILE:HG21	2.50	0.47
1:A:20:TYR:OH	3:A:302:NCA:H6	2.15	0.46
1:B:173:LEU:N	1:B:174:PRO:CD	2.79	0.46
1:C:243:SER:C	1:C:245:THR:N	2.68	0.46
1:A:193:LEU:HD21	1:A:195:ILE:HD11	1.96	0.46
1:D:234:TRP:HD1	1:D:235:PHE:N	2.12	0.46
1:C:95:GLU:HA	1:C:98:LEU:HD23	1.96	0.46
1:B:34:GLU:OE2	1:B:246:MET:HG3	2.15	0.46
1:C:11:TYR:OH	1:C:168:ALA:HB1	2.15	0.46
1:D:128:GLU:HB3	1:D:132:ARG:NH1	2.30	0.46
1:D:142:ASP:HA	2:D:301:SAH:N1	2.30	0.46
1:B:208:GLU:O	1:B:208:GLU:CG	2.63	0.46
1:C:119:GLY:O	1:C:120:ASN:C	2.54	0.46
1:C:171:PRO:O	1:C:172:ASP:HB3	2.16	0.46
1:A:184:GLY:O	1:A:259:LYS:NZ	2.41	0.46
1:B:218:ARG:HG2	1:B:235:PHE:HE2	1.78	0.46
1:D:47:LYS:CG	1:D:234:TRP:CH2	2.95	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:71:LEU:HD13	1:D:81:ILE:HG21	1.96	0.46
1:D:164:LEU:HB3	3:D:302:NCA:C2	2.45	0.46
1:D:230:TYR:N	1:D:230:TYR:CD2	2.84	0.46
1:B:85:ASP:OD2	2:B:301:SAH:O2'	2.32	0.46
1:A:189:PRO:CB	1:A:261:SER:HA	2.46	0.45
1:A:203:TYR:HD1	1:A:204:TYR:N	2.14	0.45
1:C:13:SER:CB	1:C:14:HIS:CE1	2.99	0.45
1:C:75:CYS:SG	1:C:75:CYS:O	2.74	0.45
1:A:60:ILE:HD12	1:A:60:ILE:N	2.31	0.45
1:C:231:THR:OG1	1:C:260:LEU:HD21	2.16	0.45
1:B:65:GLY:HA3	2:B:301:SAH:HB1	1.98	0.45
1:C:83:VAL:HG21	1:C:94:LEU:HD13	1.98	0.45
1:C:139:LEU:HD11	1:C:152:VAL:HG11	1.98	0.45
1:D:57:ASP:CG	1:D:79:LYS:NZ	2.70	0.45
1:B:134:ALA:O	1:B:136:LYS:HE2	2.17	0.45
1:C:238:ILE:HD11	1:C:252:LEU:HB2	1.98	0.45
1:D:258:ARG:HG3	1:D:259:LYS:H	1.82	0.45
1:A:84:THR:HB	1:A:141:CYS:HB3	1.99	0.45
1:B:178:ARG:O	1:B:182:ASN:N	2.47	0.45
1:D:202:SER:HB3	1:D:248:ASN:HD21	1.82	0.45
1:A:45:LEU:CD2	1:A:196:MET:HE1	2.46	0.45
1:D:225:VAL:HG11	1:D:257:ALA:HB2	1.97	0.45
1:C:74:ALA:C	1:C:76:GLU:H	2.19	0.45
1:D:46:PHE:CE2	1:D:51:LEU:CD2	2.99	0.45
1:D:241:SER:HA	1:D:249:ASN:HD21	1.82	0.45
1:D:249:ASN:ND2	1:D:251:GLY:H	2.14	0.45
1:A:121:ARG:HB3	1:A:121:ARG:CZ	2.47	0.44
1:C:47:LYS:HG2	1:D:47:LYS:HD3	1.96	0.44
1:D:218:ARG:HE	1:D:218:ARG:HB3	1.37	0.44
1:B:6:THR:HG21	1:B:211:PHE:HD1	1.82	0.44
1:B:142:ASP:O	1:B:148:PRO:HB3	2.17	0.44
1:B:205:MET:HE1	1:B:208:GLU:OE1	2.16	0.44
1:A:189:PRO:HB2	1:A:261:SER:HA	1.99	0.44
1:D:199:LEU:HD22	1:D:217:GLY:HA2	2.00	0.44
1:C:87:SER:OG	1:C:89:GLN:HG2	2.17	0.44
1:B:258:ARG:NH1	1:B:258:ARG:HG2	2.32	0.44
1:D:56:GLY:O	1:D:78:PHE:HA	2.18	0.44
1:B:71:LEU:CD1	1:B:83:VAL:HG11	2.48	0.44
1:C:47:LYS:O	1:C:47:LYS:HD3	2.18	0.44
1:D:37:ILE:HD13	1:D:252:LEU:HD11	1.99	0.44
1:A:30:ARG:O	1:A:32:SER:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:173:LEU:N	1:D:174:PRO:CD	2.81	0.44
1:A:30:ARG:HA	1:A:30:ARG:HD3	1.79	0.44
1:A:62:ILE:HG13	1:A:183:LEU:CD2	2.47	0.44
1:B:108:SER:N	1:B:109:PRO:HD2	2.32	0.44
1:B:170:CYS:SG	1:B:176:TYR:HA	2.58	0.44
1:C:222:GLU:O	1:C:226:LYS:HG3	2.18	0.44
1:D:57:ASP:CG	1:D:79:LYS:HZ3	2.20	0.44
1:D:177:CYS:O	1:D:181:ARG:NH1	2.50	0.44
1:D:258:ARG:CG	1:D:259:LYS:H	2.31	0.44
1:B:214:LEU:HG	1:B:216:LEU:HG	2.00	0.43
1:C:121:ARG:HA	1:C:121:ARG:HH11	1.83	0.43
1:D:83:VAL:O	1:D:138:VAL:HA	2.18	0.43
1:D:252:LEU:HD12	1:D:252:LEU:N	2.33	0.43
1:C:136:LYS:HA	1:C:136:LYS:HD3	1.57	0.43
1:C:207:GLY:O	1:C:208:GLU:OE1	2.35	0.43
1:D:253:PHE:CD1	1:D:253:PHE:C	2.90	0.43
1:D:258:ARG:HH11	1:D:258:ARG:CG	2.29	0.43
1:D:35:SER:O	1:D:39:LYS:HB2	2.17	0.43
1:C:110:VAL:O	1:C:114:VAL:HG23	2.19	0.43
1:D:184:GLY:O	1:D:259:LYS:HE3	2.18	0.43
1:D:83:VAL:HG23	1:D:138:VAL:HG13	1.99	0.43
1:A:60:ILE:CD1	1:A:157:ALA:HB2	2.48	0.43
1:D:29:SER:O	1:D:30:ARG:C	2.56	0.43
1:D:46:PHE:CE2	1:D:51:LEU:HD22	2.54	0.43
1:B:45:LEU:HD13	1:B:70:GLN:HA	2.01	0.43
1:D:255:LEU:HD12	1:D:257:ALA:N	2.34	0.43
1:B:192:PHE:CE1	1:B:258:ARG:HD2	2.53	0.43
1:D:241:SER:OG	1:D:249:ASN:O	2.21	0.43
1:D:256:VAL:O	1:D:256:VAL:HG12	2.18	0.43
1:A:163:THR:HG22	1:A:196:MET:HE3	2.01	0.42
1:A:243:SER:O	1:A:246:MET:HB2	2.19	0.42
1:D:136:LYS:HA	1:D:136:LYS:HD3	1.71	0.42
1:B:23:LYS:HZ2	1:B:23:LYS:HG2	1.76	0.42
1:B:224:ALA:HA	1:B:227:GLU:HG3	2.01	0.42
1:C:144:THR:O	1:C:182:ASN:ND2	2.52	0.42
1:A:60:ILE:HD13	1:A:157:ALA:CB	2.49	0.42
1:B:72:LEU:HD23	1:B:72:LEU:HA	1.87	0.42
1:C:13:SER:HB3	1:C:14:HIS:CE1	2.54	0.42
1:D:62:ILE:HG13	1:D:183:LEU:HD21	2.01	0.42
1:D:58:LEU:HD11	1:D:82:VAL:HG23	2.02	0.42
1:A:255:LEU:HD12	1:A:255:LEU:C	2.40	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:202:SER:C	1:C:213:SER:HB3	2.40	0.42
1:C:251:GLY:O	1:C:252:LEU:HD12	2.19	0.42
1:A:108:SER:HA	1:A:111:VAL:HB	2.01	0.42
1:A:240:GLN:NE2	1:A:241:SER:O	2.50	0.42
1:D:83:VAL:O	1:D:83:VAL:HG23	2.19	0.42
1:D:230:TYR:HB2	1:D:257:ALA:HB1	2.02	0.42
1:A:178:ARG:O	1:A:182:ASN:ND2	2.53	0.42
1:B:31:HIS:CE1	1:B:36:GLN:HE21	2.37	0.42
1:C:30:ARG:O	1:C:31:HIS:HB2	2.18	0.42
1:C:23:LYS:NZ	1:C:246:MET:CG	2.82	0.42
1:C:108:SER:HB2	1:C:109:PRO:CD	2.50	0.42
1:A:66:PRO:C	1:A:94:LEU:CD2	2.88	0.41
1:B:243:SER:O	1:B:246:MET:HB2	2.20	0.41
1:C:217:GLY:O	1:C:218:ARG:C	2.58	0.41
1:C:237:VAL:C	1:C:238:ILE:HG23	2.40	0.41
1:D:11:TYR:CE2	1:D:211:PHE:CD1	3.08	0.41
1:B:145:GLN:O	1:B:148:PRO:HG3	2.20	0.41
1:B:45:LEU:CD2	1:B:196:MET:CE	2.95	0.41
1:D:98:LEU:HD12	1:D:98:LEU:HA	1.92	0.41
1:B:63:GLY:O	2:B:301:SAH:N	2.53	0.41
1:B:141:CYS:HA	1:B:148:PRO:O	2.20	0.41
1:C:13:SER:C	1:C:14:HIS:ND1	2.73	0.41
1:A:92:GLN:O	1:A:96:LYS:HG3	2.20	0.41
1:C:13:SER:CB	1:C:14:HIS:ND1	2.84	0.41
1:A:34:GLU:OE2	1:A:246:MET:HG3	2.20	0.41
1:C:5:PHE:HB3	1:C:171:PRO:HB3	2.03	0.41
1:C:6:THR:N	1:C:212:SER:OG	2.53	0.41
1:C:8:LYS:HB3	1:C:86:TYR:CZ	2.56	0.41
1:C:41:LEU:O	1:C:44:ASN:HB2	2.20	0.41
1:A:235:PHE:CD1	1:A:255:LEU:HD23	2.56	0.41
1:D:37:ILE:HD12	1:D:242:TYR:CD1	2.56	0.41
1:A:69:TYR:CD1	1:A:70:GLN:N	2.88	0.41
1:A:147:GLN:HA	1:A:148:PRO:HD2	1.78	0.41
1:A:172:ASP:HA	1:A:214:LEU:HD13	2.01	0.41
1:B:29:SER:CB	1:C:104:ALA:O	2.69	0.41
1:C:146:SER:HB2	1:C:147:GLN:NE2	2.35	0.41
1:C:241:SER:HA	1:C:249:ASN:HD21	1.85	0.41
1:A:57:ASP:N	1:A:158:ASP:OD2	2.52	0.41
1:A:141:CYS:HB2	1:A:149:LEU:HD23	2.03	0.41
1:C:13:SER:HB2	1:C:14:HIS:CE1	2.56	0.41
1:C:31:HIS:CE1	1:C:39:LYS:HZ2	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:184:GLY:HA2	1:C:230:TYR:OH	2.21	0.41
1:C:238:ILE:HD13	1:C:238:ILE:N	2.36	0.41
1:A:87:SER:OG	1:A:89:GLN:OE1	2.37	0.41
1:C:16:ASN:HB3	1:C:19:ASP:HB2	2.03	0.41
1:A:136:LYS:HA	1:A:136:LYS:HD3	1.82	0.40
1:D:36:GLN:OE1	1:D:39:LYS:NZ	2.44	0.40
1:B:17:PRO:HD2	1:B:18:ARG:HD2	2.03	0.40
1:B:19:ASP:O	1:B:22:GLU:HB3	2.21	0.40
1:B:142:ASP:HA	2:B:301:SAH:N1	2.36	0.40
1:C:181:ARG:HB3	1:C:228:ALA:HB1	2.02	0.40
1:C:207:GLY:O	1:C:208:GLU:CG	2.69	0.40
1:D:222:GLU:O	1:D:223:ALA:C	2.58	0.40
1:A:34:GLU:H	1:A:34:GLU:CD	2.25	0.40
1:A:86:TYR:O	1:A:86:TYR:CG	2.74	0.40
1:A:152:VAL:HG13	1:A:153:PRO:HD2	2.03	0.40
1:A:203:TYR:CD1	1:A:204:TYR:N	2.88	0.40
1:B:8:LYS:O	1:B:11:TYR:N	2.45	0.40
1:D:62:ILE:HG13	1:D:183:LEU:HD22	2.03	0.40
1:D:218:ARG:O	1:D:222:GLU:HG3	2.21	0.40
1:B:48:ILE:O	1:B:54:VAL:HG23	2.21	0.40
1:C:143:VAL:HG12	1:C:183:LEU:HD21	2.04	0.40
1:C:229:GLY:O	1:C:260:LEU:HG	2.21	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	257/283 (91%)	226 (88%)	28 (11%)	3 (1%)	13 30
1	B	257/283 (91%)	232 (90%)	21 (8%)	4 (2%)	9 23
1	C	257/283 (91%)	209 (81%)	37 (14%)	11 (4%)	2 5

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	D	255/283 (90%)	215 (84%)	32 (12%)	8 (3%)	4 9
All	All	1026/1132 (91%)	882 (86%)	118 (12%)	26 (2%)	5 13

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	31	HIS
1	B	31	HIS
1	C	120	ASN
1	C	218	ARG
1	A	6	THR
1	A	74	ALA
1	C	9	ASP
1	C	31	HIS
1	C	52	ASP
1	C	240	GLN
1	D	52	ASP
1	D	249	ASN
1	C	6	THR
1	D	224	ALA
1	B	6	THR
1	B	212	SER
1	C	172	ASP
1	C	151	ALA
1	D	68	ILE
1	D	124	GLY
1	D	218	ARG
1	D	240	GLN
1	B	215	PRO
1	C	28	GLY
1	D	54	VAL
1	C	135	VAL

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	224/245 (91%)	204 (91%)	20 (9%)	9 22
1	B	224/245 (91%)	206 (92%)	18 (8%)	12 26
1	C	224/245 (91%)	204 (91%)	20 (9%)	9 22
1	D	223/245 (91%)	201 (90%)	22 (10%)	8 17
All	All	895/980 (91%)	815 (91%)	80 (9%)	9 22

All (80) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	3	SER
1	A	18	ARG
1	A	19	ASP
1	A	22	GLU
1	A	51	LEU
1	A	59	LEU
1	A	79	LYS
1	A	88	ASP
1	A	121	ARG
1	A	125	PRO
1	A	126	GLU
1	A	127	LYS
1	A	133	GLN
1	A	140	LYS
1	A	141	CYS
1	A	162	SER
1	A	167	ASP
1	A	173	LEU
1	A	231	THR
1	A	258	ARG
1	B	18	ARG
1	B	26	LYS
1	B	30	ARG
1	B	51	LEU
1	B	54	VAL
1	B	80	GLU
1	B	87	SER
1	B	141	CYS
1	B	172	ASP
1	B	209	GLN
1	B	218	ARG
1	B	219	GLU
1	B	227	GLU

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Mol	Chain	Res	Type
1	B	231	THR
1	B	238	ILE
1	B	246	MET
1	B	255	LEU
1	B	258	ARG
1	C	18	ARG
1	C	26	LYS
1	C	31	HIS
1	C	37	ILE
1	C	55	LYS
1	C	77	SER
1	C	94	LEU
1	C	159	CYS
1	C	167	ASP
1	C	178	ARG
1	C	188	LYS
1	C	197	ASP
1	C	212	SER
1	C	218	ARG
1	C	219	GLU
1	C	227	GLU
1	C	234	TRP
1	C	238	ILE
1	C	245	THR
1	C	255	LEU
1	D	12	LEU
1	D	18	ARG
1	D	19	ASP
1	D	22	GLU
1	D	23	LYS
1	D	30	ARG
1	D	51	LEU
1	D	87	SER
1	D	98	LEU
1	D	117	LEU
1	D	152	VAL
1	D	218	ARG
1	D	219	GLU
1	D	230	TYR
1	D	231	THR
1	D	232	ILE
1	D	234	TRP

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Mol	Chain	Res	Type
1	D	238	ILE
1	D	245	THR
1	D	246	MET
1	D	255	LEU
1	D	258	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	120	ASN
1	A	209	GLN
1	B	36	GLN
1	B	90	ASN
1	C	31	HIS
1	C	147	GLN
1	D	120	ASN
1	D	133	GLN
1	D	147	GLN

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 monosaccharides 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	SAH	D	301	-	24,28,28	0.89	0	25,40,40	1.62	4 (16%)
3	NCA	B	302	-	9,9,9	0.59	0	11,11,11	1.89	4 (36%)
2	SAH	B	301	-	24,28,28	0.83	0	25,40,40	1.44	4 (16%)
2	SAH	A	301	-	24,28,28	1.31	4 (16%)	25,40,40	2.18	9 (36%)
3	NCA	C	302	-	9,9,9	1.14	1 (11%)	11,11,11	1.82	3 (27%)
2	SAH	C	301	-	24,28,28	1.15	2 (8%)	25,40,40	1.67	5 (20%)
3	NCA	D	302	-	9,9,9	1.10	1 (11%)	11,11,11	1.81	3 (27%)
3	NCA	A	302	-	9,9,9	0.97	1 (11%)	11,11,11	1.85	3 (27%)

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	SAH	D	301	-	-	5/11/31/31	0/3/3/3
3	NCA	B	302	-	-	0/4/4/4	0/1/1/1
2	SAH	B	301	-	-	3/11/31/31	0/3/3/3
2	SAH	A	301	-	-	0/11/31/31	0/3/3/3
3	NCA	C	302	-	-	0/4/4/4	0/1/1/1
2	SAH	C	301	-	-	5/11/31/31	0/3/3/3
3	NCA	D	302	-	-	0/4/4/4	0/1/1/1
3	NCA	A	302	-	-	4/4/4/4	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	301	SAH	O4'-C1'	3.25	1.45	1.41
2	A	301	SAH	C2'-C1'	-3.16	1.49	1.53
3	C	302	NCA	C3-C7	3.14	1.55	1.50
2	A	301	SAH	C4-N3	-2.77	1.31	1.35
2	A	301	SAH	O4'-C1'	2.72	1.44	1.41
3	D	302	NCA	C3-C7	2.70	1.54	1.50
3	A	302	NCA	C3-C7	2.60	1.54	1.50
2	A	301	SAH	OXT-C	-2.38	1.22	1.30
2	C	301	SAH	OXT-C	-2.05	1.23	1.30

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	301	SAH	O4'-C1'-C2'	-5.86	98.36	106.93
2	A	301	SAH	N3-C2-N1	-5.49	120.09	128.68
2	D	301	SAH	O4'-C1'-C2'	-4.76	99.98	106.93
2	B	301	SAH	N3-C2-N1	-4.41	121.79	128.68
2	D	301	SAH	N3-C2-N1	-4.38	121.83	128.68
2	C	301	SAH	O4'-C1'-C2'	-4.14	100.88	106.93
2	C	301	SAH	N3-C2-N1	-4.11	122.26	128.68
2	A	301	SAH	OXT-C-O	-3.72	115.63	124.09
3	D	302	NCA	O7-C7-C3	3.67	124.03	119.63
3	C	302	NCA	O7-C7-N7	-3.56	117.52	122.58
3	A	302	NCA	C6-N1-C2	3.45	122.81	116.85
3	B	302	NCA	C6-N1-C2	3.38	122.69	116.85
3	A	302	NCA	O7-C7-N7	-3.32	117.86	122.58
3	B	302	NCA	O7-C7-N7	-3.24	117.97	122.58
3	B	302	NCA	C3-C7-N7	3.14	121.52	117.75
3	C	302	NCA	C6-N1-C2	3.14	122.27	116.85
3	D	302	NCA	C6-N1-C2	2.98	122.01	116.85
2	D	301	SAH	C4-C5-N7	-2.92	106.36	109.40
2	C	301	SAH	OXT-C-O	-2.67	118.02	124.09
3	A	302	NCA	O7-C7-C3	2.63	122.78	119.63
2	C	301	SAH	C1'-N9-C4	2.55	131.11	126.64
2	A	301	SAH	O4'-C4'-C5'	-2.51	102.37	108.83
2	B	301	SAH	O4'-C1'-C2'	-2.48	103.30	106.93
2	B	301	SAH	OXT-C-CA	2.44	121.68	113.38
3	C	302	NCA	C3-C7-N7	2.43	120.67	117.75
2	B	301	SAH	C5'-C4'-C3'	-2.36	109.16	115.06
3	D	302	NCA	O7-C7-N7	-2.33	119.26	122.58
2	A	301	SAH	C4-C5-N7	-2.30	107.00	109.40
2	A	301	SAH	C5'-C4'-C3'	2.29	120.78	115.06
2	A	301	SAH	OXT-C-CA	2.20	120.89	113.38
2	D	301	SAH	OXT-C-CA	2.13	120.65	113.38
2	A	301	SAH	O4'-C4'-C3'	-2.07	101.02	105.11
2	A	301	SAH	C3'-C2'-C1'	-2.06	97.88	100.98
3	B	302	NCA	C3-C2-N1	-2.03	120.49	123.49
2	C	301	SAH	C4-C5-N7	-2.03	107.29	109.40

There are no chirality outliers.

All (17) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	302	NCA	C2-C3-C7-O7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
3	A	302	NCA	C2-C3-C7-N7
3	A	302	NCA	C4-C3-C7-O7
3	A	302	NCA	C4-C3-C7-N7
2	C	301	SAH	C-CA-CB-CG
2	B	301	SAH	CB-CG-SD-C5'
2	C	301	SAH	N-CA-CB-CG
2	D	301	SAH	N-CA-CB-CG
2	D	301	SAH	C-CA-CB-CG
2	C	301	SAH	CB-CG-SD-C5'
2	D	301	SAH	OXT-C-CA-CB
2	D	301	SAH	O-C-CA-CB
2	D	301	SAH	CB-CG-SD-C5'
2	B	301	SAH	OXT-C-CA-CB
2	B	301	SAH	O-C-CA-CB
2	C	301	SAH	OXT-C-CA-CB
2	C	301	SAH	O-C-CA-CB

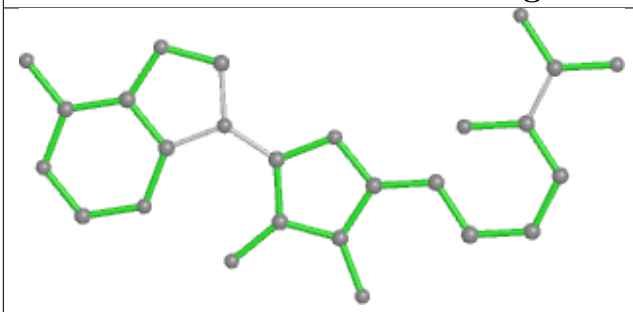
There are no ring outliers.

7 monomers are involved in 14 short contacts:

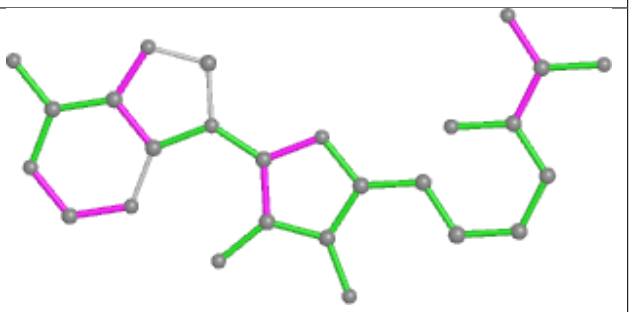
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	301	SAH	2	0
2	B	301	SAH	4	0
2	A	301	SAH	2	0
3	C	302	NCA	1	0
2	C	301	SAH	2	0
3	D	302	NCA	2	0
3	A	302	NCA	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

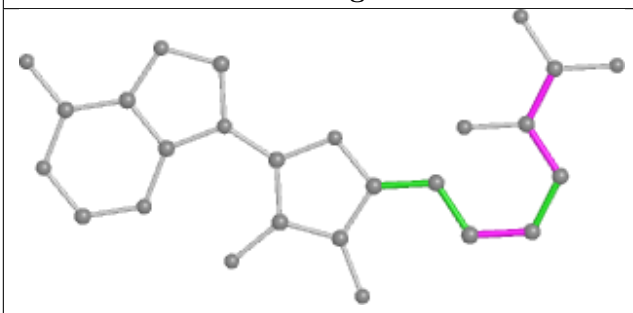
Ligand SAH D 301



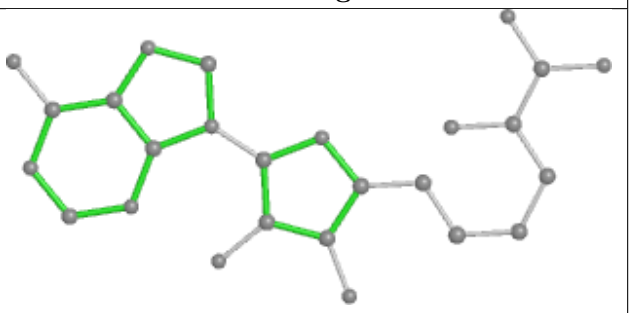
Bond lengths



Bond angles

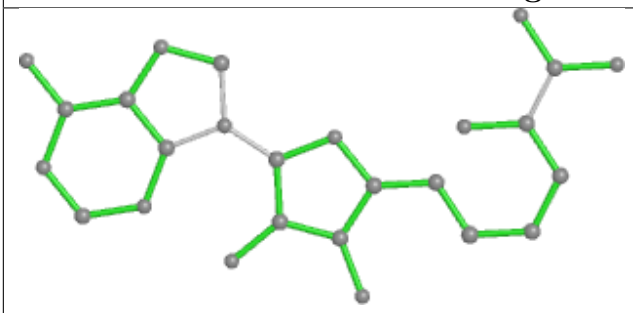


Torsions

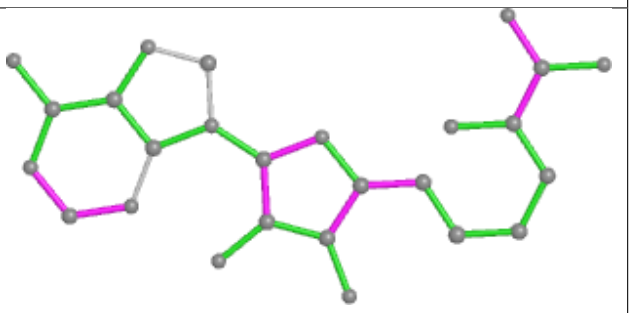


Rings

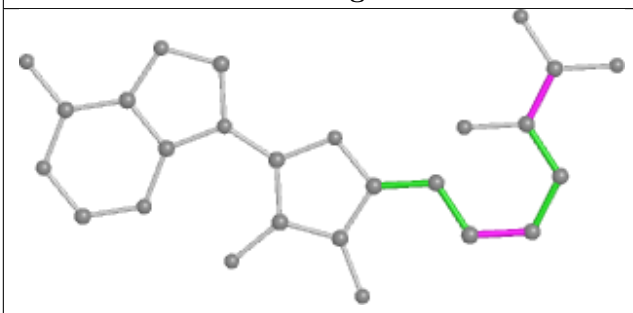
Ligand SAH B 301



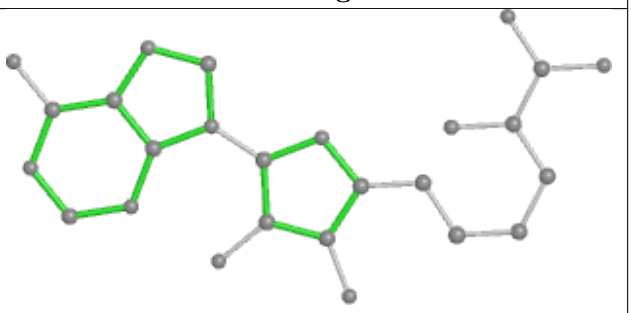
Bond lengths



Bond angles

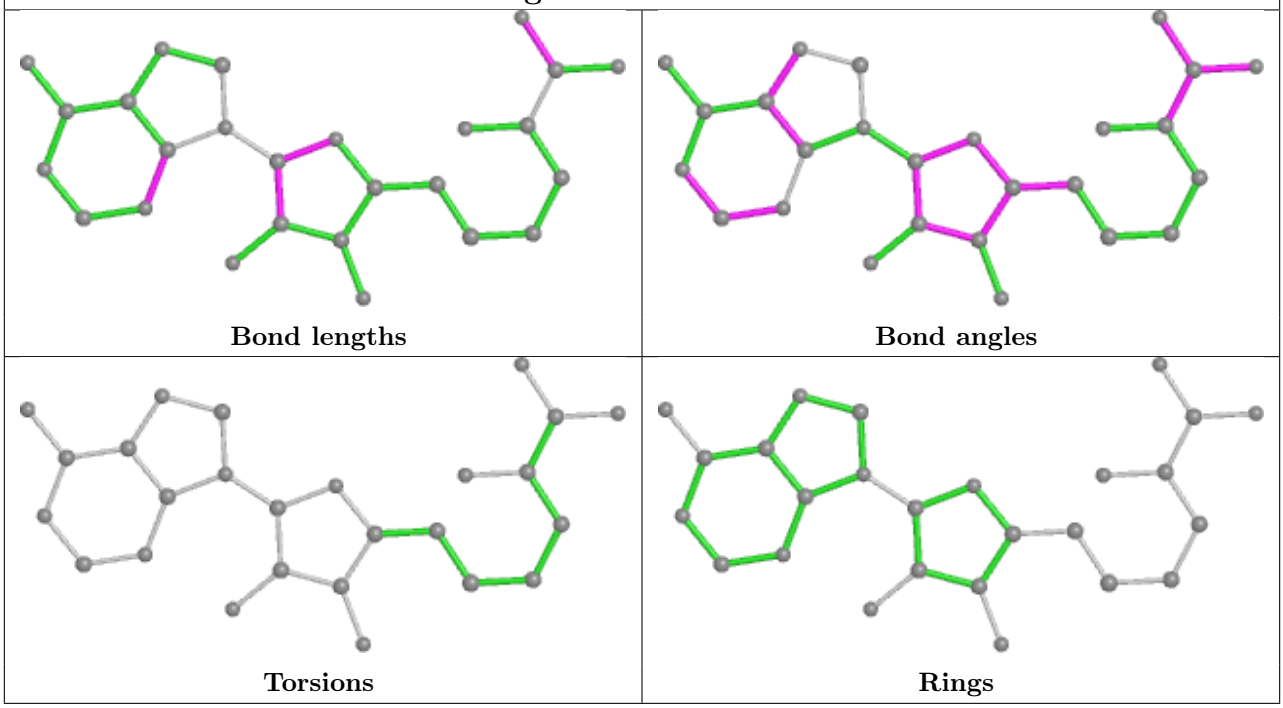


Torsions

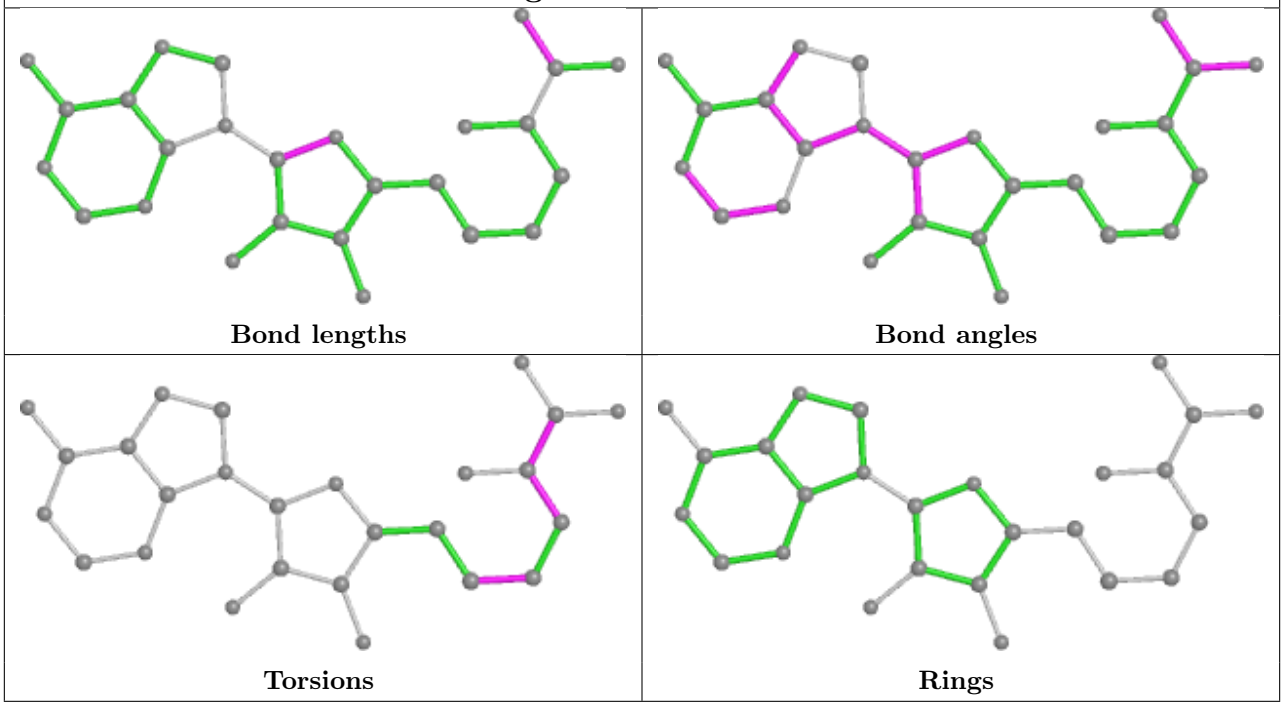


Rings

Ligand SAH A 301



Ligand SAH C 301



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	259/283 (91%)	-0.56	4 (1%)	73	76	14, 30, 46, 63	1 (0%)
1	B	259/283 (91%)	-0.53	3 (1%)	79	80	11, 31, 49, 65	1 (0%)
1	C	259/283 (91%)	-0.26	6 (2%)	60	62	17, 42, 69, 80	1 (0%)
1	D	257/283 (90%)	-0.29	5 (1%)	66	69	13, 44, 70, 81	1 (0%)
All	All	1034/1132 (91%)	-0.41	18 (1%)	70	72	11, 34, 62, 81	4 (0%)

All (18) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	5	PHE	4.1
1	C	28	GLY	3.9
1	A	234	TRP	3.9
1	D	234	TRP	3.8
1	A	4	GLY	3.6
1	A	3	SER	3.2
1	C	234	TRP	3.1
1	B	234	TRP	3.1
1	B	3	SER	2.7
1	D	14	HIS	2.4
1	C	27	PHE	2.4
1	C	3	SER	2.3
1	D	207	GLY	2.3
1	C	29	SER	2.3
1	D	29	SER	2.3
1	C	14	HIS	2.0
1	B	31	HIS	2.0
1	A	30	ARG	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 monosaccharides in this entry.

6.4 Ligands (i)

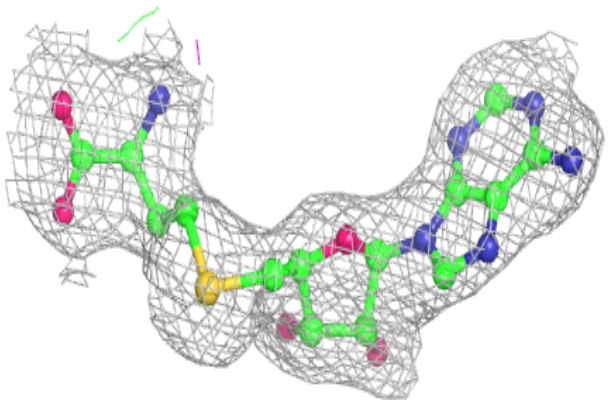
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

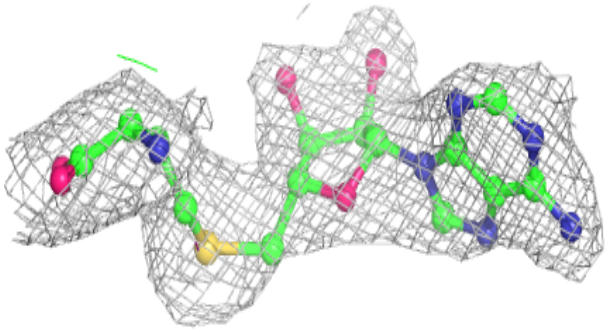
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	NCA	C	302	9/9	0.81	0.37	56,57,57,58	0
3	NCA	D	302	9/9	0.83	0.38	66,66,68,68	0
3	NCA	A	302	9/9	0.90	0.25	29,30,33,33	0
2	SAH	C	301	26/26	0.91	0.16	37,42,43,45	0
3	NCA	B	302	9/9	0.91	0.26	35,37,42,43	0
2	SAH	D	301	26/26	0.94	0.12	36,38,39,39	0
2	SAH	B	301	26/26	0.95	0.13	19,20,25,25	0
2	SAH	A	301	26/26	0.96	0.12	24,26,27,29	0

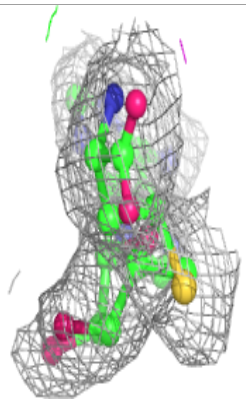
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around SAH C 301:

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

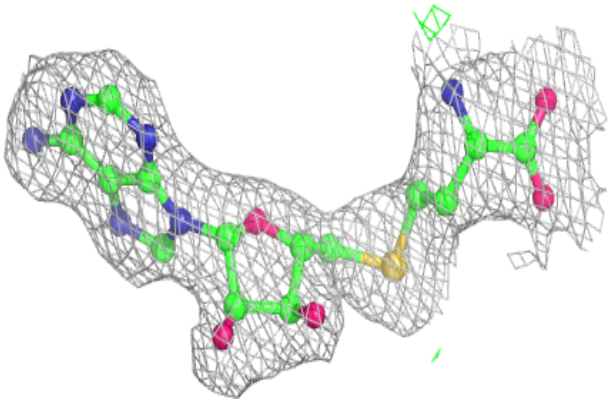


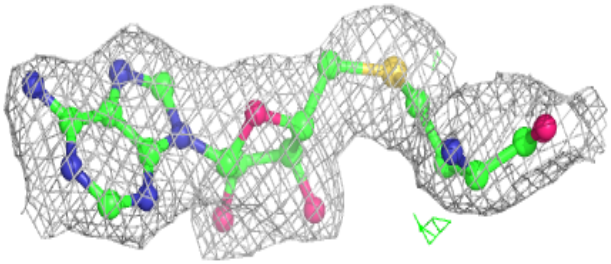


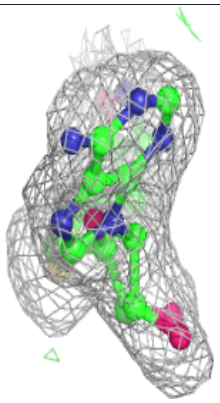


Electron density around SAH D 301:

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

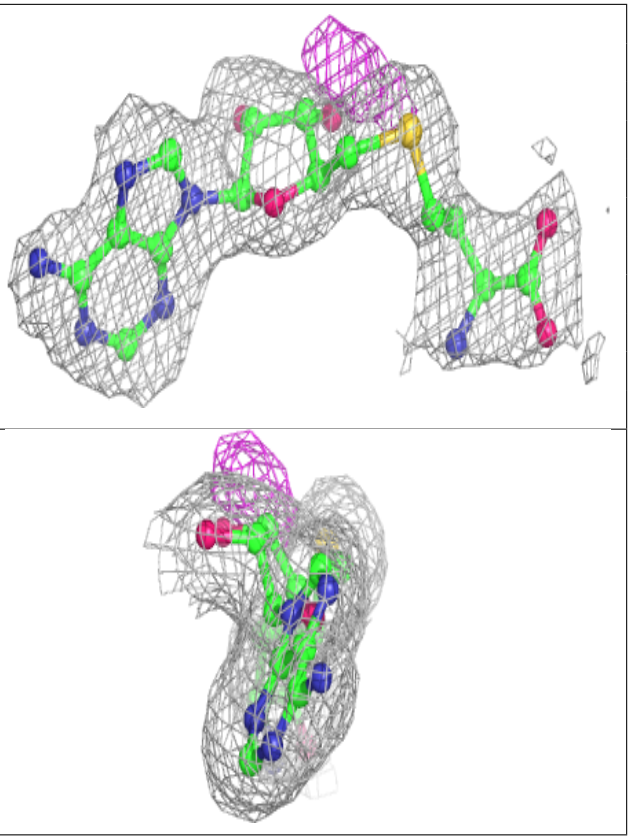






Electron density around SAH B 301:

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



Electron density around SAH A 301:

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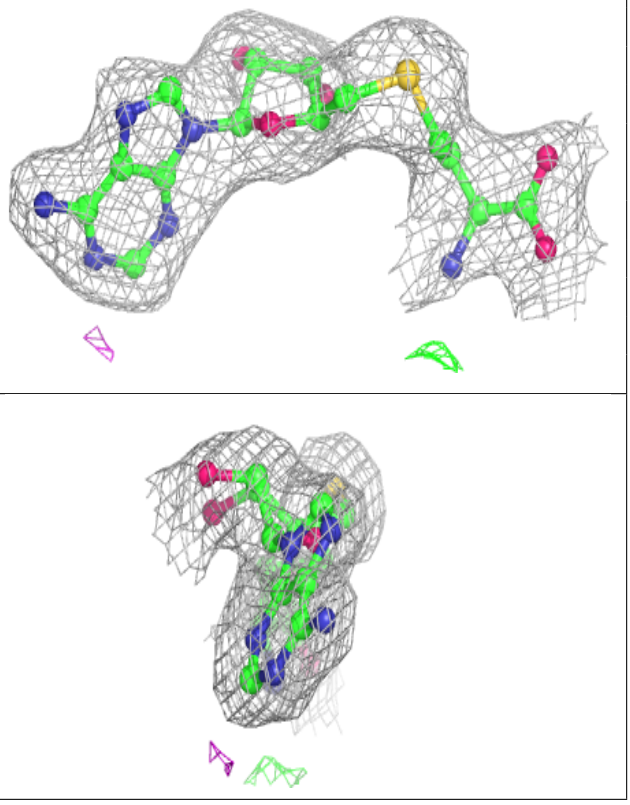
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers (i)

There are no such residues in this entry.