Full wwPDB X-ray Structure Validation Report (i)

Feb 15, 2024 – 08:34 PM EST

PDB ID	:	3R0Q
Title	:	A Uniquely Open Conformation Revealed in the Crystal Structure of Arabidopsis Thaliana Protein Arginine Methyltransferase 10
Authors	:	Cheng, Y.; Redinbo, M.R.
Deposited on	:	2011-03-08
Resolution	:	2.61 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:

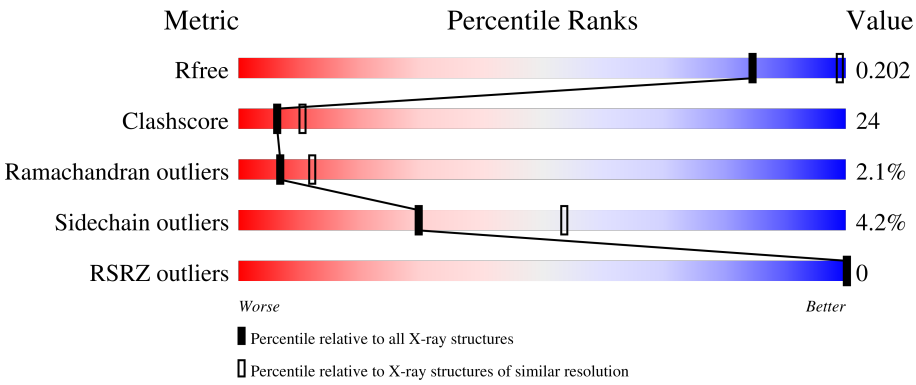
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.61 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	3797 (2.64-2.60)
Clashscore	141614	4168 (2.64-2.60)
Ramachandran outliers	138981	4093 (2.64-2.60)
Sidechain outliers	138945	4093 (2.64-2.60)
RSRZ outliers	127900	3731 (2.64-2.60)

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	376	57% 32% • 7%
1	C	376	55% 36% • 7%
1	E	376	55% 34% • 7%
1	G	376	59% 32% • • 6%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 11025 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.

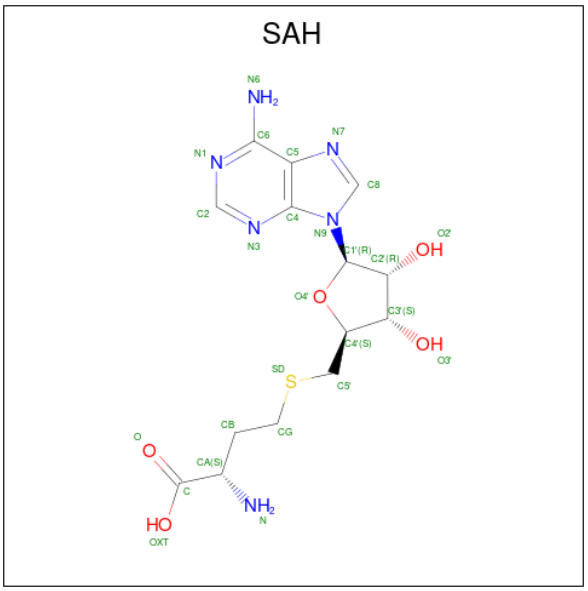
- Molecule 1 is a protein called Probable protein arginine N-methyltransferase 4.2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	C	349	2682	1708	444	513	17	0	0	0
1	G	353	2688	1718	446	507	17	0	0	0
1	A	350	2696	1718	447	514	17	0	0	0
1	E	349	2687	1713	443	514	17	0	0	0

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	8	SER	-	expression tag	UNP Q9MAT5
C	9	ASN	-	expression tag	UNP Q9MAT5
C	10	ALA	-	expression tag	UNP Q9MAT5
G	8	SER	-	expression tag	UNP Q9MAT5
G	9	ASN	-	expression tag	UNP Q9MAT5
G	10	ALA	-	expression tag	UNP Q9MAT5
A	8	SER	-	expression tag	UNP Q9MAT5
A	9	ASN	-	expression tag	UNP Q9MAT5
A	10	ALA	-	expression tag	UNP Q9MAT5
E	8	SER	-	expression tag	UNP Q9MAT5
E	9	ASN	-	expression tag	UNP Q9MAT5
E	10	ALA	-	expression tag	UNP Q9MAT5

- 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
			Total	C	N	O	S		
2	C	1	26	14	6	5	1	0	0
			Total	C	N	O	S		
2	G	1	26	14	6	5	1	0	0
			Total	C	N	O	S		
2	A	1	26	14	6	5	1	0	0
			Total	C	N	O	S		
2	E	1	26	14	6	5	1	0	0

- Molecule 3 is water.

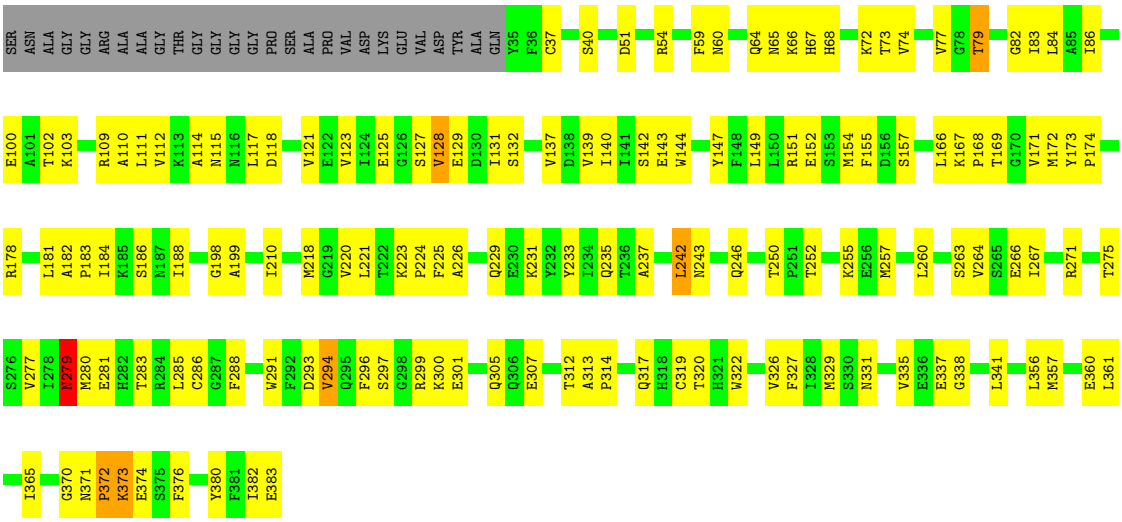
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
3	C	45	45	45	0	0
			Total	O		
3	G	39	39	39	0	0
			Total	O		
3	A	35	35	35	0	0
			Total	O		
3	E	49	49	49	0	0

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.

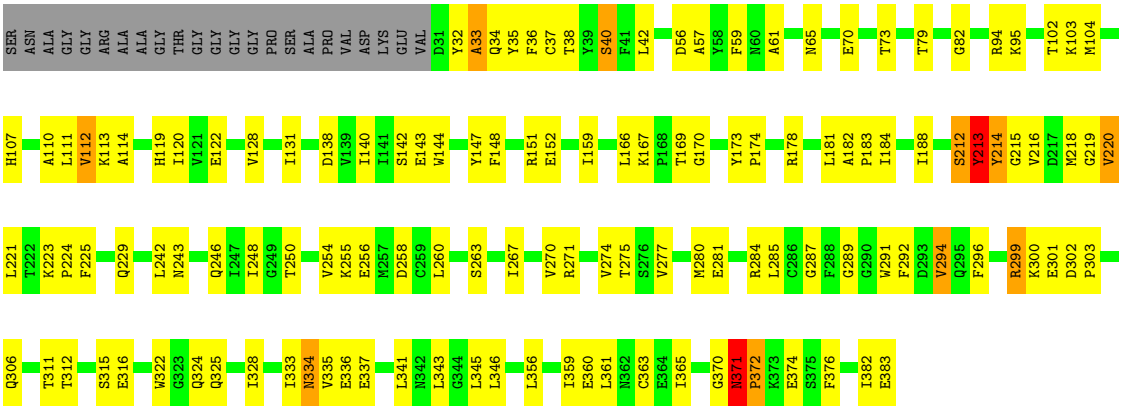
• Molecule 1: Probable protein arginine N-methyltransferase 4.2

Chain C: 55% 36% • 7%



• Molecule 1: Probable protein arginine N-methyltransferase 4.2

Chain G: 59% 32% • • 6%



• Molecule 1: Probable protein arginine N-methyltransferase 4.2

Chain A: 57% 32% • 7%

SER ASN ALA GLY GLY ARG ALA ALA GLY THR GLY GLY GLY GLY PRO SER ALA PRO VAL ASP LYS GLU VAL ASP TYR ALA Q34 Y35 Y39 S40 F41 L42 Y43 H44 Q45 K46 Y58 F59 V62 F63 Q64 N65 K66 H67 H68 F69 K72 L75 D76 V77 G78 T79 G80 S81 G82

I86 Q90 A93 R94 K95 E100 A101 T102 K103 M104 H107 A108 R109 A110 L111 V112 I120 V121 E122 V123 I124 S127 V128 E129 D130 I131 S132 L133 P134 E135 K136 V137 D138 V139 I140 W144 Y147 F148 L149 L150 R151 E152 S153 M154 F155 I159 R162 W165

L166 G170 V171 P174 A177 R178 A182 P183 I184 K185 S186 N187 I188 K192 D195 F206 I210 Y213 Y214 G215 V216 D217 M218 K223 P224 F225 A226 N240 D241 I247 T252 I253 C259 V264 S265 E266 I267 E268 E269 V270 N273 V274 T275 S276

V277 I278 N279 M280 E281 H282 W291 F292 D293 V294 G298 T312 A313 P314 S315 H318 F327 I328 I333 N334 V335 E336 E337 N340 L346 M347 S348 R349 E352 N353 H354 R355 I359 C363 E367 N371 P372 K373 E374 S375 F376 I382 E383

• Molecule 1: Probable protein arginine N-methyltransferase 4.2

Chain E: 55% 34% • 7%

SER ASN ALA GLY GLY ARG ALA ALA GLY THR GLY GLY GLY GLY PRO SER ALA PRO VAL ASP LYS GLU VAL ASP TYR ALA GLN Y35 F36 C37 S40 F41 L42 Q45 Y58 F59 N60 A61 V62 N65 K66 H67 T73 V74 L75 D76 V77 G78 T79 G80 S81 G82 I86 W87

Q90 K95 A98 V99 E100 A101 T102 K103 M104 A108 L111 V112 K113 A114 N115 N116 L117 E125 V128 I131 S132 V137 I140 I141 S142 E143 W144 M145 L149 L150 R151 E152 S153 M154 F155 R162 W165 L166 K167 P168 T169 G170 V171 M172 Y173 P174 S175

R178 P183 S186 N187 I188 A189 M200 W203 S212 Y213 Y214 V220 K223 K231 Q235 N240 D241 L242 N243 P244 Q245 Q246 I247 I248 G249 T250 P251 T252 I253 V254 A262 E266 I267 E268 E269 N273 V274 T275 S276 V277 E281 H282 T283 R284 L285

C286 F292 D293 V294 S297 G298 R299 K300 E301 A304 Q305 Q306 E307 I308 T312 A313 P314 S315 E316 W322 G323 Q324 Q325 V326 F327 I328 I333 N334 V335 L341 N342 L343 G344 L345 R349 H354 R355 L356 E360 L361 N362 C363 E364 I365 K366 E367 N371 P372 K373

E374 S375 F376 K377 Y380 F381 I382 E383

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	80.55Å 86.69Å 114.73Å 90.00° 89.97° 90.00°	Depositor
Resolution (Å)	32.97 – 2.61 32.97 – 2.61	Depositor EDS
% Data completeness (in resolution range)	96.6 (32.97-2.61) 92.2 (32.97-2.61)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.12	Depositor
$< I/\sigma(I) >$ [1]	3.68 (at 2.61Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, R_{free}	0.182 , 0.224 0.171 , 0.202	Depositor DCC
R_{free} test set	1992 reflections (4.26%)	wwPDB-VP
Wilson B-factor (Å^2)	36.4	Xtriage
Anisotropy	0.350	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 29.1	EDS
L-test for twinning[2]	$< \|L\| > = 0.42$, $< L^2 > = 0.24$	Xtriage
Estimated twinning fraction	0.457 for h,-k,-l	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11025	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 4.65% 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

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	0.44	0/2761	0.56	0/3756
1	C	0.42	0/2745	0.56	0/3734
1	E	0.50	0/2751	0.61	0/3742
1	G	0.45	0/2753	0.62	4/3748 (0.1%)
All	All	0.45	0/11010	0.59	4/14980 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	G	0	3

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	212	SER	O-C-N	-8.61	108.92	122.70
1	G	212	SER	C-N-CA	5.54	135.56	121.70
1	G	213	TYR	CA-C-N	-5.48	105.13	117.20
1	G	371	ASN	C-N-CD	-5.13	109.31	120.60

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	G	212	SER	Mainchain
1	G	213	TYR	Peptide,Mainchain

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	2696	0	2492	122	1
1	C	2682	0	2484	125	1
1	E	2687	0	2485	143	0
1	G	2688	0	2470	127	0
2	A	26	0	19	3	0
2	C	26	0	19	1	0
2	E	26	0	19	2	0
2	G	26	0	19	0	0
3	A	35	0	0	3	0
3	C	45	0	0	8	0
3	E	49	0	0	6	0
3	G	39	0	0	2	0
All	All	11025	0	10007	503	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 24.

All (503) 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:G:333:ILE:HD11	1:G:365:ILE:CD1	1.68	1.22
1:G:333:ILE:HD11	1:G:365:ILE:HD13	1.29	1.15
1:C:40:SER:HB3	1:C:102:THR:HG21	1.26	1.13
1:G:370:GLY:HA2	1:G:371:ASN:CB	1.78	1.12
1:E:356:LEU:HD23	3:E:413:HOH:O	1.52	1.10
1:G:333:ILE:CD1	1:G:365:ILE:CD1	2.38	1.01
1:A:247:ILE:HD11	1:A:314:PRO:HG2	1.42	1.00
1:E:343:LEU:HD21	1:E:363:CYS:SG	2.01	0.99
1:G:277:VAL:HG21	1:G:335:VAL:CG2	1.94	0.98
1:C:40:SER:HB3	1:C:102:THR:CG2	1.93	0.97
1:G:277:VAL:HG21	1:G:335:VAL:HG21	1.45	0.96
1:E:102:THR:HG22	1:E:103:LYS:H	1.31	0.96
1:C:255:LYS:HD3	1:C:271:ARG:HH21	1.31	0.95
1:A:267:ILE:HG21	1:A:349:ARG:HH21	1.30	0.94
1:C:365:ILE:O	1:C:373:LYS:HA	1.68	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:240:ASN:HD22	1:E:326:VAL:HG21	1.35	0.92
1:E:277:VAL:HG21	1:E:335:VAL:HG11	1.48	0.92
1:A:68:HIS:O	1:A:72:LYS:HG3	1.71	0.90
1:C:280:MET:N	1:C:281:GLU:HA	1.87	0.88
1:G:333:ILE:CD1	1:G:365:ILE:HD12	2.03	0.88
1:C:231:LYS:HA	1:C:235:GLN:HB2	1.56	0.87
1:C:279:ASN:C	1:C:281:GLU:HA	1.98	0.84
1:E:178:ARG:HD2	1:E:253:ILE:HD13	1.60	0.84
1:E:102:THR:HG22	1:E:103:LYS:N	1.92	0.84
1:C:199:ALA:HB1	1:C:229:GLN:HE22	1.42	0.84
1:G:370:GLY:CA	1:G:371:ASN:CB	2.55	0.82
1:E:40:SER:HB3	1:E:102:THR:HG21	1.60	0.82
1:E:343:LEU:CD2	1:E:363:CYS:SG	2.68	0.82
1:G:181:LEU:HD22	1:G:345:LEU:HD21	1.60	0.82
1:A:174:PRO:HB3	1:A:294:VAL:HG13	1.62	0.81
1:G:140:ILE:HG13	1:G:166:LEU:HD13	1.60	0.81
1:G:184:ILE:HG12	1:G:287:GLY:O	1.79	0.81
1:C:199:ALA:HB1	1:C:229:GLN:NE2	1.96	0.81
1:C:169:THR:HG23	3:C:412:HOH:O	1.79	0.80
1:C:40:SER:CB	1:C:102:THR:HG21	2.11	0.80
1:C:263:SER:HB2	3:C:424:HOH:O	1.81	0.80
1:G:301:GLU:O	1:G:303:PRO:HD3	1.82	0.79
1:A:280:MET:CB	1:A:337:GLU:HA	2.13	0.79
1:E:188:ILE:HG23	1:E:328:ILE:HD11	1.65	0.79
1:E:247:ILE:HD11	1:E:314:PRO:HG2	1.65	0.79
1:C:255:LYS:HD3	1:C:271:ARG:NH2	1.97	0.79
1:E:356:LEU:HD22	1:E:383:GLU:HB2	1.65	0.79
1:E:79:THR:HG22	1:E:100:GLU:HB2	1.66	0.77
1:E:315:SER:O	1:E:316:GLU:HB2	1.82	0.77
1:E:373:LYS:O	1:E:374:GLU:HB2	1.83	0.77
1:G:284:ARG:HB2	1:G:333:ILE:O	1.84	0.76
1:C:220:VAL:HG22	3:C:399:HOH:O	1.84	0.76
1:C:243:ASN:HB3	1:C:246:GLN:HG3	1.67	0.76
1:A:77:VAL:HG13	1:A:128:VAL:HG21	1.68	0.76
1:G:250:THR:O	1:G:275:THR:HG23	1.84	0.76
1:E:242:LEU:HB2	1:E:324:GLN:OE1	1.86	0.75
1:C:229:GLN:HG2	3:C:417:HOH:O	1.87	0.74
1:G:102:THR:HG22	1:G:103:LYS:H	1.53	0.74
1:G:281:GLU:HA	1:G:336:GLU:HA	1.69	0.73
1:C:299:ARG:C	1:C:301:GLU:H	1.92	0.72
1:A:140:ILE:HG13	1:A:166:LEU:HD13	1.70	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:250:THR:O	1:E:275:THR:HG23	1.88	0.72
1:A:151:ARG:CZ	1:A:383:GLU:OE1	2.37	0.72
1:C:74:VAL:HG13	1:C:139:VAL:HB	1.70	0.72
1:A:46:LYS:HD3	3:A:403:HOH:O	1.89	0.72
1:C:140:ILE:HG13	1:C:166:LEU:HD13	1.72	0.71
1:G:333:ILE:HD13	1:G:365:ILE:HD12	1.71	0.71
1:E:231:LYS:HA	1:E:235:GLN:HB2	1.72	0.71
1:A:267:ILE:HG21	1:A:349:ARG:NH2	2.05	0.70
1:E:275:THR:O	1:E:341:LEU:HD12	1.90	0.70
1:G:333:ILE:CD1	1:G:365:ILE:HD13	2.11	0.70
1:C:252:THR:HG23	1:C:275:THR:HG22	1.72	0.70
1:C:178:ARG:HB3	1:C:293:ASP:HB2	1.74	0.69
1:E:102:THR:CG2	1:E:103:LYS:H	2.04	0.69
1:G:277:VAL:HG21	1:G:335:VAL:HG22	1.74	0.69
1:G:215:GLY:C	3:G:407:HOH:O	2.31	0.68
1:G:299:ARG:HG3	1:G:301:GLU:H	1.56	0.68
1:C:223:LYS:HG2	1:G:306:GLN:OE1	1.94	0.67
1:G:334:ASN:H	1:G:334:ASN:HD22	1.42	0.67
1:G:371:ASN:N	1:G:372:PRO:HD3	2.10	0.66
1:C:67:HIS:CE1	1:C:305:GLN:HG3	2.30	0.66
1:G:151:ARG:HH12	1:G:383:GLU:CD	1.98	0.66
1:G:174:PRO:HB3	1:G:294:VAL:HG13	1.76	0.66
1:A:327:PHE:CE2	1:A:359:ILE:HD12	2.30	0.66
1:A:188:ILE:HG23	1:A:328:ILE:HD11	1.76	0.66
1:C:223:LYS:HB3	1:C:224:PRO:HD3	1.77	0.66
1:A:86:ILE:O	1:A:90:GLN:HG3	1.95	0.66
1:C:279:ASN:O	1:C:337:GLU:HB2	1.96	0.66
1:E:267:ILE:HG12	3:E:401:HOH:O	1.96	0.66
1:A:223:LYS:HB3	1:A:224:PRO:HD3	1.78	0.65
1:A:280:MET:O	1:A:337:GLU:N	2.28	0.65
1:C:109:ARG:HD2	3:C:385:HOH:O	1.96	0.65
1:E:128:VAL:HG23	2:E:1:SAH:N1	2.12	0.65
1:C:181:LEU:HD21	1:C:288:PHE:HB3	1.78	0.65
1:A:279:ASN:O	1:A:281:GLU:N	2.26	0.65
1:C:102:THR:HG22	1:C:103:LYS:H	1.62	0.65
1:G:371:ASN:H	1:G:372:PRO:HD3	1.61	0.65
1:E:151:ARG:O	1:E:152:GLU:HB2	1.97	0.64
1:A:281:GLU:O	1:A:282:HIS:CG	2.50	0.64
1:G:114:ALA:HB2	1:E:220:VAL:HG11	1.78	0.64
1:A:213:TYR:O	1:A:214:TYR:CB	2.46	0.64
1:G:169:THR:HG22	1:G:169:THR:O	1.97	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:242:LEU:HB2	1:G:324:GLN:OE1	1.98	0.64
1:E:244:PRO:HD2	1:E:316:GLU:HG3	1.80	0.64
1:C:242:LEU:HD21	1:C:326:VAL:CG2	2.28	0.63
1:G:221:LEU:HD11	1:E:111:LEU:HD13	1.80	0.63
1:G:151:ARG:O	1:G:152:GLU:HB2	1.98	0.63
1:A:102:THR:HG22	1:A:104:MET:H	1.63	0.63
1:A:281:GLU:O	1:A:282:HIS:CD2	2.52	0.63
1:E:67:HIS:CE1	1:E:305:GLN:HG3	2.34	0.63
1:G:281:GLU:H	1:G:337:GLU:H	1.44	0.63
1:A:315:SER:HB2	1:A:318:HIS:H	1.64	0.63
1:C:181:LEU:CD2	1:C:288:PHE:HB3	2.29	0.63
1:E:188:ILE:HG23	1:E:328:ILE:CD1	2.29	0.62
1:A:349:ARG:HD3	1:A:354:HIS:O	1.99	0.62
1:E:342:ASN:N	1:E:342:ASN:OD1	2.30	0.62
1:E:174:PRO:HB3	1:E:294:VAL:HG13	1.80	0.62
1:E:213:TYR:O	1:E:214:TYR:CB	2.48	0.62
1:A:213:TYR:O	1:A:214:TYR:HB2	2.00	0.61
1:C:331:ASN:HB2	1:G:70:GLU:HG2	1.82	0.61
1:G:181:LEU:CD2	1:G:345:LEU:HD21	2.28	0.61
1:E:315:SER:O	1:E:316:GLU:CB	2.47	0.61
1:C:102:THR:HG22	1:C:103:LYS:N	2.15	0.61
1:G:356:LEU:HD22	1:G:383:GLU:HB2	1.81	0.61
1:A:132:SER:HA	1:A:165:TRP:CZ2	2.36	0.61
1:A:132:SER:HA	1:A:165:TRP:HZ2	1.65	0.61
1:E:343:LEU:HD13	1:E:361:LEU:HD11	1.83	0.61
1:C:260:LEU:HD21	1:C:299:ARG:HH22	1.65	0.61
1:G:79:THR:OG1	1:G:82:GLY:HA2	2.01	0.60
1:G:280:MET:HA	1:G:337:GLU:CB	2.31	0.60
1:E:183:PRO:CD	1:E:275:THR:HG21	2.31	0.60
1:G:215:GLY:O	1:G:216:VAL:HG23	2.01	0.60
1:C:280:MET:N	1:C:281:GLU:CA	2.62	0.60
1:A:373:LYS:O	1:A:374:GLU:HB2	2.01	0.60
1:C:266:GLU:O	1:C:266:GLU:HG2	2.02	0.60
1:C:297:SER:HA	1:C:307:GLU:HG2	1.84	0.60
1:G:183:PRO:HG2	1:G:275:THR:HG21	1.84	0.60
1:G:73:THR:OG1	1:G:94:ARG:NH1	2.35	0.60
1:E:151:ARG:HD2	1:E:383:GLU:OE1	2.02	0.60
1:A:269:GLU:O	1:A:347:MET:N	2.35	0.60
1:A:277:VAL:HG11	1:A:335:VAL:CG1	2.32	0.59
1:G:143:GLU:OE2	1:G:322:TRP:HZ2	1.85	0.59
1:G:151:ARG:NH1	1:G:383:GLU:OE1	2.34	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:40:SER:HB3	1:E:102:THR:CG2	2.30	0.59
1:E:213:TYR:CD1	1:E:213:TYR:N	2.69	0.59
1:G:334:ASN:N	1:G:334:ASN:ND2	2.51	0.59
1:E:186:SER:OG	1:E:188:ILE:HG22	2.03	0.59
1:G:243:ASN:HB3	1:G:246:GLN:HG3	1.84	0.59
1:G:214:TYR:O	1:G:215:GLY:C	2.39	0.59
1:E:143:GLU:OE2	1:E:322:TRP:HZ2	1.86	0.59
1:E:58:TYR:O	1:E:62:VAL:HG23	2.03	0.59
1:E:145:MET:CE	1:E:294:VAL:HG21	2.33	0.59
1:G:102:THR:HG22	1:G:103:LYS:N	2.17	0.58
1:C:291:TRP:HB2	1:C:312:THR:OG1	2.03	0.58
1:G:223:LYS:HB3	1:G:224:PRO:HD3	1.85	0.58
1:E:375:SER:O	1:E:376:PHE:HB3	2.04	0.58
1:E:367:GLU:CB	1:E:372:PRO:HD3	2.33	0.58
1:G:361:LEU:HD23	1:G:376:PHE:HE1	1.69	0.58
1:A:102:THR:HG22	1:A:103:LYS:N	2.19	0.58
1:A:264:VAL:O	1:A:267:ILE:HB	2.03	0.58
1:A:34:GLN:CG	1:A:35:TYR:N	2.66	0.57
1:G:151:ARG:HD2	1:G:382:ILE:HG22	1.85	0.57
1:E:213:TYR:O	1:E:214:TYR:HB2	2.05	0.57
1:C:223:LYS:O	1:C:226:ALA:HB3	2.05	0.57
1:E:171:VAL:HG12	1:E:172:MET:H	1.70	0.57
1:A:373:LYS:O	1:A:374:GLU:CB	2.53	0.57
1:A:122:GLU:HG2	3:A:395:HOH:O	2.04	0.57
1:C:299:ARG:O	1:C:301:GLU:N	2.37	0.57
1:C:266:GLU:O	1:C:266:GLU:CG	2.53	0.56
1:A:178:ARG:HD3	1:A:253:ILE:HD13	1.85	0.56
1:E:372:PRO:O	1:E:373:LYS:CB	2.52	0.56
1:G:40:SER:OG	1:G:102:THR:HG21	2.04	0.56
1:G:334:ASN:H	1:G:334:ASN:ND2	2.01	0.56
1:E:80:GLY:O	1:E:108:ALA:HB2	2.05	0.56
1:G:223:LYS:HB3	1:G:224:PRO:CD	2.34	0.56
1:E:189:ALA:HB2	1:E:286:CYS:HB3	1.86	0.56
1:G:128:VAL:HA	1:G:131:ILE:HG12	1.88	0.56
1:E:174:PRO:CB	1:E:294:VAL:HG13	2.36	0.56
1:G:32:TYR:O	1:G:33:ALA:C	2.43	0.56
1:C:77:VAL:HB	1:C:142:SER:HB2	1.86	0.56
1:G:59:PHE:CE1	1:E:214:TYR:HA	2.41	0.56
1:E:235:GLN:O	1:E:380:TYR:HA	2.06	0.56
1:E:281:GLU:O	1:E:282:HIS:CB	2.54	0.55
1:C:356:LEU:HD22	1:C:383:GLU:HB2	1.87	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:299:ARG:HG2	1:E:300:LYS:H	1.71	0.55
1:C:183:PRO:HB3	1:C:285:LEU:HD11	1.89	0.55
1:A:267:ILE:HG22	1:A:268:GLU:OE1	2.07	0.55
1:C:299:ARG:C	1:C:301:GLU:N	2.60	0.55
1:G:42:LEU:HD11	1:G:107:HIS:CD2	2.42	0.55
1:A:277:VAL:HG12	1:A:280:MET:CB	2.37	0.54
1:E:143:GLU:OE2	1:E:322:TRP:CZ2	2.59	0.54
1:C:151:ARG:O	1:C:152:GLU:HB2	2.07	0.54
1:A:155:PHE:O	1:A:159:ILE:HG13	2.07	0.54
1:E:367:GLU:HB2	1:E:372:PRO:CD	2.37	0.54
1:E:140:ILE:HG13	1:E:166:LEU:HD13	1.88	0.54
1:E:162:ARG:HG3	1:E:166:LEU:HD22	1.88	0.54
1:E:171:VAL:HG12	1:E:172:MET:N	2.23	0.54
1:G:32:TYR:O	1:G:36:PHE:N	2.38	0.54
1:A:174:PRO:CB	1:A:294:VAL:HG13	2.36	0.54
1:C:151:ARG:HD2	1:C:382:ILE:HG22	1.90	0.54
1:C:341:LEU:HD23	1:C:365:ILE:HG23	1.90	0.54
1:C:250:THR:O	1:C:275:THR:HB	2.07	0.54
1:A:100:GLU:OE2	1:A:102:THR:HB	2.07	0.54
1:E:382:ILE:O	1:E:383:GLU:HB2	2.08	0.54
1:E:178:ARG:HB3	1:E:293:ASP:HB2	1.90	0.54
1:C:111:LEU:O	1:C:115:ASN:ND2	2.30	0.53
1:G:167:LYS:C	1:G:169:THR:H	2.11	0.53
1:E:188:ILE:CG2	1:E:328:ILE:HD11	2.37	0.53
1:E:306:GLN:HG2	1:E:308:ILE:HD11	1.90	0.53
1:E:250:THR:O	1:E:275:THR:CG2	2.57	0.53
1:C:186:SER:OG	1:C:188:ILE:HG22	2.08	0.53
1:A:210:ILE:HG22	1:A:216:VAL:O	2.08	0.53
1:C:144:TRP:CH2	1:C:149:LEU:HD11	2.44	0.53
1:C:341:LEU:CD2	1:C:365:ILE:HG12	2.38	0.53
1:A:138:ASP:O	1:A:170:GLY:HA2	2.09	0.53
1:C:79:THR:HG22	1:C:100:GLU:HB2	1.91	0.52
1:A:186:SER:OG	1:A:188:ILE:HG22	2.09	0.52
1:E:188:ILE:HD13	1:E:328:ILE:HD11	1.90	0.52
1:C:243:ASN:CB	1:C:246:GLN:HG3	2.38	0.52
1:G:151:ARG:NH1	1:G:383:GLU:CD	2.63	0.52
1:A:112:VAL:HG21	1:A:121:VAL:HG11	1.92	0.52
1:E:73:THR:HG22	1:E:137:VAL:HG22	1.92	0.52
1:G:254:VAL:O	1:G:271:ARG:HG2	2.09	0.52
1:A:127:SER:C	1:A:129:GLU:H	2.13	0.52
1:C:181:LEU:HD23	1:C:182:ALA:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:45:GLN:HG3	1:A:104:MET:SD	2.50	0.52
1:E:141:ILE:HG13	1:E:173:TYR:HB3	1.90	0.52
1:C:314:PRO:HA	3:C:384:HOH:O	2.10	0.52
1:G:215:GLY:O	1:G:216:VAL:CG2	2.58	0.52
1:C:79:THR:OG1	1:C:82:GLY:HA2	2.09	0.52
1:G:159:ILE:HD13	1:G:263:SER:HA	1.90	0.52
1:E:189:ALA:HA	1:E:328:ILE:HD12	1.92	0.52
1:G:112:VAL:O	1:G:113:LYS:C	2.49	0.52
1:G:34:GLN:CG	1:G:35:TYR:N	2.73	0.51
1:G:173:TYR:CD1	1:G:296:PHE:HD2	2.28	0.51
1:E:108:ALA:O	1:E:112:VAL:HG23	2.10	0.51
1:C:235:GLN:O	1:C:380:TYR:HA	2.09	0.51
1:A:65:ASN:O	1:A:67:HIS:N	2.43	0.51
1:G:292:PHE:HZ	1:G:322:TRP:CD2	2.28	0.51
1:A:144:TRP:CH2	1:A:149:LEU:HD11	2.46	0.51
1:G:221:LEU:CD1	1:E:111:LEU:HD13	2.40	0.51
1:A:75:LEU:HB2	1:A:137:VAL:HG21	1.92	0.51
1:C:225:PHE:O	1:C:229:GLN:HG3	2.11	0.51
1:G:147:TYR:HB2	1:G:151:ARG:HD3	1.93	0.51
1:E:65:ASN:OD1	1:E:305:GLN:N	2.43	0.51
1:G:114:ALA:CB	1:E:220:VAL:HG11	2.41	0.51
1:G:299:ARG:HG3	1:G:301:GLU:N	2.25	0.51
1:E:183:PRO:HB2	1:E:248:ILE:CG1	2.41	0.51
1:E:213:TYR:O	1:E:214:TYR:CG	2.64	0.51
1:C:373:LYS:O	1:C:374:GLU:HG2	2.10	0.51
1:E:115:ASN:O	1:E:117:LEU:HG	2.11	0.51
1:E:143:GLU:OE1	1:E:143:GLU:O	2.28	0.51
1:E:167:LYS:HB2	1:E:168:PRO:HD2	1.93	0.51
1:E:149:LEU:HD13	1:E:292:PHE:CD1	2.47	0.50
1:C:51:ASP:HB3	1:C:54:ARG:HB3	1.94	0.50
1:G:178:ARG:HG3	1:G:256:GLU:HG3	1.93	0.50
1:E:67:HIS:ND1	1:E:305:GLN:HG3	2.25	0.50
1:E:200:MET:O	1:E:203:TRP:HB3	2.09	0.50
1:G:183:PRO:CG	1:G:275:THR:HG21	2.41	0.50
1:G:225:PHE:O	1:G:229:GLN:HG2	2.12	0.50
1:E:131:ILE:CG2	1:E:132:SER:N	2.74	0.50
1:C:118:ASP:OD2	1:C:118:ASP:N	2.45	0.50
1:C:174:PRO:HB3	1:C:294:VAL:HG13	1.94	0.50
1:A:79:THR:OG1	1:A:82:GLY:HA2	2.11	0.50
1:A:192:LYS:O	1:A:195:ASP:HB2	2.11	0.50
1:E:284:ARG:HA	1:E:333:ILE:O	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:220:VAL:HG21	1:E:114:ALA:HB3	1.94	0.50
1:A:151:ARG:HD2	1:A:382:ILE:HG22	1.94	0.50
1:E:213:TYR:O	1:E:214:TYR:CD2	2.64	0.50
1:E:367:GLU:H	1:E:372:PRO:HD2	1.76	0.50
1:C:37:CYS:O	1:C:40:SER:OG	2.30	0.49
1:C:299:ARG:HG2	1:C:301:GLU:HB3	1.93	0.49
1:G:102:THR:C	1:G:104:MET:H	2.13	0.49
1:E:277:VAL:HG11	1:E:335:VAL:CG1	2.42	0.49
1:C:59:PHE:CE1	1:A:214:TYR:HA	2.47	0.49
1:G:188:ILE:HG23	1:G:328:ILE:HD11	1.94	0.49
1:G:274:VAL:HA	1:G:341:LEU:O	2.13	0.49
1:G:341:LEU:HD22	1:G:365:ILE:HG12	1.94	0.49
1:G:302:ASP:OD1	3:G:411:HOH:O	2.19	0.49
1:E:40:SER:CB	1:E:102:THR:HG21	2.38	0.49
1:A:69:PHE:O	1:A:93:ALA:HA	2.13	0.49
1:E:366:LYS:HB3	1:E:371:ASN:O	2.12	0.49
1:E:367:GLU:HB2	1:E:372:PRO:HD3	1.93	0.49
1:A:128:VAL:HG23	2:A:1:SAH:N1	2.28	0.49
1:E:154:MET:O	1:E:154:MET:HG2	2.12	0.49
1:A:277:VAL:HG21	1:A:335:VAL:HG11	1.94	0.49
1:G:301:GLU:C	1:G:303:PRO:HD3	2.31	0.48
1:A:34:GLN:CG	1:A:35:TYR:H	2.26	0.48
1:A:315:SER:CB	1:A:318:HIS:O	2.61	0.48
1:C:147:TYR:HB2	1:C:151:ARG:HD3	1.95	0.48
1:A:43:TYR:O	1:A:46:LYS:HB3	2.14	0.48
1:E:183:PRO:HD3	1:E:275:THR:HG21	1.95	0.48
1:G:42:LEU:HD11	1:G:107:HIS:NE2	2.28	0.48
1:G:151:ARG:O	1:G:152:GLU:CB	2.60	0.48
1:A:188:ILE:HG23	1:A:328:ILE:CD1	2.43	0.48
1:C:229:GLN:OE1	1:C:233:TYR:HE2	1.96	0.48
1:G:34:GLN:CG	1:G:35:TYR:H	2.27	0.48
1:G:270:VAL:HG22	1:G:346:LEU:HD12	1.96	0.48
1:C:286:CYS:O	1:C:329:MET:HB2	2.14	0.48
1:G:33:ALA:O	1:G:37:CYS:N	2.39	0.48
1:G:299:ARG:HG3	1:G:300:LYS:N	2.29	0.48
1:G:214:TYR:HB3	1:E:87:TRP:HZ2	1.79	0.48
1:G:291:TRP:HB2	1:G:312:THR:OG1	2.14	0.48
1:E:297:SER:OG	1:E:307:GLU:OE1	2.28	0.48
1:E:361:LEU:O	1:E:377:LYS:HA	2.14	0.48
1:C:279:ASN:OD1	1:C:283:THR:HG21	2.14	0.47
1:C:337:GLU:HG3	1:C:338:GLY:N	2.28	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:MET:HE3	1:A:107:HIS:HB2	1.95	0.47
1:A:109:ARG:NH2	1:A:123:VAL:O	2.47	0.47
1:C:103:LYS:HD3	1:C:125:GLU:OE2	2.14	0.47
1:C:242:LEU:HD21	1:C:326:VAL:HG22	1.96	0.47
1:A:151:ARG:C	1:A:153:SER:H	2.18	0.47
1:E:252:THR:HB	1:E:273:ASN:OD1	2.14	0.47
1:C:109:ARG:NH2	1:C:123:VAL:O	2.47	0.47
1:C:112:VAL:HG11	1:C:121:VAL:HB	1.96	0.47
1:G:183:PRO:HB2	1:G:248:ILE:HG13	1.96	0.47
1:E:42:LEU:HD12	1:E:42:LEU:H	1.79	0.47
1:E:277:VAL:HG21	1:E:335:VAL:CG1	2.34	0.47
1:E:299:ARG:HE	1:E:301:GLU:CD	2.17	0.47
1:G:32:TYR:HB2	1:G:36:PHE:HD1	1.80	0.47
1:A:252:THR:HB	1:A:273:ASN:ND2	2.30	0.47
1:E:367:GLU:H	1:E:372:PRO:CD	2.28	0.47
1:C:221:LEU:HD13	1:A:42:LEU:HD21	1.96	0.47
1:A:327:PHE:HE2	1:A:359:ILE:HD12	1.76	0.47
1:E:74:VAL:HG12	1:E:75:LEU:N	2.30	0.47
1:A:206:PHE:CZ	1:A:210:ILE:CD1	2.98	0.47
1:A:367:GLU:HB2	1:A:371:ASN:O	2.15	0.47
1:E:162:ARG:HG3	1:E:166:LEU:CD2	2.45	0.47
1:E:213:TYR:C	1:E:214:TYR:CG	2.88	0.47
1:A:102:THR:CG2	1:A:103:LYS:N	2.77	0.46
1:C:60:ASN:O	1:C:64:GLN:HB2	2.15	0.46
1:C:72:LYS:HD3	3:C:410:HOH:O	2.16	0.46
1:C:198:GLY:O	1:C:199:ALA:C	2.54	0.46
1:A:270:VAL:HG22	1:A:346:LEU:HG	1.97	0.46
1:A:40:SER:HB3	1:A:102:THR:CG2	2.46	0.46
1:A:183:PRO:HG2	1:A:275:THR:HG21	1.98	0.46
1:E:145:MET:HE2	1:E:294:VAL:HG21	1.97	0.46
1:G:183:PRO:HB3	1:G:285:LEU:HD13	1.96	0.46
1:C:143:GLU:OE2	1:C:322:TRP:CZ2	2.68	0.46
1:E:137:VAL:N	1:E:165:TRP:O	2.48	0.46
1:E:175:SER:HB2	3:E:406:HOH:O	2.15	0.46
1:G:280:MET:O	1:G:281:GLU:C	2.54	0.46
1:A:124:ILE:HG21	1:A:131:ILE:HD13	1.98	0.46
1:C:341:LEU:HD23	1:C:365:ILE:HG12	1.98	0.46
1:C:365:ILE:HD12	1:C:374:GLU:HB2	1.96	0.46
1:E:86:ILE:O	1:E:90:GLN:HG3	2.15	0.46
1:E:171:VAL:HG11	1:E:298:GLY:HA2	1.97	0.46
1:A:40:SER:CA	1:A:102:THR:HG21	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:199:ALA:HB1	1:C:229:GLN:CD	2.35	0.45
1:C:260:LEU:HD23	1:C:260:LEU:O	2.15	0.45
1:A:213:TYR:O	1:A:214:TYR:CG	2.69	0.45
1:A:177:ALA:O	1:A:178:ARG:HB2	2.17	0.45
1:E:141:ILE:HG13	1:E:173:TYR:CB	2.46	0.45
1:C:337:GLU:HG2	3:C:426:HOH:O	2.16	0.45
1:E:254:VAL:HG11	1:E:345:LEU:CD2	2.45	0.45
1:C:221:LEU:HD22	1:A:107:HIS:HB3	1.99	0.45
1:A:291:TRP:HB2	1:A:312:THR:OG1	2.16	0.45
1:G:33:ALA:O	1:G:34:GLN:C	2.54	0.45
1:G:289:GLY:HA2	1:G:325:GLN:O	2.16	0.45
1:A:162:ARG:NH1	1:A:259:CYS:O	2.50	0.45
1:C:68:HIS:ND1	1:C:173:TYR:OH	2.44	0.45
1:A:223:LYS:O	1:A:226:ALA:HB3	2.17	0.45
1:E:60:ASN:O	1:E:61:ALA:C	2.53	0.45
1:E:144:TRP:CE3	1:E:155:PHE:HB2	2.52	0.45
1:E:365:ILE:O	1:E:373:LYS:HA	2.16	0.45
1:C:237:ALA:HB2	1:C:327:PHE:CE2	2.51	0.45
1:A:39:TYR:CG	2:A:1:SAH:H3'	2.52	0.45
1:E:212:SER:HB3	1:E:213:TYR:CD1	2.52	0.45
1:E:245:GLN:OE1	1:E:245:GLN:HA	2.16	0.45
1:E:349:ARG:HD3	3:E:388:HOH:O	2.17	0.45
1:C:86:ILE:HG23	1:C:117:LEU:HD11	1.98	0.44
1:C:147:TYR:O	1:C:151:ARG:HB2	2.17	0.44
1:C:173:TYR:CD1	1:C:296:PHE:HD2	2.35	0.44
1:A:133:LEU:HA	1:A:134:PRO:HD3	1.87	0.44
1:A:154:MET:O	1:A:154:MET:HG2	2.16	0.44
1:E:100:GLU:HG2	1:E:104:MET:HB3	1.99	0.44
1:E:373:LYS:O	1:E:374:GLU:CB	2.60	0.44
1:C:264:VAL:HA	1:C:267:ILE:HG12	1.98	0.44
1:G:102:THR:C	1:G:104:MET:N	2.70	0.44
1:A:58:TYR:O	1:A:62:VAL:HG23	2.18	0.44
1:E:65:ASN:OD1	1:E:304:ALA:HB1	2.17	0.44
1:C:167:LYS:HB2	1:C:168:PRO:CD	2.47	0.44
1:G:32:TYR:HB2	1:G:36:PHE:CD1	2.53	0.44
1:E:100:GLU:O	1:E:125:GLU:HA	2.17	0.44
1:E:243:ASN:O	1:E:246:GLN:HG3	2.17	0.44
1:A:40:SER:CB	1:A:102:THR:HG21	2.47	0.44
1:A:363:CYS:O	1:A:375:SER:HA	2.17	0.44
1:G:169:THR:O	1:G:169:THR:CG2	2.66	0.44
1:A:133:LEU:HD22	1:A:134:PRO:HD2	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:GLU:C	1:A:282:HIS:CG	2.90	0.44
1:C:86:ILE:HG23	1:C:117:LEU:CD1	2.48	0.44
1:C:127:SER:O	1:C:129:GLU:N	2.51	0.44
1:C:277:VAL:HG21	1:C:335:VAL:HG13	2.00	0.44
1:A:147:TYR:HB2	1:A:151:ARG:HD3	1.99	0.44
1:A:280:MET:CB	1:A:337:GLU:CA	2.90	0.44
1:A:334:ASN:O	1:A:335:VAL:HG23	2.18	0.44
1:A:376:PHE:CD1	1:A:376:PHE:C	2.91	0.44
1:C:373:LYS:O	1:G:119:HIS:NE2	2.50	0.44
1:G:138:ASP:O	1:G:170:GLY:HA2	2.18	0.44
1:G:167:LYS:C	1:G:169:THR:N	2.71	0.44
1:A:153:SER:HB3	3:A:407:HOH:O	2.18	0.44
1:A:134:PRO:O	1:A:135:GLU:HB3	2.17	0.44
1:E:79:THR:OG1	1:E:98:ALA:HB1	2.18	0.44
1:C:372:PRO:O	1:C:373:LYS:CB	2.66	0.43
1:G:32:TYR:O	1:G:35:TYR:N	2.51	0.43
1:G:182:ALA:HA	1:G:183:PRO:HD3	1.78	0.43
1:G:95:LYS:HE2	1:G:122:GLU:HB2	2.01	0.43
1:E:245:GLN:OE1	1:E:245:GLN:CA	2.66	0.43
1:C:129:GLU:OE2	1:C:157:SER:HA	2.18	0.43
1:C:218:MET:HE1	1:A:111:LEU:HD21	2.01	0.43
1:A:39:TYR:CD1	2:A:1:SAH:H3'	2.53	0.43
1:E:151:ARG:O	1:E:152:GLU:CB	2.66	0.43
1:G:56:ASP:O	1:G:57:ALA:C	2.56	0.43
1:C:184:ILE:HD11	1:C:326:VAL:HG13	1.99	0.43
1:C:210:ILE:O	1:C:210:ILE:HG22	2.18	0.43
1:G:95:LYS:HG3	1:G:120:ILE:O	2.17	0.43
1:C:155:PHE:CD2	1:C:257:MET:HE1	2.54	0.43
1:A:100:GLU:HG3	1:A:102:THR:H	1.83	0.43
1:A:277:VAL:HG21	1:A:335:VAL:CG1	2.48	0.43
1:C:151:ARG:CZ	1:C:383:GLU:OE1	2.67	0.43
1:A:133:LEU:HA	1:A:133:LEU:HD23	1.69	0.43
1:A:133:LEU:N	1:A:165:TRP:CH2	2.80	0.43
1:A:267:ILE:O	1:A:267:ILE:CG2	2.66	0.43
1:E:77:VAL:HG13	1:E:128:VAL:HG21	2.00	0.43
1:C:260:LEU:HD11	1:C:299:ARG:CZ	2.49	0.43
1:C:312:THR:O	1:C:313:ALA:C	2.58	0.43
1:A:127:SER:C	1:A:129:GLU:N	2.71	0.43
1:G:267:ILE:CG2	1:G:267:ILE:O	2.66	0.43
1:A:178:ARG:O	1:A:292:PHE:HA	2.19	0.43
1:E:79:THR:OG1	1:E:82:GLY:HA2	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:277:VAL:HG11	1:E:335:VAL:HG12	2.01	0.42
1:C:83:ILE:HG23	1:C:84:LEU:N	2.34	0.42
1:G:218:MET:O	1:G:219:GLY:C	2.57	0.42
1:A:188:ILE:HG12	1:A:188:ILE:O	2.19	0.42
1:E:45:GLN:HG3	1:E:104:MET:SD	2.59	0.42
1:E:243:ASN:OD1	1:E:245:GLN:HB2	2.19	0.42
1:C:199:ALA:CB	1:C:229:GLN:OE1	2.67	0.42
1:C:376:PHE:C	1:C:376:PHE:CD1	2.93	0.42
1:A:382:ILE:O	1:A:383:GLU:HB2	2.19	0.42
1:C:186:SER:CB	1:C:188:ILE:HG22	2.49	0.42
1:G:32:TYR:HB3	1:G:35:TYR:HB3	2.02	0.42
1:A:40:SER:HA	1:A:102:THR:HG21	2.02	0.42
1:A:279:ASN:C	1:A:281:GLU:H	2.21	0.42
1:C:357:MET:HB2	1:C:382:ILE:HB	2.02	0.42
1:A:69:PHE:N	1:A:69:PHE:CD1	2.88	0.42
1:A:171:VAL:CG1	1:A:298:GLY:HA2	2.50	0.42
1:A:240:ASN:OD1	1:A:241:ASP:N	2.52	0.42
1:E:266:GLU:HG2	1:E:266:GLU:O	2.20	0.42
1:E:250:THR:N	1:E:275:THR:HG23	2.35	0.42
1:E:322:TRP:O	1:E:323:GLY:C	2.58	0.42
1:C:301:GLU:O	1:C:301:GLU:HG2	2.18	0.42
1:G:61:ALA:O	1:G:65:ASN:HB2	2.20	0.42
1:A:81:SER:O	1:A:108:ALA:HA	2.20	0.42
1:C:51:ASP:OD1	1:C:54:ARG:HB2	2.20	0.41
1:E:186:SER:CB	1:E:188:ILE:HG22	2.50	0.41
1:C:73:THR:HG22	1:C:137:VAL:HG22	2.02	0.41
1:C:174:PRO:CB	1:C:294:VAL:HG13	2.51	0.41
1:C:370:GLY:HA2	1:C:371:ASN:HA	1.91	0.41
1:G:359:ILE:HD11	1:G:382:ILE:HD11	2.02	0.41
1:A:182:ALA:O	1:A:184:ILE:HG23	2.20	0.41
1:E:183:PRO:HB2	1:E:248:ILE:HG13	2.01	0.41
1:A:65:ASN:C	1:A:67:HIS:H	2.23	0.41
1:E:58:TYR:OH	1:E:174:PRO:HD3	2.19	0.41
1:E:307:GLU:C	1:E:308:ILE:HD12	2.40	0.41
1:C:154:MET:O	1:C:154:MET:HG2	2.20	0.41
1:G:174:PRO:CB	1:G:294:VAL:HG13	2.47	0.41
1:G:315:SER:O	1:G:316:GLU:CB	2.68	0.41
1:A:65:ASN:C	1:A:67:HIS:N	2.74	0.41
1:E:171:VAL:CG1	1:E:298:GLY:HA2	2.51	0.41
1:E:343:LEU:HD22	1:E:363:CYS:HA	2.02	0.41
1:C:110:ALA:O	1:C:114:ALA:CB	2.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:341:LEU:CD2	1:G:365:ILE:HG12	2.51	0.41
1:G:343:LEU:CD2	1:G:363:CYS:HB2	2.51	0.41
1:C:171:VAL:HG12	1:C:172:MET:N	2.35	0.41
1:G:110:ALA:O	1:E:220:VAL:HG21	2.20	0.41
1:A:112:VAL:HG11	1:A:121:VAL:HB	2.03	0.41
1:A:152:GLU:O	1:A:355:ARG:NH1	2.47	0.41
1:A:333:ILE:HD13	1:A:374:GLU:HG2	2.03	0.41
1:G:346:LEU:HB3	1:G:360:GLU:HB2	2.03	0.41
1:A:59:PHE:CE1	1:A:63:PHE:CE2	3.09	0.41
1:E:223:LYS:HB3	3:E:427:HOH:O	2.21	0.41
1:E:349:ARG:HD2	1:E:354:HIS:O	2.20	0.41
1:C:54:ARG:HH22	2:C:1:SAH:C	2.31	0.41
1:C:229:GLN:OE1	1:C:233:TYR:CE2	2.74	0.41
1:G:144:TRP:HE3	1:G:144:TRP:O	2.03	0.41
1:G:255:LYS:HD2	1:G:271:ARG:HH21	1.86	0.41
1:G:258:ASP:OD2	1:G:260:LEU:HB2	2.20	0.41
1:G:270:VAL:HG22	1:G:346:LEU:CD1	2.50	0.41
1:A:40:SER:HB3	1:A:102:THR:HG21	2.02	0.41
1:E:167:LYS:NZ	3:E:414:HOH:O	2.53	0.41
1:E:273:ASN:O	1:E:342:ASN:HA	2.20	0.41
2:E:1:SAH:HG2	2:E:1:SAH:H4'	1.30	0.41
1:C:65:ASN:C	1:C:67:HIS:H	2.25	0.41
1:G:343:LEU:HD23	1:G:363:CYS:HB2	2.03	0.41
1:A:278:ILE:O	1:A:279:ASN:C	2.59	0.41
1:A:35:TYR:CE1	1:A:152:GLU:HB3	2.56	0.40
1:A:95:LYS:HG3	1:A:120:ILE:O	2.21	0.40
1:E:162:ARG:NH2	1:E:262:ALA:O	2.46	0.40
1:G:143:GLU:OE2	1:G:322:TRP:CZ2	2.71	0.40
1:C:131:ILE:HG22	1:C:132:SER:N	2.37	0.40
1:C:260:LEU:HD11	1:C:299:ARG:NH2	2.36	0.40
1:G:376:PHE:CD1	1:G:376:PHE:C	2.95	0.40
1:A:206:PHE:CZ	1:A:210:ILE:HD12	2.55	0.40
1:E:244:PRO:CD	1:E:316:GLU:HG3	2.50	0.40
1:C:260:LEU:HD21	1:C:299:ARG:NH2	2.33	0.40
1:G:42:LEU:HD12	1:G:42:LEU:H	1.87	0.40
1:G:181:LEU:HD22	1:G:254:VAL:HG11	2.02	0.40
1:G:292:PHE:HZ	1:G:322:TRP:CE2	2.40	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:C:243:ASN:ND2	1:A:265:SER:OG[2_445]	2.09	0.11

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	348/376 (93%)	313 (90%)	27 (8%)	8 (2%)	6	10
1	C	347/376 (92%)	311 (90%)	29 (8%)	7 (2%)	7	13
1	E	347/376 (92%)	302 (87%)	39 (11%)	6 (2%)	9	16
1	G	351/376 (93%)	310 (88%)	33 (9%)	8 (2%)	6	10
All	All	1393/1504 (93%)	1236 (89%)	128 (9%)	29 (2%)	7	12

All (29) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	372	PRO
1	G	213	TYR
1	G	372	PRO
1	A	280	MET
1	A	371	ASN
1	A	374	GLU
1	E	282	HIS
1	E	316	GLU
1	E	372	PRO
1	E	373	LYS
1	E	374	GLU
1	C	300	LYS
1	A	373	LYS
1	A	352	GLU
1	C	66	LYS
1	C	242	LEU
1	G	214	TYR

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Mol	Chain	Res	Type
1	G	371	ASN
1	G	374	GLU
1	A	135	GLU
1	C	373	LYS
1	G	142	SER
1	E	152	GLU
1	C	128	VAL
1	C	279	ASN
1	G	33	ALA
1	A	178	ARG
1	A	372	PRO
1	G	112	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	273/320 (85%)	261 (96%)	12 (4%)	28	52
1	C	272/320 (85%)	263 (97%)	9 (3%)	38	62
1	E	272/320 (85%)	256 (94%)	16 (6%)	19	37
1	G	266/320 (83%)	257 (97%)	9 (3%)	37	61
All	All	1083/1280 (85%)	1037 (96%)	46 (4%)	30	53

All (46) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	79	THR
1	C	128	VAL
1	C	279	ASN
1	C	294	VAL
1	C	317	GLN
1	C	319	CYS
1	C	320	THR
1	C	360	GLU
1	C	361	LEU

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Mol	Chain	Res	Type
1	G	38	THR
1	G	40	SER
1	G	111	LEU
1	G	148	PHE
1	G	220	VAL
1	G	294	VAL
1	G	299	ARG
1	G	311	THR
1	G	334	ASN
1	A	79	THR
1	A	127	SER
1	A	137	VAL
1	A	210	ILE
1	A	217	ASP
1	A	218	MET
1	A	265	SER
1	A	268	GLU
1	A	294	VAL
1	A	335	VAL
1	A	340	ASN
1	A	347	MET
1	E	37	CYS
1	E	95	LYS
1	E	137	VAL
1	E	169	THR
1	E	172	MET
1	E	212	SER
1	E	213	TYR
1	E	245	GLN
1	E	269	GLU
1	E	283	THR
1	E	301	GLU
1	E	312	THR
1	E	341	LEU
1	E	342	ASN
1	E	343	LEU
1	E	360	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	G	334	ASN

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)

4 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	E	1	-	24,28,28	1.20	3 (12%)	25,40,40	1.61	4 (16%)
2	SAH	A	1	-	24,28,28	1.15	2 (8%)	25,40,40	1.72	4 (16%)
2	SAH	C	1	-	24,28,28	1.14	3 (12%)	25,40,40	1.73	4 (16%)
2	SAH	G	1	-	24,28,28	1.16	3 (12%)	25,40,40	1.74	2 (8%)

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	E	1	-	-	7/11/31/31	0/3/3/3
2	SAH	A	1	-	-	3/11/31/31	0/3/3/3
2	SAH	C	1	-	-	3/11/31/31	0/3/3/3
2	SAH	G	1	-	-	1/11/31/31	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1	SAH	C2-N3	4.17	1.38	1.32
2	G	1	SAH	C2-N3	3.70	1.38	1.32
2	A	1	SAH	C2-N3	3.58	1.37	1.32
2	C	1	SAH	C2-N3	3.52	1.37	1.32
2	C	1	SAH	C2-N1	2.39	1.38	1.33
2	E	1	SAH	C2-N1	2.36	1.38	1.33
2	G	1	SAH	C2-N1	2.23	1.38	1.33
2	A	1	SAH	C2-N1	2.18	1.38	1.33
2	C	1	SAH	OXT-C	-2.12	1.23	1.30
2	E	1	SAH	OXT-C	-2.09	1.23	1.30
2	G	1	SAH	OXT-C	-2.06	1.23	1.30

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	1	SAH	N3-C2-N1	-5.93	119.40	128.68
2	A	1	SAH	N3-C2-N1	-5.66	119.83	128.68
2	C	1	SAH	N3-C2-N1	-5.59	119.94	128.68
2	E	1	SAH	N3-C2-N1	-5.30	120.39	128.68
2	G	1	SAH	C5'-SD-CG	-4.02	90.21	102.27
2	A	1	SAH	C5'-SD-CG	-3.65	91.31	102.27
2	E	1	SAH	C5'-SD-CG	-3.60	91.45	102.27
2	C	1	SAH	C5'-SD-CG	-3.59	91.50	102.27
2	A	1	SAH	OXT-C-CA	2.63	122.33	113.38
2	E	1	SAH	OXT-C-O	-2.32	118.83	124.09
2	C	1	SAH	C1'-N9-C4	-2.23	122.72	126.64
2	C	1	SAH	OXT-C-O	-2.12	119.28	124.09
2	A	1	SAH	OXT-C-O	-2.09	119.35	124.09
2	E	1	SAH	C4-C5-N7	-2.06	107.26	109.40

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	E	1	SAH	N-CA-CB-CG
2	E	1	SAH	C-CA-CB-CG
2	E	1	SAH	O4'-C4'-C5'-SD
2	E	1	SAH	C3'-C4'-C5'-SD
2	A	1	SAH	C-CA-CB-CG
2	E	1	SAH	C4'-C5'-SD-CG
2	A	1	SAH	CB-CG-SD-C5'

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Mol	Chain	Res	Type	Atoms
2	E	1	SAH	CB-CG-SD-C5'
2	C	1	SAH	C-CA-CB-CG
2	E	1	SAH	CA-CB-CG-SD
2	C	1	SAH	CB-CG-SD-C5'
2	G	1	SAH	CB-CG-SD-C5'
2	C	1	SAH	N-CA-CB-CG
2	A	1	SAH	N-CA-CB-CG

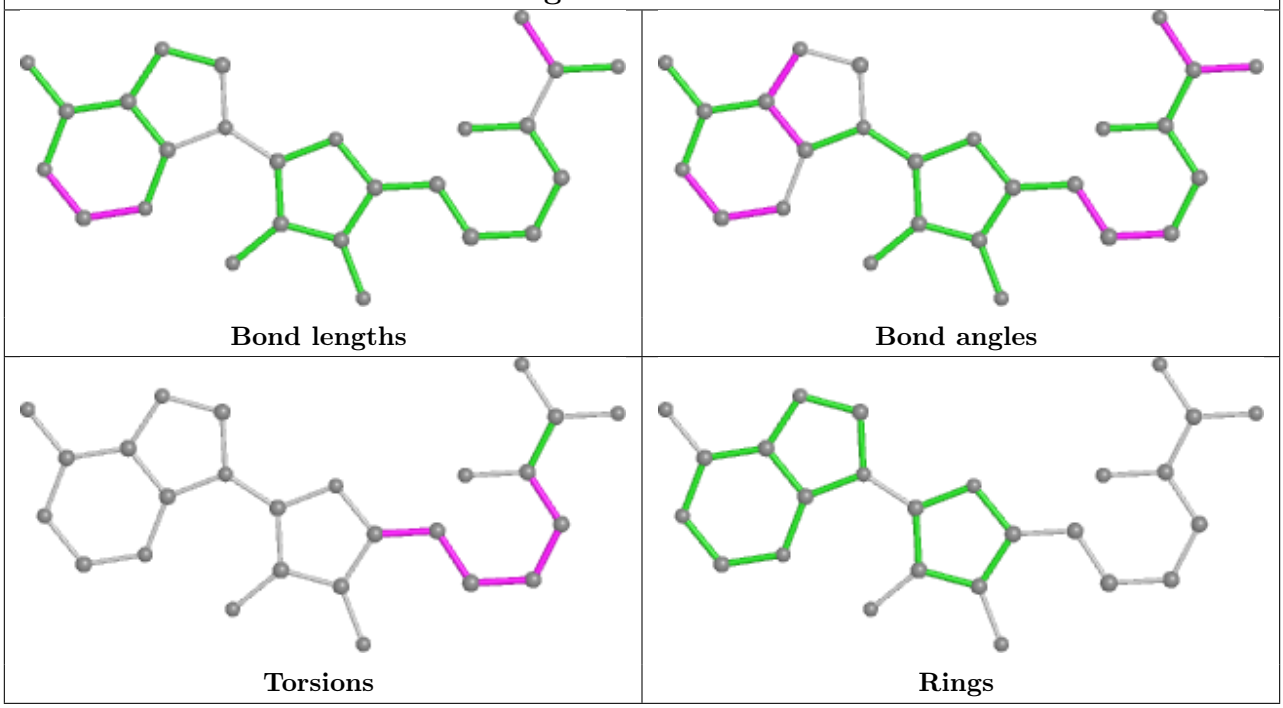
There are no ring outliers.

3 monomers are involved in 6 short contacts:

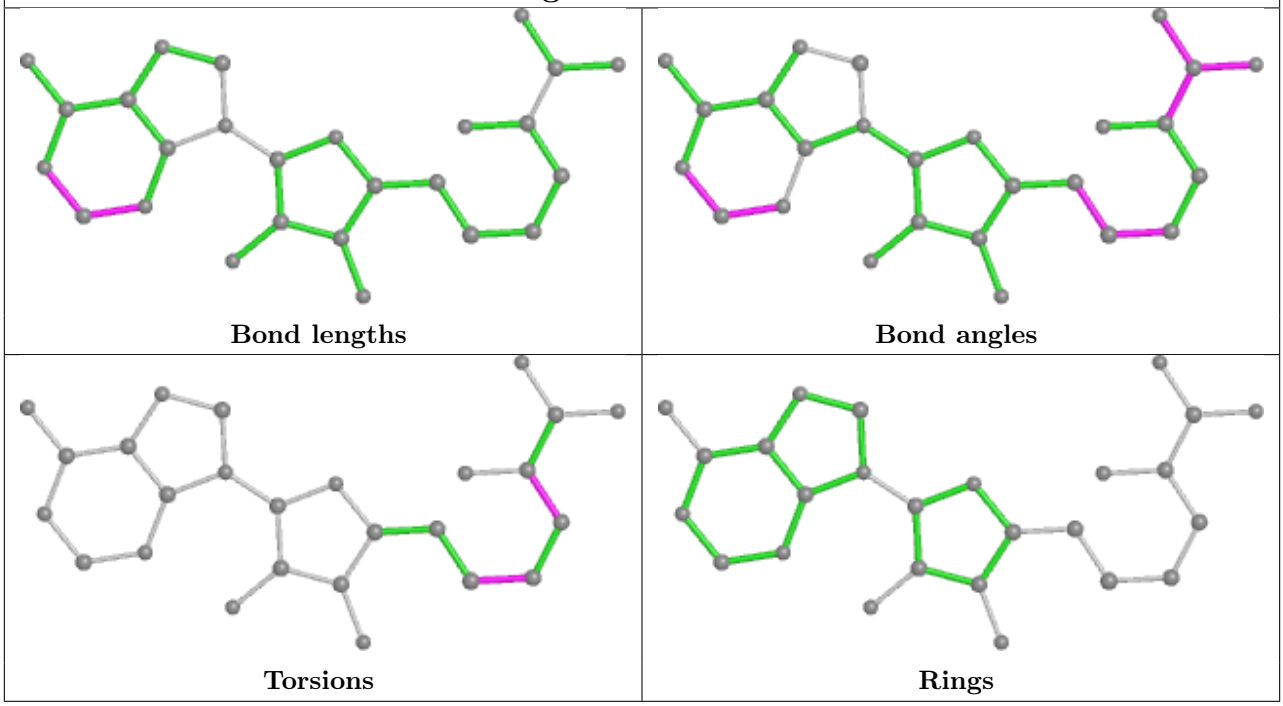
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	SAH	2	0
2	A	1	SAH	3	0
2	C	1	SAH	1	0

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.

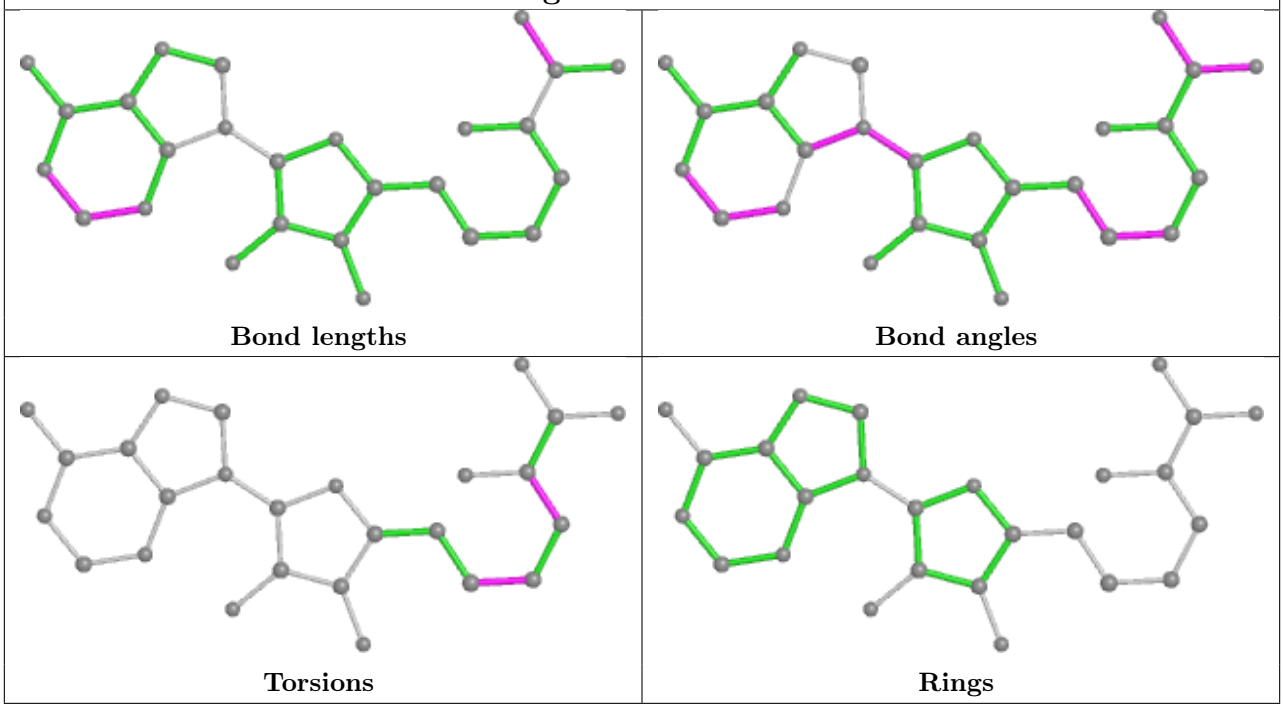
Ligand SAH E 1



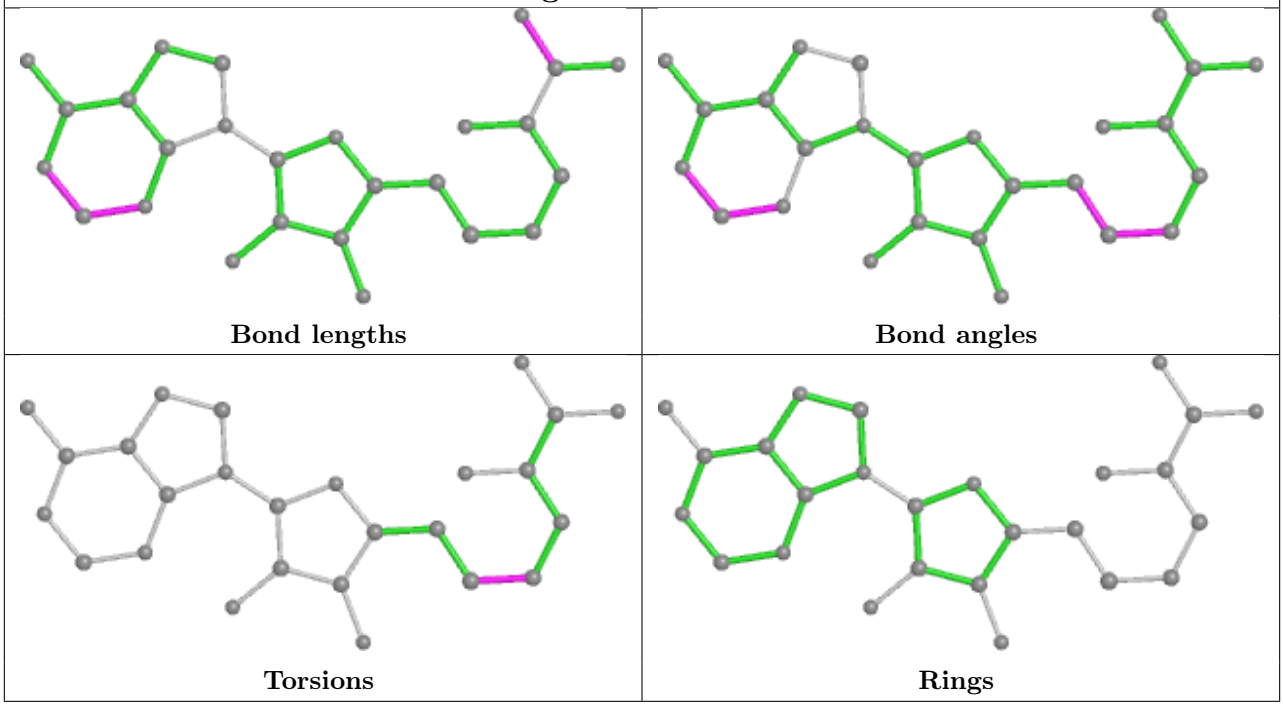
Ligand SAH A 1



Ligand SAH C 1



Ligand SAH G 1



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	350/376 (93%)	-0.89	0	100	100	26, 37, 49, 61	0
1	C	349/376 (92%)	-0.88	0	100	100	25, 37, 48, 74	0
1	E	349/376 (92%)	-0.90	0	100	100	24, 34, 47, 69	0
1	G	353/376 (93%)	-0.92	0	100	100	25, 34, 45, 53	0
All	All	1401/1504 (93%)	-0.90	0	100	100	24, 35, 48, 74	0

There are no RSRZ outliers to report.

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)

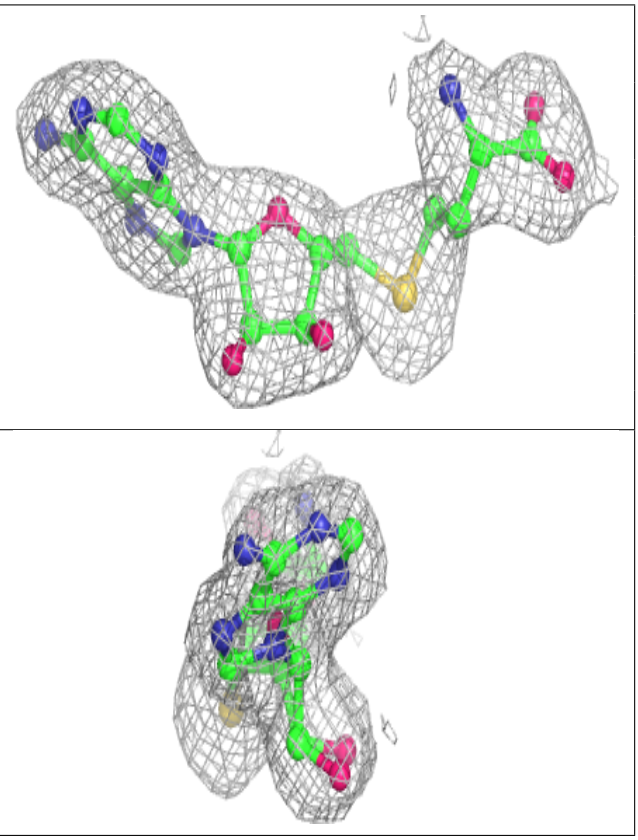
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	SAH	C	1	26/26	0.98	0.12	26,34,36,37	0
2	SAH	G	1	26/26	0.98	0.12	24,29,32,34	0
2	SAH	A	1	26/26	0.98	0.10	22,32,36,38	0
2	SAH	E	1	26/26	0.98	0.11	26,33,38,39	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.

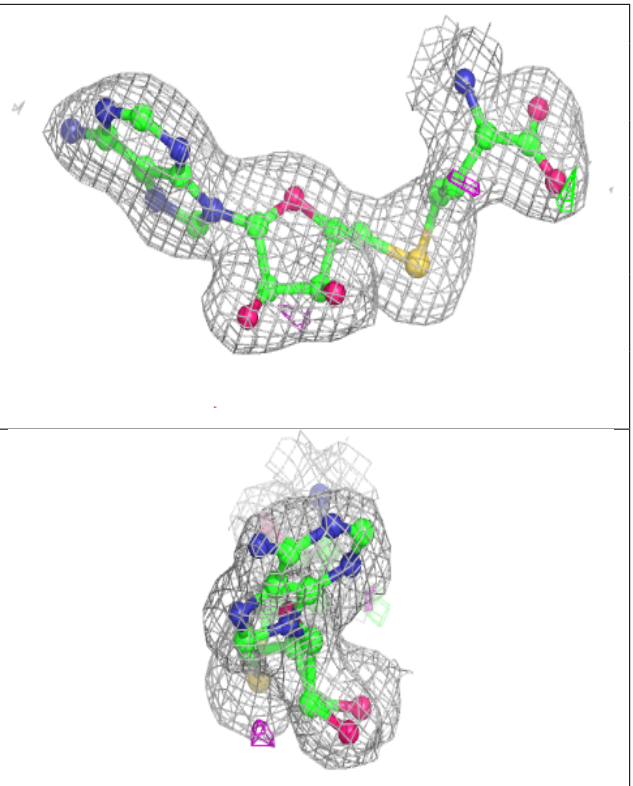
Electron density around SAH C 1:

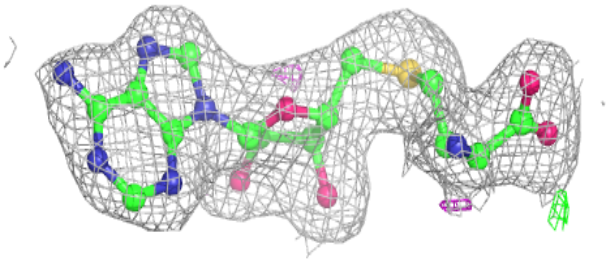
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around SAH G 1:

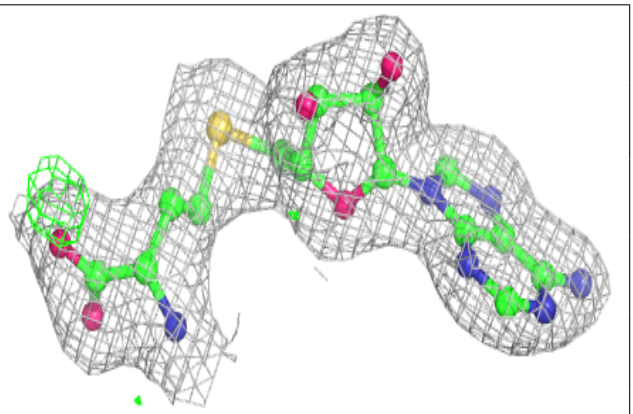
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

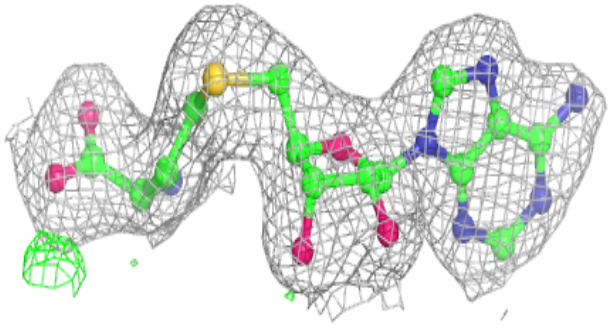


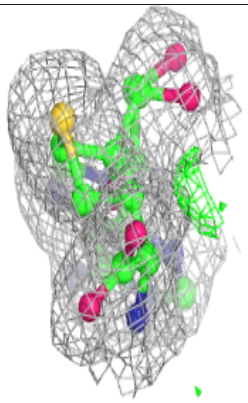


Electron density around SAH A 1:

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

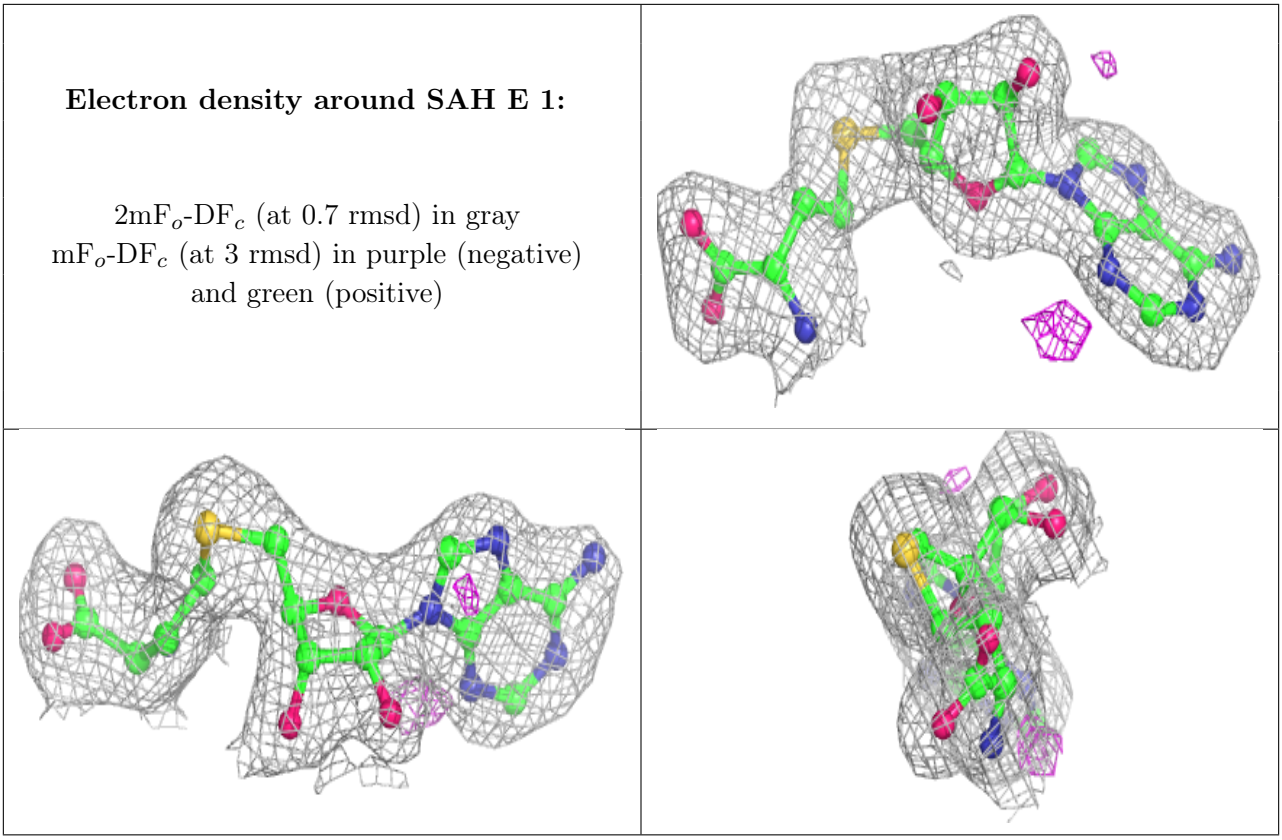






Electron density around SAH E 1:

$2mF_o$-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.