Full wwPDB X-ray Structure Validation Report ⓘ

Mar 23, 2024 – 11:08 AM EDT

PDB ID	:	1KYW
Title	:	Crystal Structure Analysis of Caffeic Acid/5-hydroxyferulic acid 3/5-O-methyltransferase in complex with 5-hydroxyconiferaldehyde
Authors	:	Zubieta, C.; Kota, P.; Ferrer, J.-L.; Dixon, R.A.; Noel, J.P.
Deposited on	:	2002-02-06
Resolution	:	2.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

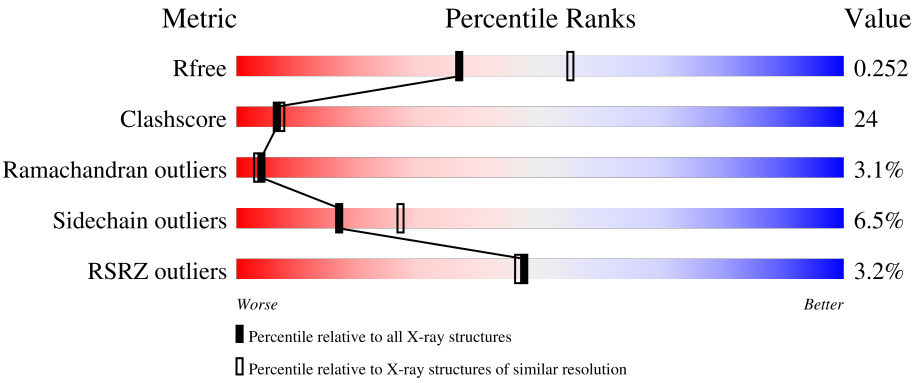
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36.1
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36.1

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 2.40 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	3907 (2.40-2.40)
Clashscore	141614	4398 (2.40-2.40)
Ramachandran outliers	138981	4318 (2.40-2.40)
Sidechain outliers	138945	4319 (2.40-2.40)
RSRZ outliers	127900	3811 (2.40-2.40)

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	365	3% 57% 35%
1	C	365	6% 58% 30% 10%
1	F	365	% 71% 24%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SAH	C	1698	X	-	-	-
2	SAH	F	1699	X	-	-	-
3	HFL	F	0	-	-	X	X

2 Entry composition

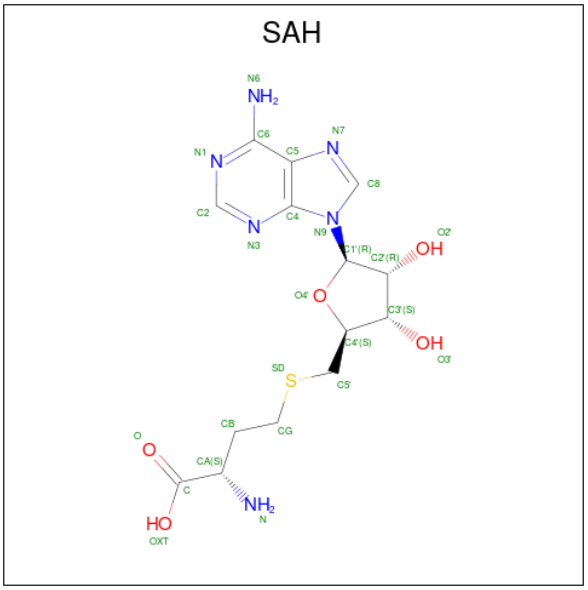
There are 4 unique types of molecules in this entry. The entry contains 8538 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Caffeic acid 3-O-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	0	0
			2693	1728	442	503	20			
1	C	361	Total	C	N	O	S	0	0	0
			2777	1780	456	521	20			
1	F	361	Total	C	N	O	S	0	0	0
			2777	1780	456	521	20			

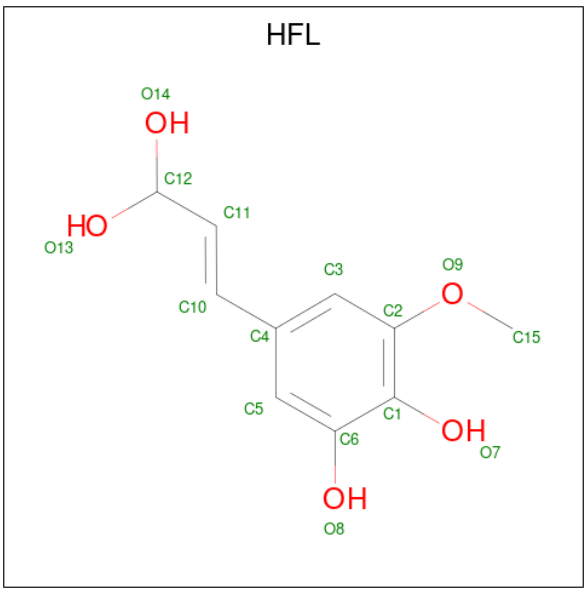
- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



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

- Molecule 3 is 5-(3,3-DIHYDROXYPROPENY)-3-METHOXY-BENZENE-1,2-DIOL

(three-letter code: HFL) (formula: $C_{10}H_{12}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	F	1	Total C O 15 10 5	0	0

- Molecule 4 is water.

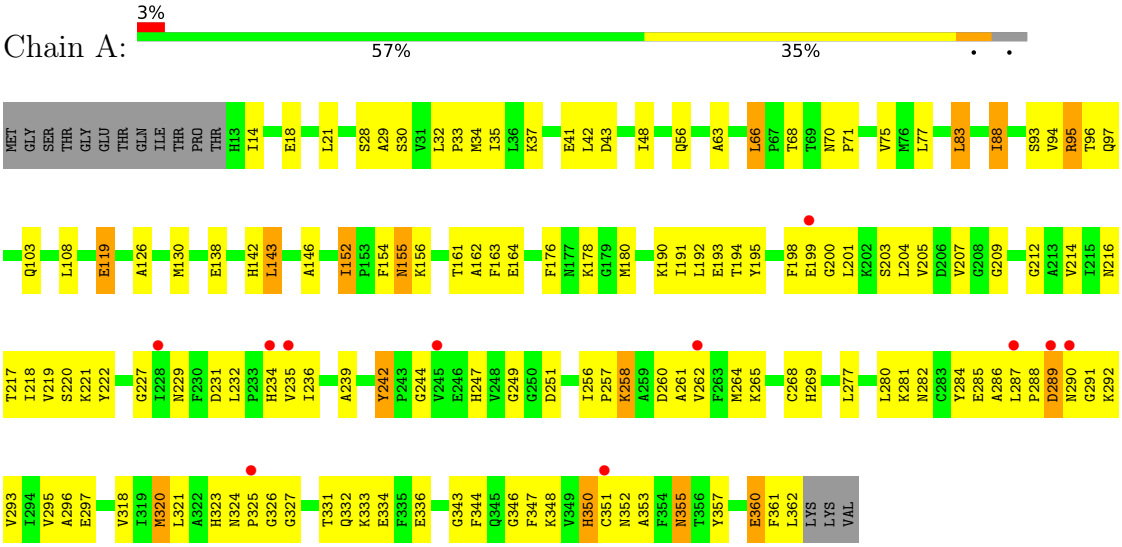
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	69	Total O 69 69	0	0
4	C	64	Total O 64 64	0	0
4	F	91	Total O 91 91	0	0

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.

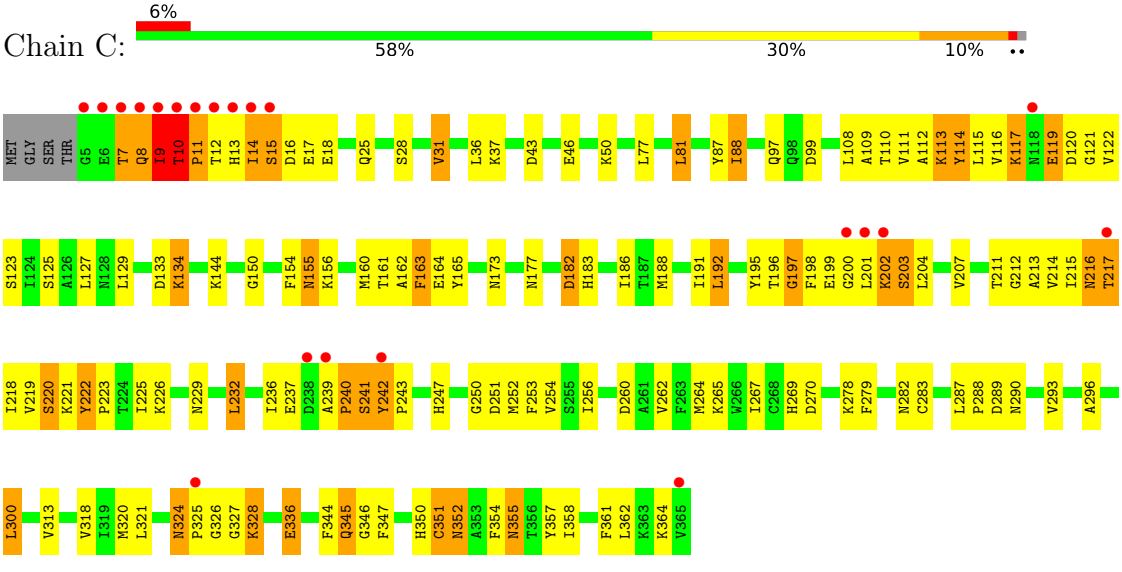
• Molecule 1: Caffeic acid 3-O-methyltransferase

Chain A:



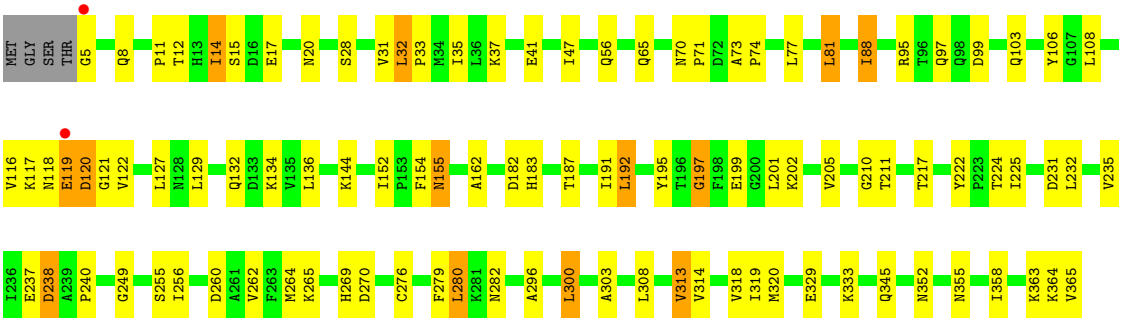
• Molecule 1: Caffeic acid 3-O-methyltransferase

Chain C:



• Molecule 1: Caffeic acid 3-O-methyltransferase

Chain F:


MET GLY SER THR G5 Q8 P11 T12 H13 I14 S15 D16 E17 N20 S28 V31 L32 P33 M34 I35 L36 K37 E41 I47 Q56 Q65 N70 P71 D72 A73 P74 L77 L81 I88 R95 T96 Q97 Q98 D99 Q103 Y106 G107 L108
V116 K117 N118 E119 D120 G121 V122 L127 N128 L129 Q132 D133 K134 V135 L136 K144 I152 P153 F154 N155 A162 D182 H183 T187 I191 L192 Y195 T196 G197 F198 E199 G200 L201 K202 V205 G210 T211 T217 Y222 P223 T224 I225 D231 L232 V235
I236 E237 D238 A239 P240 G249 S255 I256 D260 A261 V262 F263 M264 K265 H269 D270 C276 F279 L280 K281 N282 A296 L300 A303 L308 V313 V314 V318 I319 M320 E329 K333 Q345 N352 N355 I358 K363 K364 V365

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	104.47Å 62.00Å 112.21Å 90.00° 111.27° 90.00°	Depositor
Resolution (Å)	97.36 – 2.40 97.36 – 2.40	Depositor EDS
% Data completeness (in resolution range)	90.1 (97.36-2.40) 90.2 (97.36-2.40)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.89 (at 2.40Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.207 , 0.261 0.197 , 0.252	Depositor DCC
R_{free} test set	2393 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å^2)	42.7	Xtriage
Anisotropy	0.078	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 57.8	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	8538	wwPDB-VP
Average B, all atoms (Å^2)	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.54% 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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: HFL, 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	0.42	0/2752	0.64	0/3730
1	C	0.51	4/2837 (0.1%)	0.72	1/3844 (0.0%)
1	F	0.46	0/2837	0.68	2/3844 (0.1%)
All	All	0.47	4/8426 (0.0%)	0.68	3/11418 (0.0%)

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	9	ILE	C-N	7.14	1.50	1.34
1	C	10	THR	N-CA	6.83	1.60	1.46
1	C	9	ILE	CA-C	6.20	1.69	1.52
1	C	9	ILE	N-CA	5.95	1.58	1.46

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	119	GLU	N-CA-C	-8.96	86.80	111.00
1	C	222	TYR	N-CA-C	-7.45	90.88	111.00
1	F	300	LEU	CA-CB-CG	5.35	127.60	115.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2693	0	2701	131	0
1	C	2777	0	2792	173	2
1	F	2777	0	2792	84	0
2	C	26	0	17	8	0
2	F	26	0	17	7	0
3	F	15	0	12	7	0
4	A	69	0	0	5	0
4	C	64	0	0	10	0
4	F	91	0	0	2	0
All	All	8538	0	8331	391	2

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 (391) 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:F:136:LEU:CD2	3:F:0:HFL:H151	1.45	1.46
1:C:9:ILE:HG22	1:C:10:THR:N	1.29	1.41
1:C:9:ILE:CG2	1:C:10:THR:H	1.34	1.40
1:F:136:LEU:HD21	3:F:0:HFL:C15	1.61	1.24
2:C:1698:SAH:C4'	2:C:1698:SAH:SD	2.32	1.18
2:C:1698:SAH:C5'	2:C:1698:SAH:C3'	2.26	1.13
2:F:1699:SAH:C5'	2:F:1699:SAH:C3'	2.27	1.11
2:F:1699:SAH:C4'	2:F:1699:SAH:SD	2.38	1.11
2:C:1698:SAH:C5'	2:C:1698:SAH:O4'	1.95	1.10
1:F:118:ASN:HA	1:F:121:GLY:H	1.12	1.08
2:F:1699:SAH:C5'	2:F:1699:SAH:O4'	1.98	1.08
1:F:136:LEU:HD22	3:F:0:HFL:C15	1.78	1.04
1:C:203:SER:HB3	1:C:260:ASP:H	1.28	0.99
1:F:136:LEU:HD22	3:F:0:HFL:H152	1.42	0.98
1:F:119:GLU:HB2	1:F:122:VAL:HB	1.42	0.98
1:C:9:ILE:CG2	1:C:10:THR:N	2.01	0.98
2:F:1699:SAH:C4'	2:F:1699:SAH:H5'1	1.47	0.98
2:C:1698:SAH:C4'	2:C:1698:SAH:H5'2	1.46	0.97
2:F:1699:SAH:C4'	2:F:1699:SAH:H5'2	1.47	0.97
2:C:1698:SAH:C4'	2:C:1698:SAH:H5'1	1.46	0.94
1:A:258:LYS:H	1:A:258:LYS:HD3	1.33	0.94
1:F:136:LEU:CD2	3:F:0:HFL:H152	1.96	0.93
1:C:9:ILE:HG12	1:C:87:TYR:HD2	1.34	0.93
1:C:216:ASN:OD1	1:C:242:TYR:HB2	1.71	0.91
1:C:10:THR:HG22	1:C:25:GLN:CD	1.90	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:THR:HG22	1:C:25:GLN:OE1	1.72	0.88
1:C:7:THR:HG22	1:C:9:ILE:H	1.39	0.87
2:F:1699:SAH:C5'	2:F:1699:SAH:C4'	0.85	0.84
1:C:324:ASN:HD22	1:C:327:GLY:N	1.74	0.84
1:C:127:LEU:HD11	1:C:183:HIS:HB2	1.58	0.83
1:C:7:THR:CB	1:C:88:ILE:HG12	2.09	0.83
1:F:199:GLU:HG2	1:F:222:TYR:HE2	1.43	0.83
1:F:136:LEU:HD21	3:F:0:HFL:H151	0.83	0.83
1:A:119:GLU:CD	1:A:119:GLU:H	1.81	0.83
2:C:1698:SAH:C4'	2:C:1698:SAH:C5'	0.83	0.82
1:A:212:GLY:HA2	1:A:229:ASN:ND2	1.94	0.81
1:C:88:ILE:O	1:C:88:ILE:HG22	1.80	0.81
1:C:9:ILE:HG12	1:C:87:TYR:CD2	2.15	0.81
1:C:117:LYS:HB3	1:C:121:GLY:HA2	1.63	0.81
1:F:345:GLN:HG2	1:F:365:VAL:HG23	1.63	0.80
1:C:324:ASN:HD22	1:C:327:GLY:H	1.31	0.79
1:C:9:ILE:HG22	1:C:10:THR:H	0.64	0.79
1:A:258:LYS:HA	1:A:286:ALA:HB1	1.63	0.78
1:C:202:LYS:HA	1:C:225:ILE:HA	1.66	0.78
1:F:199:GLU:HG2	1:F:222:TYR:CE2	2.18	0.78
1:C:232:LEU:HD12	1:C:250:GLY:O	1.84	0.78
1:F:127:LEU:HD21	1:F:183:HIS:HB2	1.64	0.77
1:C:202:LYS:HG3	1:C:226:LYS:HG2	1.66	0.77
1:A:261:ALA:HA	1:A:287:LEU:HD21	1.67	0.77
1:A:95:ARG:HH11	1:A:97:GLN:HE21	1.33	0.76
1:C:7:THR:HG21	1:C:88:ILE:HD13	1.66	0.76
1:A:130:MET:HE2	1:A:176:PHE:HA	1.68	0.76
1:C:14:ILE:HA	1:C:18:GLU:OE2	1.86	0.76
1:C:7:THR:HB	1:C:88:ILE:HG12	1.65	0.76
1:C:7:THR:HG21	1:C:88:ILE:CD1	2.17	0.74
1:C:242:TYR:CG	1:C:243:PRO:HD2	2.22	0.74
1:C:122:VAL:HA	1:C:182:ASP:OD2	1.87	0.73
1:A:331:THR:HG22	1:A:334:GLU:HG3	1.68	0.73
1:F:118:ASN:HA	1:F:121:GLY:N	1.97	0.73
1:C:110:THR:O	1:C:113:LYS:HB2	1.87	0.73
1:A:331:THR:HG22	1:A:334:GLU:CG	2.19	0.72
1:A:344:PHE:HD2	1:A:362:LEU:HB2	1.56	0.71
1:C:134:LYS:CE	1:C:134:LYS:H	2.03	0.71
1:C:77:LEU:O	1:C:81:LEU:HD22	1.91	0.70
1:F:300:LEU:HD13	1:F:313:VAL:HG22	1.74	0.70
1:C:215:ILE:O	1:C:217:THR:N	2.21	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:47:ILE:HD13	1:F:65:GLN:HB2	1.74	0.69
1:A:236:ILE:HG21	1:A:247:HIS:HB3	1.75	0.69
1:C:265:LYS:NZ	4:C:1713:HOH:O	2.23	0.69
1:F:118:ASN:C	1:F:120:ASP:H	1.90	0.69
1:F:154:PHE:CE2	1:F:162:ALA:HA	2.28	0.69
1:C:320:MET:O	1:C:324:ASN:HB3	1.93	0.68
1:C:265:LYS:HG2	4:C:1713:HOH:O	1.93	0.68
1:C:9:ILE:HG23	1:C:10:THR:N	2.08	0.67
1:A:332:GLN:HE21	1:A:347:PHE:HE2	1.42	0.67
1:C:7:THR:HG21	1:C:88:ILE:CG1	2.25	0.67
1:C:364:LYS:O	1:C:364:LYS:HD3	1.94	0.67
1:F:155:ASN:HD22	1:F:155:ASN:N	1.93	0.67
1:C:218:ILE:N	4:C:1731:HOH:O	2.20	0.66
1:F:119:GLU:O	1:F:120:ASP:HB2	1.95	0.66
1:C:119:GLU:O	1:C:122:VAL:HB	1.95	0.66
1:C:191:ILE:HD13	1:C:358:ILE:HD11	1.77	0.65
1:C:7:THR:CG2	1:C:88:ILE:HG12	2.27	0.65
1:C:112:ALA:O	1:C:116:VAL:HG23	1.97	0.65
1:C:8:GLN:O	1:C:9:ILE:HB	1.96	0.65
1:C:213:ALA:HA	1:C:216:ASN:HB2	1.79	0.65
1:A:14:ILE:HG13	1:A:18:GLU:OE1	1.98	0.64
1:A:119:GLU:CD	1:A:119:GLU:N	2.51	0.64
1:C:15:SER:H	1:C:18:GLU:CD	2.01	0.63
1:A:88:ILE:O	1:A:88:ILE:HG22	1.98	0.63
1:C:344:PHE:O	1:C:346:GLY:N	2.31	0.63
1:A:289:ASP:HA	1:A:362:LEU:HD21	1.79	0.63
1:A:95:ARG:HH11	1:A:97:GLN:NE2	1.96	0.62
1:A:83:LEU:HD12	1:F:314:VAL:HG12	1.81	0.62
1:C:256:ILE:HG12	1:C:282:ASN:HB3	1.81	0.62
1:A:292:LYS:NZ	1:A:360:GLU:HG2	2.14	0.62
1:C:10:THR:HG22	1:C:25:GLN:NE2	2.13	0.62
1:C:160:MET:HE1	1:C:165:TYR:HA	1.81	0.62
1:C:220:SER:C	1:C:222:TYR:H	2.02	0.61
1:A:277:LEU:O	1:A:281:LYS:HG3	2.01	0.61
1:C:7:THR:HG21	1:C:88:ILE:HG12	1.82	0.61
1:F:187:THR:O	1:F:191:ILE:HG13	2.00	0.61
1:A:152:ILE:HG23	1:A:155:ASN:HB2	1.82	0.60
1:C:212:GLY:O	1:C:216:ASN:N	2.29	0.60
1:C:300:LEU:HD12	1:C:313:VAL:HG22	1.82	0.60
1:C:110:THR:O	1:C:113:LYS:CB	2.48	0.60
1:A:204:LEU:HD12	1:A:261:ALA:O	2.02	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:12:THR:O	1:C:12:THR:HG22	2.01	0.60
1:C:214:VAL:O	1:C:218:ILE:HB	2.03	0.59
1:C:300:LEU:CD1	1:C:313:VAL:HG22	2.32	0.59
1:C:217:THR:HA	1:C:220:SER:HB2	1.84	0.59
1:C:336:GLU:HG2	1:C:347:PHE:CD2	2.37	0.59
1:A:282:ASN:O	1:A:285:GLU:HB2	2.03	0.59
1:C:111:VAL:C	1:C:113:LYS:H	2.06	0.58
1:C:251:ASP:OD2	1:C:254:VAL:HG23	2.02	0.58
1:A:236:ILE:CG2	1:A:247:HIS:HB3	2.33	0.58
1:C:344:PHE:O	1:C:362:LEU:O	2.21	0.58
1:A:201:LEU:HD22	1:A:203:SER:O	2.03	0.58
1:C:119:GLU:O	1:C:122:VAL:N	2.34	0.58
1:C:213:ALA:CA	1:C:216:ASN:HB2	2.33	0.58
1:A:264:MET:HE1	1:A:280:LEU:HD21	1.86	0.58
1:C:9:ILE:CG1	1:C:87:TYR:HD2	2.10	0.58
1:C:88:ILE:O	1:C:88:ILE:CG2	2.50	0.58
1:A:48:ILE:HB	1:A:108:LEU:HD21	1.86	0.58
1:A:75:VAL:HG23	4:A:373:HOH:O	2.04	0.58
1:A:288:PRO:C	1:A:290:ASN:H	2.07	0.57
1:F:95:ARG:HE	1:F:103:GLN:NE2	2.01	0.57
1:A:258:LYS:HD3	1:A:258:LYS:N	2.12	0.57
1:C:111:VAL:C	1:C:113:LYS:N	2.57	0.57
1:A:201:LEU:HD23	1:A:260:ASP:HB3	1.86	0.57
1:C:251:ASP:OD1	2:C:1698:SAH:N6	2.30	0.57
1:A:288:PRO:O	1:A:290:ASN:N	2.36	0.57
1:A:293:VAL:HB	1:A:361:PHE:HB2	1.87	0.57
1:A:130:MET:HE1	1:A:180:MET:HG2	1.85	0.57
1:C:195:TYR:CZ	1:C:197:GLY:HA3	2.40	0.57
1:C:8:GLN:O	1:C:8:GLN:OE1	2.23	0.56
1:A:95:ARG:NH1	1:A:97:GLN:HE21	1.99	0.56
1:A:256:ILE:O	1:A:286:ALA:HB2	2.05	0.56
1:A:344:PHE:CD2	1:A:362:LEU:HB2	2.39	0.56
1:C:240:PRO:O	1:C:241:SER:HB3	2.04	0.56
1:C:320:MET:O	1:C:324:ASN:CB	2.53	0.56
1:A:95:ARG:NH1	1:A:97:GLN:NE2	2.53	0.56
1:A:258:LYS:H	1:A:258:LYS:CD	2.13	0.56
1:A:209:GLY:HA3	1:A:229:ASN:ND2	2.20	0.56
1:C:218:ILE:HG13	4:C:1731:HOH:O	2.04	0.56
1:A:231:ASP:O	1:A:249:GLY:HA2	2.06	0.56
1:A:288:PRO:C	1:A:290:ASN:N	2.59	0.56
1:F:37:LYS:HE3	1:F:132:GLN:O	2.05	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:232:LEU:HB2	1:A:235:VAL:HG23	1.86	0.56
1:A:161:THR:OG1	1:A:164:GLU:HG3	2.06	0.55
1:A:190:LYS:O	1:A:194:THR:HG23	2.07	0.55
1:F:97:GLN:HB3	1:F:99:ASP:OD1	2.06	0.55
1:A:154:PHE:CE2	1:A:162:ALA:HA	2.42	0.55
1:A:344:PHE:C	1:A:346:GLY:H	2.10	0.55
1:F:5:GLY:N	1:F:308:LEU:H	2.05	0.55
1:F:231:ASP:O	1:F:249:GLY:HA2	2.05	0.55
1:F:313:VAL:HG23	1:F:329:GLU:HG3	1.88	0.55
1:C:236:ILE:HG23	1:C:247:HIS:HB3	1.88	0.55
1:A:260:ASP:O	1:A:291:GLY:HA3	2.07	0.55
1:C:196:THR:O	1:C:198:PHE:N	2.40	0.55
1:C:200:GLY:HA3	4:C:1699:HOH:O	2.07	0.54
1:F:202:LYS:HD3	1:F:260:ASP:OD2	2.06	0.54
1:C:15:SER:HB3	1:C:18:GLU:HG2	1.88	0.54
1:C:155:ASN:N	1:C:155:ASN:HD22	2.03	0.54
1:C:196:THR:O	1:C:199:GLU:HG2	2.08	0.54
1:C:253:PHE:HD2	1:C:278:LYS:HG2	1.72	0.54
1:A:155:ASN:N	1:A:155:ASN:HD22	2.06	0.53
1:F:97:GLN:NE2	1:F:103:GLN:HE22	2.05	0.53
1:F:32:LEU:HB3	1:F:33:PRO:CD	2.39	0.53
1:F:238:ASP:OD2	1:F:238:ASP:N	2.39	0.53
1:F:264:MET:O	1:F:265:LYS:HB3	2.08	0.53
1:C:212:GLY:C	1:C:216:ASN:HB2	2.29	0.53
1:F:88:ILE:HG22	1:F:88:ILE:O	2.08	0.53
1:C:9:ILE:HG23	1:C:87:TYR:CE2	2.44	0.53
1:C:15:SER:H	1:C:18:GLU:CG	2.23	0.52
1:A:30:SER:O	1:A:34:MET:HG2	2.09	0.52
1:A:142:HIS:HD2	4:A:409:HOH:O	1.91	0.52
1:A:37:LYS:O	1:A:41:GLU:HG3	2.10	0.52
1:A:318:VAL:HG13	1:F:35:ILE:HD11	1.90	0.52
1:C:324:ASN:ND2	1:C:327:GLY:H	2.02	0.52
2:C:1698:SAH:O4'	2:C:1698:SAH:H5'1	1.80	0.52
1:F:152:ILE:HD12	1:F:152:ILE:N	2.24	0.52
1:F:195:TYR:CZ	1:F:197:GLY:HA3	2.44	0.52
1:A:265:LYS:HB2	1:A:296:ALA:HB3	1.91	0.52
1:C:155:ASN:HD22	1:C:155:ASN:H	1.56	0.52
1:C:204:LEU:CD2	1:C:219:VAL:HG11	2.40	0.52
1:C:215:ILE:C	1:C:217:THR:H	2.06	0.52
1:C:293:VAL:HB	1:C:361:PHE:HB2	1.91	0.52
1:A:95:ARG:NH1	1:A:103:GLN:OE1	2.43	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:264:MET:HE3	1:C:267:ILE:HB	1.90	0.52
1:A:293:VAL:O	1:A:360:GLU:HA	2.10	0.51
1:C:10:THR:O	1:C:11:PRO:O	2.29	0.51
1:C:123:SER:OG	1:C:125:SER:HB2	2.10	0.51
1:F:276:CYS:O	1:F:280:LEU:HB2	2.10	0.51
1:C:324:ASN:ND2	1:C:327:GLY:N	2.50	0.51
1:A:143:LEU:HD21	1:A:321:LEU:HD11	1.91	0.51
1:A:205:VAL:CG1	1:A:262:VAL:HG22	2.41	0.51
1:C:113:LYS:HD3	1:C:114:TYR:CE1	2.45	0.51
1:C:134:LYS:H	1:C:134:LYS:HE2	1.74	0.51
1:C:217:THR:N	4:C:1731:HOH:O	2.43	0.51
1:C:161:THR:OG1	1:C:164:GLU:HG3	2.12	0.50
1:A:94:VAL:HG21	1:F:303:ALA:HB2	1.92	0.50
1:C:202:LYS:HG3	1:C:226:LYS:CG	2.39	0.50
1:C:9:ILE:HG23	1:C:87:TYR:CD2	2.46	0.50
1:C:108:LEU:HD22	1:C:112:ALA:HB1	1.94	0.50
1:A:216:ASN:ND2	1:A:242:TYR:HB3	2.25	0.50
1:C:212:GLY:O	1:C:216:ASN:HB2	2.12	0.50
1:A:66:LEU:HB3	1:A:68:THR:HG22	1.92	0.49
1:C:262:VAL:HG23	1:C:287:LEU:HD21	1.93	0.49
1:A:286:ALA:O	1:A:288:PRO:HD3	2.12	0.49
1:F:205:VAL:CG1	1:F:262:VAL:HG22	2.43	0.49
1:A:264:MET:O	1:A:265:LYS:HB3	2.12	0.49
1:C:211:THR:HG23	1:C:240:PRO:HD2	1.95	0.49
1:A:152:ILE:HD11	1:A:323:HIS:C	2.33	0.49
1:A:292:LYS:HB2	1:A:361:PHE:O	2.13	0.49
1:C:202:LYS:O	1:C:203:SER:HB2	2.12	0.49
2:F:1699:SAH:O4'	2:F:1699:SAH:H5'1	1.81	0.49
1:A:219:VAL:HG11	1:A:244:GLY:HA3	1.94	0.49
1:A:292:LYS:HD2	1:A:360:GLU:HB2	1.95	0.49
1:A:321:LEU:HD13	1:A:321:LEU:O	2.13	0.48
1:A:130:MET:CE	1:A:180:MET:HG2	2.43	0.48
1:C:239:ALA:O	1:C:240:PRO:O	2.30	0.48
1:F:28:SER:O	1:F:31:VAL:HB	2.13	0.48
1:F:265:LYS:HA	1:F:296:ALA:HB3	1.96	0.48
1:A:264:MET:CE	1:A:295:VAL:HG22	2.43	0.48
1:C:221:LYS:HE3	1:C:221:LYS:HA	1.94	0.48
1:F:265:LYS:HA	1:F:296:ALA:O	2.14	0.48
1:F:255:SER:C	1:F:256:ILE:HD12	2.34	0.48
1:A:56:GLN:NE2	1:A:93:SER:OG	2.36	0.48
1:A:192:LEU:HD11	1:A:217:THR:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:37:LYS:O	1:F:41:GLU:HG3	2.14	0.48
1:A:21:LEU:HB3	1:F:308:LEU:HB3	1.96	0.48
1:C:9:ILE:HG12	1:C:87:TYR:HB3	1.94	0.48
1:A:352:ASN:OD1	1:A:352:ASN:O	2.32	0.48
1:F:256:ILE:HD13	1:F:282:ASN:HB3	1.96	0.47
1:F:333:LYS:HE2	4:F:1733:HOH:O	2.14	0.47
1:C:160:MET:HE2	1:C:164:GLU:HB3	1.96	0.47
1:F:345:GLN:HB2	1:F:364:LYS:HG2	1.97	0.47
1:C:12:THR:O	1:C:12:THR:CG2	2.63	0.47
1:A:268:CYS:HB2	1:A:297:GLU:OE2	2.14	0.47
1:F:192:LEU:CD2	1:F:217:THR:HG22	2.44	0.47
1:A:221:LYS:HG2	1:A:222:TYR:CE1	2.50	0.47
1:A:336:GLU:HG2	1:A:347:PHE:CD2	2.49	0.47
1:A:190:LYS:HB3	1:A:353:ALA:HB1	1.96	0.47
1:C:216:ASN:O	1:C:217:THR:CB	2.63	0.47
1:C:345:GLN:NE2	1:C:364:LYS:H	2.13	0.47
1:F:201:LEU:O	1:F:225:ILE:HG12	2.15	0.47
1:F:345:GLN:OE1	1:F:363:LYS:HA	2.15	0.47
1:A:143:LEU:HD21	1:A:321:LEU:CD1	2.45	0.47
1:C:318:VAL:O	1:C:321:LEU:HB3	2.14	0.47
1:C:14:ILE:HD13	1:C:14:ILE:C	2.35	0.47
1:C:37:LYS:HG3	1:C:129:LEU:HD23	1.97	0.47
1:C:364:LYS:HD3	1:C:364:LYS:C	2.35	0.47
1:A:63:ALA:HB2	1:A:77:LEU:HD12	1.96	0.46
1:C:213:ALA:HA	1:C:216:ASN:CB	2.45	0.46
1:F:8:GLN:HG2	1:F:308:LEU:HD21	1.96	0.46
1:A:35:ILE:HD11	1:F:318:VAL:HG13	1.97	0.46
1:C:154:PHE:CE2	1:C:162:ALA:HA	2.50	0.46
1:C:264:MET:O	1:C:265:LYS:HB3	2.15	0.46
1:A:138:GLU:OE1	1:F:134:LYS:HE2	2.15	0.46
1:F:11:PRO:CG	1:F:14:ILE:HD13	2.46	0.46
1:F:276:CYS:HA	1:F:279:PHE:CE2	2.51	0.46
1:A:152:ILE:HG23	1:A:155:ASN:CB	2.45	0.46
1:C:28:SER:O	1:C:31:VAL:HB	2.16	0.46
1:A:195:TYR:HD2	1:A:198:PHE:CE1	2.33	0.46
1:A:333:LYS:HG3	4:A:415:HOH:O	2.16	0.46
1:C:223:PRO:C	1:C:225:ILE:H	2.19	0.46
1:A:88:ILE:HG13	1:F:12:THR:O	2.15	0.45
1:A:95:ARG:HG2	1:A:96:THR:N	2.30	0.45
1:C:188:MET:SD	1:C:265:LYS:HE3	2.55	0.45
1:C:283:CYS:O	1:C:287:LEU:HG	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:37:LYS:HE3	1:F:132:GLN:C	2.36	0.45
1:F:211:THR:OG1	1:F:240:PRO:HD2	2.17	0.45
1:A:70:ASN:HA	1:A:71:PRO:HD3	1.83	0.45
1:A:324:ASN:HA	1:A:325:PRO:HD3	1.65	0.45
1:C:97:GLN:HB3	1:C:99:ASP:OD1	2.17	0.45
1:A:195:TYR:HA	4:A:374:HOH:O	2.15	0.45
1:A:331:THR:CG2	1:A:334:GLU:HG3	2.41	0.45
1:C:212:GLY:HA2	1:C:229:ASN:ND2	2.32	0.45
1:F:300:LEU:HD13	1:F:313:VAL:CG2	2.45	0.45
1:C:252:MET:O	1:C:282:ASN:ND2	2.42	0.45
1:C:192:LEU:HD21	1:C:218:ILE:HG22	1.99	0.45
1:F:155:ASN:N	1:F:155:ASN:ND2	2.63	0.45
1:A:352:ASN:HB3	1:A:357:TYR:CD2	2.51	0.44
1:C:211:THR:HG23	1:C:240:PRO:CD	2.47	0.44
1:C:216:ASN:O	1:C:217:THR:HB	2.16	0.44
1:C:264:MET:HE2	1:C:279:PHE:CE1	2.52	0.44
1:C:328:LYS:HD2	1:C:328:LYS:O	2.17	0.44
1:F:276:CYS:HA	1:F:279:PHE:CZ	2.52	0.44
1:A:126:ALA:HB1	1:A:178:LYS:HD2	1.98	0.44
1:A:346:GLY:O	1:A:361:PHE:HA	2.17	0.44
1:C:119:GLU:O	1:C:122:VAL:CB	2.65	0.44
1:C:188:MET:SD	1:C:214:VAL:HG13	2.58	0.44
1:F:122:VAL:HG13	1:F:182:ASP:CG	2.38	0.44
1:A:37:LYS:HE2	1:A:41:GLU:OE2	2.17	0.44
1:A:344:PHE:HD2	1:A:362:LEU:CB	2.25	0.44
1:C:264:MET:CE	1:C:279:PHE:CE1	3.00	0.44
1:F:37:LYS:HG3	1:F:129:LEU:HD23	1.99	0.44
1:A:292:LYS:HZ2	1:A:360:GLU:HG2	1.83	0.44
1:C:288:PRO:C	1:C:290:ASN:H	2.21	0.44
1:F:191:ILE:HD13	1:F:358:ILE:HD11	1.99	0.44
1:C:350:HIS:O	1:C:351:CYS:O	2.35	0.44
1:A:152:ILE:HG23	1:A:155:ASN:CG	2.38	0.44
1:A:191:ILE:C	1:A:193:GLU:H	2.21	0.44
1:C:215:ILE:C	4:C:1731:HOH:O	2.56	0.44
1:C:216:ASN:O	1:C:217:THR:HG22	2.18	0.44
1:C:288:PRO:O	1:C:290:ASN:N	2.51	0.44
1:A:251:ASP:OD2	1:A:251:ASP:C	2.55	0.43
1:C:216:ASN:N	4:C:1731:HOH:O	2.50	0.43
1:A:178:LYS:HE3	4:A:401:HOH:O	2.17	0.43
1:A:264:MET:HE3	1:A:295:VAL:HG22	2.01	0.43
1:A:284:TYR:CE1	1:A:343:GLY:O	2.72	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:320:MET:CE	3:F:0:HFL:O8	2.66	0.43
1:A:296:ALA:O	1:A:297:GLU:HG2	2.18	0.43
1:A:348:LYS:HB2	1:A:360:GLU:OE1	2.18	0.43
1:C:240:PRO:O	1:C:241:SER:CB	2.65	0.43
1:C:242:TYR:CB	1:C:243:PRO:HD2	2.45	0.43
1:F:363:LYS:O	1:F:363:LYS:HG3	2.18	0.43
1:A:207:VAL:HG23	1:A:262:VAL:HG13	2.00	0.43
1:A:28:SER:HB2	1:F:319:ILE:HD11	2.00	0.43
1:C:109:ALA:O	1:C:112:ALA:N	2.51	0.43
1:A:216:ASN:O	1:A:220:SER:HB2	2.19	0.43
1:C:46:GLU:O	1:C:50:LYS:HG3	2.19	0.43
1:C:150:GLY:O	1:C:156:LYS:HE2	2.18	0.43
1:C:109:ALA:O	1:C:110:THR:C	2.57	0.43
1:F:37:LYS:HD2	1:F:132:GLN:HB3	2.00	0.43
1:C:350:HIS:HB3	1:C:351:CYS:H	1.70	0.43
1:A:205:VAL:HG13	1:A:205:VAL:O	2.19	0.43
1:F:108:LEU:HD13	1:F:116:VAL:HG21	2.01	0.43
1:A:355:ASN:HD22	1:A:355:ASN:HA	1.69	0.43
1:C:201:LEU:O	1:C:202:LYS:O	2.37	0.43
1:C:328:LYS:HD2	1:C:328:LYS:C	2.39	0.43
1:A:146:ALA:HA	1:A:156:LYS:HE3	2.00	0.42
1:A:350:HIS:NE2	1:A:360:GLU:OE1	2.52	0.42
1:A:236:ILE:HA	1:A:239:ALA:HB2	2.01	0.42
1:A:227:GLY:N	1:A:244:GLY:O	2.51	0.42
1:C:18:GLU:HA	4:C:1703:HOH:O	2.17	0.42
1:C:134:LYS:H	1:C:134:LYS:HE3	1.80	0.42
1:C:182:ASP:O	1:C:186:ILE:HG13	2.19	0.42
1:F:20:ASN:HB3	4:F:1722:HOH:O	2.19	0.42
1:C:113:LYS:O	1:C:115:LEU:N	2.52	0.42
1:C:113:LYS:C	1:C:115:LEU:H	2.21	0.42
1:C:355:ASN:HD22	1:C:355:ASN:HA	1.69	0.42
1:A:29:ALA:HB3	1:F:33:PRO:HB3	2.01	0.42
1:C:264:MET:HE2	1:C:279:PHE:HE1	1.84	0.42
1:A:265:LYS:HA	1:A:296:ALA:O	2.20	0.42
1:C:320:MET:HG3	1:C:324:ASN:HB3	2.01	0.42
1:F:77:LEU:O	1:F:81:LEU:HD22	2.20	0.42
1:F:345:GLN:HG2	1:F:365:VAL:CG2	2.43	0.42
1:A:214:VAL:O	1:A:218:ILE:HG13	2.19	0.42
1:C:219:VAL:C	1:C:221:LYS:H	2.23	0.42
1:C:163:PHE:CD1	1:C:163:PHE:N	2.86	0.42
1:A:32:LEU:HB3	1:A:33:PRO:CD	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:119:GLU:N	1:A:119:GLU:OE1	2.52	0.42
1:C:223:PRO:C	1:C:225:ILE:N	2.74	0.42
1:F:119:GLU:H	1:F:122:VAL:H	1.68	0.42
1:A:231:ASP:HB3	1:A:236:ILE:HD11	2.02	0.41
1:C:265:LYS:HA	1:C:296:ALA:HB3	2.01	0.41
1:C:354:PHE:O	1:C:355:ASN:CB	2.67	0.41
1:F:280:LEU:HD12	1:F:280:LEU:HA	1.85	0.41
1:A:21:LEU:HD21	1:F:355:ASN:HB2	2.01	0.41
1:F:56:GLN:HA	1:F:106:TYR:O	2.20	0.41
1:A:209:GLY:HA3	1:A:229:ASN:HD21	1.86	0.41
1:C:222:TYR:HA	4:C:1740:HOH:O	2.19	0.41
1:F:73:ALA:HB3	1:F:74:PRO:HD3	2.02	0.41
1:C:108:LEU:HB3	1:C:112:ALA:HB3	2.03	0.41
1:C:173:ASN:ND2	1:C:177:ASN:HD21	2.18	0.41
1:C:352:ASN:HB2	1:C:357:TYR:CE2	2.55	0.41
1:C:216:ASN:O	1:C:242:TYR:HD1	2.04	0.41
1:F:210:GLY:HA2	1:F:235:VAL:HG11	2.02	0.41
1:C:221:LYS:HA	1:C:221:LYS:CE	2.48	0.41
1:F:70:ASN:HA	1:F:71:PRO:HD3	1.87	0.41
1:A:201:LEU:CD2	1:A:260:ASP:HB3	2.51	0.41
1:C:15:SER:OG	1:C:16:ASP:N	2.51	0.41
1:C:222:TYR:N	1:C:223:PRO:HD3	2.36	0.41
1:A:265:LYS:CB	1:A:296:ALA:HB3	2.51	0.41
1:A:332:GLN:NE2	1:A:347:PHE:HE2	2.15	0.41
1:A:346:GLY:O	1:A:362:LEU:N	2.51	0.41
1:C:133:ASP:CG	1:C:134:LYS:HE3	2.40	0.41
1:A:195:TYR:CD2	1:A:198:PHE:CE1	3.09	0.41
1:A:232:LEU:O	1:A:236:ILE:HG12	2.21	0.41
1:C:216:ASN:O	1:C:242:TYR:CD1	2.74	0.40
1:F:37:LYS:HD2	1:F:132:GLN:CB	2.51	0.40
1:A:42:LEU:HD21	1:F:144:LYS:HG2	2.03	0.40
1:A:296:ALA:C	1:A:297:GLU:HG2	2.42	0.40
1:A:320:MET:HG2	1:A:327:GLY:C	2.42	0.40
1:C:14:ILE:HD13	1:C:15:SER:O	2.22	0.40
1:C:207:VAL:HG23	1:C:262:VAL:HG13	2.04	0.40
1:F:231:ASP:OD2	1:F:232:LEU:N	2.48	0.40
1:C:344:PHE:C	1:C:346:GLY:H	2.23	0.40
1:C:344:PHE:C	1:C:346:GLY:N	2.75	0.40

All (2) 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:10:THR:OG1	1:C:10:THR:OG1[2_556]	1.59	0.61
1:C:10:THR:N	1:C:10:THR:OG1[2_556]	2.17	0.03

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	348/365 (95%)	325 (93%)	16 (5%)	7 (2%)	7 9
1	C	359/365 (98%)	310 (86%)	27 (8%)	22 (6%)	1 0
1	F	359/365 (98%)	336 (94%)	19 (5%)	4 (1%)	14 20
All	All	1066/1095 (97%)	971 (91%)	62 (6%)	33 (3%)	4 3

All (33) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	GLU
1	A	289	ASP
1	C	11	PRO
1	C	202	LYS
1	C	216	ASN
1	C	240	PRO
1	C	241	SER
1	C	345	GLN
1	C	351	CYS
1	F	120	ASP
1	A	350	HIS
1	C	9	ILE
1	C	119	GLU
1	C	197	GLY
1	C	217	THR
1	C	289	ASP
1	F	117	LYS
1	C	7	THR

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Mol	Chain	Res	Type
1	C	113	LYS
1	C	114	TYR
1	C	117	LYS
1	F	197	GLY
1	C	10	THR
1	C	15	SER
1	C	220	SER
1	C	326	GLY
1	A	200	GLY
1	A	326	GLY
1	C	324	ASN
1	C	325	PRO
1	A	88	ILE
1	A	257	PRO
1	F	88	ILE

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	294/307 (96%)	277 (94%)	17 (6%)	20 32
1	C	304/307 (99%)	277 (91%)	27 (9%)	9 14
1	F	304/307 (99%)	289 (95%)	15 (5%)	25 40
All	All	902/921 (98%)	843 (94%)	59 (6%)	17 27

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	43	ASP
1	A	66	LEU
1	A	83	LEU
1	A	95	ARG
1	A	119	GLU
1	A	143	LEU
1	A	152	ILE

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Mol	Chain	Res	Type
1	A	155	ASN
1	A	163	PHE
1	A	234	HIS
1	A	242	TYR
1	A	258	LYS
1	A	269	HIS
1	A	320	MET
1	A	351	CYS
1	A	355	ASN
1	A	360	GLU
1	C	8	GLN
1	C	13	HIS
1	C	14	ILE
1	C	17	GLU
1	C	31	VAL
1	C	36	LEU
1	C	43	ASP
1	C	81	LEU
1	C	88	ILE
1	C	120	ASP
1	C	134	LYS
1	C	144	LYS
1	C	155	ASN
1	C	163	PHE
1	C	182	ASP
1	C	192	LEU
1	C	203	SER
1	C	232	LEU
1	C	237	GLU
1	C	242	TYR
1	C	269	HIS
1	C	270	ASP
1	C	300	LEU
1	C	328	LYS
1	C	336	GLU
1	C	352	ASN
1	C	355	ASN
1	F	14	ILE
1	F	15	SER
1	F	17	GLU
1	F	32	LEU
1	F	81	LEU

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Mol	Chain	Res	Type
1	F	155	ASN
1	F	192	LEU
1	F	224	THR
1	F	237	GLU
1	F	238	ASP
1	F	269	HIS
1	F	270	ASP
1	F	280	LEU
1	F	313	VAL
1	F	352	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (30) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	56	GLN
1	A	97	GLN
1	A	131	ASN
1	A	132	GLN
1	A	142	HIS
1	A	155	ASN
1	A	216	ASN
1	A	229	ASN
1	A	234	HIS
1	A	275	HIS
1	A	282	ASN
1	A	332	GLN
1	A	355	ASN
1	C	98	GLN
1	C	155	ASN
1	C	177	ASN
1	C	229	ASN
1	C	234	HIS
1	C	247	HIS
1	C	269	HIS
1	C	315	HIS
1	C	324	ASN
1	C	345	GLN
1	C	355	ASN
1	F	103	GLN
1	F	131	ASN
1	F	155	ASN
1	F	229	ASN

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Mol	Chain	Res	Type
1	F	323	HIS
1	F	352	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

3 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	C	1698	-	24,28,28	4.14	9 (37%)	25,40,40	3.15	8 (32%)
3	HFL	F	0	1	15,15,15	1.98	6 (40%)	19,20,20	2.16	5 (26%)
2	SAH	F	1699	-	24,28,28	4.06	7 (29%)	25,40,40	3.27	9 (36%)

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	C	1698	-	2/2/6/6	4/11/31/31	0/3/3/3
3	HFL	F	0	1	-	3/7/7/7	0/1/1/1
2	SAH	F	1699	-	2/2/6/6	4/11/31/31	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	1698	SAH	C5'-C4'	-17.45	0.83	1.52
2	F	1699	SAH	C5'-C4'	-17.03	0.85	1.52
2	F	1699	SAH	C2'-C3'	-5.31	1.38	1.53
2	C	1698	SAH	C2'-C3'	-5.21	1.39	1.53
2	C	1698	SAH	C2-N3	3.94	1.38	1.32
2	C	1698	SAH	C2-N1	3.76	1.40	1.33
2	F	1699	SAH	C8-N7	-3.65	1.28	1.34
2	F	1699	SAH	C4-N3	3.63	1.40	1.35
3	F	0	HFL	C5-C6	3.60	1.44	1.38
3	F	0	HFL	C2-C1	3.57	1.45	1.40
2	F	1699	SAH	C2-N3	3.49	1.37	1.32
2	C	1698	SAH	C4-N3	3.48	1.40	1.35
2	F	1699	SAH	C2-N1	3.45	1.40	1.33
2	C	1698	SAH	C8-N7	-3.34	1.28	1.34
3	F	0	HFL	C3-C2	3.09	1.44	1.38
2	C	1698	SAH	O-C	2.52	1.29	1.22
3	F	0	HFL	C6-C1	2.48	1.43	1.40
3	F	0	HFL	C3-C4	2.30	1.43	1.39
2	C	1698	SAH	C2'-C1'	-2.29	1.50	1.53
2	F	1699	SAH	O-C	2.29	1.29	1.22
3	F	0	HFL	C5-C4	2.23	1.43	1.39
2	C	1698	SAH	C6-C5	2.04	1.50	1.43

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1699	SAH	C5'-C4'-C3'	9.52	138.86	115.06
2	C	1698	SAH	C5'-C4'-C3'	9.49	138.78	115.06
2	F	1699	SAH	C3'-C2'-C1'	9.10	114.68	100.98
2	C	1698	SAH	C3'-C2'-C1'	8.80	114.23	100.98
3	F	0	HFL	O9-C2-C1	6.24	120.84	114.54
2	F	1699	SAH	N3-C2-N1	-4.88	121.04	128.68
2	C	1698	SAH	N3-C2-N1	-4.65	121.40	128.68
3	F	0	HFL	O13-C12-O14	-3.82	99.38	111.88
2	F	1699	SAH	C2-N1-C6	3.81	125.27	118.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	C	1698	SAH	C2-N1-C6	3.70	125.08	118.75
2	F	1699	SAH	C4-C5-N7	3.52	113.07	109.40
2	F	1699	SAH	C1'-N9-C4	3.36	132.54	126.64
2	C	1698	SAH	C4-C5-N7	3.30	112.84	109.40
2	F	1699	SAH	N6-C6-N1	3.01	124.82	118.57
2	C	1698	SAH	C1'-N9-C4	2.94	131.81	126.64
2	C	1698	SAH	N6-C6-N1	2.82	124.43	118.57
3	F	0	HFL	C3-C2-C1	-2.51	118.12	120.60
3	F	0	HFL	C15-O9-C2	-2.40	113.91	117.53
2	F	1699	SAH	C5-C6-N1	-2.36	115.01	120.35
2	C	1698	SAH	C5-C6-N1	-2.29	115.17	120.35
2	F	1699	SAH	O4'-C4'-C5'	2.07	114.17	108.83
3	F	0	HFL	C4-C3-C2	2.04	122.92	120.17

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	C	1698	SAH	C1'
2	C	1698	SAH	C4'
2	F	1699	SAH	C1'
2	F	1699	SAH	C4'

All (11) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	1698	SAH	O4'-C4'-C5'-SD
2	F	1699	SAH	O4'-C4'-C5'-SD
2	F	1699	SAH	CA-CB-CG-SD
3	F	0	HFL	C3-C2-O9-C15
2	C	1698	SAH	CA-CB-CG-SD
3	F	0	HFL	C1-C2-O9-C15
3	F	0	HFL	C10-C11-C12-O14
2	C	1698	SAH	OXT-C-CA-N
2	C	1698	SAH	O-C-CA-N
2	F	1699	SAH	O-C-CA-N
2	F	1699	SAH	OXT-C-CA-N

There are no ring outliers.

3 monomers are involved in 22 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	1698	SAH	8	0

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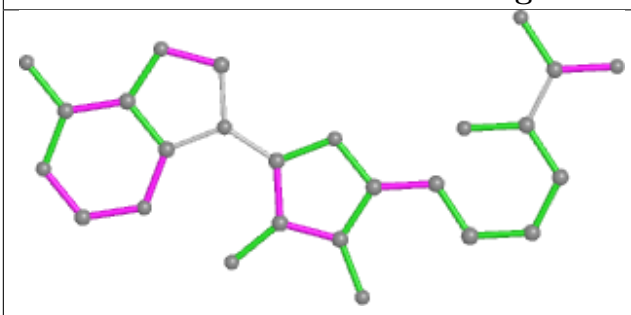
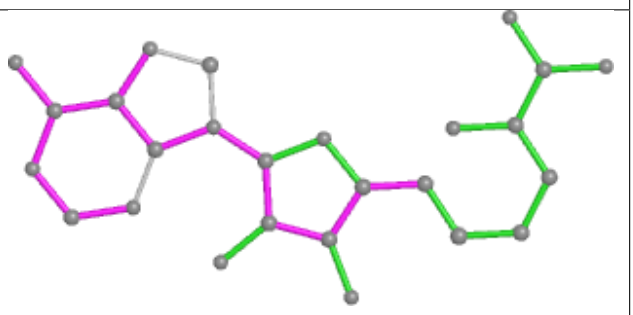
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	F	0	HFL	7	0
2	F	1699	SAH	7	0

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.

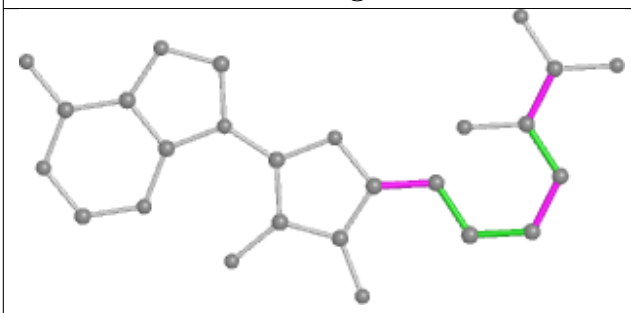
Ligand SAH C 1698



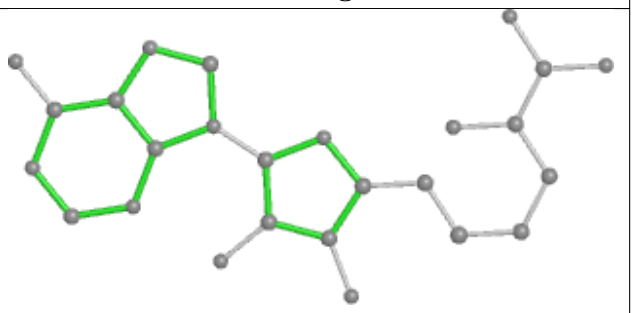
Bond lengths



Bond angles

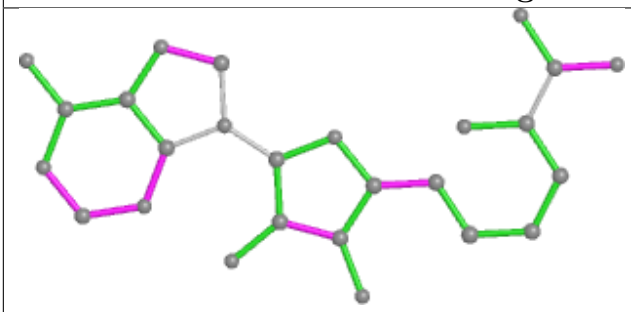


Torsions

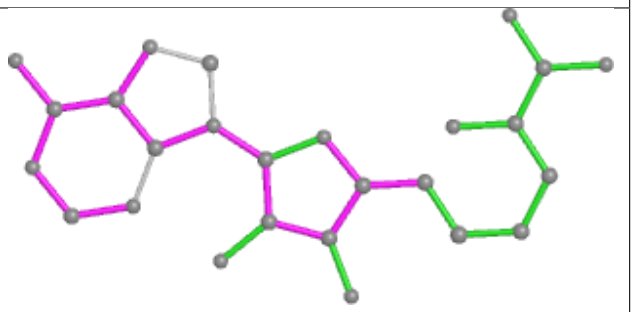


Rings

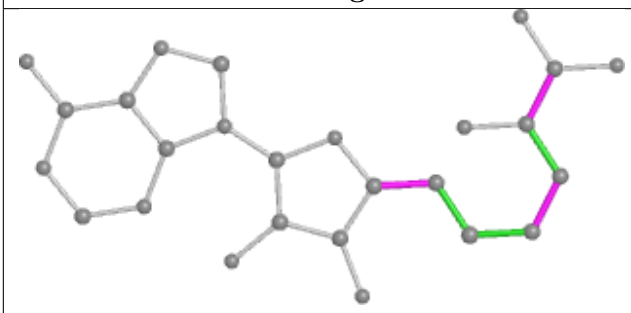
Ligand SAH F 1699



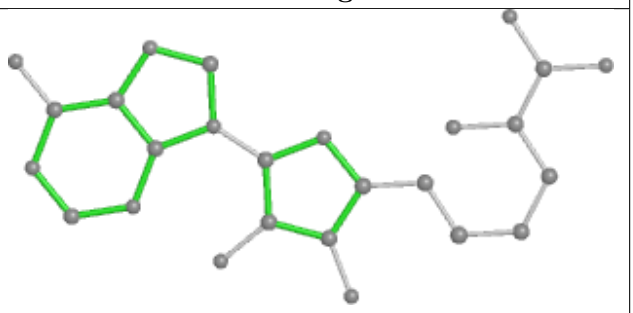
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	350/365 (95%)	0.13	11 (3%) 49 47	19, 47, 90, 109	0
1	C	361/365 (98%)	0.24	21 (5%) 23 22	26, 48, 86, 128	0
1	F	361/365 (98%)	-0.13	2 (0%) 89 88	21, 41, 65, 98	0
All	All	1072/1095 (97%)	0.08	34 (3%) 47 46	19, 45, 86, 128	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	9	ILE	13.5
1	C	12	THR	7.8
1	C	6	GLU	6.8
1	C	5	GLY	6.8
1	C	11	PRO	6.4
1	C	7	THR	5.7
1	C	14	ILE	5.3
1	C	242	TYR	5.3
1	C	10	THR	5.2
1	C	13	HIS	4.6
1	C	217	THR	4.6
1	A	351	CYS	4.5
1	A	325	PRO	4.3
1	A	290	ASN	4.2
1	F	119	GLU	3.5
1	C	238	ASP	3.5
1	C	8	GLN	3.2
1	A	234	HIS	3.2
1	A	235	VAL	3.2
1	C	15	SER	3.0
1	C	201	LEU	3.0
1	C	239	ALA	3.0
1	A	228	ILE	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	199	GLU	2.7
1	C	325	PRO	2.7
1	C	202	LYS	2.5
1	F	5	GLY	2.4
1	C	200	GLY	2.4
1	A	287	LEU	2.4
1	A	245	VAL	2.4
1	C	118	ASN	2.4
1	A	289	ASP	2.2
1	C	365	VAL	2.1
1	A	262	VAL	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)

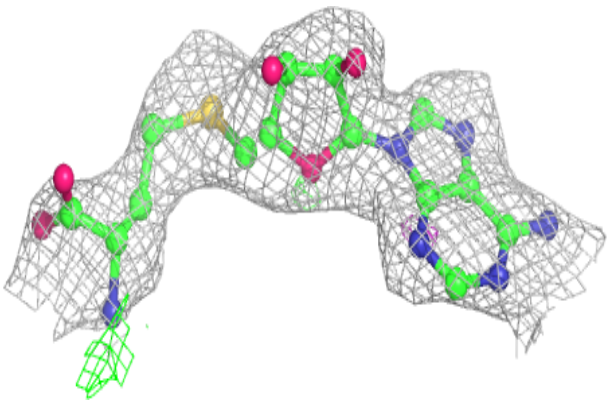
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

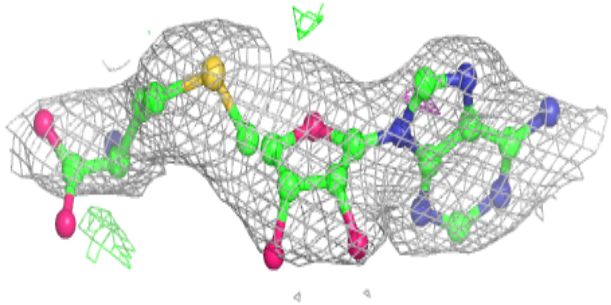
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	HFL	F	0	15/15	0.65	0.48	87,98,104,111	0
2	SAH	C	1698	26/26	0.88	0.24	70,76,102,105	0
2	SAH	F	1699	26/26	0.92	0.20	53,72,85,89	0

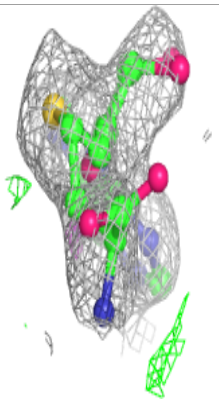
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around SAH C 1698:

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

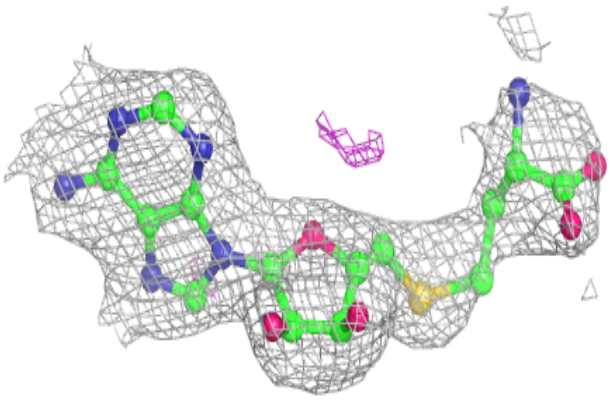


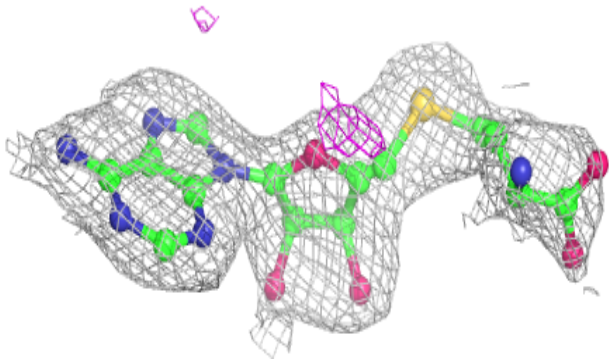


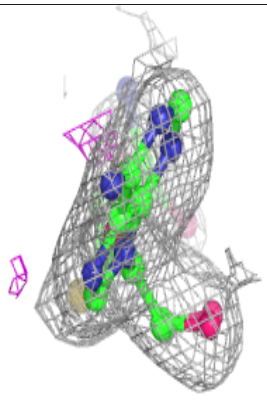


Electron density around SAH F 1699:

$2mF_o$-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.