Full wwPDB X-ray Structure Validation Report (i)

Aug 8, 2023 – 02:49 PM EDT

PDB ID	:	1OZV
Title	:	Crystal structure of the SET domain of LSMT bound to Lysine and AdoHcy
Authors	:	Trievel, R.C.; Flynn, E.M.; Houtz, R.L.; Hurley, J.H.
Deposited on	:	2003-04-09
Resolution	:	2.65 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:

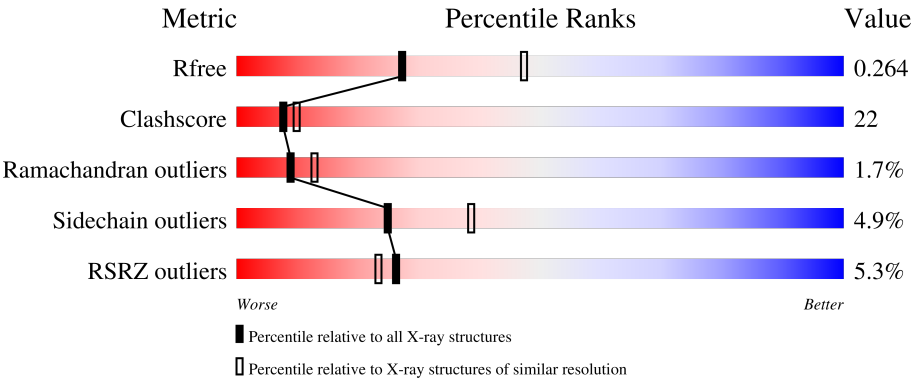
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.35
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (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 2.65 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	1332 (2.68-2.64)
Clashscore	141614	1374 (2.68-2.64)
Ramachandran outliers	138981	1349 (2.68-2.64)
Sidechain outliers	138945	1349 (2.68-2.64)
RSRZ outliers	127900	1318 (2.68-2.64)

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	444	8% 57% 36%
1	B	444	5% 64% 32%
1	C	444	2% 63% 32% 5%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 11304 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.

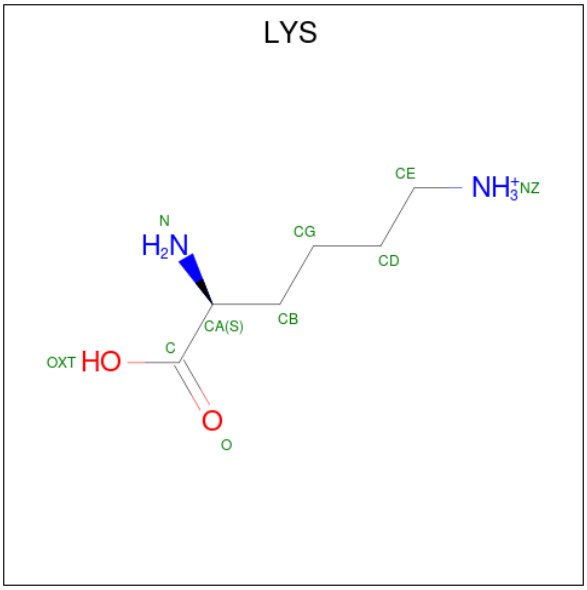
- Molecule 1 is a protein called Ribulose-1,5 bisphosphate carboxylase/oxygenase large subunit N-methyltransferase, chloroplast.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	429	Total	C	N	O	S	0	0	0
			3461	2219	572	663	7			
1	B	441	Total	C	N	O	S	0	0	0
			3549	2275	586	681	7			
1	C	440	Total	C	N	O	S	0	0	0
			3542	2270	585	680	7			

There are 21 discrepancies between the modelled and reference sequences:

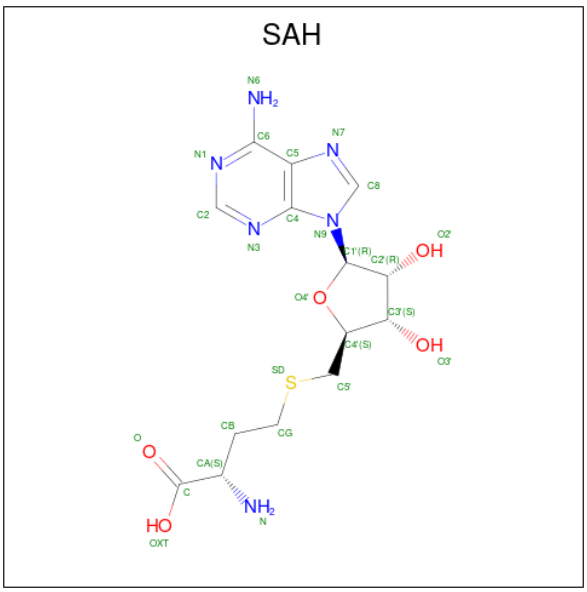
Chain	Residue	Modelled	Actual	Comment	Reference
A	45	MET	-	initiating methionine	UNP Q43088
A	483	GLU	-	engineered mutation	UNP Q43088
A	484	ASN	-	engineered mutation	UNP Q43088
A	485	LEU	-	engineered mutation	UNP Q43088
A	486	TYR	-	engineered mutation	UNP Q43088
A	487	PHE	-	engineered mutation	UNP Q43088
A	488	GLN	-	engineered mutation	UNP Q43088
B	45	MET	-	initiating methionine	UNP Q43088
B	483	GLU	-	engineered mutation	UNP Q43088
B	484	ASN	-	engineered mutation	UNP Q43088
B	485	LEU	-	engineered mutation	UNP Q43088
B	486	TYR	-	engineered mutation	UNP Q43088
B	487	PHE	-	engineered mutation	UNP Q43088
B	488	GLN	-	engineered mutation	UNP Q43088
C	45	MET	-	initiating methionine	UNP Q43088
C	483	GLU	-	engineered mutation	UNP Q43088
C	484	ASN	-	engineered mutation	UNP Q43088
C	485	LEU	-	engineered mutation	UNP Q43088
C	486	TYR	-	engineered mutation	UNP Q43088
C	487	PHE	-	engineered mutation	UNP Q43088
C	488	GLN	-	engineered mutation	UNP Q43088

- Molecule 2 is LYSINE (three-letter code: LYS) (formula: $C_6H_{15}N_2O_2$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C N O 10 6 2 2	0	0
2	A	1	Total C N O 10 6 2 2	0	0
2	A	1	Total C N O 10 6 2 2	0	0

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



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

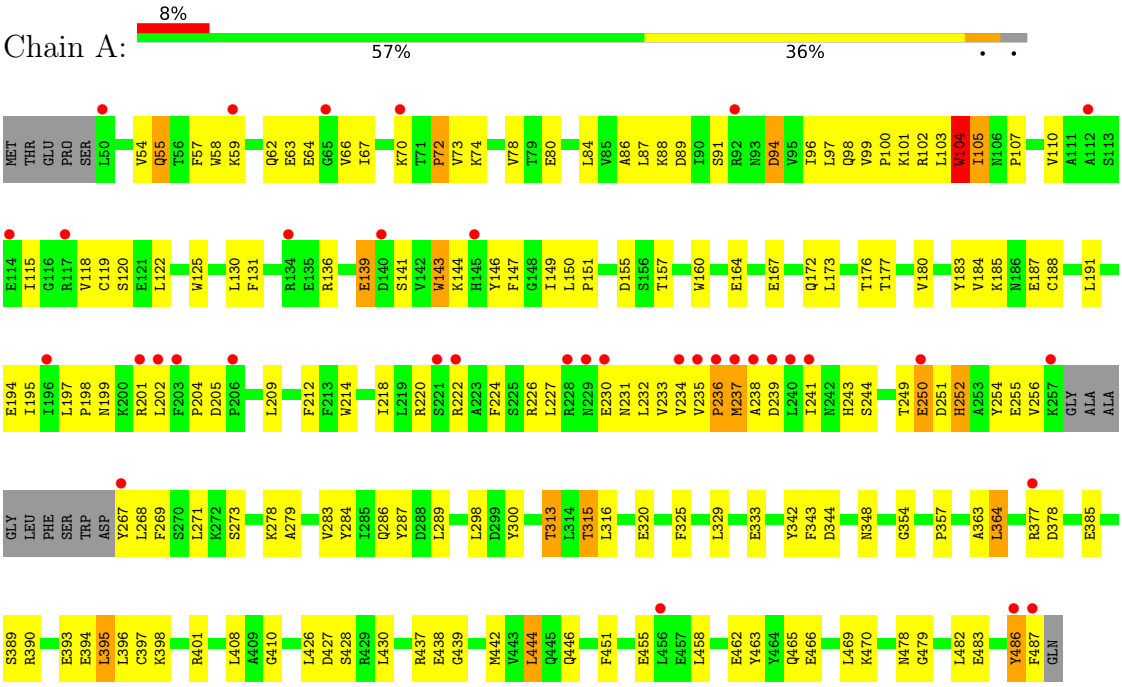
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	199	Total	O	0	0
			199	199		
4	B	212	Total	O	0	0
			212	212		
4	C	233	Total	O	0	0
			233	233		

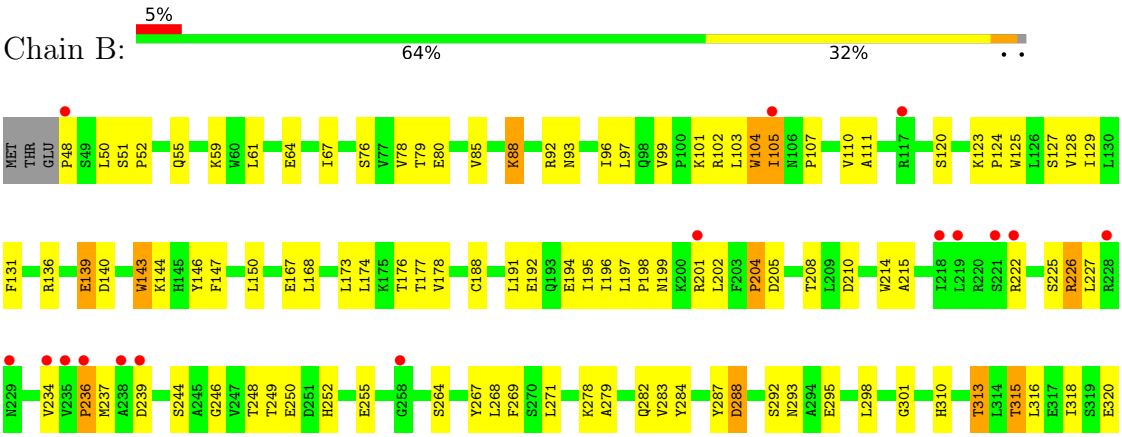
3 Residue-property plots (i)

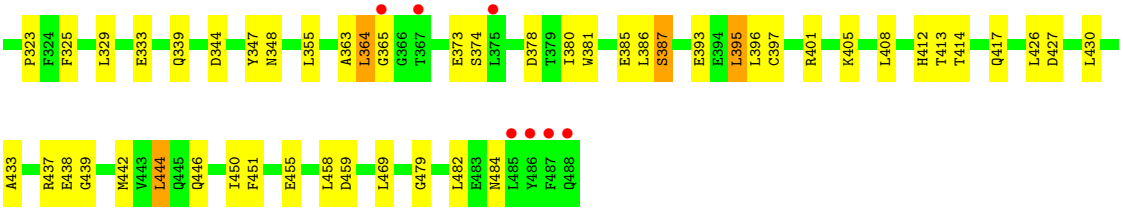
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. 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: Ribulose-1,5 bisphosphate carboxylase/oxygenase large subunit N-methyltransferase, chloroplast



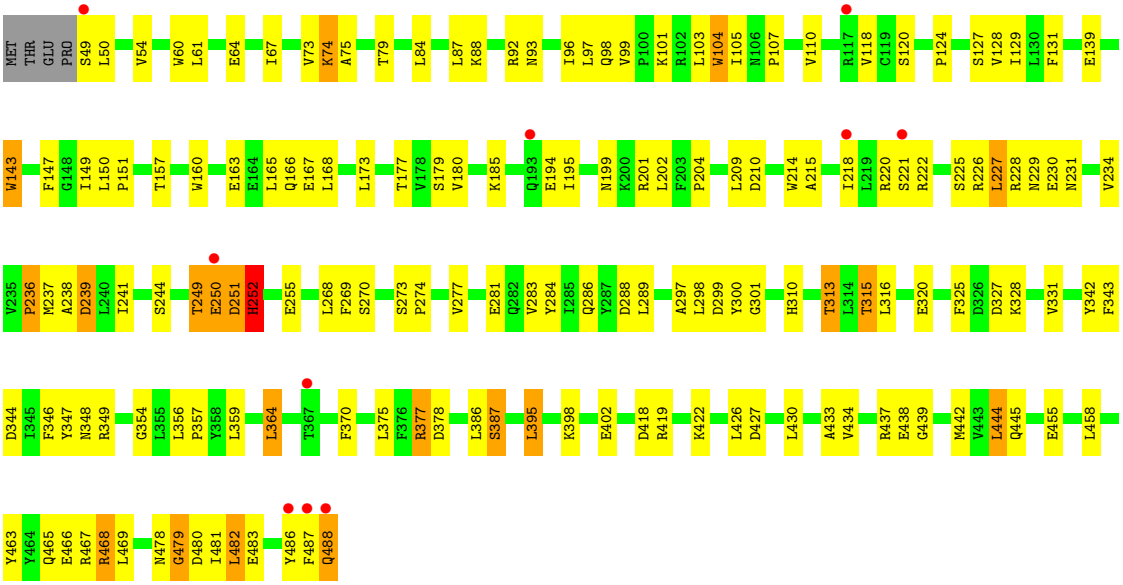
• Molecule 1: Ribulose-1,5 bisphosphate carboxylase/oxygenase large subunit N-methyltransferase, chloroplast





• Molecule 1: Ribulose-1,5 bisphosphate carboxylase/oxygenase large subunit N-methyltransferase, chloroplast

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α, β, γ	131.96Å 156.90Å 267.55Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.76 – 2.65 29.76 – 2.65	Depositor EDS
% Data completeness (in resolution range)	89.8 (29.76-2.65) 89.9 (29.76-2.65)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.06	Depositor
$< I/\sigma(I) >$ [1]	2.99 (at 2.64Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.227 , 0.266 0.222 , 0.264	Depositor DCC
R_{free} test set	3664 reflections (4.59%)	wwPDB-VP
Wilson B-factor (Å^2)	54.5	Xtriage
Anisotropy	0.511	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 55.9	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	11304	wwPDB-VP
Average B, all atoms (Å^2)	67.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.75% 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: 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	0.38	0/3532	0.59	0/4790
1	B	0.40	0/3625	0.61	1/4917 (0.0%)
1	C	0.41	0/3617	0.65	1/4906 (0.0%)
All	All	0.39	0/10774	0.62	2/14613 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	251	ASP	N-CA-C	9.28	136.05	111.00
1	B	105	ILE	N-CA-C	-5.13	97.14	111.00

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	3461	0	3432	179	0
1	B	3549	0	3509	141	0
1	C	3542	0	3501	161	0
2	A	30	0	36	7	0
3	A	26	0	19	0	0
3	B	26	0	19	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	C	26	0	19	1	0
4	A	199	0	0	17	0
4	B	212	0	0	22	0
4	C	233	0	0	18	0
All	All	11304	0	10535	464	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 22.

All (464) 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:395:LEU:HD22	1:C:469:LEU:HD12	1.47	0.95
1:C:50:LEU:HD22	1:C:54:VAL:HG11	1.46	0.95
1:B:48:PRO:HD2	4:B:1204:HOH:O	1.68	0.92
1:B:438:GLU:HG2	1:B:442:MET:HE2	1.51	0.91
1:A:177:THR:HG22	1:A:298:LEU:HD12	1.53	0.90
1:C:250:GLU:HA	4:C:1029:HOH:O	1.71	0.88
1:C:468:ARG:HH11	1:C:468:ARG:HB3	1.43	0.84
1:B:173:LEU:O	1:B:177:THR:HG23	1.76	0.84
1:C:73:VAL:HG21	1:C:84:LEU:HB3	1.59	0.83
1:C:105:ILE:HB	1:C:234:VAL:HB	1.60	0.83
1:A:439:GLY:HA2	1:A:442:MET:HE3	1.62	0.82
1:C:97:LEU:HD13	1:C:237:MET:HE3	1.62	0.82
1:B:78:VAL:HG11	1:B:282:GLN:HE22	1.43	0.81
1:A:395:LEU:HD22	1:B:469:LEU:HD12	1.62	0.80
1:A:226:ARG:HG2	1:A:252:HIS:NE2	1.96	0.79
1:A:486:TYR:HD2	1:A:487:PHE:N	1.79	0.79
1:C:479:GLY:O	1:C:483:GLU:HG2	1.82	0.78
1:A:73:VAL:HG21	1:A:84:LEU:HB3	1.66	0.78
1:A:199:ASN:HB3	1:A:202:LEU:HD13	1.64	0.78
1:A:486:TYR:CD2	1:A:487:PHE:N	2.52	0.77
1:B:199:ASN:HB3	1:B:202:LEU:HD13	1.64	0.77
1:A:185:LYS:HE3	1:A:209:LEU:HD11	1.66	0.76
1:A:54:VAL:HA	1:A:149:ILE:HD11	1.65	0.76
1:B:104:TRP:CH2	1:B:269:PHE:HB2	2.21	0.76
1:C:199:ASN:HB3	1:C:202:LEU:HD13	1.69	0.74
1:A:315:THR:HG21	4:A:1033:HOH:O	1.88	0.74
1:B:226:ARG:HD3	4:B:1179:HOH:O	1.85	0.74
1:A:130:LEU:HD11	1:A:191:LEU:HD22	1.70	0.74
1:B:67:ILE:HD11	1:B:237:MET:SD	2.28	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:THR:HB	1:C:344:ASP:OD1	1.89	0.72
1:B:105:ILE:HB	1:B:234:VAL:HB	1.72	0.72
1:A:97:LEU:HD22	1:A:237:MET:HG3	1.71	0.71
1:A:101:LYS:HA	1:A:104:TRP:CD2	2.25	0.71
1:C:54:VAL:HA	1:C:149:ILE:HD11	1.73	0.71
1:A:143:TRP:HB2	1:A:147:PHE:CE1	2.25	0.71
1:A:315:THR:HG22	4:A:1001:HOH:O	1.90	0.71
1:B:92:ARG:O	1:B:93:ASN:HB2	1.89	0.71
1:B:278:LYS:HE2	4:B:1158:HOH:O	1.89	0.70
1:A:469:LEU:HD12	1:C:395:LEU:HD22	1.72	0.70
1:B:249:THR:HA	4:B:1162:HOH:O	1.91	0.70
1:B:315:THR:HG22	4:B:1002:HOH:O	1.90	0.70
1:A:222:ARG:NH1	1:A:239:ASP:OD2	2.25	0.70
1:A:96:ILE:HD11	1:A:273:SER:HB2	1.73	0.69
1:A:167:GLU:HG3	1:A:437:ARG:NH1	2.07	0.69
1:C:226:ARG:HD3	1:C:252:HIS:CE1	2.28	0.69
2:A:900:LYS:HE3	1:C:221:SER:O	1.93	0.68
1:A:486:TYR:HD2	1:A:487:PHE:H	1.40	0.68
1:B:107:PRO:O	1:B:110:VAL:HG22	1.94	0.68
1:A:73:VAL:CG2	1:A:84:LEU:HB3	2.24	0.68
1:C:67:ILE:HD11	1:C:237:MET:SD	2.34	0.68
1:A:100:PRO:HA	1:A:268:LEU:CD1	2.25	0.67
1:A:104:TRP:CH2	1:A:269:PHE:HB2	2.30	0.67
1:C:74:LYS:HD2	1:C:75:ALA:O	1.94	0.67
1:C:222:ARG:NH2	3:C:1002:SAH:O	2.25	0.67
1:A:96:ILE:HD13	1:A:283:VAL:HG11	1.76	0.67
1:B:103:LEU:O	1:B:143:TRP:HZ3	1.79	0.66
1:B:101:LYS:HA	1:B:104:TRP:CD2	2.30	0.66
1:A:54:VAL:HG22	1:A:149:ILE:HD12	1.77	0.65
1:C:97:LEU:HB2	1:C:237:MET:HE1	1.78	0.65
1:A:173:LEU:O	1:A:177:THR:HG23	1.96	0.65
1:C:346:PHE:HB2	1:C:349:ARG:HD2	1.78	0.65
1:B:55:GLN:HE22	1:B:59:LYS:NZ	1.92	0.65
1:C:227:LEU:HB3	1:C:230:GLU:HB2	1.79	0.65
1:B:97:LEU:HB2	1:B:237:MET:HE1	1.79	0.64
1:A:479:GLY:O	1:A:483:GLU:HG2	1.98	0.64
1:A:188:CYS:HB3	1:A:212:PHE:CD1	2.33	0.64
1:C:104:TRP:CH2	1:C:269:PHE:HB2	2.33	0.64
1:A:97:LEU:HD22	1:A:237:MET:CG	2.27	0.64
1:C:222:ARG:HD3	1:C:239:ASP:OD2	1.99	0.63
1:A:59:LYS:HD3	1:A:62:GLN:OE1	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:226:ARG:HG2	1:C:226:ARG:HH11	1.63	0.63
1:A:101:LYS:HA	1:A:104:TRP:CE3	2.34	0.63
1:C:167:GLU:HG3	1:C:437:ARG:NH1	2.14	0.63
1:A:167:GLU:HG3	1:A:437:ARG:HH12	1.62	0.63
1:A:194:GLU:C	1:A:195:ILE:HD12	2.19	0.63
1:C:250:GLU:HB3	4:C:1029:HOH:O	1.98	0.63
1:A:73:VAL:HG11	1:A:96:ILE:HG22	1.78	0.63
1:B:264:SER:HA	1:B:267:TYR:CZ	2.34	0.63
1:A:151:PRO:CD	1:A:222:ARG:HH21	2.12	0.62
1:B:167:GLU:HG2	1:B:430:LEU:HD12	1.81	0.62
1:C:50:LEU:HD22	1:C:54:VAL:CG1	2.27	0.62
1:B:103:LEU:O	1:B:143:TRP:CZ3	2.52	0.62
1:A:107:PRO:HB3	4:A:1049:HOH:O	2.00	0.62
1:A:107:PRO:O	1:A:110:VAL:HG22	2.00	0.62
1:C:320:GLU:HA	1:C:325:PHE:CD1	2.35	0.62
1:B:320:GLU:HA	1:B:325:PHE:CD1	2.35	0.62
1:B:78:VAL:HG12	1:B:80:GLU:H	1.65	0.61
1:B:202:LEU:HD12	1:B:202:LEU:N	2.16	0.61
1:B:123:LYS:HG2	1:C:488:GLN:OXT	2.01	0.61
1:B:99:VAL:O	1:B:104:TRP:CH2	2.54	0.61
1:C:251:ASP:O	1:C:252:HIS:O	2.18	0.60
1:A:88:LYS:HA	1:A:279:ALA:HB2	1.84	0.60
1:A:218:ILE:HG23	1:A:222:ARG:HD2	1.84	0.60
1:C:107:PRO:O	1:C:110:VAL:HG22	2.01	0.60
1:B:395:LEU:CD2	1:C:469:LEU:HD12	2.28	0.60
1:B:414:THR:HG23	1:B:417:GLN:OE1	2.01	0.60
1:A:227:LEU:HD11	1:A:256:VAL:HG23	1.83	0.60
1:A:250:GLU:HG2	1:A:289:LEU:HD12	1.82	0.60
1:A:479:GLY:HA3	1:C:342:TYR:CZ	2.36	0.60
1:A:398:LYS:HB3	4:A:1084:HOH:O	2.01	0.60
1:B:401:ARG:O	1:B:405:LYS:HG3	2.02	0.60
1:C:185:LYS:HE3	1:C:209:LEU:HD11	1.83	0.60
1:A:100:PRO:HA	1:A:268:LEU:HD12	1.84	0.60
1:B:92:ARG:HD2	4:B:1151:HOH:O	2.00	0.60
1:A:202:LEU:O	1:A:204:PRO:HD3	2.02	0.59
1:C:194:GLU:C	1:C:195:ILE:HD12	2.22	0.59
1:B:329:LEU:O	1:B:333:GLU:HG3	2.01	0.59
1:C:250:GLU:CA	4:C:1029:HOH:O	2.38	0.59
1:B:78:VAL:CG1	1:B:282:GLN:HE22	2.16	0.59
1:B:439:GLY:HA2	1:B:442:MET:HE3	1.83	0.59
1:B:99:VAL:O	1:B:104:TRP:HH2	1.86	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:252:HIS:CE1	4:C:1135:HOH:O	2.56	0.59
1:C:227:LEU:HB2	4:C:1019:HOH:O	2.03	0.58
1:C:96:ILE:HD11	1:C:273:SER:HB2	1.85	0.58
1:A:465:GLN:HB3	1:C:395:LEU:HD11	1.85	0.58
1:C:220:ARG:HD3	1:C:299:ASP:OD1	2.03	0.58
1:A:313:THR:HB	1:A:344:ASP:OD1	2.04	0.58
1:C:103:LEU:O	1:C:143:TRP:CZ3	2.56	0.58
1:C:157:THR:OG1	1:C:177:THR:HG21	2.04	0.58
1:C:252:HIS:HE1	4:C:1135:HOH:O	1.84	0.58
1:C:298:LEU:HD23	1:C:298:LEU:C	2.23	0.58
1:A:482:LEU:HD21	1:C:180:VAL:HA	1.86	0.58
1:B:143:TRP:HB2	1:B:147:PHE:CE1	2.39	0.58
1:C:315:THR:HG22	4:C:1003:HOH:O	2.03	0.58
1:A:250:GLU:HG2	1:A:289:LEU:CD1	2.33	0.58
1:C:104:TRP:HH2	1:C:269:PHE:H	1.52	0.58
2:A:900:LYS:NZ	4:A:1003:HOH:O	2.36	0.57
1:C:96:ILE:HD13	1:C:283:VAL:HG11	1.87	0.57
1:C:201:ARG:HB3	1:C:201:ARG:HH11	1.69	0.57
1:B:292:SER:OG	1:B:295:GLU:HG3	2.03	0.57
1:A:250:GLU:HB2	4:A:1106:HOH:O	2.03	0.57
1:A:194:GLU:HG3	4:A:1094:HOH:O	2.03	0.57
1:C:226:ARG:HB3	1:C:252:HIS:CE1	2.39	0.57
1:B:97:LEU:HD13	1:B:237:MET:HE3	1.87	0.56
1:A:98:GLN:HA	1:A:269:PHE:O	2.04	0.56
1:C:455:GLU:O	1:C:458:LEU:HB2	2.06	0.56
1:C:150:LEU:HD13	1:C:218:ILE:HD13	1.86	0.56
1:A:101:LYS:HG3	1:A:104:TRP:CD1	2.41	0.56
1:B:197:LEU:HB2	1:B:198:PRO:HD3	1.87	0.56
1:A:70:LYS:O	1:A:72:PRO:HD3	2.06	0.55
1:B:226:ARG:HG3	4:B:1191:HOH:O	2.06	0.55
1:B:97:LEU:HB2	1:B:237:MET:CE	2.36	0.55
1:B:202:LEU:HD12	1:B:202:LEU:H	1.71	0.55
1:B:264:SER:HA	1:B:267:TYR:CE1	2.42	0.55
1:B:96:ILE:CD1	1:B:283:VAL:HG11	2.37	0.55
1:B:313:THR:HG21	1:C:478:ASN:CG	2.26	0.55
1:C:398:LYS:O	1:C:402:GLU:HG2	2.06	0.55
1:A:220:ARG:HB3	4:A:1160:HOH:O	2.06	0.55
1:B:318:ILE:O	1:B:339:GLN:NE2	2.38	0.55
1:A:103:LEU:O	1:A:143:TRP:CZ3	2.59	0.55
1:B:78:VAL:HG11	1:B:282:GLN:NE2	2.16	0.55
1:C:386:LEU:O	1:C:387:SER:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:243:HIS:CE1	1:A:286:GLN:HE22	2.25	0.55
1:B:174:LEU:O	1:B:178:VAL:HG23	2.07	0.55
1:A:99:VAL:O	1:A:104:TRP:CH2	2.60	0.55
1:C:483:GLU:O	1:C:487:PHE:HD1	1.90	0.54
1:A:105:ILE:HB	1:A:234:VAL:HB	1.89	0.54
1:A:99:VAL:O	1:A:104:TRP:HH2	1.90	0.54
1:C:97:LEU:HD11	1:C:238:ALA:HB2	1.90	0.54
1:C:327:ASP:O	1:C:331:VAL:HG23	2.07	0.54
1:C:99:VAL:O	1:C:104:TRP:HH2	1.90	0.54
1:B:313:THR:HB	1:B:344:ASP:OD1	2.07	0.54
1:C:468:ARG:HH11	1:C:468:ARG:CB	2.18	0.54
1:A:74:LYS:HB3	1:A:87:LEU:HD21	1.88	0.54
1:C:163:GLU:O	1:C:166:GLN:HB2	2.07	0.54
1:C:466:GLU:HB2	4:C:1192:HOH:O	2.07	0.54
1:B:51:SER:N	1:B:52:PRO:HD2	2.23	0.54
1:B:55:GLN:NE2	1:B:59:LYS:NZ	2.56	0.54
1:C:167:GLU:HG3	1:C:437:ARG:HH12	1.73	0.53
1:A:97:LEU:HD11	1:A:238:ALA:HB2	1.89	0.53
1:C:118:VAL:HG13	4:C:1065:HOH:O	2.08	0.53
1:C:482:LEU:HD22	1:C:486:TYR:CZ	2.43	0.53
1:A:202:LEU:C	1:A:204:PRO:HD3	2.29	0.53
1:B:363:ALA:O	1:B:364:LEU:C	2.47	0.53
1:A:54:VAL:CA	1:A:149:ILE:HD11	2.36	0.53
1:A:144:LYS:HA	4:A:1098:HOH:O	2.08	0.53
1:B:140:ASP:HA	4:B:1147:HOH:O	2.07	0.53
1:A:70:LYS:C	1:A:72:PRO:HD3	2.29	0.53
1:B:250:GLU:OE2	1:B:288:ASP:HA	2.09	0.53
1:A:110:VAL:HG12	1:A:131:PHE:CG	2.44	0.53
1:A:320:GLU:HA	1:A:325:PHE:CD1	2.44	0.53
1:A:438:GLU:HG2	1:A:442:MET:HE2	1.90	0.53
1:C:50:LEU:CD2	1:C:54:VAL:HG11	2.30	0.53
1:A:231:ASN:C	1:A:232:LEU:HD12	2.30	0.52
2:A:800:LYS:HE3	1:B:222:ARG:O	2.09	0.52
1:A:105:ILE:HG22	1:A:105:ILE:O	2.09	0.52
1:A:119:CYS:HA	1:A:122:LEU:HD12	1.91	0.52
1:C:92:ARG:HG2	1:C:93:ASN:ND2	2.24	0.52
1:C:99:VAL:O	1:C:104:TRP:CH2	2.61	0.52
1:A:146:TYR:CE2	1:A:150:LEU:HD11	2.44	0.52
1:C:54:VAL:HG22	1:C:149:ILE:HD12	1.90	0.52
1:C:298:LEU:HD23	1:C:298:LEU:O	2.10	0.52
1:A:97:LEU:HD12	1:A:97:LEU:O	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:227:LEU:HD23	1:A:230:GLU:HB2	1.92	0.52
1:B:48:PRO:N	4:B:1099:HOH:O	2.42	0.52
1:B:298:LEU:HD23	4:B:1043:HOH:O	2.09	0.52
1:A:91:SER:O	1:A:94:ASP:HB2	2.09	0.52
1:A:188:CYS:HB3	1:A:212:PHE:CE1	2.45	0.52
1:A:243:HIS:HE1	1:A:286:GLN:HE22	1.58	0.51
1:A:58:TRP:CZ2	1:A:74:LYS:HA	2.44	0.51
1:C:129:ILE:HG23	1:C:215:ALA:HB3	1.92	0.51
1:A:226:ARG:HB2	1:A:226:ARG:NH1	2.26	0.51
1:C:103:LEU:O	1:C:143:TRP:HZ3	1.93	0.51
1:B:227:LEU:HA	4:B:1092:HOH:O	2.10	0.51
1:A:197:LEU:HB2	1:A:198:PRO:HD3	1.92	0.51
1:C:105:ILE:HD11	1:C:143:TRP:CE2	2.46	0.51
1:C:225:SER:HA	4:C:1019:HOH:O	2.10	0.51
1:C:244:SER:HB2	1:C:284:TYR:CG	2.46	0.51
1:A:72:PRO:O	1:A:86:ALA:HA	2.11	0.51
1:A:316:LEU:HD12	1:A:343:PHE:CE1	2.46	0.51
1:B:78:VAL:CG1	1:B:80:GLU:OE2	2.59	0.51
1:B:136:ARG:HD2	1:B:214:TRP:CZ3	2.46	0.51
1:C:482:LEU:HD22	1:C:486:TYR:OH	2.11	0.51
1:A:104:TRP:O	1:A:105:ILE:HG12	2.11	0.50
1:C:74:LYS:HE3	4:C:1047:HOH:O	2.11	0.50
1:C:104:TRP:HH2	1:C:269:PHE:N	2.08	0.50
1:C:202:LEU:N	1:C:202:LEU:HD12	2.27	0.50
1:B:110:VAL:HG12	1:B:131:PHE:CG	2.47	0.50
1:A:99:VAL:CG2	1:A:237:MET:HB3	2.42	0.50
1:A:122:LEU:HA	4:A:1039:HOH:O	2.12	0.50
1:B:50:LEU:HD23	1:B:51:SER:N	2.27	0.50
1:B:225:SER:HB2	4:B:1191:HOH:O	2.11	0.50
1:A:451:PHE:O	1:A:455:GLU:HG3	2.12	0.50
1:A:218:ILE:O	1:A:222:ARG:HB2	2.12	0.50
1:A:410:GLY:HA3	4:A:1021:HOH:O	2.10	0.50
1:B:386:LEU:O	1:B:387:SER:HB3	2.12	0.50
1:C:438:GLU:HG2	1:C:442:MET:CE	2.41	0.50
1:A:103:LEU:O	1:A:143:TRP:HZ3	1.95	0.49
1:A:329:LEU:O	1:A:333:GLU:HG3	2.12	0.49
1:A:462:GLU:HB3	4:A:1164:HOH:O	2.11	0.49
1:C:277:VAL:HG13	1:C:281:GLU:HB2	1.94	0.49
1:C:167:GLU:HG2	1:C:430:LEU:HD12	1.95	0.49
1:B:96:ILE:HD11	1:B:283:VAL:HG11	1.93	0.49
1:B:101:LYS:HA	1:B:104:TRP:CE3	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:97:LEU:HB2	1:C:237:MET:CE	2.42	0.49
1:C:226:ARG:HG2	1:C:226:ARG:NH1	2.26	0.49
1:C:249:THR:HG22	1:C:250:GLU:OE1	2.12	0.49
1:C:124:PRO:O	1:C:128:VAL:HG23	2.13	0.49
1:A:315:THR:HB	1:A:342:TYR:CE2	2.48	0.49
1:A:342:TYR:CZ	1:B:479:GLY:HA3	2.48	0.49
1:A:115:ILE:O	1:A:118:VAL:HG22	2.13	0.49
1:C:482:LEU:HD22	1:C:486:TYR:CE2	2.48	0.49
1:A:88:LYS:O	1:A:89:ASP:C	2.51	0.49
1:A:96:ILE:HD11	1:A:273:SER:CA	2.43	0.49
1:A:100:PRO:HA	1:A:268:LEU:HD11	1.94	0.49
1:A:479:GLY:HA3	1:C:342:TYR:CE2	2.48	0.48
1:B:412:HIS:CD2	1:B:413:THR:HG23	2.48	0.48
1:B:88:LYS:HA	1:B:279:ALA:HB2	1.93	0.48
1:B:167:GLU:HG3	1:B:437:ARG:NH1	2.28	0.48
1:A:96:ILE:HD11	1:A:273:SER:CB	2.40	0.48
1:C:310:HIS:CD2	1:C:439:GLY:HA3	2.48	0.48
1:A:70:LYS:O	1:A:72:PRO:CD	2.61	0.48
1:B:167:GLU:HG3	1:B:437:ARG:HH12	1.77	0.48
1:C:143:TRP:HB2	1:C:147:PHE:CE1	2.48	0.48
1:B:61:LEU:HB3	1:B:67:ILE:HG12	1.95	0.48
1:C:157:THR:HA	1:C:160:TRP:CD1	2.48	0.48
1:C:222:ARG:HH11	1:C:239:ASP:CG	2.17	0.48
1:A:201:ARG:HH12	1:A:202:LEU:HD11	1.79	0.48
1:A:97:LEU:HD22	1:A:237:MET:SD	2.54	0.48
1:A:455:GLU:O	1:A:458:LEU:HB2	2.14	0.48
1:C:73:VAL:HG22	1:C:74:LYS:N	2.28	0.48
1:C:92:ARG:HG3	1:C:274:PRO:O	2.13	0.48
1:C:438:GLU:HG2	1:C:442:MET:HE3	1.95	0.48
1:B:255:GLU:HA	1:B:268:LEU:O	2.14	0.48
1:C:201:ARG:HH12	1:C:202:LEU:HD11	1.79	0.48
1:B:78:VAL:CG1	1:B:79:THR:N	2.77	0.48
1:C:202:LEU:HD12	1:C:202:LEU:H	1.77	0.48
1:B:192:GLU:HA	1:B:196:ILE:HB	1.96	0.48
1:A:105:ILE:HD11	1:A:143:TRP:CE2	2.49	0.47
1:B:136:ARG:HD2	1:B:214:TRP:CH2	2.49	0.47
1:A:73:VAL:HG11	1:A:96:ILE:CG2	2.45	0.47
1:C:101:LYS:HA	1:C:104:TRP:CD2	2.50	0.47
1:A:393:GLU:O	1:A:396:LEU:HG	2.14	0.47
1:B:225:SER:O	1:B:226:ARG:C	2.53	0.47
1:A:243:HIS:CE1	1:A:286:GLN:NE2	2.82	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:482:LEU:HD11	1:C:179:SER:OG	2.15	0.47
1:B:264:SER:HA	1:B:267:TYR:CE2	2.49	0.47
1:A:176:THR:O	1:A:180:VAL:HG23	2.13	0.47
1:B:105:ILE:HD11	1:B:143:TRP:CE2	2.50	0.47
1:B:139:GLU:O	1:B:144:LYS:HD2	2.15	0.47
1:B:167:GLU:HG2	1:B:430:LEU:CD1	2.43	0.47
1:B:459:ASP:HB2	4:B:1066:HOH:O	2.15	0.47
1:C:214:TRP:O	1:C:218:ILE:HG13	2.14	0.47
1:B:323:PRO:CB	1:C:375:LEU:HD21	2.44	0.47
1:A:238:ALA:HB1	1:A:271:LEU:HD22	1.97	0.47
1:B:395:LEU:HD11	1:C:465:GLN:HB3	1.97	0.47
1:A:389:SER:HA	1:A:463:TYR:CG	2.49	0.47
1:B:64:GLU:OE1	1:B:102:ARG:NH1	2.47	0.47
1:B:315:THR:HG21	4:C:1092:HOH:O	2.15	0.47
1:B:373:GLU:HG3	4:B:1081:HOH:O	2.15	0.47
1:C:173:LEU:O	1:C:177:THR:HG23	2.14	0.47
1:C:201:ARG:HB3	1:C:201:ARG:NH1	2.29	0.47
1:C:251:ASP:O	1:C:252:HIS:C	2.53	0.47
1:B:188:CYS:O	1:B:191:LEU:HB2	2.16	0.46
1:B:396:LEU:HD12	1:B:397:CYS:N	2.29	0.46
1:A:439:GLY:HA2	1:A:442:MET:CE	2.41	0.46
1:B:381:TRP:O	1:B:385:GLU:HG3	2.15	0.46
1:C:73:VAL:CG2	1:C:84:LEU:HB3	2.38	0.46
1:B:482:LEU:HD12	4:B:1192:HOH:O	2.15	0.46
1:B:301:GLY:HA3	4:B:1021:HOH:O	2.16	0.46
1:B:408:LEU:HD21	1:B:444:LEU:HB3	1.98	0.46
1:C:286:GLN:HG2	1:C:289:LEU:HG	1.98	0.46
1:A:278:LYS:HB3	4:A:1074:HOH:O	2.15	0.46
1:A:224:PHE:HB3	1:A:254:TYR:CZ	2.50	0.46
1:B:316:LEU:HD11	1:B:355:LEU:HD12	1.98	0.46
1:A:96:ILE:CD1	1:A:273:SER:HB2	2.45	0.46
1:B:147:PHE:HA	1:B:150:LEU:HD12	1.97	0.46
1:B:347:TYR:CE2	1:B:348:ASN:ND2	2.84	0.46
1:B:365:GLY:C	4:B:1019:HOH:O	2.54	0.46
1:B:446:GLN:O	1:B:450:ILE:HG13	2.15	0.46
1:A:125:TRP:HZ2	1:A:183:TYR:OH	1.99	0.46
1:A:202:LEU:N	1:A:202:LEU:HD12	2.29	0.46
1:A:466:GLU:O	1:A:470:LYS:HG2	2.16	0.46
1:A:107:PRO:HA	1:A:110:VAL:HG22	1.97	0.45
1:B:393:GLU:O	1:B:396:LEU:HG	2.15	0.45
1:C:241:ILE:HD11	1:C:283:VAL:HG12	1.97	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:123:LYS:HD3	1:C:486:TYR:O	2.16	0.45
1:B:146:TYR:CE1	1:B:236:PRO:HA	2.51	0.45
1:C:347:TYR:O	1:C:348:ASN:HB2	2.15	0.45
1:C:226:ARG:NH2	1:C:288:ASP:HA	2.31	0.45
1:C:316:LEU:HD21	1:C:359:LEU:HD23	1.98	0.45
1:A:146:TYR:CE1	1:A:236:PRO:HA	2.50	0.45
1:B:176:THR:HG21	1:C:481:ILE:HD12	1.97	0.45
1:B:287:TYR:O	1:B:288:ASP:HB2	2.15	0.45
1:C:478:ASN:O	1:C:480:ASP:N	2.50	0.45
1:A:151:PRO:HD2	1:A:222:ARG:HH21	1.81	0.45
1:A:183:TYR:CZ	1:A:187:GLU:HG3	2.51	0.45
1:C:110:VAL:HG12	1:C:131:PHE:CG	2.52	0.45
1:B:194:GLU:C	1:B:195:ILE:HD12	2.37	0.45
1:C:98:GLN:HA	1:C:269:PHE:O	2.17	0.45
1:C:444:LEU:HD12	1:C:444:LEU:HA	1.86	0.45
1:A:241:ILE:HG23	1:A:241:ILE:O	2.16	0.44
1:C:168:LEU:HD21	1:C:433:ALA:HA	1.99	0.44
1:C:250:GLU:CB	4:C:1029:HOH:O	2.55	0.44
1:B:78:VAL:HG12	1:B:79:THR:N	2.31	0.44
1:B:101:LYS:HA	1:B:104:TRP:CE2	2.51	0.44
1:C:316:LEU:HD12	1:C:343:PHE:CE1	2.52	0.44
1:B:125:TRP:O	1:B:129:ILE:HG13	2.17	0.44
1:C:157:THR:OG1	1:C:177:THR:CG2	2.65	0.44
1:C:316:LEU:HD21	1:C:359:LEU:CD2	2.47	0.44
1:B:313:THR:HG22	4:B:1188:HOH:O	2.18	0.44
1:A:99:VAL:HA	1:A:100:PRO:HD3	1.83	0.44
2:A:900:LYS:N	1:C:300:TYR:HH	2.15	0.44
1:B:455:GLU:O	1:B:458:LEU:HB2	2.17	0.44
1:A:243:HIS:HE1	1:A:286:GLN:NE2	2.16	0.44
1:C:103:LEU:HA	1:C:143:TRP:CH2	2.53	0.44
1:C:445:GLN:NE2	4:C:1162:HOH:O	2.49	0.44
1:A:99:VAL:O	1:A:268:LEU:HG	2.18	0.44
1:B:143:TRP:CD1	1:B:143:TRP:N	2.85	0.44
1:A:172:GLN:NE2	1:A:313:THR:HG23	2.33	0.44
1:B:129:ILE:HG23	1:B:215:ALA:HB3	2.00	0.44
1:C:301:GLY:HA3	4:C:1013:HOH:O	2.17	0.44
1:A:141:SER:HB3	4:A:1098:HOH:O	2.18	0.43
1:A:354:GLY:HA2	1:A:357:PRO:HG2	1.99	0.43
1:C:486:TYR:HB2	1:C:487:PHE:H	1.36	0.43
1:A:408:LEU:HD21	1:A:444:LEU:HB3	2.00	0.43
1:B:110:VAL:HG23	1:B:111:ALA:N	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:195:ILE:HD12	1:B:195:ILE:N	2.33	0.43
1:B:244:SER:C	1:B:246:GLY:H	2.20	0.43
1:C:167:GLU:HG2	1:C:430:LEU:CD1	2.48	0.43
1:C:356:LEU:N	1:C:357:PRO:HD2	2.33	0.43
1:A:99:VAL:HG21	1:A:237:MET:HB3	2.00	0.43
1:A:103:LEU:HA	1:A:143:TRP:CH2	2.53	0.43
1:A:249:THR:C	1:A:251:ASP:H	2.21	0.43
1:C:225:SER:HB3	1:C:231:ASN:O	2.18	0.43
1:C:320:GLU:HG2	1:C:325:PHE:CE1	2.54	0.43
1:A:300:TYR:HH	2:A:700:LYS:N	2.15	0.43
1:C:60:TRP:O	1:C:64:GLU:HG2	2.18	0.43
1:C:370:PHE:HB3	4:C:1098:HOH:O	2.18	0.43
1:C:438:GLU:OE2	1:C:442:MET:HE2	2.18	0.43
1:A:139:GLU:O	1:A:144:LYS:HD2	2.19	0.43
1:A:396:LEU:HD12	1:A:397:CYS:N	2.33	0.43
1:A:486:TYR:CD2	1:A:486:TYR:C	2.91	0.43
1:B:380:ILE:HG23	1:B:381:TRP:N	2.33	0.43
1:B:110:VAL:HG21	1:B:127:SER:HB3	2.00	0.43
1:B:123:LYS:CG	1:C:488:GLN:OXT	2.65	0.43
1:C:73:VAL:HG11	1:C:96:ILE:HG22	2.01	0.43
1:C:160:TRP:HB2	1:C:165:LEU:HD21	2.00	0.43
1:A:250:GLU:HB3	1:A:286:GLN:CG	2.49	0.43
1:C:110:VAL:HG21	1:C:127:SER:HB3	2.00	0.43
1:A:149:ILE:HD13	1:A:149:ILE:HA	1.78	0.43
1:B:252:HIS:O	1:B:271:LEU:HD12	2.19	0.43
1:C:74:LYS:HG2	1:C:87:LEU:HD21	2.01	0.43
1:A:155:ASP:OD2	1:A:428:SER:HB3	2.18	0.43
1:A:195:ILE:HD12	1:A:195:ILE:N	2.33	0.43
1:C:226:ARG:HD3	1:C:252:HIS:ND1	2.34	0.43
1:C:419:ARG:NH1	4:C:1055:HOH:O	2.52	0.43
1:A:99:VAL:HG21	1:A:235:VAL:CG1	2.49	0.42
1:A:287:TYR:CZ	2:A:700:LYS:HE2	2.54	0.42
1:A:401:ARG:HD3	4:A:1060:HOH:O	2.17	0.42
1:B:124:PRO:O	1:B:128:VAL:HG23	2.19	0.42
1:B:244:SER:HB2	1:B:284:TYR:CG	2.54	0.42
1:A:136:ARG:HD3	4:A:1077:HOH:O	2.18	0.42
1:B:451:PHE:O	1:B:455:GLU:HG3	2.19	0.42
1:C:92:ARG:O	1:C:93:ASN:HB2	2.18	0.42
1:A:101:LYS:HA	1:A:104:TRP:CE2	2.53	0.42
1:A:157:THR:HA	1:A:160:TRP:CD1	2.54	0.42
1:B:50:LEU:C	1:B:52:PRO:HD2	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:96:ILE:CD1	1:C:283:VAL:HG11	2.48	0.42
1:C:438:GLU:CD	1:C:442:MET:HE2	2.40	0.42
1:A:238:ALA:CB	1:A:271:LEU:HD22	2.50	0.42
1:B:244:SER:C	1:B:246:GLY:N	2.72	0.42
1:A:478:ASN:CG	1:C:313:THR:HG21	2.40	0.42
1:A:55:GLN:HE21	1:A:55:GLN:HB2	1.64	0.42
1:A:230:GLU:HB3	1:A:233:VAL:CG2	2.49	0.42
1:B:320:GLU:HG2	1:B:325:PHE:CE1	2.53	0.42
1:A:315:THR:HB	1:A:342:TYR:CD2	2.55	0.42
1:A:363:ALA:O	1:A:364:LEU:C	2.58	0.42
1:A:455:GLU:HA	1:A:458:LEU:HD13	2.02	0.42
1:B:278:LYS:NZ	4:B:1050:HOH:O	2.53	0.42
1:A:78:VAL:HG23	1:A:80:GLU:HG2	2.01	0.42
1:A:180:VAL:O	1:A:184:VAL:HG23	2.20	0.42
1:B:310:HIS:CD2	1:B:439:GLY:HA3	2.55	0.42
1:C:150:LEU:HA	1:C:151:PRO:HD3	1.86	0.42
1:A:150:LEU:HA	1:A:151:PRO:HD3	1.79	0.41
1:A:151:PRO:HD3	1:A:222:ARG:HH21	1.83	0.41
1:A:390:ARG:HA	1:A:463:TYR:CZ	2.55	0.41
1:C:61:LEU:HB3	1:C:67:ILE:HG12	2.01	0.41
1:A:160:TRP:HA	1:A:164:GLU:OE2	2.20	0.41
1:B:222:ARG:HH11	1:B:239:ASP:CG	2.23	0.41
1:C:377:ARG:HA	1:C:377:ARG:HD3	1.86	0.41
1:B:225:SER:O	1:B:227:LEU:HG	2.19	0.41
1:C:354:GLY:HA2	1:C:357:PRO:CG	2.49	0.41
1:A:377:ARG:HA	1:A:377:ARG:HD3	1.92	0.41
1:C:98:GLN:HG2	1:C:270:SER:HA	2.02	0.41
1:C:297:ALA:O	1:C:300:TYR:O	2.38	0.41
1:A:255:GLU:HG2	1:A:256:VAL:N	2.36	0.41
2:A:900:LYS:HE3	1:C:222:ARG:HA	2.02	0.41
1:A:244:SER:HB2	1:A:284:TYR:CG	2.55	0.41
1:A:394:GLU:HB2	1:A:458:LEU:HD21	2.02	0.41
1:B:59:LYS:HB2	1:B:59:LYS:HZ2	1.85	0.41
1:B:168:LEU:HD21	1:B:433:ALA:HA	2.02	0.41
1:B:202:LEU:C	1:B:204:PRO:HD3	2.40	0.41
1:B:104:TRP:CZ2	1:B:269:PHE:HB2	2.55	0.41
1:C:54:VAL:HA	1:C:149:ILE:CD1	2.47	0.41
1:C:463:TYR:O	1:C:467:ARG:HG3	2.20	0.41
1:A:100:PRO:C	1:A:102:ARG:N	2.74	0.41
1:C:418:ASP:O	1:C:422:LYS:HG3	2.21	0.41
1:A:62:GLN:HA	1:A:67:ILE:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:101:LYS:HG3	1:B:104:TRP:CD1	2.56	0.41
1:B:248:THR:HB	4:B:1091:HOH:O	2.21	0.41
1:C:88:LYS:HE3	4:C:1093:HOH:O	2.21	0.41
1:A:63:GLU:O	1:A:64:GLU:HG2	2.21	0.41
1:A:99:VAL:HG21	1:A:235:VAL:HG12	2.02	0.41
1:C:228:ARG:O	1:C:229:ASN:HB2	2.20	0.41
1:C:430:LEU:O	1:C:434:VAL:HG23	2.21	0.41
1:A:57:PHE:CE1	1:A:146:TYR:HA	2.56	0.40
1:A:214:TRP:CZ2	1:A:218:ILE:HD12	2.56	0.40
1:B:76:SER:HB3	1:B:85:VAL:HG23	2.03	0.40
1:B:110:VAL:CG2	1:B:111:ALA:N	2.83	0.40
1:B:201:ARG:HH12	1:B:202:LEU:HD11	1.86	0.40
1:A:64:GLU:OE1	1:A:102:ARG:NH1	2.55	0.40
1:A:201:ARG:NH1	1:A:202:LEU:HD11	2.36	0.40
1:B:226:ARG:HB3	4:B:1116:HOH:O	2.21	0.40
1:B:293:ASN:HD22	1:B:310:HIS:CD2	2.38	0.40
1:C:328:LYS:HE2	1:C:364:LEU:HB3	2.03	0.40
1:A:167:GLU:HG2	1:A:430:LEU:CD1	2.51	0.40
1:A:348:ASN:H	1:A:446:GLN:HE22	1.69	0.40
1:A:390:ARG:HG2	4:A:1025:HOH:O	2.21	0.40
1:A:202:LEU:HD12	1:A:202:LEU:H	1.87	0.40
1:A:267:TYR:O	1:A:268:LEU:HD12	2.21	0.40
1:B:208:THR:HG23	4:B:1045:HOH:O	2.20	0.40
1:C:92:ARG:CB	1:C:92:ARG:NH1	2.85	0.40
1:C:202:LEU:C	1:C:204:PRO:HD3	2.42	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	425/444 (96%)	375 (88%)	41 (10%)	9 (2%)	7 10

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	B	439/444 (99%)	400 (91%)	33 (8%)	6 (1%)	11 16
1	C	438/444 (99%)	405 (92%)	26 (6%)	7 (2%)	9 14
All	All	1302/1332 (98%)	1180 (91%)	100 (8%)	22 (2%)	9 13

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	252	HIS
1	B	364	LEU
1	C	252	HIS
1	A	105	ILE
1	B	226	ARG
1	B	288	ASP
1	C	387	SER
1	A	104	TRP
1	A	364	LEU
1	B	387	SER
1	C	479	GLY
1	A	120	SER
1	C	236	PRO
1	C	377	ARG
1	A	250	GLU
1	A	236	PRO
1	B	120	SER
1	C	120	SER
1	C	364	LEU
1	A	72	PRO
1	A	66	VAL
1	B	204	PRO

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	379/390 (97%)	363 (96%)	16 (4%)	30 45

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	B	387/390 (99%)	371 (96%)	16 (4%)	30 46
1	C	386/390 (99%)	361 (94%)	25 (6%)	17 26
All	All	1152/1170 (98%)	1095 (95%)	57 (5%)	25 38

All (57) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	94	ASP
1	A	104	TRP
1	A	139	GLU
1	A	143	TRP
1	A	205	ASP
1	A	237	MET
1	A	313	THR
1	A	315	THR
1	A	378	ASP
1	A	385	GLU
1	A	395	LEU
1	A	426	LEU
1	A	427	ASP
1	A	444	LEU
1	A	486	TYR
1	B	88	LYS
1	B	104	TRP
1	B	139	GLU
1	B	143	TRP
1	B	205	ASP
1	B	210	ASP
1	B	236	PRO
1	B	313	THR
1	B	315	THR
1	B	374	SER
1	B	378	ASP
1	B	395	LEU
1	B	426	LEU
1	B	427	ASP
1	B	444	LEU
1	B	484	ASN
1	C	49	SER
1	C	74	LYS

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Mol	Chain	Res	Type
1	C	79	THR
1	C	104	TRP
1	C	139	GLU
1	C	143	TRP
1	C	210	ASP
1	C	227	LEU
1	C	236	PRO
1	C	239	ASP
1	C	249	THR
1	C	250	GLU
1	C	252	HIS
1	C	255	GLU
1	C	268	LEU
1	C	313	THR
1	C	315	THR
1	C	378	ASP
1	C	395	LEU
1	C	426	LEU
1	C	427	ASP
1	C	444	LEU
1	C	468	ARG
1	C	482	LEU
1	C	488	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	55	GLN
1	A	93	ASN
1	A	145	HIS
1	A	166	GLN
1	A	169	GLN
1	A	243	HIS
1	B	55	GLN
1	B	152	GLN
1	B	169	GLN
1	B	310	HIS
1	B	348	ASN
1	B	412	HIS
1	B	484	ASN
1	B	488	GLN
1	C	55	GLN

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Mol	Chain	Res	Type
1	C	145	HIS
1	C	152	GLN
1	C	166	GLN
1	C	169	GLN
1	C	310	HIS

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

6 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	LYS	A	900	-	8,9,9	0.70	0	9,10,10	0.93	0
3	SAH	C	1002	-	24,28,28	1.09	3 (12%)	25,40,40	1.01	0
3	SAH	A	1000	-	24,28,28	1.01	2 (8%)	25,40,40	1.05	1 (4%)
3	SAH	B	1001	-	24,28,28	0.99	3 (12%)	25,40,40	1.00	1 (4%)
2	LYS	A	700	-	8,9,9	0.69	0	9,10,10	0.74	0
2	LYS	A	800	-	8,9,9	0.72	0	9,10,10	0.58	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	LYS	A	900	-	-	2/9/9/9	-
3	SAH	C	1002	-	-	3/11/31/31	0/3/3/3
3	SAH	A	1000	-	-	5/11/31/31	0/3/3/3
3	SAH	B	1001	-	-	4/11/31/31	0/3/3/3
2	LYS	A	700	-	-	0/9/9/9	-
2	LYS	A	800	-	-	1/9/9/9	-

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	1001	SAH	C2-N3	2.42	1.36	1.32
3	A	1000	SAH	C2-N3	2.39	1.35	1.32
3	C	1002	SAH	C8-N7	-2.35	1.30	1.34
3	C	1002	SAH	C4-N3	2.25	1.38	1.35
3	C	1002	SAH	C2-N3	2.19	1.35	1.32
3	A	1000	SAH	C8-N7	-2.19	1.30	1.34
3	B	1001	SAH	C4-N3	2.14	1.38	1.35
3	B	1001	SAH	OXT-C	-2.11	1.23	1.30

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	B	1001	SAH	C5-C6-N6	2.46	124.09	120.35
3	A	1000	SAH	OXT-C-CA	2.07	120.44	113.38

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	1000	SAH	CA-CB-CG-SD
2	A	900	LYS	CA-CB-CG-CD
3	A	1000	SAH	C3'-C4'-C5'-SD
3	B	1001	SAH	OXT-C-CA-CB
3	C	1002	SAH	O-C-CA-CB
3	C	1002	SAH	OXT-C-CA-CB
3	A	1000	SAH	CB-CG-SD-C5'
3	C	1002	SAH	CB-CG-SD-C5'
2	A	900	LYS	CG-CD-CE-NZ

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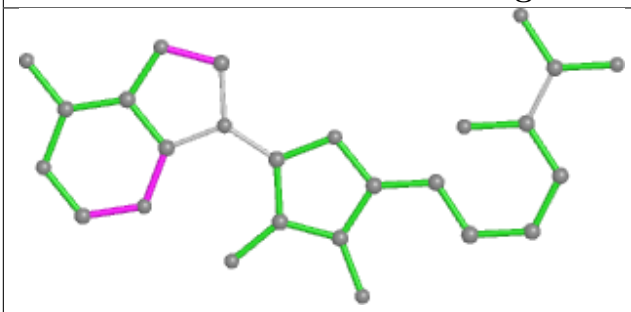
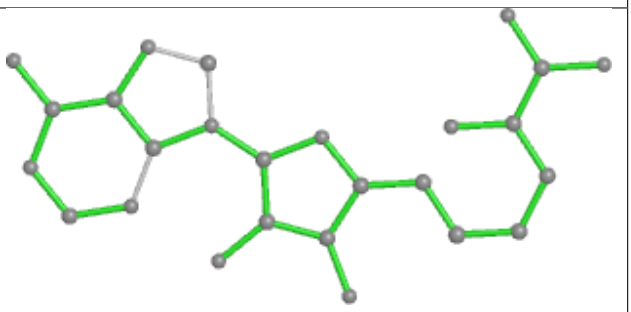
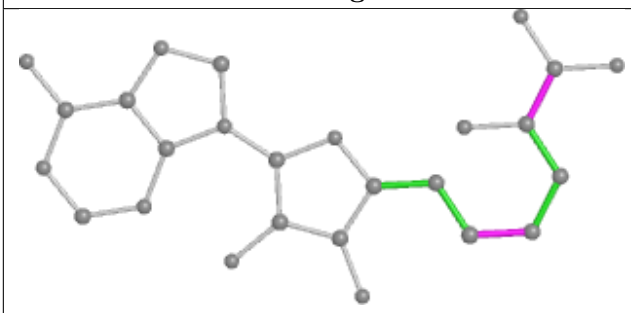
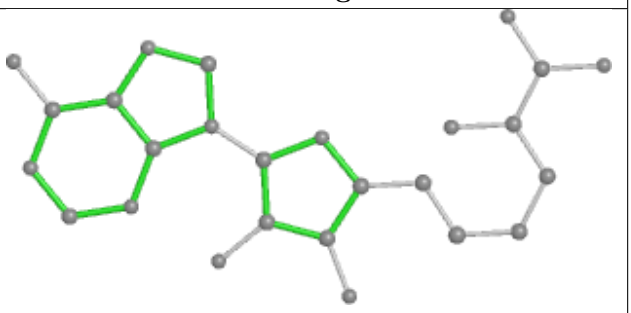
Mol	Chain	Res	Type	Atoms
3	B	1001	SAH	CB-CG-SD-C5'
3	A	1000	SAH	O-C-CA-CB
3	A	1000	SAH	OXT-C-CA-CB
3	B	1001	SAH	O-C-CA-CB
2	A	800	LYS	O-C-CA-N
3	B	1001	SAH	C3'-C4'-C5'-SD

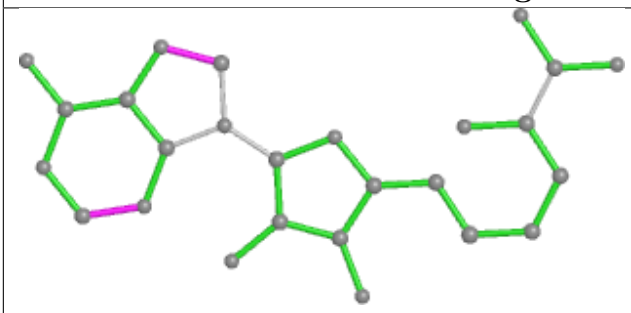
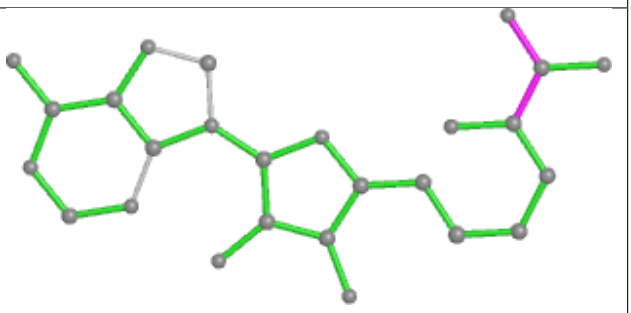
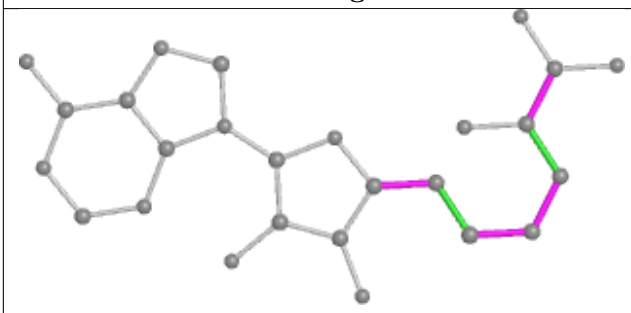
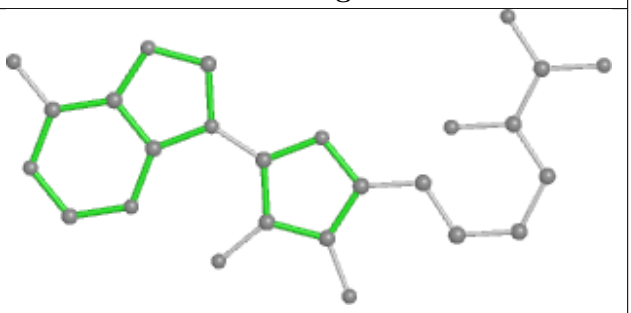
There are no ring outliers.

4 monomers are involved in 8 short contacts:

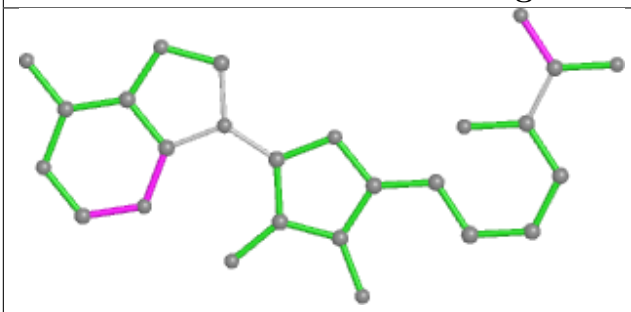
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	900	LYS	4	0
3	C	1002	SAH	1	0
2	A	700	LYS	2	0
2	A	800	LYS	1	0

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.

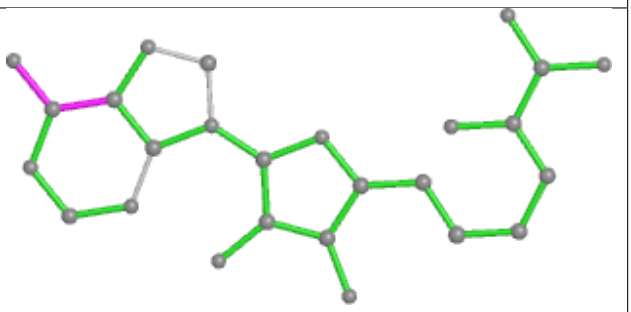
Ligand SAH C 1002	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SAH A 1000	
 Bond lengths	 Bond angles
 Torsions	 Rings

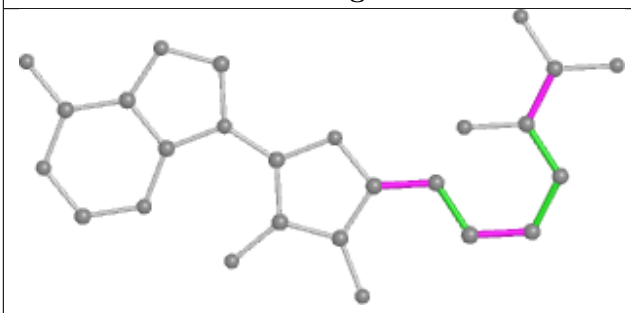
Ligand SAH B 1001



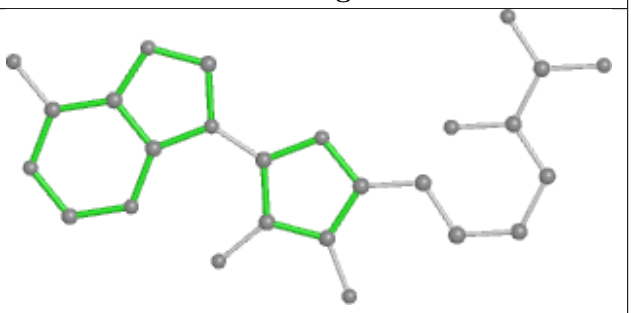
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 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	429/444 (96%)	0.27	36 (8%)	11	8	42, 67, 117, 130	0
1	B	441/444 (99%)	0.05	23 (5%)	27	24	36, 60, 100, 132	0
1	C	440/444 (99%)	-0.08	10 (2%)	60	56	37, 61, 95, 114	0
All	All	1310/1332 (98%)	0.08	69 (5%)	26	23	36, 63, 105, 132	0

All (69) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	487	PHE	8.0
1	A	487	PHE	5.9
1	A	267	TYR	5.9
1	A	239	ASP	5.8
1	A	234	VAL	5.3
1	A	202	LEU	5.2
1	B	229	ASN	4.9
1	A	222	ARG	4.8
1	A	140	ASP	4.5
1	A	112	ALA	4.4
1	A	70	LYS	4.3
1	A	201	ARG	4.2
1	B	228	ARG	4.2
1	B	487	PHE	4.2
1	C	486	TYR	4.0
1	A	221	SER	3.9
1	A	236	PRO	3.9
1	B	375	LEU	3.8
1	B	488	GLN	3.6
1	A	240	LEU	3.5
1	A	228	ARG	3.4
1	B	486	TYR	3.4
1	A	229	ASN	3.4

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Mol	Chain	Res	Type	RSRZ
1	A	235	VAL	3.3
1	A	117	ARG	3.3
1	B	236	PRO	3.2
1	B	238	ALA	3.2
1	B	48	PRO	3.1
1	C	250	GLU	3.1
1	A	59	LYS	3.1
1	A	238	ALA	3.1
1	A	250	GLU	3.0
1	B	258	GLY	2.8
1	A	486	TYR	2.7
1	A	145	HIS	2.7
1	A	241	ILE	2.7
1	B	218	ILE	2.6
1	A	237	MET	2.6
1	A	377	ARG	2.6
1	B	235	VAL	2.6
1	A	114	GLU	2.6
1	A	456	LEU	2.6
1	A	203	PHE	2.5
1	B	219	LEU	2.5
1	B	485	LEU	2.5
1	C	221	SER	2.5
1	B	365	GLY	2.4
1	C	488	GLN	2.4
1	B	201	ARG	2.4
1	B	105	ILE	2.3
1	C	218	ILE	2.2
1	A	230	GLU	2.2
1	B	117	ARG	2.2
1	B	239	ASP	2.2
1	C	193	GLN	2.2
1	C	49	SER	2.1
1	A	50	LEU	2.1
1	A	65	GLY	2.1
1	A	134	ARG	2.1
1	B	222	ARG	2.1
1	B	367	THR	2.1
1	A	92	ARG	2.1
1	B	221	SER	2.1
1	A	257	LYS	2.1
1	A	196	ILE	2.1

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Mol	Chain	Res	Type	RSRZ
1	B	234	VAL	2.0
1	C	367	THR	2.0
1	A	206	PRO	2.0
1	C	117	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)

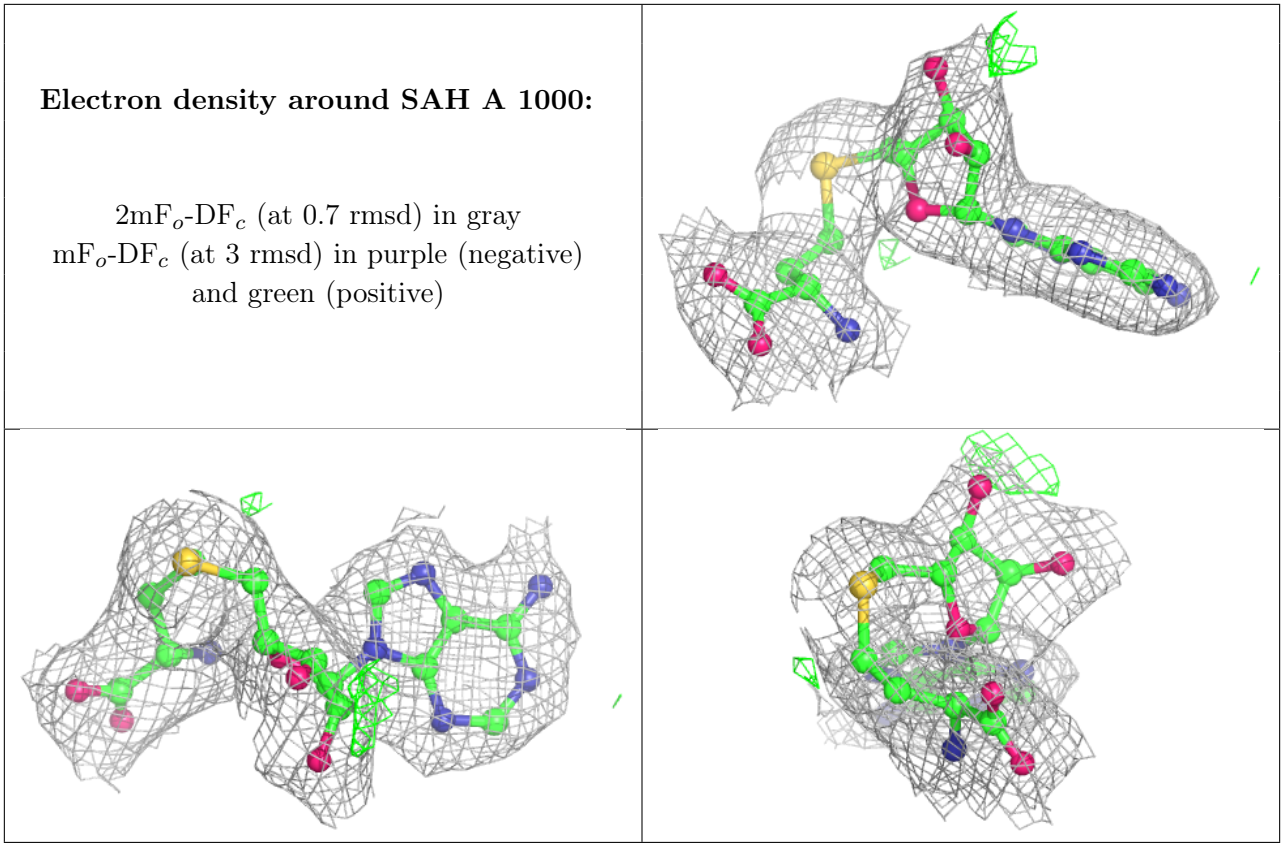
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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
2	LYS	A	700	10/10	0.89	0.43	76,77,80,80	0
2	LYS	A	800	10/10	0.93	0.27	55,58,60,60	0
3	SAH	A	1000	26/26	0.93	0.25	58,61,63,64	0
2	LYS	A	900	10/10	0.94	0.27	45,48,50,51	0
3	SAH	B	1001	26/26	0.95	0.20	37,43,46,48	0
3	SAH	C	1002	26/26	0.95	0.19	48,53,55,56	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.

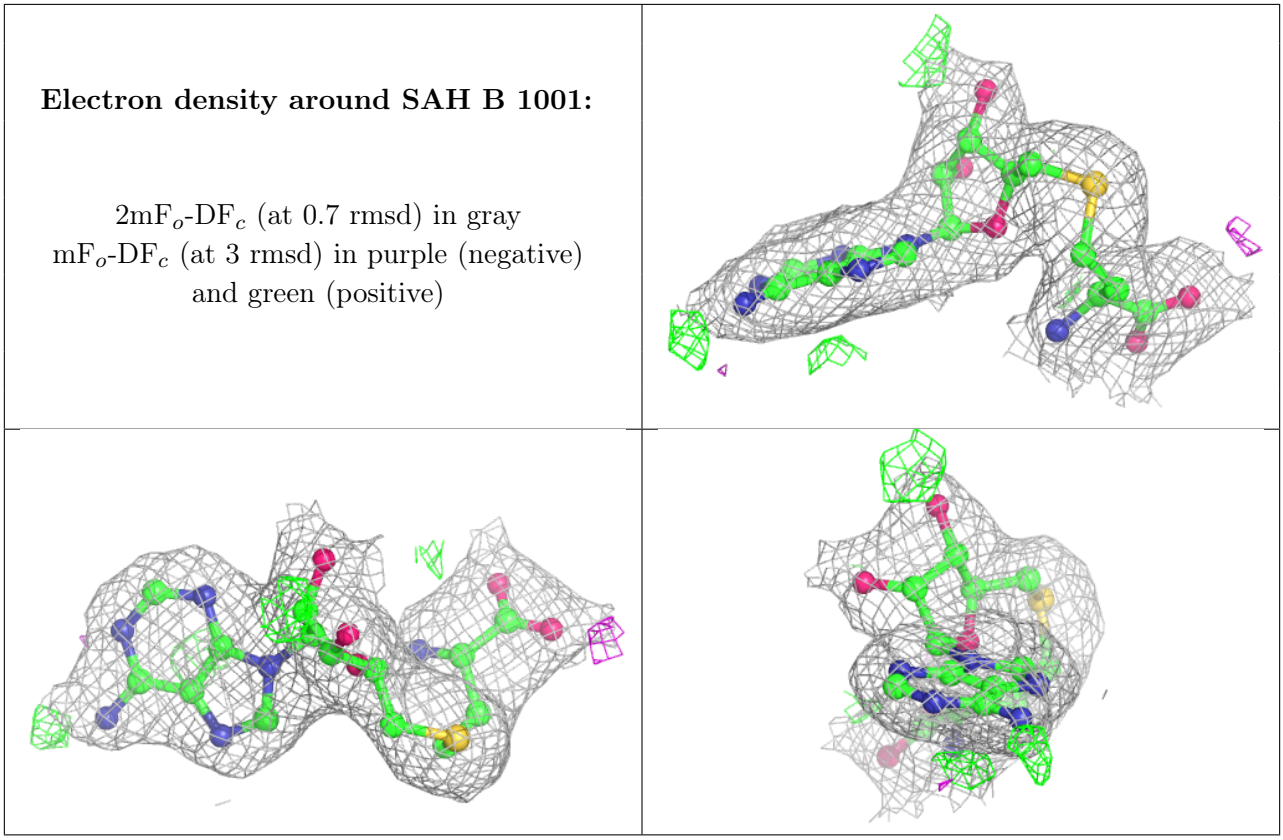
Electron density around SAH A 1000:

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



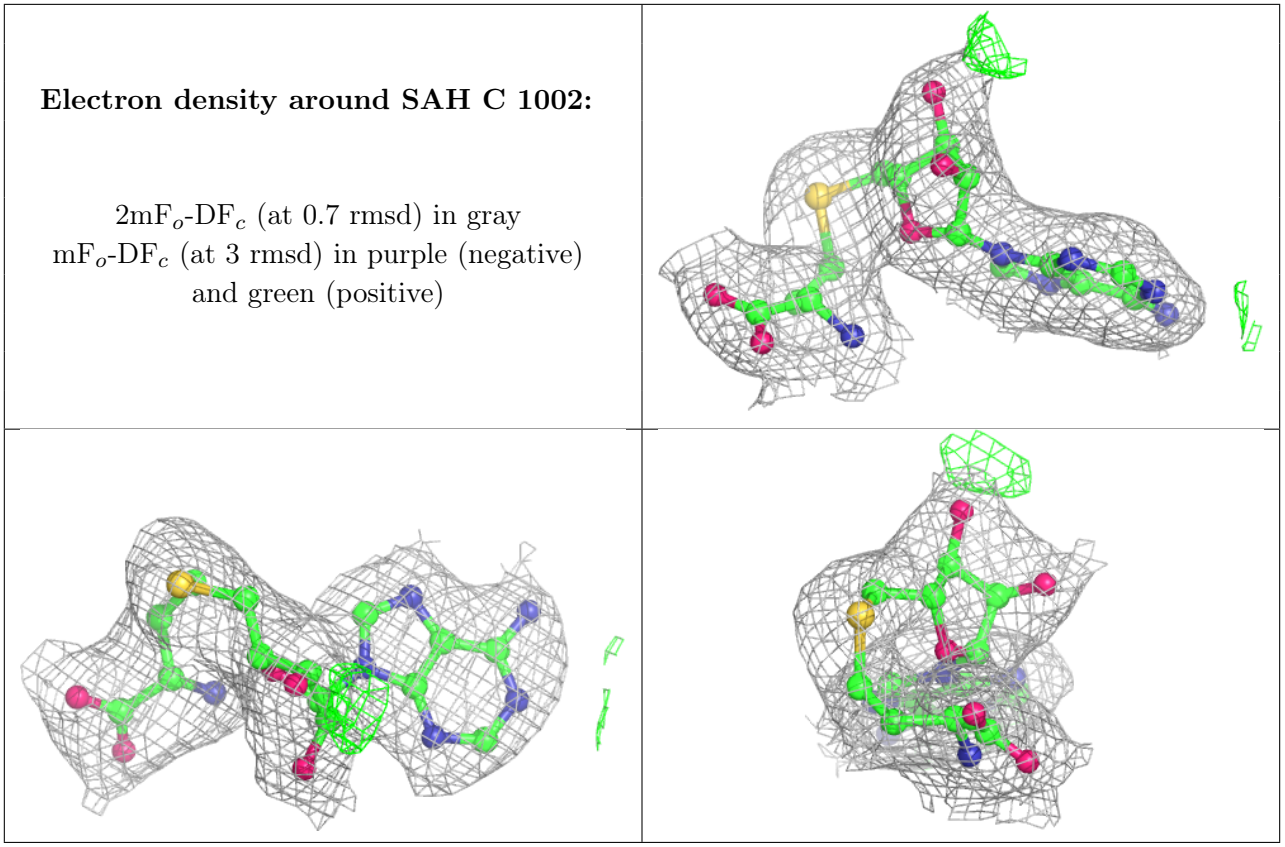
Electron density around SAH B 1001:

$2mF_o$-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 C 1002:

$2mF_o$-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

There are no such residues in this entry.