



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:26 PM UTC

PDB ID : 1M6E / pdb_00001m6e
Title : CRYSTAL STRUCTURE OF SALICYLIC ACID CARBOXYL METHYL-TRANSFERASE (SAMT)
Authors : Zubieta, C.; Ross, J.R.; Koscheski, P.; Yang, Y.; Pichersky, E.; Noel, J.P.
Deposited on : 2002-07-16
Resolution : 3.00 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 : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

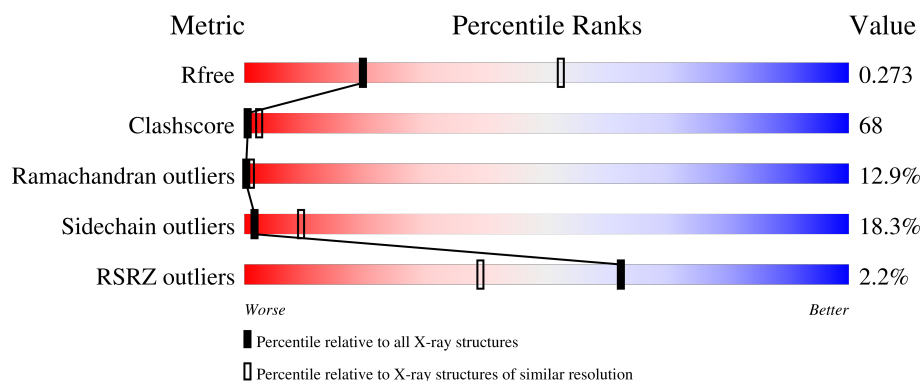
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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}	180053	2672 (3.00-3.00)
Clashscore	190562	2977 (3.00-3.00)
Ramachandran outliers	187476	2877 (3.00-3.00)
Sidechain outliers	187428	2880 (3.00-3.00)
RSRZ outliers	180081	2671 (3.00-3.00)

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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	X	359	

2 Entry composition [i](#)

There are 5 unique types of molecules in this entry. The entry contains 2877 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.

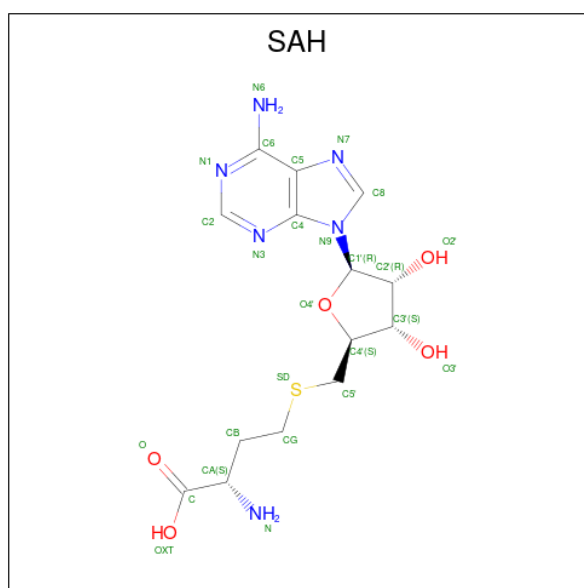
- Molecule 1 is a protein called S-adenosyl-L-methionine:salicylic acid carboxyl methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	X	359	Total	C	N	O	S	0	0	0
			2826	1788	479	539	20			

- Molecule 2 is LUTETIUM (III) ION (CCD ID: LU) (formula: Lu).

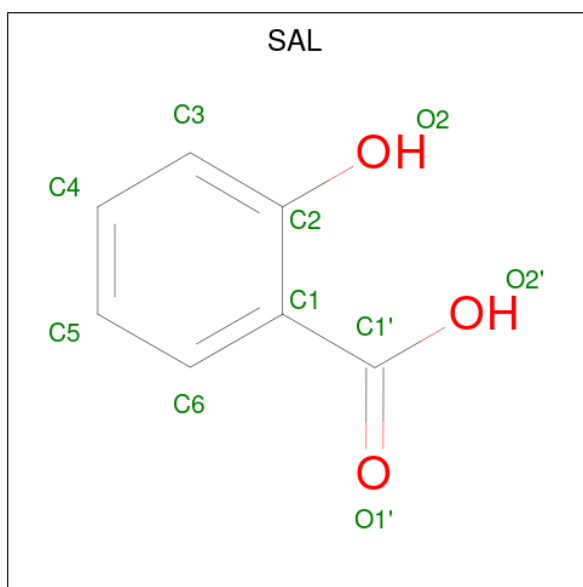
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	X	1	Total	Lu	0	0
			1	1		

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (CCD ID: SAH) (formula: C₁₄H₂₀N₆O₅S).



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

- Molecule 4 is 2-HYDROXYBENZOIC ACID (CCD ID: SAL) (formula: C₇H₆O₃).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	X	1	Total	C	O	0	0
			10	7	3		

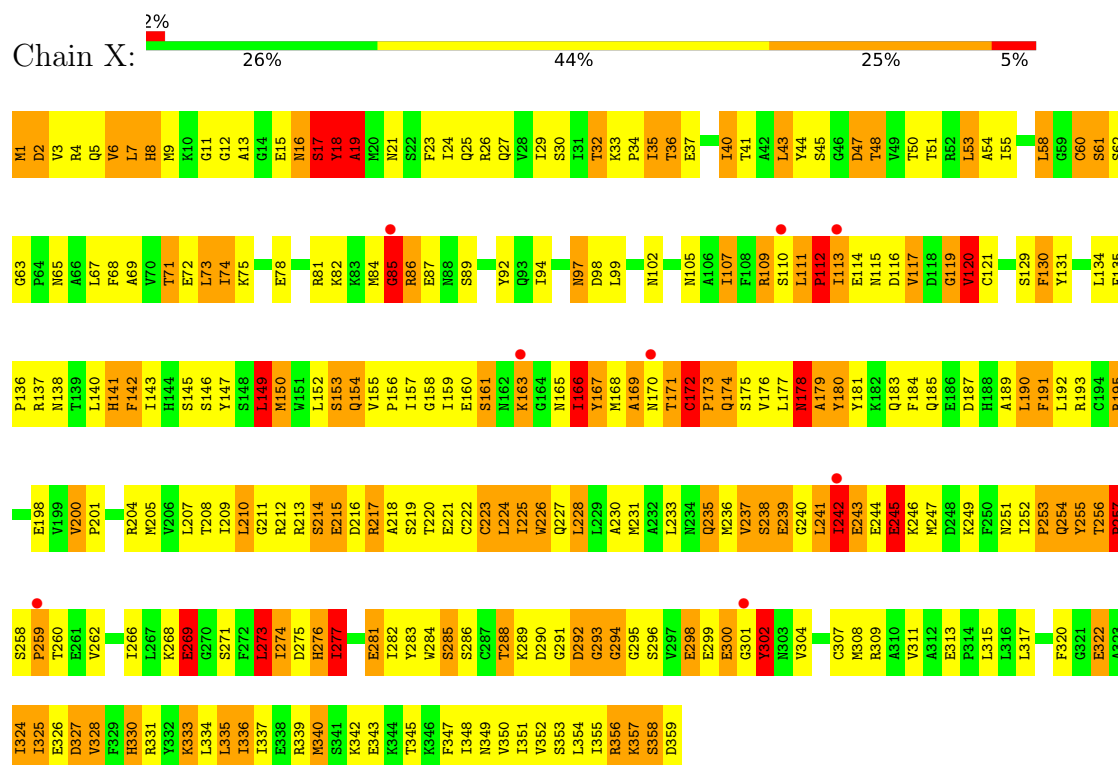
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	X	14	Total	O	0	0
			14	14		

3 Residue-property plots

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: S-adenosyl-L-methionine:salicylic acid carboxyl methyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 43 21 2	Depositor
Cell constants a, b, c, α , β , γ	141.74Å 141.74Å 63.98Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	24.81 – 3.00 24.81 – 3.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (24.81-3.00) 99.7 (24.81-3.00)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.06 (at 2.89Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, R_{free}	0.225 , 0.288 0.217 , 0.273	Depositor DCC
R_{free} test set	673 reflections (4.54%)	wwPDB-VP
Wilson B-factor (Å ²)	75.0	Xtriage
Anisotropy	0.131	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 77.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	2877	wwPDB-VP
Average B, all atoms (Å ²)	66.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.42% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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	X	0.85	2/2880 (0.1%)	1.45	51/3891 (1.3%)

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	X	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	256	THR	CA-CB	7.02	1.65	1.54
1	X	357	LYS	CA-C	-6.77	1.49	1.53

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	179	ALA	N-CA-C	-11.99	97.23	113.30
1	X	356	ARG	N-CA-C	-9.63	96.27	110.23
1	X	285	SER	N-CA-C	-9.46	100.94	111.07
1	X	102	ASN	N-CA-C	-9.33	96.08	110.17
1	X	140	LEU	N-CA-C	9.18	123.85	109.07
1	X	47	ASP	N-CA-C	8.73	123.11	110.10
1	X	19	ALA	N-CA-C	-8.37	92.98	110.80
1	X	180	TYR	N-CA-C	-8.33	101.23	111.40
1	X	48	THR	N-CA-C	-8.25	93.23	110.80
1	X	245	GLU	N-CA-C	-8.08	93.58	110.80
1	X	7	LEU	N-CA-C	7.75	120.86	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	X	256	THR	CA-C-N	7.71	129.47	119.84
1	X	256	THR	C-N-CA	7.71	129.47	119.84
1	X	241	LEU	N-CA-C	7.61	120.97	110.24
1	X	269	GLU	N-CA-C	-7.57	97.66	109.25
1	X	73	LEU	N-CA-C	-7.54	103.06	112.72
1	X	119	GLY	N-CA-C	-7.51	104.68	115.27
1	X	167	TYR	N-CA-C	7.35	118.88	108.74
1	X	8	HIS	N-CA-C	7.31	121.94	110.17
1	X	300	GLU	N-CA-C	-7.02	104.58	113.43
1	X	172	CYS	CA-C-N	-6.96	111.15	119.84
1	X	172	CYS	C-N-CA	-6.96	111.15	119.84
1	X	273	LEU	N-CA-C	6.79	120.00	111.24
1	X	237	VAL	N-CA-C	-6.67	103.98	110.72
1	X	94	ILE	N-CA-C	6.58	118.87	108.87
1	X	243	GLU	N-CA-C	-6.55	97.38	108.26
1	X	12	GLY	N-CA-C	6.54	121.17	110.97
1	X	322	GLU	N-CA-C	6.53	119.22	111.71
1	X	160	GLU	N-CA-C	-6.31	104.89	112.59
1	X	242	ILE	N-CA-C	6.21	122.25	109.34
1	X	223	CYS	N-CA-C	6.16	120.06	112.54
1	X	353	SER	N-CA-C	-6.07	100.30	109.95
1	X	72	GLU	N-CA-C	-5.99	104.15	112.30
1	X	60	CYS	N-CA-C	-5.57	101.07	109.60
1	X	226	TRP	N-CA-C	-5.56	104.04	112.04
1	X	41	THR	N-CA-C	-5.53	104.89	111.03
1	X	149	LEU	N-CA-C	5.49	119.72	113.19
1	X	74	ILE	N-CA-C	-5.47	104.21	111.05
1	X	131	TYR	N-CA-C	-5.44	99.22	110.80
1	X	9	MET	N-CA-C	-5.42	101.06	108.38
1	X	327	ASP	N-CA-C	5.42	117.19	111.28
1	X	53	LEU	N-CA-C	-5.40	100.89	109.59
1	X	85	GLY	N-CA-C	-5.38	100.42	113.18
1	X	17	SER	CA-C-N	5.26	131.60	121.54
1	X	17	SER	C-N-CA	5.26	131.60	121.54
1	X	260	THR	N-CA-C	-5.20	106.78	113.23
1	X	107	ILE	CB-CA-C	-5.20	105.17	111.87
1	X	191	PHE	N-CA-C	-5.19	105.07	111.40
1	X	330	HIS	N-CA-C	-5.12	105.78	111.36
1	X	268	LYS	N-CA-C	-5.07	105.03	111.11
1	X	97	ASN	N-CA-C	5.06	117.74	109.59

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	18	TYR	Sidechain
1	X	255	TYR	Sidechain

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	X	2826	0	2805	389	0
2	X	1	0	0	0	0
3	X	26	0	19	2	0
4	X	10	0	5	0	0
5	X	14	0	0	3	0
All	All	2877	0	2829	389	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 68.

All (389) 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:X:24:ILE:HD11	1:X:286:SER:H	1.06	1.15
1:X:254:GLN:CD	1:X:254:GLN:H	1.56	1.10
1:X:184:PHE:HB2	1:X:256:THR:HG21	1.19	1.10
1:X:169:ALA:HA	1:X:223:CYS:HB3	1.38	1.01
1:X:24:ILE:HD11	1:X:286:SER:N	1.76	0.99
1:X:15:GLU:HG2	1:X:16:ASN:H	1.28	0.98
1:X:4:ARG:HD2	1:X:254:GLN:HG2	1.47	0.96
1:X:117:VAL:HB	1:X:121:CYS:SG	2.06	0.95
1:X:173:PRO:O	1:X:174:GLN:HB3	1.66	0.94
1:X:296:SER:HA	1:X:340:MET:HE1	1.49	0.94
1:X:244:GLU:O	1:X:245:GLU:HB2	1.65	0.93
1:X:35:ILE:HD12	1:X:35:ILE:H	1.34	0.92
1:X:15:GLU:HG2	1:X:16:ASN:N	1.82	0.91
1:X:107:ILE:O	1:X:112:PRO:HD2	1.69	0.91
1:X:275:ASP:O	1:X:277:ILE:N	2.02	0.91

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:320:PHE:HB3	1:X:324:ILE:HD12	1.49	0.91
1:X:167:TYR:OH	1:X:257:PRO:HD3	1.71	0.91
1:X:254:GLN:CD	1:X:254:GLN:N	2.20	0.90
1:X:24:ILE:HG12	1:X:286:SER:HA	1.54	0.90
1:X:150:MET:HE3	1:X:210:LEU:HB3	1.53	0.88
1:X:40:ILE:HD11	1:X:73:LEU:HD13	1.56	0.88
1:X:117:VAL:HG21	1:X:121:CYS:HB2	1.55	0.88
1:X:195:ARG:NH1	1:X:198:GLU:OE1	2.08	0.85
1:X:245:GLU:O	1:X:249:LYS:HD2	1.76	0.85
1:X:166:ILE:O	1:X:253:PRO:HD2	1.77	0.85
1:X:178:ASN:N	1:X:178:ASN:HD22	1.73	0.84
1:X:117:VAL:CG2	1:X:121:CYS:HB2	2.08	0.84
1:X:24:ILE:CG1	1:X:286:SER:HA	2.07	0.84
1:X:254:GLN:H	1:X:254:GLN:NE2	1.75	0.83
1:X:155:VAL:HA	1:X:254:GLN:HB3	1.60	0.82
1:X:2:ASP:HB3	1:X:4:ARG:HH21	1.46	0.81
1:X:190:LEU:HD22	1:X:190:LEU:O	1.80	0.81
1:X:2:ASP:HB3	1:X:4:ARG:NH2	1.95	0.81
1:X:165:ASN:OD1	1:X:252:ILE:HG12	1.79	0.81
1:X:159:ILE:HG21	1:X:252:ILE:CD1	2.10	0.81
1:X:217:ARG:HG3	1:X:217:ARG:HH11	1.46	0.80
1:X:1:MET:O	1:X:2:ASP:HB2	1.81	0.80
1:X:143:ILE:HB	1:X:205:MET:HG2	1.63	0.79
1:X:169:ALA:HA	1:X:223:CYS:CB	2.15	0.77
1:X:50:THR:HG22	1:X:51:THR:HG23	1.64	0.77
1:X:174:GLN:HE21	1:X:176:VAL:HG23	1.50	0.77
1:X:213:ARG:NH1	1:X:281:GLU:HG2	2.00	0.77
1:X:116:ASP:O	1:X:117:VAL:HG22	1.85	0.77
1:X:4:ARG:NH2	1:X:7:LEU:HD13	2.01	0.76
1:X:357:LYS:HG3	1:X:358:SER:H	1.51	0.75
1:X:317:LEU:HD13	1:X:325:ILE:CD1	2.16	0.75
1:X:184:PHE:CB	1:X:256:THR:HG21	2.10	0.75
1:X:85:GLY:C	1:X:86:ARG:HG2	2.12	0.74
1:X:242:ILE:HD11	1:X:324:ILE:HG13	1.70	0.74
1:X:317:LEU:HD13	1:X:325:ILE:HD11	1.69	0.74
1:X:212:ARG:HG3	1:X:212:ARG:HH11	1.51	0.73
1:X:150:MET:O	1:X:255:TYR:HB2	1.87	0.73
1:X:153:SER:HB3	1:X:187:ASP:OD1	1.87	0.73
1:X:241:LEU:O	1:X:243:GLU:N	2.21	0.73
1:X:68:PHE:O	1:X:71:THR:HG22	1.87	0.73
1:X:44:TYR:OH	1:X:86:ARG:HG3	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:82:LYS:C	1:X:84:MET:H	1.94	0.73
1:X:111:LEU:O	1:X:113:ILE:N	2.22	0.72
1:X:161:SER:HB2	1:X:177:LEU:HD11	1.70	0.72
1:X:214:SER:C	1:X:216:ASP:H	1.98	0.71
1:X:35:ILE:HD12	1:X:35:ILE:N	2.05	0.71
1:X:4:ARG:HD2	1:X:254:GLN:CG	2.20	0.71
1:X:317:LEU:HD11	1:X:322:GLU:HG2	1.73	0.71
1:X:112:PRO:C	1:X:114:GLU:N	2.41	0.71
1:X:213:ARG:CZ	1:X:281:GLU:HG2	2.21	0.71
1:X:317:LEU:CD1	1:X:322:GLU:HG2	2.21	0.70
1:X:109:ARG:O	1:X:113:ILE:HG13	1.90	0.70
1:X:167:TYR:C	1:X:169:ALA:H	2.00	0.70
1:X:214:SER:O	1:X:216:ASP:N	2.25	0.70
1:X:257:PRO:O	1:X:258:SER:OG	2.08	0.70
1:X:67:LEU:O	1:X:71:THR:HB	1.92	0.69
1:X:189:ALA:O	1:X:193:ARG:HG2	1.91	0.69
1:X:245:GLU:HG2	1:X:249:LYS:NZ	2.07	0.69
1:X:216:ASP:O	1:X:218:ALA:N	2.25	0.69
1:X:159:ILE:HG21	1:X:252:ILE:HD13	1.71	0.69
1:X:35:ILE:H	1:X:35:ILE:CD1	2.05	0.69
1:X:15:GLU:CG	1:X:16:ASN:H	2.04	0.69
1:X:322:GLU:HA	1:X:325:ILE:HD12	1.73	0.69
1:X:112:PRO:C	1:X:114:GLU:H	2.01	0.69
1:X:150:MET:HG3	1:X:255:TYR:HD1	1.58	0.69
1:X:284:TRP:CD2	1:X:345:THR:HB	2.28	0.68
1:X:130:PHE:HA	1:X:134:LEU:HD11	1.75	0.68
1:X:171:THR:O	1:X:172:CYS:HB2	1.92	0.68
1:X:170:ASN:HA	1:X:218:ALA:HB1	1.74	0.68
1:X:324:ILE:HG22	1:X:325:ILE:N	2.07	0.68
1:X:167:TYR:OH	1:X:257:PRO:CD	2.42	0.68
1:X:24:ILE:CD1	1:X:286:SER:HA	2.24	0.68
1:X:150:MET:HG3	1:X:255:TYR:CD1	2.29	0.68
1:X:180:TYR:OH	1:X:252:ILE:HG22	1.93	0.67
1:X:155:VAL:HG22	1:X:254:GLN:HG3	1.75	0.67
1:X:296:SER:OG	1:X:340:MET:SD	2.47	0.67
1:X:166:ILE:N	1:X:166:ILE:HD13	2.08	0.67
1:X:116:ASP:C	1:X:117:VAL:HG22	2.20	0.67
1:X:200:VAL:HG22	1:X:201:PRO:HD2	1.74	0.67
1:X:112:PRO:O	1:X:114:GLU:N	2.28	0.67
1:X:217:ARG:HG3	1:X:217:ARG:NH1	2.07	0.67
1:X:178:ASN:N	1:X:178:ASN:ND2	2.38	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:40:ILE:CD1	1:X:73:LEU:HD22	2.24	0.67
1:X:288:THR:HA	5:X:2822:HOH:O	1.95	0.67
1:X:167:TYR:HH	1:X:257:PRO:HD3	1.59	0.66
1:X:119:GLY:O	1:X:120:VAL:HG12	1.95	0.66
1:X:184:PHE:HB2	1:X:256:THR:CG2	2.12	0.66
1:X:43:LEU:O	1:X:43:LEU:HD22	1.94	0.66
1:X:296:SER:HA	1:X:340:MET:CE	2.25	0.66
1:X:24:ILE:HD11	1:X:286:SER:CA	2.26	0.65
1:X:74:ILE:HG12	1:X:92:TYR:CD2	2.30	0.65
1:X:337:ILE:O	1:X:340:MET:HB3	1.96	0.65
1:X:222:CYS:HB2	1:X:257:PRO:HG2	1.77	0.65
1:X:165:ASN:HD22	1:X:249:LYS:HA	1.62	0.65
1:X:254:GLN:N	1:X:254:GLN:NE2	2.39	0.64
1:X:258:SER:O	1:X:350:VAL:HG21	1.97	0.64
1:X:275:ASP:C	1:X:277:ILE:H	2.05	0.64
1:X:301:GLY:O	1:X:302:TYR:CB	2.43	0.64
1:X:296:SER:C	1:X:298:GLU:H	2.04	0.64
1:X:111:LEU:C	1:X:113:ILE:H	2.04	0.64
1:X:78:GLU:OE2	1:X:89:SER:HB3	1.96	0.64
1:X:150:MET:CE	1:X:210:LEU:HB3	2.27	0.64
1:X:153:SER:CB	1:X:187:ASP:OD1	2.44	0.64
1:X:159:ILE:HD13	1:X:252:ILE:CD1	2.28	0.64
1:X:349:ASN:O	1:X:351:ILE:HD12	1.97	0.63
1:X:150:MET:CG	1:X:255:TYR:HD1	2.11	0.63
1:X:159:ILE:HD13	1:X:252:ILE:HD13	1.81	0.63
1:X:167:TYR:CG	1:X:168:MET:N	2.67	0.63
1:X:253:PRO:HA	1:X:254:GLN:NE2	2.14	0.63
1:X:296:SER:CB	1:X:340:MET:SD	2.88	0.62
1:X:173:PRO:O	1:X:174:GLN:CB	2.44	0.62
1:X:11:GLY:HA3	5:X:2817:HOH:O	1.98	0.61
1:X:294:GLY:HA3	1:X:298:GLU:HG3	1.83	0.61
1:X:236:MET:HB3	1:X:241:LEU:HD12	1.83	0.61
1:X:112:PRO:HA	1:X:114:GLU:CG	2.31	0.61
1:X:168:MET:HE3	1:X:180:TYR:HB3	1.83	0.61
1:X:212:ARG:NH1	1:X:259:PRO:HD3	2.16	0.61
1:X:7:LEU:HD23	1:X:7:LEU:C	2.26	0.60
1:X:251:ASN:O	1:X:252:ILE:HG12	2.01	0.60
1:X:159:ILE:HG23	1:X:161:SER:HB2	1.83	0.60
1:X:167:TYR:C	1:X:169:ALA:N	2.57	0.60
1:X:357:LYS:HG3	1:X:358:SER:N	2.17	0.60
1:X:112:PRO:HA	1:X:114:GLU:HG3	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:300:GLU:HB2	1:X:340:MET:HE3	1.84	0.59
1:X:224:LEU:O	1:X:225:ILE:HB	2.02	0.59
1:X:130:PHE:O	1:X:191:PHE:HD1	1.85	0.59
1:X:212:ARG:HD3	1:X:222:CYS:SG	2.42	0.59
1:X:226:TRP:NE1	1:X:255:TYR:OH	2.32	0.59
1:X:111:LEU:C	1:X:113:ILE:N	2.61	0.59
1:X:339:ARG:NH2	1:X:343:GLU:OE1	2.35	0.59
1:X:214:SER:HB2	1:X:221:GLU:OE1	2.02	0.59
1:X:262:VAL:O	1:X:266:ILE:HG13	2.03	0.59
1:X:301:GLY:CA	1:X:337:ILE:HG12	2.33	0.59
1:X:214:SER:C	1:X:216:ASP:N	2.58	0.58
1:X:40:ILE:HD11	1:X:73:LEU:HD22	1.86	0.58
1:X:159:ILE:HG21	1:X:252:ILE:HD11	1.85	0.58
1:X:244:GLU:O	1:X:245:GLU:CB	2.44	0.58
1:X:61:SER:O	1:X:107:ILE:HD11	2.03	0.58
1:X:340:MET:O	1:X:343:GLU:O	2.21	0.58
1:X:40:ILE:HG12	1:X:142:PHE:CE1	2.39	0.58
1:X:58:LEU:HD12	1:X:97:ASN:HB3	1.84	0.58
1:X:116:ASP:C	1:X:117:VAL:CG2	2.77	0.58
1:X:161:SER:CB	1:X:177:LEU:HD11	2.34	0.58
1:X:24:ILE:HD11	1:X:286:SER:HA	1.84	0.58
1:X:152:LEU:HB2	1:X:254:GLN:O	2.03	0.58
1:X:170:ASN:CG	1:X:171:THR:N	2.60	0.58
1:X:236:MET:CB	1:X:241:LEU:HD12	2.34	0.58
1:X:173:PRO:CB	1:X:177:LEU:HD22	2.34	0.57
1:X:262:VAL:HG12	1:X:266:ILE:HD11	1.86	0.57
1:X:111:LEU:HB3	1:X:112:PRO:HD3	1.87	0.57
1:X:85:GLY:O	1:X:86:ARG:NE	2.28	0.56
1:X:82:LYS:C	1:X:84:MET:N	2.63	0.56
1:X:213:ARG:NH2	1:X:281:GLU:CG	2.69	0.56
1:X:301:GLY:O	1:X:302:TYR:HB2	2.04	0.56
1:X:317:LEU:HD11	1:X:322:GLU:CG	2.35	0.56
1:X:111:LEU:O	1:X:114:GLU:HG2	2.05	0.56
1:X:228:LEU:HD23	1:X:335:LEU:HB3	1.88	0.56
1:X:149:LEU:HD11	1:X:191:PHE:CE2	2.40	0.56
1:X:238:SER:C	1:X:240:GLY:H	2.14	0.55
1:X:168:MET:HE3	1:X:180:TYR:CB	2.37	0.55
1:X:170:ASN:CA	1:X:218:ALA:HB1	2.36	0.55
1:X:177:LEU:O	1:X:179:ALA:N	2.36	0.55
1:X:107:ILE:O	1:X:112:PRO:CD	2.50	0.55
1:X:317:LEU:CD1	1:X:325:ILE:HD11	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:216:ASP:C	1:X:218:ALA:H	2.15	0.55
1:X:342:LYS:O	1:X:343:GLU:HG3	2.07	0.55
1:X:296:SER:C	1:X:298:GLU:N	2.60	0.55
1:X:211:GLY:HA2	1:X:257:PRO:HB3	1.88	0.55
1:X:212:ARG:HG3	1:X:212:ARG:NH1	2.18	0.55
1:X:220:THR:HG23	1:X:224:LEU:HD13	1.88	0.55
1:X:259:PRO:HA	1:X:350:VAL:HG21	1.89	0.55
1:X:227:GLN:O	1:X:231:MET:HG3	2.07	0.54
1:X:245:GLU:HG2	1:X:249:LYS:HZ1	1.71	0.54
1:X:71:THR:O	1:X:71:THR:HG23	2.08	0.54
1:X:105:ASN:O	1:X:109:ARG:HG3	2.07	0.54
1:X:262:VAL:HG21	1:X:350:VAL:HG11	1.89	0.54
1:X:242:ILE:HG13	1:X:324:ILE:HD11	1.89	0.54
1:X:274:ILE:HA	1:X:354:LEU:HD23	1.90	0.54
1:X:245:GLU:O	1:X:249:LYS:HB2	2.08	0.54
1:X:178:ASN:ND2	1:X:178:ASN:H	2.06	0.53
1:X:17:SER:HA	1:X:21:ASN:HD22	1.73	0.53
1:X:276:HIS:CG	1:X:276:HIS:O	2.62	0.53
1:X:152:LEU:HG	1:X:255:TYR:HA	1.90	0.53
1:X:273:LEU:O	1:X:274:ILE:HB	2.07	0.53
1:X:152:LEU:HD22	1:X:183:GLN:HG3	1.91	0.53
1:X:307:CYS:O	1:X:311:VAL:HG23	2.08	0.53
1:X:69:ALA:C	1:X:71:THR:H	2.17	0.53
1:X:153:SER:HB3	1:X:187:ASP:CG	2.33	0.53
1:X:292:ASP:O	1:X:293:GLY:C	2.52	0.52
1:X:172:CYS:N	1:X:173:PRO:CD	2.73	0.52
1:X:352:VAL:HG11	1:X:354:LEU:HD21	1.92	0.52
1:X:33:LYS:O	1:X:37:GLU:HG2	2.10	0.52
1:X:213:ARG:O	1:X:215:GLU:N	2.42	0.52
1:X:224:LEU:O	1:X:225:ILE:CB	2.58	0.52
1:X:330:HIS:HA	1:X:333:LYS:HZ3	1.74	0.52
1:X:16:ASN:N	1:X:16:ASN:OD1	2.41	0.52
1:X:212:ARG:HA	1:X:348:ILE:HB	1.90	0.52
1:X:324:ILE:O	1:X:326:GLU:HG2	2.10	0.52
1:X:109:ARG:O	1:X:111:LEU:N	2.43	0.52
1:X:273:LEU:O	1:X:274:ILE:CB	2.56	0.52
1:X:291:GLY:O	1:X:292:ASP:CB	2.57	0.52
1:X:98:ASP:OD1	1:X:99:LEU:N	2.38	0.52
1:X:112:PRO:O	1:X:113:ILE:C	2.53	0.52
1:X:165:ASN:O	1:X:166:ILE:C	2.52	0.52
1:X:358:SER:O	1:X:359:ASP:HB3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:117:VAL:HB	1:X:121:CYS:HG	1.75	0.52
1:X:44:TYR:OH	1:X:81:ARG:HB2	2.10	0.52
1:X:50:THR:HG22	1:X:51:THR:N	2.24	0.52
1:X:239:GLU:CD	1:X:331:ARG:HH12	2.17	0.52
1:X:166:ILE:HD13	1:X:166:ILE:H	1.72	0.51
1:X:227:GLN:HG2	1:X:231:MET:HE2	1.93	0.51
1:X:181:TYR:CE2	1:X:185:GLN:NE2	2.78	0.51
1:X:330:HIS:HA	1:X:333:LYS:NZ	2.25	0.51
1:X:192:LEU:HB3	1:X:269:GLU:HG2	1.93	0.51
1:X:288:THR:CA	5:X:2822:HOH:O	2.57	0.51
1:X:352:VAL:HG12	1:X:354:LEU:HG	1.93	0.51
1:X:226:TRP:CH2	1:X:308:MET:HE1	2.45	0.51
1:X:228:LEU:CD2	1:X:335:LEU:HB3	2.41	0.51
1:X:54:ALA:H	1:X:141:HIS:HD2	1.59	0.50
1:X:283:TYR:C	1:X:285:SER:H	2.18	0.50
1:X:32:THR:HG23	1:X:32:THR:O	2.11	0.50
1:X:317:LEU:HD13	1:X:322:GLU:HG2	1.94	0.50
1:X:300:GLU:HA	1:X:304:VAL:HG23	1.94	0.49
1:X:282:ILE:HG22	1:X:349:ASN:HD21	1.76	0.49
1:X:82:LYS:O	1:X:84:MET:HE2	2.12	0.49
1:X:226:TRP:NE1	1:X:255:TYR:CE2	2.79	0.49
1:X:295:GLY:O	1:X:299:GLU:HB3	2.13	0.49
1:X:296:SER:HB3	1:X:340:MET:SD	2.53	0.49
1:X:7:LEU:HD22	1:X:315:LEU:HD23	1.94	0.49
1:X:171:THR:O	1:X:172:CYS:CB	2.59	0.49
1:X:142:PHE:HA	1:X:204:ARG:O	2.12	0.49
1:X:326:GLU:HG3	1:X:327:ASP:H	1.77	0.49
1:X:213:ARG:HH22	1:X:281:GLU:CD	2.21	0.49
1:X:292:ASP:O	1:X:294:GLY:N	2.45	0.49
1:X:7:LEU:HD23	1:X:7:LEU:O	2.13	0.48
1:X:33:LYS:HB3	1:X:34:PRO:HD3	1.95	0.48
1:X:154:GLN:HG3	1:X:155:VAL:O	2.12	0.48
1:X:309:ARG:O	1:X:313:GLU:HB2	2.13	0.48
1:X:325:ILE:O	1:X:326:GLU:C	2.57	0.48
1:X:339:ARG:HD2	1:X:339:ARG:O	2.12	0.48
1:X:349:ASN:O	1:X:351:ILE:CD1	2.61	0.48
1:X:29:ILE:HD11	3:X:2814:SAH:O	2.12	0.48
1:X:220:THR:HG23	1:X:224:LEU:HB2	1.94	0.48
1:X:236:MET:HE1	1:X:328:VAL:HB	1.96	0.48
1:X:212:ARG:O	1:X:259:PRO:HB3	2.13	0.48
1:X:40:ILE:HD11	1:X:73:LEU:CD1	2.36	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:4:ARG:NH1	1:X:315:LEU:HD22	2.29	0.48
1:X:181:TYR:O	1:X:185:GLN:HG3	2.15	0.47
1:X:35:ILE:HG13	1:X:276:HIS:HD2	1.80	0.47
1:X:271:SER:HA	1:X:356:ARG:HH12	1.79	0.47
1:X:212:ARG:HH12	1:X:259:PRO:HD3	1.78	0.47
1:X:327:ASP:O	1:X:331:ARG:HG3	2.15	0.47
1:X:173:PRO:HB2	1:X:177:LEU:HD22	1.97	0.47
1:X:238:SER:C	1:X:240:GLY:N	2.73	0.47
1:X:237:VAL:HG22	1:X:243:GLU:HB2	1.95	0.46
1:X:242:ILE:CD1	1:X:324:ILE:HG13	2.43	0.46
1:X:74:ILE:HG23	1:X:92:TYR:CZ	2.50	0.46
1:X:340:MET:O	1:X:340:MET:HG2	2.11	0.46
1:X:78:GLU:OE2	1:X:92:TYR:OH	2.32	0.46
1:X:112:PRO:O	1:X:114:GLU:C	2.58	0.46
1:X:158:GLY:O	1:X:159:ILE:HG13	2.15	0.46
1:X:317:LEU:HB2	1:X:325:ILE:HD11	1.97	0.46
1:X:145:SER:HB3	1:X:207:LEU:HD22	1.97	0.46
1:X:155:VAL:HG12	1:X:156:PRO:N	2.31	0.46
1:X:228:LEU:HD13	1:X:336:ILE:HG23	1.97	0.46
1:X:333:LYS:O	1:X:337:ILE:HG13	2.16	0.46
1:X:284:TRP:HB3	1:X:304:VAL:HG21	1.98	0.46
1:X:216:ASP:C	1:X:218:ALA:N	2.73	0.46
1:X:149:LEU:HB3	1:X:209:ILE:HG12	1.98	0.46
1:X:288:THR:OG1	1:X:289:LYS:N	2.49	0.46
1:X:2:ASP:CB	1:X:4:ARG:HH21	2.21	0.45
1:X:53:LEU:HA	1:X:141:HIS:HD2	1.81	0.45
1:X:212:ARG:O	1:X:259:PRO:HG3	2.16	0.45
1:X:244:GLU:HG2	1:X:246:LYS:HG3	1.97	0.45
1:X:326:GLU:CG	1:X:327:ASP:H	2.29	0.45
1:X:168:MET:O	1:X:169:ALA:C	2.59	0.45
1:X:180:TYR:O	1:X:183:GLN:HB3	2.16	0.45
1:X:357:LYS:CG	1:X:358:SER:N	2.78	0.45
1:X:120:VAL:O	1:X:120:VAL:CG1	2.64	0.45
1:X:107:ILE:HG23	1:X:111:LEU:HD13	1.97	0.45
1:X:225:ILE:CG2	1:X:226:TRP:N	2.79	0.45
1:X:159:ILE:CD1	1:X:252:ILE:HD12	2.46	0.45
1:X:224:LEU:HD21	1:X:339:ARG:HG2	1.99	0.45
1:X:266:ILE:O	1:X:269:GLU:O	2.35	0.45
1:X:18:TYR:O	1:X:19:ALA:HB2	2.16	0.45
1:X:145:SER:HB3	1:X:207:LEU:CD2	2.46	0.45
1:X:224:LEU:HG	1:X:228:LEU:HD12	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:269:GLU:CD	1:X:271:SER:OG	2.60	0.45
1:X:2:ASP:CB	1:X:4:ARG:NH2	2.76	0.45
1:X:26:ARG:NH2	1:X:68:PHE:CE1	2.85	0.45
1:X:17:SER:CA	1:X:21:ASN:HD22	2.29	0.45
1:X:347:PHE:C	1:X:348:ILE:HD12	2.42	0.45
1:X:357:LYS:CG	1:X:358:SER:H	2.17	0.45
1:X:169:ALA:CA	1:X:223:CYS:HB3	2.27	0.44
1:X:238:SER:O	1:X:240:GLY:N	2.50	0.44
1:X:53:LEU:HA	1:X:141:HIS:CD2	2.53	0.44
1:X:40:ILE:HD12	1:X:73:LEU:HB3	1.99	0.44
1:X:54:ALA:H	1:X:141:HIS:CD2	2.36	0.44
1:X:141:HIS:O	1:X:142:PHE:CB	2.65	0.44
1:X:30:SER:O	1:X:33:LYS:HB2	2.17	0.44
1:X:220:THR:CG2	1:X:224:LEU:HD22	2.48	0.44
1:X:165:ASN:ND2	1:X:249:LYS:HA	2.29	0.44
1:X:170:ASN:HB2	1:X:218:ALA:HB1	1.99	0.44
1:X:1:MET:O	1:X:2:ASP:CB	2.58	0.43
1:X:169:ALA:HA	1:X:223:CYS:SG	2.58	0.43
1:X:53:LEU:HD23	1:X:92:TYR:CE2	2.54	0.43
1:X:65:ASN:HA	1:X:68:PHE:HB3	2.01	0.43
1:X:146:SER:HA	1:X:208:THR:HB	2.01	0.43
1:X:251:ASN:O	1:X:252:ILE:CG1	2.67	0.43
1:X:233:LEU:HD23	1:X:236:MET:HE2	1.99	0.43
1:X:283:TYR:C	1:X:285:SER:N	2.77	0.43
1:X:299:GLU:HB3	1:X:340:MET:HE1	1.99	0.43
1:X:44:TYR:CE1	1:X:86:ARG:HD2	2.53	0.43
1:X:150:MET:HE3	1:X:210:LEU:CD2	2.49	0.43
1:X:150:MET:CG	1:X:255:TYR:CD1	2.96	0.43
1:X:166:ILE:O	1:X:253:PRO:CD	2.58	0.43
1:X:273:LEU:O	1:X:274:ILE:HG22	2.19	0.43
1:X:153:SER:HB2	1:X:187:ASP:OD1	2.19	0.43
1:X:352:VAL:CG1	1:X:354:LEU:HD21	2.48	0.43
1:X:7:LEU:C	1:X:7:LEU:CD2	2.92	0.43
1:X:193:ARG:HG3	1:X:193:ARG:NH1	2.34	0.43
1:X:283:TYR:O	1:X:285:SER:N	2.45	0.43
1:X:284:TRP:CE2	1:X:345:THR:HB	2.54	0.43
1:X:218:ALA:HA	1:X:223:CYS:SG	2.59	0.42
1:X:235:GLN:HE21	1:X:235:GLN:HB2	1.57	0.42
1:X:324:ILE:O	1:X:325:ILE:C	2.62	0.42
1:X:40:ILE:O	1:X:40:ILE:HG22	2.19	0.42
1:X:129:SER:HA	3:X:2814:SAH:N1	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:214:SER:CB	1:X:221:GLU:OE1	2.67	0.42
1:X:36:THR:CG2	1:X:73:LEU:HD21	2.49	0.42
1:X:65:ASN:HA	1:X:68:PHE:CB	2.49	0.42
1:X:170:ASN:OD1	1:X:171:THR:N	2.48	0.42
1:X:277:ILE:O	1:X:277:ILE:HG12	2.20	0.42
1:X:284:TRP:CD1	1:X:347:PHE:CE1	3.08	0.42
1:X:168:MET:CE	1:X:180:TYR:HB3	2.48	0.42
1:X:134:LEU:HB2	1:X:135:PHE:CE1	2.55	0.42
1:X:137:ARG:O	1:X:138:ASN:C	2.62	0.42
1:X:336:ILE:O	1:X:337:ILE:C	2.63	0.42
1:X:23:PHE:N	1:X:23:PHE:CD1	2.87	0.42
1:X:237:VAL:HG11	1:X:245:GLU:HG3	2.02	0.42
1:X:55:ILE:HG21	1:X:73:LEU:HD12	2.01	0.42
1:X:237:VAL:HG22	1:X:243:GLU:CB	2.50	0.41
1:X:300:GLU:HA	1:X:304:VAL:CG2	2.51	0.41
1:X:326:GLU:HG3	1:X:327:ASP:N	2.35	0.41
1:X:111:LEU:O	1:X:112:PRO:C	2.61	0.41
1:X:81:ARG:HD2	1:X:89:SER:OG	2.21	0.41
1:X:166:ILE:HG12	1:X:230:ALA:CB	2.51	0.41
1:X:63:GLY:C	1:X:111:LEU:HD11	2.45	0.41
1:X:180:TYR:OH	1:X:252:ILE:CG2	2.64	0.41
1:X:61:SER:HB3	1:X:62:SER:H	1.60	0.41
1:X:165:ASN:O	1:X:252:ILE:HG23	2.19	0.41
1:X:5:GLN:HA	1:X:99:LEU:HD13	2.03	0.41
1:X:205:MET:HE3	1:X:354:LEU:HD12	2.03	0.41
1:X:245:GLU:O	1:X:249:LYS:CD	2.59	0.41
1:X:85:GLY:C	1:X:86:ARG:CG	2.87	0.41
1:X:163:LYS:C	1:X:165:ASN:H	2.29	0.41
1:X:235:GLN:O	1:X:239:GLU:HG3	2.21	0.41
1:X:63:GLY:O	1:X:111:LEU:HD11	2.21	0.41
1:X:219:SER:C	1:X:221:GLU:N	2.76	0.41
1:X:225:ILE:HD11	1:X:308:MET:HG3	2.03	0.41
1:X:291:GLY:O	1:X:292:ASP:HB2	2.21	0.41
1:X:3:VAL:HG13	1:X:6:VAL:HB	2.03	0.40
1:X:109:ARG:C	1:X:111:LEU:H	2.29	0.40
1:X:166:ILE:HG12	1:X:230:ALA:HB2	2.02	0.40
1:X:109:ARG:C	1:X:111:LEU:N	2.78	0.40
1:X:112:PRO:HA	1:X:114:GLU:HG2	2.04	0.40
1:X:150:MET:C	1:X:255:TYR:HB2	2.46	0.40
1:X:165:ASN:ND2	1:X:249:LYS:C	2.79	0.40
1:X:212:ARG:C	1:X:348:ILE:HG21	2.46	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:252:ILE:O	1:X:253:PRO:C	2.63	0.40
1:X:47:ASP:N	1:X:86:ARG:HH22	2.19	0.40
1:X:60:CYS:O	1:X:98:ASP:OD2	2.39	0.40
1:X:154:GLN:HE21	1:X:154:GLN:HB3	1.63	0.40
1:X:251:ASN:C	1:X:252:ILE:CG1	2.94	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	X	357/359 (99%)	255 (71%)	56 (16%)	46 (13%)	0 1

All (46) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	2	ASP
1	X	13	ALA
1	X	17	SER
1	X	19	ALA
1	X	111	LEU
1	X	115	ASN
1	X	147	TYR
1	X	157	ILE
1	X	171	THR
1	X	172	CYS
1	X	214	SER
1	X	215	GLU
1	X	217	ARG
1	X	225	ILE
1	X	242	ILE
1	X	259	PRO

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Mol	Chain	Res	Type
1	X	274	ILE
1	X	276	HIS
1	X	294	GLY
1	X	325	ILE
1	X	110	SER
1	X	178	ASN
1	X	239	GLU
1	X	245	GLU
1	X	257	PRO
1	X	292	ASP
1	X	293	GLY
1	X	302	TYR
1	X	324	ILE
1	X	358	SER
1	X	18	TYR
1	X	48	THR
1	X	112	PRO
1	X	113	ILE
1	X	142	PHE
1	X	169	ALA
1	X	45	SER
1	X	166	ILE
1	X	75	LYS
1	X	120	VAL
1	X	163	LYS
1	X	173	PRO
1	X	174	GLN
1	X	175	SER
1	X	85	GLY
1	X	277	ILE

5.3.2 Protein sidechains ⓘ

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	X	311/311 (100%)	254 (82%)	57 (18%)	2 9

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

Mol	Chain	Res	Type
1	X	1	MET
1	X	6	VAL
1	X	8	HIS
1	X	16	ASN
1	X	25	GLN
1	X	27	GLN
1	X	32	THR
1	X	35	ILE
1	X	36	THR
1	X	40	ILE
1	X	43	LEU
1	X	58	LEU
1	X	61	SER
1	X	71	THR
1	X	86	ARG
1	X	87	GLU
1	X	109	ARG
1	X	112	PRO
1	X	117	VAL
1	X	120	VAL
1	X	130	PHE
1	X	136	PRO
1	X	141	HIS
1	X	149	LEU
1	X	150	MET
1	X	153	SER
1	X	154	GLN
1	X	161	SER
1	X	166	ILE
1	X	178	ASN
1	X	190	LEU
1	X	195	ARG
1	X	200	VAL
1	X	210	LEU
1	X	224	LEU
1	X	228	LEU
1	X	235	GLN
1	X	238	SER
1	X	247	MET
1	X	253	PRO
1	X	254	GLN
1	X	257	PRO

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Mol	Chain	Res	Type
1	X	269	GLU
1	X	273	LEU
1	X	277	ILE
1	X	281	GLU
1	X	288	THR
1	X	290	ASP
1	X	298	GLU
1	X	302	TYR
1	X	328	VAL
1	X	333	LYS
1	X	334	LEU
1	X	335	LEU
1	X	336	ILE
1	X	340	MET
1	X	355	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	8	HIS
1	X	25	GLN
1	X	105	ASN
1	X	141	HIS
1	X	154	GLN
1	X	174	GLN
1	X	178	ASN
1	X	185	GLN
1	X	197	GLN
1	X	235	GLN
1	X	251	ASN
1	X	276	HIS
1	X	303	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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	$\# Z > 2$
3	SAH	X	2814	-	27,28,28	1.91	6 (22%)	36,40,40	1.47	7 (19%)
4	SAL	X	2000	-	10,10,10	3.16	3 (30%)	13,13,13	2.06	4 (30%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	SAH	X	2814	-	-	2/15/31/31	0/3/3/3
4	SAL	X	2000	-	-	0/4/4/4	0/1/1/1

All (9) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	X	2000	SAL	C5-C6	8.06	1.52	1.38
3	X	2814	SAH	O4'-C1'	-5.49	1.29	1.42
3	X	2814	SAH	O3'-C3'	4.70	1.54	1.43
4	X	2000	SAL	C1-C2	4.19	1.47	1.40
3	X	2814	SAH	C4-N3	2.46	1.39	1.34
3	X	2814	SAH	C2'-C3'	-2.44	1.46	1.53
3	X	2814	SAH	C2'-C1'	2.38	1.60	1.53
4	X	2000	SAL	C6-C1	2.37	1.43	1.39
3	X	2814	SAH	C2-N1	2.10	1.37	1.33

All (11) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	X	2000	SAL	C2-C1-C1'	4.06	124.17	120.00
3	X	2814	SAH	O4'-C4'-C5'	-3.17	100.67	108.83
4	X	2000	SAL	O2'-C1'-C1	3.07	124.02	115.28
3	X	2814	SAH	O2'-C2'-C3'	3.04	121.55	111.82
4	X	2000	SAL	C4-C3-C2	2.98	123.72	120.05
4	X	2000	SAL	O2'-C1'-O1'	-2.94	117.04	123.35
3	X	2814	SAH	O4'-C1'-N9	2.73	113.34	108.09
3	X	2814	SAH	CB-CA-C	-2.60	103.56	110.45
3	X	2814	SAH	O2'-C2'-C1'	2.32	118.08	110.10
3	X	2814	SAH	CB-CG-SD	2.31	118.62	113.45
3	X	2814	SAH	C5'-SD-CG	-2.28	95.49	102.26

There are no chirality outliers.

All (2) torsion outliers are listed below:

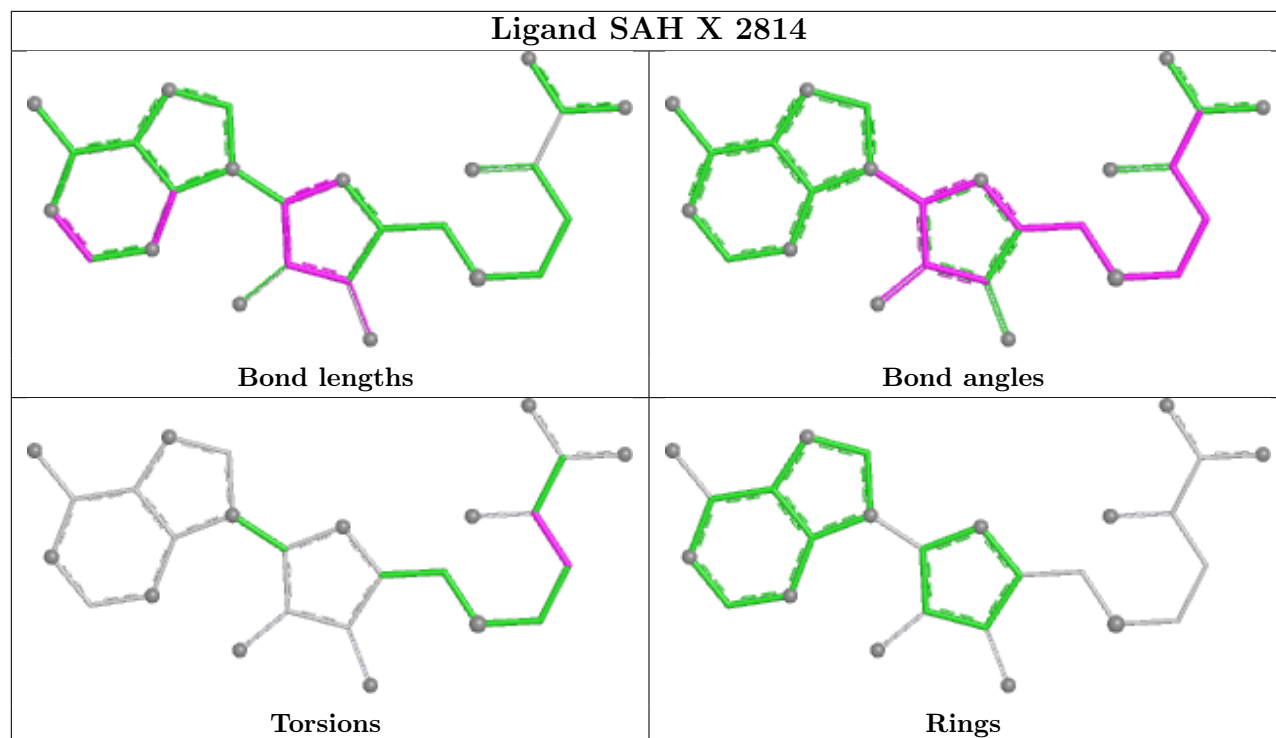
Mol	Chain	Res	Type	Atoms
3	X	2814	SAH	N-CA-CB-CG
3	X	2814	SAH	C-CA-CB-CG

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	X	2814	SAH	2	0

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



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [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	X	359/359 (100%)	-0.16	8 (2%) 62 39	26, 62, 115, 171	0

All (8) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	X	113	ILE	3.1
1	X	85	GLY	2.6
1	X	259	PRO	2.6
1	X	301	GLY	2.5
1	X	242	ILE	2.4
1	X	110	SER	2.4
1	X	163	LYS	2.2
1	X	170	ASN	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](#)

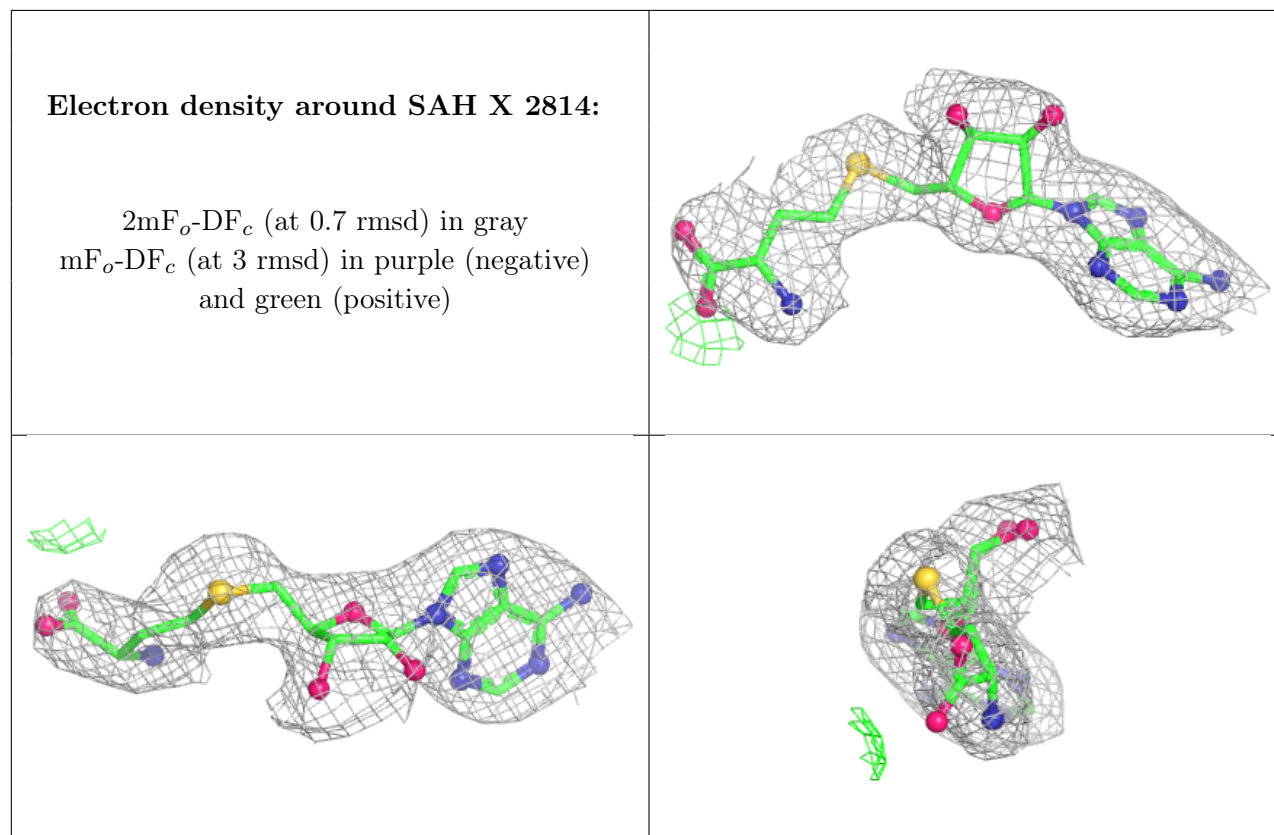
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
2	LU	X	999	1/1	0.95	0.14	81,81,81,81	1
4	SAL	X	2000	10/10	0.95	0.14	71,75,82,92	0
3	SAH	X	2814	26/26	0.97	0.07	28,39,65,83	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.