



# Full wwPDB X-ray Structure Validation Report ⓘ

May 22, 2020 – 11:05 pm BST

PDB ID : 1SUI  
Title : Alfalfa caffeoyl coenzyme A 3-O-methyltransferase  
Authors : Ferrer, J.-L.; Zubieta, C.; Dixon, R.A.; Noel, J.P.  
Deposited on : 2004-03-26  
Resolution : 2.70 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](mailto: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.

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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 : 2.11  
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) : 2.11

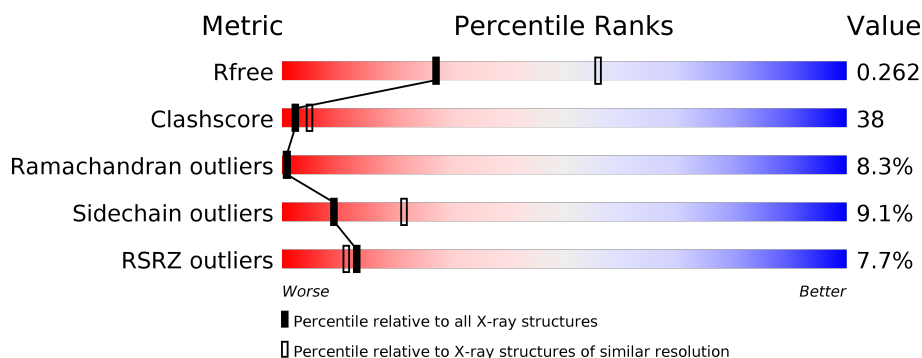
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 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	A	247	<div> <div>2%</div> <div> <div>48%</div> <div>35%</div> <div>9%</div> <div>8%</div> </div> </div>
1	B	247	<div> <div>4%</div> <div> <div>47%</div> <div>38%</div> <div>6%</div> <div>8%</div> </div> </div>
1	C	247	<div> <div>8%</div> <div> <div>35%</div> <div>45%</div> <div>12%</div> <div>8%</div> </div> </div>
1	D	247	<div> <div>15%</div> <div> <div>25%</div> <div>56%</div> <div>10%</div> <div>8%</div> </div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SAH	B	302	-	-	-	X
3	SAH	C	303	-	-	-	X
4	FRE	A	306	X	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 7446 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 Caffeoyle-CoA O-methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	227	Total	C	N	O	S	0	0	0
			1807	1162	301	335	9			
1	B	227	Total	C	N	O	S	0	0	0
			1807	1162	301	335	9			
1	C	227	Total	C	N	O	S	0	0	0
			1807	1162	301	335	9			
1	D	227	Total	C	N	O	S	0	0	0
			1789	1150	295	335	9			

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

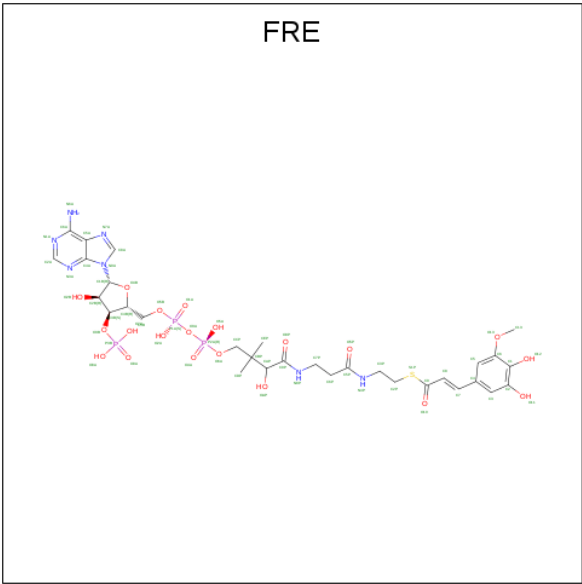
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		
2	D	1	Total	Ca	0	0
			1	1		
2	C	1	Total	Ca	0	0
			1	1		

- Molecule 3 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C<sub>14</sub>H<sub>20</sub>N<sub>6</sub>O<sub>5</sub>S).



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		
3	D	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

- Molecule 4 is FERULOYL COENZYME A (three-letter code: FRE) (formula: C<sub>31</sub>H<sub>44</sub>N<sub>7</sub>O<sub>20</sub>P<sub>3</sub>S).



Mol	Chain	Residues	Atoms						ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	S	1	0
			62	31	7	20	3	1		

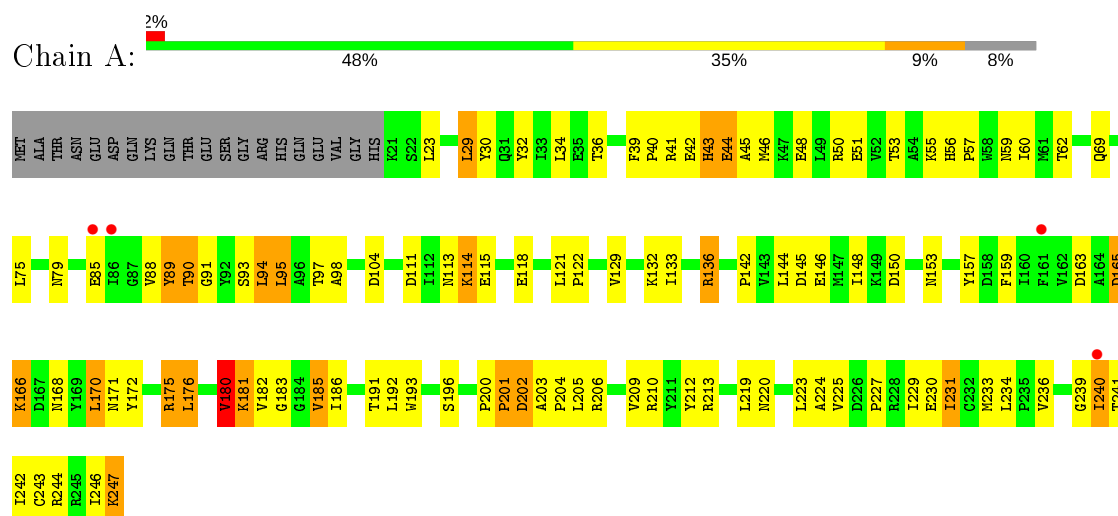
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	19	Total	O	0	0
			19	19		
5	B	31	Total	O	0	0
			31	31		
5	C	11	Total	O	0	0
			11	11		
5	D	5	Total	O	0	0
			5	5		

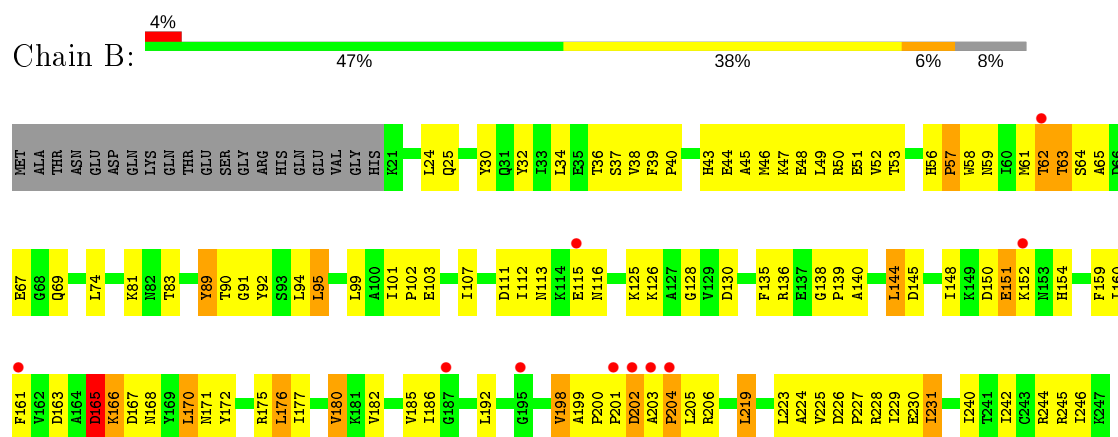
### 3 Residue-property plots [i](#)

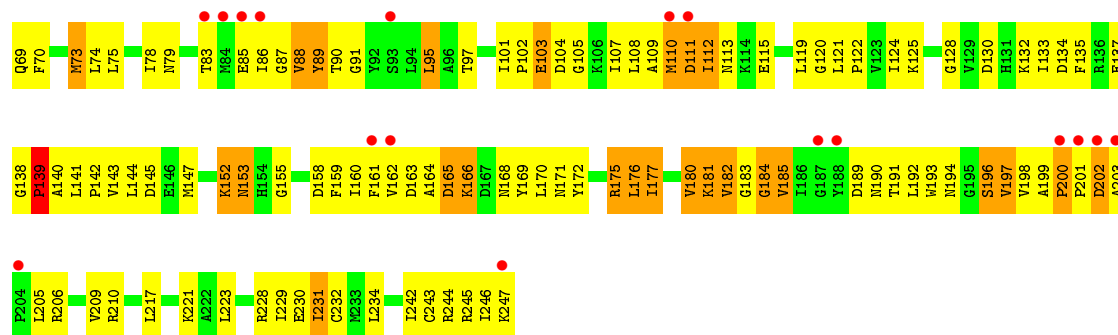
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Caffeoyl-CoA O-methyltransferase

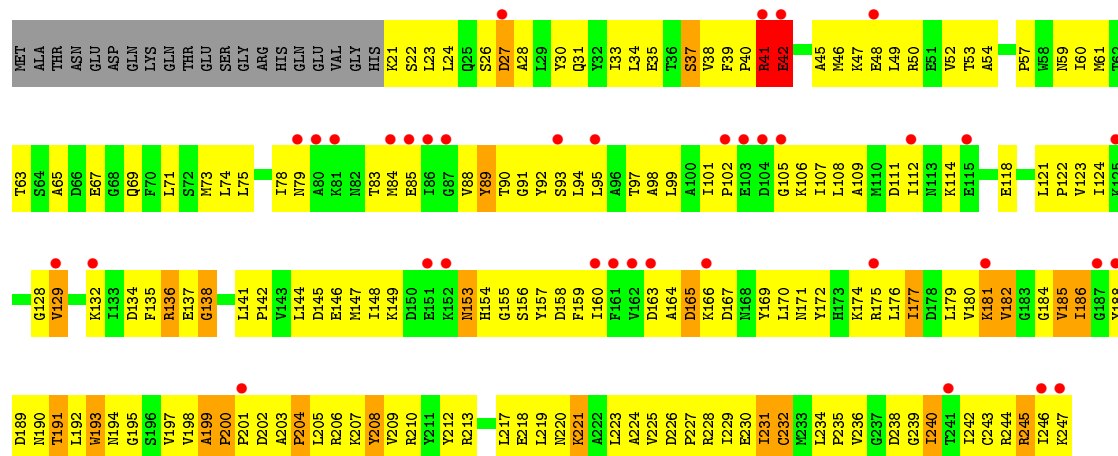


#### • Molecule 1: Caffeoyl-CoA O-methyltransferase





● Molecule 1: Caffeoyl-CoA O-methyltransferase





## 4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	60.85Å 136.49Å 332.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	25.00 – 2.70 25.08 – 2.67	Depositor EDS
% Data completeness (in resolution range)	(Not available) (25.00-2.70) 87.8 (25.08-2.67)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.06	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.13 (at 2.68Å)	Xtriage
Refinement program	CNS	Depositor
R, $R_{free}$	0.235 , 0.285 0.220 , 0.262	Depositor DCC
$R_{free}$ test set	1766 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	78.4	Xtriage
Anisotropy	0.327	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 54.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	7446	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	81.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.16% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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 [i](#)

### 5.1 Standard geometry [i](#)

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

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	0.46	0/1844	0.73	1/2496 (0.0%)
1	B	0.45	0/1844	0.71	1/2496 (0.0%)
1	C	0.37	0/1844	0.66	0/2496
1	D	0.30	0/1824	0.57	0/2472
All	All	0.40	0/7356	0.67	2/9960 (0.0%)

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	64	SER	N-CA-C	-5.83	95.27	111.00
1	A	180	VAL	CB-CA-C	-5.50	100.95	111.40

There are no chirality outliers.

There are no planarity outliers.

### 5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1807	0	1831	106	0
1	B	1807	0	1831	90	0
1	C	1807	0	1831	166	0
1	D	1789	0	1799	215	0
2	A	1	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	26	0	19	3	0
3	B	26	0	19	2	0
3	C	26	0	19	6	0
3	D	26	0	19	4	0
4	A	62	0	38	6	0
5	A	19	0	0	0	0
5	B	31	0	0	0	0
5	C	11	0	0	0	0
5	D	5	0	0	0	0
All	All	7446	0	7406	566	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 38.

All (566) 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)
4:A:306:FRE:O9P	4:A:306:FRE:H62	1.45	1.12
1:D:185:VAL:HG13	1:D:186:ILE:H	1.12	1.11
1:C:182:VAL:HG13	1:C:183:GLY:H	1.24	1.03
1:B:165:ASP:O	1:B:166:LYS:HB2	1.64	0.97
1:B:53:THR:OG1	1:B:90:THR:HG21	1.65	0.97
1:C:141:LEU:H	1:C:141:LEU:HD12	1.30	0.97
1:A:165:ASP:O	1:A:166:LYS:HB2	1.62	0.95
1:C:185:VAL:HA	1:C:243:CYS:O	1.69	0.91
1:C:60:ILE:HG13	1:C:61:MET:HG3	1.52	0.91
4:A:306:FRE:C6P	4:A:306:FRE:O9P	2.20	0.90
1:D:38:VAL:HG23	1:D:39:PHE:H	1.37	0.90
1:A:180:VAL:HG21	1:A:186:ILE:HD11	1.55	0.87
1:D:185:VAL:HG13	1:D:186:ILE:N	1.89	0.86
1:D:21:LYS:HG2	1:D:22:SER:H	1.37	0.86
1:D:199:ALA:HB3	1:D:203:ALA:HB2	1.57	0.86
1:D:182:VAL:H	1:D:245:ARG:HH11	1.22	0.86
1:D:141:LEU:HD21	1:D:175:ARG:HH21	1.40	0.85
1:C:143:VAL:O	1:C:147:MET:HG3	1.75	0.84
1:C:60:ILE:HG23	1:C:61:MET:HE2	1.59	0.84
1:D:146:GLU:HG3	1:D:147:MET:HG3	1.60	0.84
1:C:46:MET:HE1	1:C:95:LEU:HB3	1.59	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:42:GLU:HG3	1:A:42:GLU:O	1.77	0.83
1:B:67:GLU:HG2	1:B:240:ILE:HD11	1.60	0.83
1:A:180:VAL:CG2	1:A:186:ILE:HD11	2.10	0.82
1:C:95:LEU:HG	1:C:124:ILE:HG12	1.61	0.81
1:A:136:ARG:HG2	1:A:136:ARG:HH11	1.45	0.81
1:C:177:ILE:HD13	1:C:177:ILE:O	1.81	0.79
1:C:87:GLY:HA2	3:C:303:SAH:H2	1.65	0.79
1:A:55:LYS:O	1:A:55:LYS:HD3	1.83	0.78
1:D:129:VAL:HG22	1:D:132:LYS:HD2	1.66	0.78
1:B:198:VAL:HG11	1:B:205:LEU:HD11	1.65	0.77
1:C:86:ILE:HG12	1:C:110:MET:HG2	1.64	0.77
1:C:181:LYS:HG3	1:C:182:VAL:H	1.49	0.77
1:C:110:MET:HG3	1:C:111:ASP:OD1	1.84	0.77
1:C:43:HIS:HD2	1:C:46:MET:HG3	1.50	0.77
1:A:163:ASP:OD1	4:A:306:FRE:C13	2.33	0.76
1:A:46:MET:SD	1:A:95:LEU:HD13	2.25	0.76
1:D:46:MET:SD	1:D:95:LEU:HD22	2.25	0.76
1:D:185:VAL:CG1	1:D:186:ILE:H	1.93	0.76
1:D:205:LEU:CD1	1:D:213:ARG:HH21	1.98	0.76
1:A:30:TYR:CE2	1:A:34:LEU:HD11	2.20	0.76
1:C:130:ASP:HA	1:C:133:ILE:HD13	1.66	0.76
1:A:53:THR:OG1	1:A:90:THR:HG21	1.86	0.76
1:C:32:TYR:O	1:C:36:THR:HG23	1.86	0.75
1:C:58:TRP:C	1:C:60:ILE:H	1.89	0.75
1:C:43:HIS:CD2	1:C:46:MET:HG3	2.22	0.74
1:D:181:LYS:HD2	1:D:245:ARG:HH12	1.50	0.74
1:C:141:LEU:HB2	1:C:142:PRO:HD3	1.69	0.74
1:A:163:ASP:OD1	4:A:306:FRE:H131	1.88	0.74
1:C:198:VAL:HG12	1:C:199:ALA:H	1.52	0.73
1:C:165:ASP:O	1:C:166:LYS:HB2	1.88	0.73
1:D:159:PHE:HD1	1:D:185:VAL:HG21	1.54	0.73
1:C:205:LEU:HD23	1:C:205:LEU:H	1.54	0.72
1:D:160:ILE:HD13	1:D:176:LEU:HD11	1.71	0.72
1:D:166:LYS:HB2	1:D:212:TYR:CD1	2.24	0.72
1:B:230:GLU:O	1:B:231:ILE:HG12	1.91	0.71
1:A:231:ILE:HD11	1:C:41:ARG:HD3	1.72	0.71
1:C:31:GLN:O	1:C:35:GLU:HG2	1.91	0.71
1:B:200:PRO:N	1:B:201:PRO:HD2	2.06	0.71
1:A:191:THR:HG21	1:A:241:THR:OG1	1.91	0.70
1:D:141:LEU:HD21	1:D:175:ARG:NH2	2.04	0.70
1:D:38:VAL:HG23	1:D:39:PHE:N	2.04	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:37:SER:O	1:B:69:GLN:NE2	2.24	0.70
1:D:135:PHE:O	1:D:136:ARG:HD2	1.91	0.70
1:C:53:THR:OG1	1:C:90:THR:HG21	1.91	0.70
1:A:43:HIS:O	1:A:44:GLU:HB3	1.92	0.70
1:B:145:ASP:O	1:B:148:ILE:HG22	1.92	0.70
1:D:192:LEU:HB2	1:D:238:ASP:O	1.91	0.70
1:C:88:VAL:O	1:C:89:TYR:HB3	1.92	0.70
1:C:44:GLU:N	1:C:44:GLU:OE1	2.24	0.69
1:A:225:VAL:HG12	1:A:225:VAL:O	1.93	0.69
1:C:133:ILE:N	1:C:133:ILE:HD12	2.06	0.69
1:B:34:LEU:HD22	1:B:65:ALA:HB3	1.75	0.69
1:C:152:LYS:HE3	1:C:152:LYS:O	1.92	0.69
1:C:182:VAL:HG13	1:C:183:GLY:N	2.03	0.69
1:D:231:ILE:HA	1:D:242:ILE:O	1.92	0.69
1:A:172:TYR:HB3	1:A:176:LEU:HD22	1.74	0.69
1:D:47:LYS:HD3	1:D:50:ARG:HH21	1.58	0.68
1:A:142:PRO:O	1:A:146:GLU:HG3	1.93	0.68
1:C:120:GLY:C	1:C:122:PRO:HD2	2.13	0.68
1:C:200:PRO:O	1:C:202:ASP:N	2.25	0.68
1:C:198:VAL:HG12	1:C:199:ALA:N	2.07	0.68
1:D:177:ILE:HD13	1:D:177:ILE:O	1.92	0.68
1:D:31:GLN:O	1:D:35:GLU:HG2	1.92	0.68
1:B:30:TYR:CE1	1:B:34:LEU:HD11	2.29	0.68
1:B:230:GLU:HG3	1:B:244:ARG:NH2	2.09	0.68
1:D:181:LYS:HA	1:D:245:ARG:NH1	2.09	0.68
1:C:60:ILE:HG23	1:C:61:MET:H	1.57	0.68
1:D:21:LYS:CG	1:D:22:SER:H	2.06	0.68
1:D:141:LEU:HB3	1:D:142:PRO:HD3	1.75	0.68
1:D:193:TRP:HE1	1:D:209:VAL:HA	1.59	0.67
1:D:159:PHE:HA	1:D:185:VAL:HG11	1.76	0.67
1:C:121:LEU:N	1:C:122:PRO:HD2	2.08	0.67
1:A:136:ARG:HG2	1:A:136:ARG:NH1	2.09	0.67
1:B:170:LEU:HD22	1:B:219:LEU:HD23	1.75	0.67
1:D:170:LEU:HD12	1:D:218:GLU:HG2	1.77	0.66
1:D:159:PHE:CD1	1:D:185:VAL:HG21	2.31	0.66
1:C:228:ARG:HH21	1:C:245:ARG:HH21	1.42	0.66
1:D:205:LEU:H	1:D:205:LEU:HD23	1.61	0.65
1:C:47:LYS:O	1:C:51:GLU:HG3	1.97	0.65
1:D:27:ASP:O	1:D:31:GLN:HB2	1.97	0.65
1:A:231:ILE:HA	1:A:242:ILE:O	1.97	0.65
1:D:229:ILE:HA	1:D:244:ARG:O	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:163:ASP:OD2	3:B:302:SAH:HG1	1.97	0.65
1:B:32:TYR:O	1:B:36:THR:HG23	1.97	0.64
1:C:103:GLU:HA	1:C:132:LYS:HE2	1.78	0.64
1:C:163:ASP:OD2	3:C:303:SAH:HG2	1.97	0.64
1:C:60:ILE:CG2	1:C:61:MET:HE2	2.28	0.64
1:D:146:GLU:HG3	1:D:147:MET:N	2.13	0.64
1:A:113:ASN:O	1:A:114:LYS:HB3	1.98	0.64
1:C:203:ALA:O	1:C:205:LEU:HD23	1.97	0.64
1:B:176:LEU:O	1:B:180:VAL:HG22	1.98	0.64
1:C:231:ILE:HA	1:C:242:ILE:O	1.98	0.64
1:D:159:PHE:HA	1:D:185:VAL:HG21	1.80	0.64
1:D:205:LEU:HD11	1:D:213:ARG:HH21	1.62	0.64
1:B:230:GLU:HG3	1:B:244:ARG:CZ	2.27	0.63
1:B:199:ALA:O	1:B:202:ASP:HB3	1.98	0.63
1:A:233:MET:CE	1:C:37:SER:HB2	2.27	0.63
1:B:151:GLU:HA	1:B:154:HIS:CD2	2.33	0.63
1:C:115:GLU:OE1	1:C:115:GLU:HA	1.98	0.63
1:D:38:VAL:HG23	1:D:39:PHE:HD1	1.64	0.63
1:C:73:MET:HA	1:C:73:MET:HE3	1.80	0.63
1:D:202:ASP:O	1:D:204:PRO:HD3	1.99	0.63
1:C:125:LYS:HA	1:C:130:ASP:OD1	1.98	0.62
1:D:200:PRO:C	1:D:202:ASP:H	2.00	0.62
1:A:43:HIS:O	1:A:44:GLU:CB	2.48	0.62
1:B:160:ILE:HD12	1:B:180:VAL:HG13	1.82	0.62
1:C:44:GLU:O	1:C:45:ALA:HB3	1.99	0.62
1:A:129:VAL:HG23	1:A:132:LYS:HE3	1.82	0.62
1:A:185:VAL:HA	1:A:243:CYS:O	1.98	0.62
1:C:34:LEU:HD23	1:C:38:VAL:HG21	1.80	0.61
1:D:184:GLY:O	1:D:185:VAL:HB	2.00	0.61
1:A:163:ASP:OD2	3:A:301:SAH:HB1	2.00	0.61
1:A:42:GLU:OE2	1:A:50:ARG:NH2	2.33	0.61
1:C:60:ILE:HG23	1:C:61:MET:CE	2.29	0.61
1:B:170:LEU:CD2	1:B:219:LEU:HA	2.31	0.61
1:A:85:GLU:OE2	1:A:93:SER:HB2	2.00	0.61
1:D:123:VAL:HG12	1:D:123:VAL:O	2.01	0.61
1:D:33:ILE:O	1:D:37:SER:HB3	2.00	0.61
1:C:172:TYR:O	1:C:176:LEU:HB2	2.01	0.60
1:C:141:LEU:CD1	1:C:141:LEU:H	2.08	0.60
1:C:139:PRO:HB3	1:C:141:LEU:HD13	1.82	0.60
1:D:49:LEU:HD11	1:D:90:THR:HG23	1.84	0.60
1:D:141:LEU:HD11	1:D:175:ARG:HH21	1.67	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:95:LEU:HD23	1:D:95:LEU:O	2.01	0.60
1:C:172:TYR:HB3	1:C:176:LEU:HD22	1.83	0.59
1:B:203:ALA:N	1:B:204:PRO:CD	2.66	0.59
1:D:197:VAL:O	1:D:197:VAL:HG13	2.03	0.59
1:A:236:VAL:HG23	1:A:240:ILE:HD11	1.82	0.59
1:C:209:VAL:HG23	1:C:210:ARG:N	2.18	0.59
1:A:163:ASP:OD1	4:A:306:FRE:H133	2.02	0.59
1:C:196:SER:O	1:C:198:VAL:HG23	2.03	0.59
1:D:200:PRO:O	1:D:202:ASP:N	2.35	0.59
1:A:191:THR:HG23	1:A:220:ASN:OD1	2.03	0.58
1:D:159:PHE:HD1	1:D:185:VAL:CG2	2.16	0.58
1:D:200:PRO:C	1:D:202:ASP:N	2.56	0.58
1:B:160:ILE:HG21	1:B:176:LEU:HG	1.85	0.58
1:B:50:ARG:HG2	1:B:63:THR:HG21	1.83	0.58
1:D:205:LEU:HD13	1:D:213:ARG:HH21	1.68	0.58
1:D:232:CYS:HB3	1:D:242:ILE:HG13	1.86	0.58
1:D:141:LEU:CD2	1:D:175:ARG:HH21	2.14	0.58
1:B:227:PRO:O	1:B:246:ILE:HD11	2.03	0.58
1:C:144:LEU:HD21	1:C:176:LEU:HD13	1.85	0.58
1:C:56:HIS:HE1	1:C:58:TRP:HB2	1.68	0.58
1:D:34:LEU:HA	1:D:38:VAL:HG22	1.84	0.58
1:C:206:ARG:O	1:C:209:VAL:HG22	2.03	0.58
1:D:63:THR:HG21	1:D:93:SER:HB3	1.85	0.57
1:A:42:GLU:CD	1:A:50:ARG:HH22	2.07	0.57
1:A:88:VAL:O	1:A:89:TYR:O	2.22	0.57
1:C:112:ILE:HG12	1:C:113:ASN:N	2.19	0.57
1:C:56:HIS:CE1	1:C:58:TRP:HB2	2.39	0.57
1:D:42:GLU:OE2	1:D:47:LYS:HE3	2.04	0.57
1:D:71:LEU:O	1:D:75:LEU:HD13	2.05	0.57
1:D:141:LEU:HD11	1:D:175:ARG:NH2	2.20	0.57
1:C:75:LEU:HD21	1:C:159:PHE:CD2	2.40	0.57
1:D:180:VAL:HG23	1:D:181:LYS:N	2.20	0.57
1:B:53:THR:HG21	1:B:62:THR:HG21	1.86	0.57
1:C:189:ASP:OD1	1:C:190:ASN:N	2.38	0.57
1:D:128:GLY:O	1:D:129:VAL:HG12	2.05	0.57
1:A:163:ASP:O	3:A:301:SAH:H5'1	2.06	0.56
1:B:39:PHE:N	1:B:40:PRO:HD2	2.20	0.56
1:C:166:LYS:HD3	1:C:169:TYR:CE2	2.40	0.56
1:B:165:ASP:OD1	1:B:168:ASN:HB2	2.04	0.56
1:A:94:LEU:HD13	1:A:133:ILE:HD13	1.88	0.56
1:A:39:PHE:HB2	1:A:40:PRO:HD3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:61:MET:HE3	1:C:61:MET:O	2.04	0.56
1:C:58:TRP:C	1:C:60:ILE:N	2.58	0.56
1:C:58:TRP:O	1:C:60:ILE:N	2.39	0.56
1:D:246:ILE:HG13	1:D:247:LYS:N	2.20	0.56
1:D:28:ALA:HA	1:D:31:GLN:HB3	1.87	0.56
1:B:101:ILE:HB	1:B:102:PRO:HD2	1.88	0.56
1:B:231:ILE:HA	1:B:242:ILE:O	2.06	0.56
1:D:114:LYS:HG3	1:D:135:PHE:HE2	1.71	0.56
1:D:155:GLY:C	1:D:157:TYR:H	2.10	0.56
1:A:196:SER:O	1:A:213:ARG:HD2	2.05	0.56
1:A:42:GLU:O	1:A:44:GLU:N	2.39	0.56
1:D:198:VAL:HG22	1:D:199:ALA:H	1.72	0.55
1:D:74:LEU:O	1:D:78:ILE:HG12	2.06	0.55
1:D:184:GLY:HA2	1:D:245:ARG:HB2	1.88	0.55
1:B:49:LEU:HD23	1:B:92:TYR:HA	1.87	0.55
1:C:229:ILE:HA	1:C:244:ARG:O	2.07	0.55
1:D:38:VAL:HG12	1:D:69:GLN:NE2	2.21	0.55
1:A:233:MET:HE3	1:C:37:SER:HB2	1.89	0.55
1:C:155:GLY:O	1:C:181:LYS:HD2	2.06	0.55
1:D:94:LEU:HD21	1:D:107:ILE:HG21	1.87	0.55
1:C:101:ILE:HB	1:C:102:PRO:HD2	1.89	0.55
1:D:141:LEU:HD21	1:D:175:ARG:HE	1.72	0.55
1:D:165:ASP:OD1	1:D:166:LYS:N	2.40	0.55
1:A:150:ASP:HB3	1:A:153:ASN:ND2	2.22	0.55
1:C:166:LYS:HE3	1:C:193:TRP:HZ3	1.71	0.55
1:D:98:ALA:O	1:D:129:VAL:HG21	2.06	0.55
1:C:109:ALA:O	1:C:110:MET:C	2.46	0.54
1:C:183:GLY:O	1:C:185:VAL:N	2.39	0.54
1:C:166:LYS:HE3	1:C:193:TRP:CZ3	2.42	0.54
1:D:198:VAL:HG22	1:D:199:ALA:N	2.23	0.54
1:D:231:ILE:HA	1:D:243:CYS:HA	1.87	0.54
1:D:39:PHE:HB2	1:D:40:PRO:HD3	1.89	0.54
1:A:44:GLU:HG3	1:A:45:ALA:N	2.21	0.54
1:C:232:CYS:SG	1:C:234:LEU:HD21	2.48	0.54
1:B:180:VAL:HG11	1:B:186:ILE:CG1	2.37	0.54
1:C:209:VAL:CG2	1:C:210:ARG:N	2.71	0.54
1:D:47:LYS:HD3	1:D:50:ARG:NH2	2.22	0.54
1:D:101:ILE:CD1	1:D:132:LYS:HD3	2.38	0.54
1:A:225:VAL:CG1	1:A:225:VAL:O	2.56	0.54
1:D:45:ALA:HB1	1:D:95:LEU:HD11	1.90	0.54
1:A:23:LEU:HD13	1:A:192:LEU:HD12	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:228:ARG:NH2	1:C:245:ARG:HH21	2.06	0.54
1:D:105:GLY:O	1:D:132:LYS:HG2	2.08	0.54
1:D:38:VAL:CG2	1:D:39:PHE:H	2.17	0.54
1:C:165:ASP:O	1:C:166:LYS:HE2	2.08	0.53
1:D:101:ILE:HD11	1:D:132:LYS:HD3	1.89	0.53
1:D:229:ILE:HB	1:D:243:CYS:HB3	1.89	0.53
1:C:203:ALA:HB3	1:C:205:LEU:HD22	1.90	0.53
1:D:160:ILE:O	1:D:186:ILE:HA	2.07	0.53
1:D:230:GLU:OE1	1:D:244:ARG:NH1	2.42	0.53
1:D:24:LEU:HD12	1:D:30:TYR:HB2	1.89	0.53
1:A:239:GLY:C	1:A:240:ILE:HD13	2.29	0.53
1:D:182:VAL:H	1:D:245:ARG:NH1	1.99	0.53
1:D:165:ASP:C	1:D:166:LYS:HD2	2.28	0.53
1:D:34:LEU:HB3	1:D:39:PHE:CE1	2.42	0.53
1:A:229:ILE:O	1:C:41:ARG:NH2	2.41	0.53
1:A:89:TYR:O	1:A:91:GLY:N	2.36	0.53
1:C:85:GLU:O	1:C:110:MET:HB3	2.09	0.53
1:C:97:THR:O	1:C:101:ILE:HG12	2.08	0.53
1:C:181:LYS:CG	1:C:182:VAL:H	2.17	0.53
1:C:87:GLY:HA2	3:C:303:SAH:C2	2.37	0.53
1:B:165:ASP:O	1:B:166:LYS:CB	2.48	0.52
1:C:109:ALA:HB3	1:C:133:ILE:HG23	1.91	0.52
1:B:46:MET:SD	1:B:95:LEU:HD13	2.49	0.52
1:C:112:ILE:HG12	1:C:113:ASN:H	1.73	0.52
1:D:105:GLY:O	1:D:106:LYS:HD2	2.10	0.52
1:D:192:LEU:O	1:D:193:TRP:C	2.47	0.52
1:D:224:ALA:HA	1:D:231:ILE:HD13	1.90	0.52
1:B:37:SER:C	1:B:69:GLN:HE22	2.12	0.52
1:C:121:LEU:N	1:C:122:PRO:CD	2.73	0.52
1:D:48:GLU:OE1	1:D:123:VAL:HG13	2.09	0.52
1:B:111:ASP:OD1	1:B:112:ILE:N	2.43	0.52
1:D:75:LEU:HD21	1:D:97:THR:HG23	1.91	0.52
1:B:30:TYR:HE1	1:B:34:LEU:HD11	1.71	0.52
1:D:144:LEU:O	1:D:148:ILE:HG12	2.10	0.52
1:D:144:LEU:HD12	1:D:147:MET:HE1	1.92	0.52
1:D:50:ARG:NH1	1:D:65:ALA:HB2	2.24	0.52
1:A:157:TYR:O	1:A:181:LYS:HD2	2.10	0.52
1:C:109:ALA:CB	1:C:133:ILE:HG23	2.40	0.52
1:C:110:MET:O	1:C:111:ASP:HB3	2.08	0.52
1:D:188:TYR:O	1:D:191:THR:HG23	2.10	0.52
1:B:202:ASP:OD1	1:B:204:PRO:HB2	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:LEU:HD22	1:C:95:LEU:HD12	1.91	0.51
1:C:89:TYR:O	1:C:90:THR:HB	2.09	0.51
1:D:217:LEU:O	1:D:221:LYS:HB2	2.10	0.51
1:A:230:GLU:O	1:A:231:ILE:HG12	2.08	0.51
1:D:53:THR:HG22	1:D:53:THR:O	2.09	0.51
1:C:133:ILE:CD1	1:C:133:ILE:N	2.73	0.51
1:D:129:VAL:CG2	1:D:132:LYS:HD2	2.37	0.51
1:D:184:GLY:O	1:D:185:VAL:CB	2.58	0.51
1:A:53:THR:OG1	1:A:90:THR:CG2	2.56	0.51
1:A:234:LEU:HD21	1:C:70:PHE:CD1	2.46	0.51
1:D:154:HIS:O	1:D:181:LYS:HE2	2.11	0.51
1:A:201:PRO:O	1:A:202:ASP:HB3	2.11	0.51
1:A:170:LEU:HD22	1:A:219:LEU:HD23	1.92	0.51
1:B:81:LYS:HG2	1:B:102:PRO:HG3	1.93	0.51
1:D:75:LEU:CD2	1:D:97:THR:HA	2.41	0.51
1:A:206:ARG:HB2	1:A:209:VAL:HG12	1.93	0.51
1:B:47:LYS:O	1:B:51:GLU:HG3	2.11	0.51
1:C:29:LEU:O	1:C:33:ILE:HG13	2.10	0.51
1:D:88:VAL:HG21	1:D:109:ALA:HB1	1.92	0.51
1:B:200:PRO:N	1:B:201:PRO:CD	2.74	0.51
1:B:43:HIS:HD2	1:B:44:GLU:N	2.09	0.51
1:C:74:LEU:O	1:C:74:LEU:HD23	2.11	0.51
1:C:60:ILE:HG21	1:C:89:TYR:CE2	2.46	0.51
1:D:112:ILE:HA	1:D:138:GLY:HA2	1.93	0.51
1:C:49:LEU:CD2	1:C:95:LEU:HD12	2.40	0.50
1:A:182:VAL:O	1:A:183:GLY:C	2.49	0.50
1:D:182:VAL:N	1:D:245:ARG:HH11	2.00	0.50
1:C:168:ASN:HA	1:C:171:ASN:HD22	1.77	0.50
1:D:108:LEU:HD13	1:D:134:ASP:HB3	1.92	0.50
1:D:154:HIS:O	1:D:181:LYS:HG3	2.10	0.50
1:D:205:LEU:HD11	1:D:213:ARG:NH2	2.25	0.50
1:A:98:ALA:HB1	1:A:129:VAL:HG22	1.94	0.50
1:B:62:THR:OG1	1:B:63:THR:N	2.43	0.50
1:D:146:GLU:CG	1:D:147:MET:HG3	2.39	0.50
1:A:233:MET:HE3	1:C:37:SER:CB	2.41	0.50
1:D:160:ILE:HD12	1:D:180:VAL:HG13	1.94	0.50
1:B:113:ASN:OD1	1:B:115:GLU:HB2	2.12	0.50
1:A:150:ASP:HB3	1:A:153:ASN:HD22	1.76	0.50
1:C:133:ILE:HG22	1:C:134:ASP:N	2.27	0.50
1:D:83:THR:O	1:D:108:LEU:HD23	2.12	0.50
1:C:88:VAL:HG12	1:C:89:TYR:N	2.27	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:43:HIS:CD2	1:B:45:ALA:H	2.30	0.49
1:C:205:LEU:HD21	1:C:210:ARG:NH2	2.27	0.49
1:D:144:LEU:HA	1:D:147:MET:HE3	1.94	0.49
1:B:62:THR:HG21	1:B:89:TYR:HE2	1.78	0.49
1:D:89:TYR:O	1:D:90:THR:HB	2.12	0.49
1:B:48:GLU:O	1:B:52:VAL:HG23	2.12	0.49
1:C:197:VAL:HG23	1:C:197:VAL:O	2.12	0.49
1:D:157:TYR:O	1:D:180:VAL:HA	2.11	0.49
1:C:177:ILE:HD11	1:C:245:ARG:HG3	1.93	0.49
1:C:181:LYS:HG3	1:C:182:VAL:N	2.22	0.49
1:C:70:PHE:CZ	1:C:234:LEU:HD12	2.46	0.49
1:A:32:TYR:CE1	1:A:36:THR:HG21	2.47	0.49
1:B:89:TYR:O	1:B:90:THR:HB	2.12	0.49
1:D:184:GLY:HA3	1:D:245:ARG:H	1.77	0.49
1:D:95:LEU:HD23	1:D:99:LEU:HG	1.94	0.49
1:B:38:VAL:HG22	1:B:69:GLN:NE2	2.27	0.48
1:C:198:VAL:CG1	1:C:199:ALA:N	2.76	0.48
1:D:146:GLU:CG	1:D:147:MET:N	2.76	0.48
1:D:219:LEU:HD13	1:D:219:LEU:C	2.33	0.48
1:B:165:ASP:HB2	1:B:167:ASP:OD1	2.12	0.48
1:B:43:HIS:HD2	1:B:45:ALA:H	1.61	0.48
1:C:74:LEU:O	1:C:78:ILE:HG12	2.12	0.48
1:D:106:LYS:HA	1:D:132:LYS:HB3	1.94	0.48
1:A:193:TRP:NE1	1:A:209:VAL:HG23	2.28	0.48
1:C:66:ASP:OD1	1:C:66:ASP:N	2.46	0.48
1:D:136:ARG:HH11	1:D:136:ARG:HG2	1.78	0.48
1:B:83:THR:OG1	1:B:107:ILE:HG12	2.13	0.48
1:B:180:VAL:HG11	1:B:186:ILE:HG13	1.95	0.48
1:C:133:ILE:HG22	1:C:135:PHE:H	1.79	0.48
1:D:180:VAL:HG11	1:D:186:ILE:HG13	1.96	0.48
1:D:219:LEU:HD21	1:D:223:LEU:HD22	1.96	0.48
1:C:198:VAL:CG1	1:C:199:ALA:H	2.23	0.48
1:C:89:TYR:C	1:C:89:TYR:CD1	2.87	0.48
1:D:188:TYR:CD1	1:D:223:LEU:HD21	2.49	0.48
1:A:166:LYS:HB3	1:A:212:TYR:CD1	2.48	0.48
1:A:60:ILE:HG12	1:A:60:ILE:O	2.13	0.48
1:A:75:LEU:CD1	1:A:97:THR:HG23	2.44	0.48
1:A:44:GLU:CG	1:A:45:ALA:N	2.77	0.47
1:D:141:LEU:HD23	1:D:141:LEU:O	2.14	0.47
1:D:234:LEU:O	1:D:236:VAL:N	2.39	0.47
1:A:113:ASN:O	1:A:114:LYS:CB	2.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:144:LEU:HA	1:D:147:MET:CE	2.44	0.47
1:D:158:ASP:O	1:D:185:VAL:HG11	2.14	0.47
1:C:217:LEU:O	1:C:221:LYS:HG2	2.14	0.47
1:A:75:LEU:HD21	1:A:159:PHE:CD2	2.50	0.47
1:B:43:HIS:CD2	1:B:44:GLU:N	2.83	0.47
1:D:118:GLU:HA	1:D:121:LEU:HB2	1.96	0.47
1:D:141:LEU:HD21	1:D:175:ARG:NE	2.28	0.47
1:A:145:ASP:CG	1:A:175:ARG:HH21	2.18	0.47
1:C:30:TYR:CE2	1:C:34:LEU:HD11	2.49	0.47
1:A:233:MET:HE2	1:C:37:SER:HB2	1.97	0.47
1:B:150:ASP:O	1:B:152:LYS:N	2.48	0.47
1:C:119:LEU:O	1:C:119:LEU:HD23	2.14	0.47
1:C:230:GLU:HG3	1:C:246:ILE:HG21	1.95	0.47
1:C:103:GLU:HA	1:C:132:LYS:CE	2.45	0.47
1:C:163:ASP:CG	3:C:303:SAH:HG2	2.35	0.47
1:D:185:VAL:CG1	1:D:186:ILE:N	2.61	0.47
1:D:189:ASP:HA	1:D:240:ILE:HG12	1.97	0.47
1:B:226:ASP:HB3	1:B:229:ILE:HG12	1.97	0.47
1:C:162:VAL:HG12	1:C:169:TYR:CE1	2.49	0.47
1:D:160:ILE:HG21	1:D:176:LEU:HD21	1.97	0.47
1:C:63:THR:O	1:C:63:THR:HG23	2.15	0.47
1:D:163:ASP:OD1	1:D:189:ASP:HB3	2.15	0.47
1:D:166:LYS:HE3	1:D:193:TRP:CZ3	2.50	0.47
1:D:21:LYS:HG2	1:D:22:SER:N	2.17	0.47
1:D:181:LYS:HD2	1:D:245:ARG:NH1	2.24	0.47
1:A:34:LEU:HB3	1:A:39:PHE:CE2	2.50	0.46
1:C:133:ILE:HG22	1:C:135:PHE:N	2.29	0.46
1:C:230:GLU:HG3	1:C:246:ILE:CG2	2.45	0.46
1:D:176:LEU:HA	1:D:179:LEU:HD23	1.95	0.46
1:A:200:PRO:HG2	1:A:203:ALA:CB	2.45	0.46
1:D:165:ASP:O	1:D:169:TYR:CE1	2.69	0.46
1:D:34:LEU:HA	1:D:38:VAL:CG2	2.44	0.46
1:D:171:ASN:O	1:D:172:TYR:C	2.54	0.46
1:C:89:TYR:O	1:C:91:GLY:N	2.43	0.46
1:B:89:TYR:C	1:B:91:GLY:H	2.18	0.46
1:D:63:THR:HG23	1:D:92:TYR:CD1	2.51	0.46
1:A:240:ILE:HD13	1:A:240:ILE:N	2.31	0.46
1:B:171:ASN:O	1:B:175:ARG:NH1	2.49	0.46
1:C:61:MET:CE	1:C:61:MET:H	2.29	0.46
1:A:234:LEU:HD21	1:C:70:PHE:HD1	1.81	0.46
1:D:141:LEU:HD21	1:D:175:ARG:CZ	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:ASN:C	1:D:192:LEU:H	2.19	0.46
1:D:200:PRO:O	1:D:203:ALA:N	2.48	0.46
1:D:111:ASP:OD2	3:D:304:SAH:H4'	2.16	0.46
1:C:196:SER:OG	1:C:197:VAL:N	2.47	0.46
1:D:121:LEU:N	1:D:122:PRO:CD	2.79	0.46
1:D:206:ARG:HB2	1:D:209:VAL:HG12	1.98	0.46
1:B:67:GLU:CG	1:B:240:ILE:HD11	2.38	0.46
1:A:29:LEU:HD21	1:C:192:LEU:HD22	1.97	0.46
1:D:239:GLY:O	1:D:240:ILE:HG13	2.16	0.46
1:D:47:LYS:CD	1:D:50:ARG:HH21	2.24	0.46
1:A:200:PRO:HA	1:A:201:PRO:HD3	1.76	0.46
1:D:227:PRO:O	1:D:246:ILE:HD11	2.16	0.46
1:B:150:ASP:C	1:B:152:LYS:H	2.19	0.46
1:D:165:ASP:O	1:D:166:LYS:HD2	2.16	0.46
1:D:28:ALA:HA	1:D:31:GLN:CB	2.45	0.46
1:B:112:ILE:HD11	1:B:139:PRO:HG3	1.97	0.45
1:D:84:MET:HB2	1:D:157:TYR:CE2	2.51	0.45
1:A:181:LYS:HE3	1:A:183:GLY:HA3	1.99	0.45
1:A:227:PRO:O	1:A:246:ILE:HD11	2.15	0.45
1:A:163:ASP:CG	4:A:306:FRE:H131	2.36	0.45
1:C:230:GLU:O	1:C:231:ILE:HG12	2.16	0.45
1:C:61:MET:SD	3:C:303:SAH:H5'1	2.56	0.45
1:D:95:LEU:C	1:D:95:LEU:HD23	2.37	0.45
1:A:59:ASN:O	1:A:62:THR:HG22	2.17	0.45
1:B:34:LEU:CD2	1:B:65:ALA:HB3	2.46	0.45
1:C:159:PHE:CZ	1:C:161:PHE:HB2	2.51	0.45
1:C:45:ALA:O	1:C:48:GLU:N	2.50	0.45
1:B:201:PRO:O	1:B:203:ALA:N	2.50	0.45
1:D:232:CYS:HB3	1:D:242:ILE:CG1	2.46	0.45
1:A:121:LEU:N	1:A:122:PRO:CD	2.80	0.45
1:B:89:TYR:O	1:B:91:GLY:N	2.48	0.45
1:C:112:ILE:CG1	1:C:113:ASN:N	2.79	0.45
1:C:246:ILE:HG13	1:C:247:LYS:HG3	1.98	0.45
1:C:112:ILE:CG1	1:C:113:ASN:H	2.28	0.45
1:D:107:ILE:C	1:D:108:LEU:HD22	2.36	0.45
1:D:89:TYR:O	1:D:91:GLY:N	2.45	0.45
1:D:106:LYS:HG3	1:D:132:LYS:HA	1.98	0.45
1:D:145:ASP:HA	1:D:148:ILE:HG12	1.99	0.45
1:D:219:LEU:HD13	1:D:220:ASN:N	2.32	0.45
1:A:244:ARG:HD3	1:C:73:MET:CE	2.47	0.45
1:B:225:VAL:O	1:B:225:VAL:HG12	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:VAL:O	1:D:89:TYR:HB3	2.16	0.45
1:A:166:LYS:C	1:A:168:ASN:H	2.20	0.45
1:B:53:THR:HG21	1:B:62:THR:CG2	2.47	0.45
1:C:158:ASP:O	1:C:184:GLY:O	2.35	0.45
1:D:145:ASP:HA	1:D:148:ILE:CG1	2.47	0.45
1:D:230:GLU:O	1:D:231:ILE:HG12	2.17	0.45
1:D:231:ILE:HG22	1:D:243:CYS:SG	2.57	0.45
1:B:24:LEU:HD12	1:B:30:TYR:HB2	1.99	0.44
1:D:107:ILE:N	1:D:132:LYS:O	2.49	0.44
1:D:184:GLY:CA	1:D:245:ARG:H	2.29	0.44
1:D:34:LEU:HD22	1:D:39:PHE:HE1	1.80	0.44
1:D:60:ILE:HG13	1:D:60:ILE:O	2.17	0.44
1:A:111:ASP:OD2	3:A:301:SAH:H4'	2.17	0.44
1:D:145:ASP:OD1	1:D:175:ARG:HD2	2.17	0.44
1:D:194:ASN:HB3	1:D:195:GLY:H	1.61	0.44
1:A:200:PRO:HG2	1:A:203:ALA:HB3	1.99	0.44
1:B:81:LYS:HG2	1:B:102:PRO:CG	2.48	0.44
1:B:95:LEU:HD22	1:B:99:LEU:HG	1.99	0.44
1:C:107:ILE:O	1:C:109:ALA:N	2.50	0.44
1:C:205:LEU:HD12	1:C:209:VAL:HG23	1.99	0.44
1:D:185:VAL:HG22	1:D:186:ILE:N	2.32	0.44
1:D:170:LEU:HD23	1:D:170:LEU:O	2.17	0.44
1:A:48:GLU:O	1:A:51:GLU:HB2	2.17	0.44
1:B:230:GLU:HG3	1:B:244:ARG:NH1	2.32	0.44
1:B:56:HIS:NE2	1:B:116:ASN:ND2	2.65	0.44
1:C:184:GLY:O	1:C:185:VAL:HB	2.18	0.44
1:D:165:ASP:HB3	3:D:304:SAH:HN61	1.83	0.44
1:D:209:VAL:HG13	1:D:210:ARG:N	2.33	0.44
1:D:52:VAL:C	1:D:54:ALA:H	2.21	0.44
1:D:95:LEU:HD21	1:D:99:LEU:HD11	1.99	0.44
1:B:53:THR:HG1	1:B:90:THR:HG21	1.77	0.44
1:A:231:ILE:CD1	1:C:41:ARG:HD3	2.44	0.44
1:C:73:MET:CE	1:C:73:MET:HA	2.46	0.44
1:D:114:LYS:HG3	1:D:135:PHE:CE2	2.51	0.44
1:D:21:LYS:CG	1:D:22:SER:N	2.75	0.44
1:C:153:ASN:HA	1:C:153:ASN:HD22	1.52	0.44
1:C:162:VAL:HG12	1:C:169:TYR:HE1	1.82	0.44
1:D:240:ILE:HG22	1:D:240:ILE:O	2.17	0.44
1:B:126:LYS:C	1:B:128:GLY:H	2.21	0.43
1:B:182:VAL:HA	1:B:245:ARG:HD3	2.00	0.43
1:A:176:LEU:O	1:A:180:VAL:CG2	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:172:TYR:HB3	1:B:176:LEU:HD22	1.99	0.43
1:D:145:ASP:O	1:D:149:LYS:HE3	2.19	0.43
1:D:180:VAL:HG11	1:D:186:ILE:CG1	2.47	0.43
1:B:140:ALA:O	1:B:144:LEU:HB2	2.19	0.43
1:B:199:ALA:C	1:B:201:PRO:HD2	2.38	0.43
1:B:228:ARG:HH21	1:B:245:ARG:HH21	1.66	0.43
1:B:61:MET:HG3	1:B:62:THR:N	2.34	0.43
1:A:244:ARG:HD3	1:C:73:MET:HE1	1.99	0.43
1:D:136:ARG:O	1:D:137:GLU:HG2	2.19	0.43
1:B:159:PHE:CE2	1:B:161:PHE:HB2	2.53	0.43
1:C:113:ASN:ND2	1:C:139:PRO:HD3	2.33	0.43
1:C:37:SER:O	1:C:69:GLN:NE2	2.51	0.43
1:A:165:ASP:HB2	1:A:168:ASN:HB2	2.01	0.43
1:D:67:GLU:OE2	1:D:240:ILE:HG13	2.19	0.43
1:B:203:ALA:O	1:B:205:LEU:N	2.52	0.43
1:D:107:ILE:HG22	1:D:108:LEU:N	2.34	0.43
1:D:170:LEU:HD12	1:D:218:GLU:CG	2.46	0.43
1:A:246:ILE:O	1:A:247:LYS:HB3	2.19	0.43
1:C:160:ILE:HD12	1:C:180:VAL:HG13	2.01	0.43
1:C:182:VAL:CG1	1:C:183:GLY:N	2.74	0.43
1:D:246:ILE:CG1	1:D:247:LYS:N	2.82	0.43
1:A:118:GLU:O	1:A:122:PRO:HD3	2.19	0.42
1:A:200:PRO:O	1:A:202:ASP:N	2.47	0.42
1:B:37:SER:C	1:B:69:GLN:NE2	2.72	0.42
1:C:130:ASP:C	1:C:132:LYS:H	2.22	0.42
1:C:175:ARG:H	1:C:175:ARG:HG2	1.52	0.42
1:D:22:SER:OG	1:D:23:LEU:N	2.52	0.42
1:B:163:ASP:CG	3:B:302:SAH:HG1	2.39	0.42
1:B:50:ARG:HG2	1:B:63:THR:CG2	2.49	0.42
1:D:26:SER:C	1:D:28:ALA:N	2.71	0.42
1:D:63:THR:CG2	1:D:93:SER:HB3	2.49	0.42
1:C:44:GLU:CD	1:C:44:GLU:H	2.21	0.42
1:C:46:MET:CE	1:C:95:LEU:HD13	2.48	0.42
1:A:244:ARG:CB	1:C:73:MET:HE1	2.48	0.42
1:A:165:ASP:CB	1:A:168:ASN:HB2	2.50	0.42
1:A:170:LEU:CD2	1:A:219:LEU:HA	2.49	0.42
1:C:42:GLU:OE2	1:C:50:ARG:NH2	2.49	0.42
1:D:180:VAL:HG23	1:D:181:LYS:H	1.83	0.42
1:D:225:VAL:O	1:D:227:PRO:HD3	2.20	0.42
1:D:181:LYS:HA	1:D:245:ARG:HG3	2.02	0.42
1:D:41:ARG:N	1:D:41:ARG:NE	2.67	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:88:VAL:O	3:D:304:SAH:HA	2.19	0.42
1:A:180:VAL:HG22	1:A:186:ILE:HD11	1.94	0.42
1:C:113:ASN:HD21	1:C:139:PRO:HD3	1.85	0.42
1:D:141:LEU:CD1	1:D:175:ARG:HH21	2.32	0.42
1:D:180:VAL:O	1:D:181:LYS:O	2.37	0.42
1:D:181:LYS:CA	1:D:245:ARG:NH1	2.81	0.42
1:D:95:LEU:HD21	1:D:99:LEU:CD1	2.49	0.42
1:B:135:PHE:CD1	1:B:136:ARG:N	2.87	0.42
1:C:177:ILE:HD12	1:C:228:ARG:CZ	2.49	0.42
1:A:181:LYS:HG2	1:A:183:GLY:H	1.84	0.42
1:C:134:ASP:O	1:C:134:ASP:OD1	2.38	0.42
1:B:175:ARG:HH11	1:B:175:ARG:HG2	1.83	0.42
1:D:203:ALA:O	1:D:205:LEU:CD2	2.67	0.42
1:D:97:THR:O	1:D:101:ILE:HG23	2.20	0.41
1:D:208:TYR:N	1:D:208:TYR:CD1	2.87	0.41
1:D:225:VAL:O	1:D:225:VAL:HG12	2.20	0.41
1:D:226:ASP:C	1:D:228:ARG:H	2.22	0.41
1:D:41:ARG:CA	1:D:41:ARG:NE	2.83	0.41
1:C:33:ILE:O	1:C:37:SER:HB3	2.21	0.41
1:D:59:ASN:C	1:D:61:MET:H	2.24	0.41
1:A:40:PRO:O	1:A:41:ARG:CB	2.68	0.41
1:C:137:GLU:HG2	1:C:138:GLY:N	2.35	0.41
1:C:140:ALA:O	1:C:141:LEU:C	2.58	0.41
1:C:46:MET:HE2	1:C:95:LEU:HD13	2.02	0.41
1:D:108:LEU:N	1:D:108:LEU:HD22	2.35	0.41
1:A:193:TRP:CD1	1:A:209:VAL:HG23	2.56	0.41
1:D:163:ASP:OD2	3:D:304:SAH:HB1	2.21	0.41
1:A:185:VAL:H	1:A:244:ARG:HA	1.86	0.41
1:A:75:LEU:HD11	1:A:97:THR:HG23	2.03	0.41
1:D:155:GLY:C	1:D:157:TYR:N	2.73	0.41
1:B:224:ALA:HA	1:B:231:ILE:HD13	2.03	0.41
1:A:148:ILE:HA	1:A:148:ILE:HD13	1.93	0.41
1:B:192:LEU:HA	1:B:192:LEU:HD23	1.77	0.41
1:D:159:PHE:CD1	1:D:185:VAL:CG2	2.99	0.41
1:D:84:MET:HG2	1:D:85:GLU:N	2.36	0.41
1:A:224:ALA:HA	1:A:231:ILE:HD13	2.03	0.40
1:C:190:ASN:C	1:C:192:LEU:H	2.25	0.40
1:C:206:ARG:HD2	1:C:206:ARG:N	2.36	0.40
1:D:158:ASP:O	1:D:185:VAL:CG1	2.69	0.40
1:A:240:ILE:HB	1:A:242:ILE:CD1	2.52	0.40
1:B:112:ILE:HD12	1:B:138:GLY:C	2.41	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:49:LEU:HD11	1:C:90:THR:CG2	2.51	0.40
1:D:73:MET:HA	1:D:73:MET:CE	2.52	0.40
1:A:171:ASN:O	1:A:175:ARG:HD3	2.20	0.40
1:B:125:LYS:HA	1:B:130:ASP:OD1	2.22	0.40
1:B:225:VAL:O	1:B:225:VAL:CG1	2.69	0.40
1:A:56:HIS:HA	1:A:57:PRO:HD3	1.89	0.40
1:A:104:ASP:OD1	1:A:104:ASP:N	2.54	0.40
1:A:40:PRO:O	1:A:41:ARG:HB2	2.22	0.40
1:A:94:LEU:HD23	1:A:94:LEU:HA	1.81	0.40
1:C:112:ILE:HG13	3:C:303:SAH:C2	2.52	0.40
1:D:180:VAL:CG2	1:D:181:LYS:N	2.84	0.40
1:D:191:THR:HB	1:D:220:ASN:OD1	2.22	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles ⓘ

### 5.3.1 Protein backbone ⓘ

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	225/247 (91%)	196 (87%)	18 (8%)	11 (5%)	2	4
1	B	225/247 (91%)	197 (88%)	18 (8%)	10 (4%)	2	5
1	C	225/247 (91%)	170 (76%)	30 (13%)	25 (11%)	0	0
1	D	225/247 (91%)	155 (69%)	41 (18%)	29 (13%)	0	0
All	All	900/988 (91%)	718 (80%)	107 (12%)	75 (8%)	1	1

All (75) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	43	HIS
1	A	89	TYR
1	A	165	ASP

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Mol	Chain	Res	Type
1	A	202	ASP
1	A	231	ILE
1	B	62	THR
1	B	63	THR
1	B	89	TYR
1	B	202	ASP
1	C	60	ILE
1	C	104	ASP
1	C	110	MET
1	C	166	LYS
1	C	182	VAL
1	C	201	PRO
1	C	231	ILE
1	D	102	PRO
1	D	153	ASN
1	D	181	LYS
1	D	185	VAL
1	D	186	ILE
1	D	207	LYS
1	D	231	ILE
1	A	44	GLU
1	A	166	LYS
1	B	151	GLU
1	B	166	LYS
1	B	231	ILE
1	C	105	GLY
1	C	165	ASP
1	C	184	GLY
1	C	194	ASN
1	C	196	SER
1	C	197	VAL
1	D	37	SER
1	D	182	VAL
1	D	193	TRP
1	A	114	LYS
1	B	204	PRO
1	C	59	ASN
1	C	139	PRO
1	C	200	PRO
1	C	202	ASP
1	D	156	SER
1	D	204	PRO

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Mol	Chain	Res	Type
1	B	165	ASP
1	C	111	ASP
1	C	164	ALA
1	C	181	LYS
1	D	41	ARG
1	D	79	ASN
1	D	89	TYR
1	D	164	ALA
1	D	165	ASP
1	D	240	ILE
1	A	185	VAL
1	C	88	VAL
1	C	185	VAL
1	C	191	THR
1	D	42	GLU
1	D	124	ILE
1	D	191	THR
1	D	232	CYS
1	D	129	VAL
1	D	199	ALA
1	B	57	PRO
1	A	204	PRO
1	C	112	ILE
1	C	128	GLY
1	D	138	GLY
1	D	201	PRO
1	A	201	PRO
1	D	200	PRO
1	D	235	PRO
1	D	57	PRO

### 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	A	196/214 (92%)	177 (90%)	19 (10%)	8 19

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	196/214 (92%)	177 (90%)	19 (10%)	8	19
1	C	196/214 (92%)	174 (89%)	22 (11%)	6	13
1	D	192/214 (90%)	181 (94%)	11 (6%)	20	44
All	All	780/856 (91%)	709 (91%)	71 (9%)	9	21

All (71) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	LEU
1	A	69	GLN
1	A	79	ASN
1	A	90	THR
1	A	94	LEU
1	A	95	LEU
1	A	115	GLU
1	A	136	ARG
1	A	144	LEU
1	A	170	LEU
1	A	175	ARG
1	A	176	LEU
1	A	180	VAL
1	A	181	LYS
1	A	205	LEU
1	A	210	ARG
1	A	223	LEU
1	A	240	ILE
1	A	247	LYS
1	B	25	GLN
1	B	57	PRO
1	B	58	TRP
1	B	59	ASN
1	B	74	LEU
1	B	94	LEU
1	B	95	LEU
1	B	103	GLU
1	B	144	LEU
1	B	165	ASP
1	B	170	LEU
1	B	176	LEU
1	B	177	ILE
1	B	180	VAL

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Mol	Chain	Res	Type
1	B	185	VAL
1	B	198	VAL
1	B	206	ARG
1	B	219	LEU
1	B	223	LEU
1	C	27	ASP
1	C	36	THR
1	C	44	GLU
1	C	61	MET
1	C	66	ASP
1	C	73	MET
1	C	79	ASN
1	C	83	THR
1	C	89	TYR
1	C	95	LEU
1	C	103	GLU
1	C	108	LEU
1	C	139	PRO
1	C	145	ASP
1	C	152	LYS
1	C	153	ASN
1	C	170	LEU
1	C	175	ARG
1	C	176	LEU
1	C	177	ILE
1	C	180	VAL
1	C	223	LEU
1	D	27	ASP
1	D	41	ARG
1	D	42	GLU
1	D	136	ARG
1	D	153	ASN
1	D	167	ASP
1	D	174	LYS
1	D	177	ILE
1	D	208	TYR
1	D	221	LYS
1	D	245	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	GLN
1	A	153	ASN
1	A	194	ASN
1	B	43	HIS
1	B	69	GLN
1	B	116	ASN
1	C	31	GLN
1	C	43	HIS
1	C	69	GLN
1	C	79	ASN
1	C	113	ASN
1	C	168	ASN
1	C	171	ASN
1	C	220	ASN
1	D	31	GLN
1	D	69	GLN
1	D	116	ASN
1	D	153	ASN
1	D	190	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

## 5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 9 ligands modelled in this entry, 4 are monoatomic - leaving 5 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	A	301	-	21,28,28	1.69	4 (19%)	20,40,40	2.26	11 (55%)
4	FRE	A	306	-	55,65,65	1.50	9 (16%)	70,96,96	2.12	14 (20%)
3	SAH	B	302	-	21,28,28	1.63	4 (19%)	20,40,40	2.15	9 (45%)
3	SAH	C	303	-	21,28,28	1.77	4 (19%)	20,40,40	2.14	8 (40%)
3	SAH	D	304	2	21,28,28	1.73	4 (19%)	20,40,40	2.13	8 (40%)

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	A	301	-	-	2/7/31/31	0/3/3/3
3	SAH	B	302	-	-	4/7/31/31	0/3/3/3
3	SAH	C	303	-	-	3/7/31/31	0/3/3/3
4	FRE	A	306	-	1/1/12/16	31/54/74/74	0/4/4/4
3	SAH	D	304	2	-	4/7/31/31	0/3/3/3

All (25) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	303	SAH	O4'-C1'	5.48	1.48	1.41
3	D	304	SAH	O4'-C1'	5.01	1.48	1.41
3	B	302	SAH	O4'-C1'	4.45	1.47	1.41
3	A	301	SAH	O4'-C1'	4.25	1.47	1.41
4	A	306	FRE	C7P-N8P	4.05	1.55	1.46
3	C	303	SAH	C8-N7	-3.96	1.27	1.34
3	D	304	SAH	C8-N7	-3.84	1.27	1.34
4	A	306	FRE	C3P-N4P	3.79	1.54	1.46
3	A	301	SAH	C8-N7	-3.73	1.28	1.34
3	B	302	SAH	C8-N7	-3.68	1.28	1.34
4	A	306	FRE	OAP-CAP	3.27	1.48	1.42
4	A	306	FRE	P3B-O9A	3.07	1.60	1.50
4	A	306	FRE	P2A-O6A	-2.63	1.48	1.59
4	A	306	FRE	C2-C1	2.59	1.43	1.40
4	A	306	FRE	C5-C4	2.52	1.44	1.39
4	A	306	FRE	C6-C1	2.37	1.43	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	301	SAH	C5-C4	-2.36	1.34	1.40
3	B	302	SAH	O2'-C2'	-2.33	1.37	1.43
3	D	304	SAH	O2'-C2'	-2.27	1.37	1.43
3	A	301	SAH	CA-N	2.25	1.52	1.47
3	D	304	SAH	CA-N	2.20	1.52	1.47
3	C	303	SAH	O2'-C2'	-2.16	1.37	1.43
4	A	306	FRE	C5-C6	2.06	1.42	1.38
3	B	302	SAH	CA-N	2.05	1.51	1.47
3	C	303	SAH	CA-N	2.03	1.51	1.47

All (50) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	A	306	FRE	C6P-C5P-N4P	6.11	126.70	116.42
4	A	306	FRE	O5P-C5P-C6P	-6.05	110.95	122.02
4	A	306	FRE	OAP-CAP-CBP	5.96	124.28	110.25
4	A	306	FRE	C3P-N4P-C5P	-5.40	112.81	122.84
4	A	306	FRE	C2P-S1P-C9	5.31	106.47	99.80
4	A	306	FRE	C7P-N8P-C9P	-5.25	113.23	122.59
4	A	306	FRE	C13-O13-C6	4.80	124.77	117.53
3	A	301	SAH	N3-C2-N1	-3.98	122.46	128.68
3	A	301	SAH	C2-N1-C6	3.83	125.31	118.75
3	C	303	SAH	C2-N1-C6	3.78	125.22	118.75
3	D	304	SAH	N3-C2-N1	-3.77	122.79	128.68
3	D	304	SAH	C2-N1-C6	3.77	125.20	118.75
3	B	302	SAH	C2-N1-C6	3.75	125.16	118.75
3	B	302	SAH	N3-C2-N1	-3.64	122.99	128.68
4	A	306	FRE	O13-C6-C1	3.58	118.15	114.54
4	A	306	FRE	C5-C6-C1	-3.54	117.11	120.60
3	C	303	SAH	N3-C2-N1	-3.49	123.22	128.68
3	C	303	SAH	C4-C5-N7	3.39	112.94	109.40
3	C	303	SAH	O2'-C2'-C3'	3.39	122.79	111.82
3	A	301	SAH	O2'-C2'-C3'	3.28	122.42	111.82
3	D	304	SAH	C4-C5-N7	3.24	112.78	109.40
3	B	302	SAH	C4-C5-N7	3.19	112.72	109.40
3	D	304	SAH	O2'-C2'-C3'	3.14	121.97	111.82
3	D	304	SAH	N6-C6-N1	3.10	125.01	118.57
3	B	302	SAH	O2'-C2'-C3'	3.02	121.58	111.82
3	C	303	SAH	N6-C6-N1	3.01	124.83	118.57
3	B	302	SAH	N6-C6-N1	2.90	124.60	118.57
3	C	303	SAH	C5-C6-N1	-2.89	113.79	120.35
4	A	306	FRE	C5A-C6A-N6A	2.88	124.73	120.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	301	SAH	C5-C6-N1	-2.86	113.87	120.35
3	D	304	SAH	C5-C6-N1	-2.83	113.94	120.35
3	B	302	SAH	C5-C6-N1	-2.82	113.96	120.35
3	B	302	SAH	C5'-C4'-C3'	2.78	122.00	115.06
4	A	306	FRE	C4-C5-C6	2.77	123.92	120.17
3	A	301	SAH	O4'-C1'-C2'	2.72	110.90	106.93
3	A	301	SAH	C4-C5-N7	2.56	112.07	109.40
3	C	303	SAH	O4'-C4'-C5'	2.51	115.30	108.83
3	A	301	SAH	N6-C6-N1	2.48	123.72	118.57
3	C	303	SAH	O2'-C2'-C1'	2.40	119.71	110.85
3	A	301	SAH	C5'-C4'-C3'	2.40	121.04	115.06
3	D	304	SAH	O2'-C2'-C1'	2.38	119.65	110.85
3	A	301	SAH	O2'-C2'-C1'	2.35	119.54	110.85
3	B	302	SAH	O2'-C2'-C1'	2.35	119.53	110.85
3	A	301	SAH	O4'-C4'-C5'	2.27	114.67	108.83
3	D	304	SAH	O4'-C4'-C5'	2.25	114.61	108.83
4	A	306	FRE	O3B-P3B-O9A	-2.16	101.05	109.39
3	A	301	SAH	O4'-C4'-C3'	-2.13	100.91	105.11
3	B	302	SAH	O4'-C4'-C3'	-2.10	100.95	105.11
4	A	306	FRE	P2A-O6A-CCP	-2.02	109.92	121.56
4	A	306	FRE	C3-C2-C1	2.01	121.85	120.47

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	A	306	FRE	CAP

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	306	FRE	C3B-C4B-C5B-O5B
4	A	306	FRE	O4B-C4B-C5B-O5B
4	A	306	FRE	C5B-O5B-P1A-O2A
4	A	306	FRE	CCP-O6A-P2A-O5A
4	A	306	FRE	CEP-CBP-CCP-O6A
4	A	306	FRE	CAP-CBP-CCP-O6A
4	A	306	FRE	OAP-CAP-CBP-CCP
4	A	306	FRE	C9P-CAP-CBP-CCP
4	A	306	FRE	C9P-CAP-CBP-CDP
4	A	306	FRE	OAP-CAP-CBP-CEP
4	A	306	FRE	C9P-CAP-CBP-CEP
4	A	306	FRE	C6P-C5P-N4P-C3P

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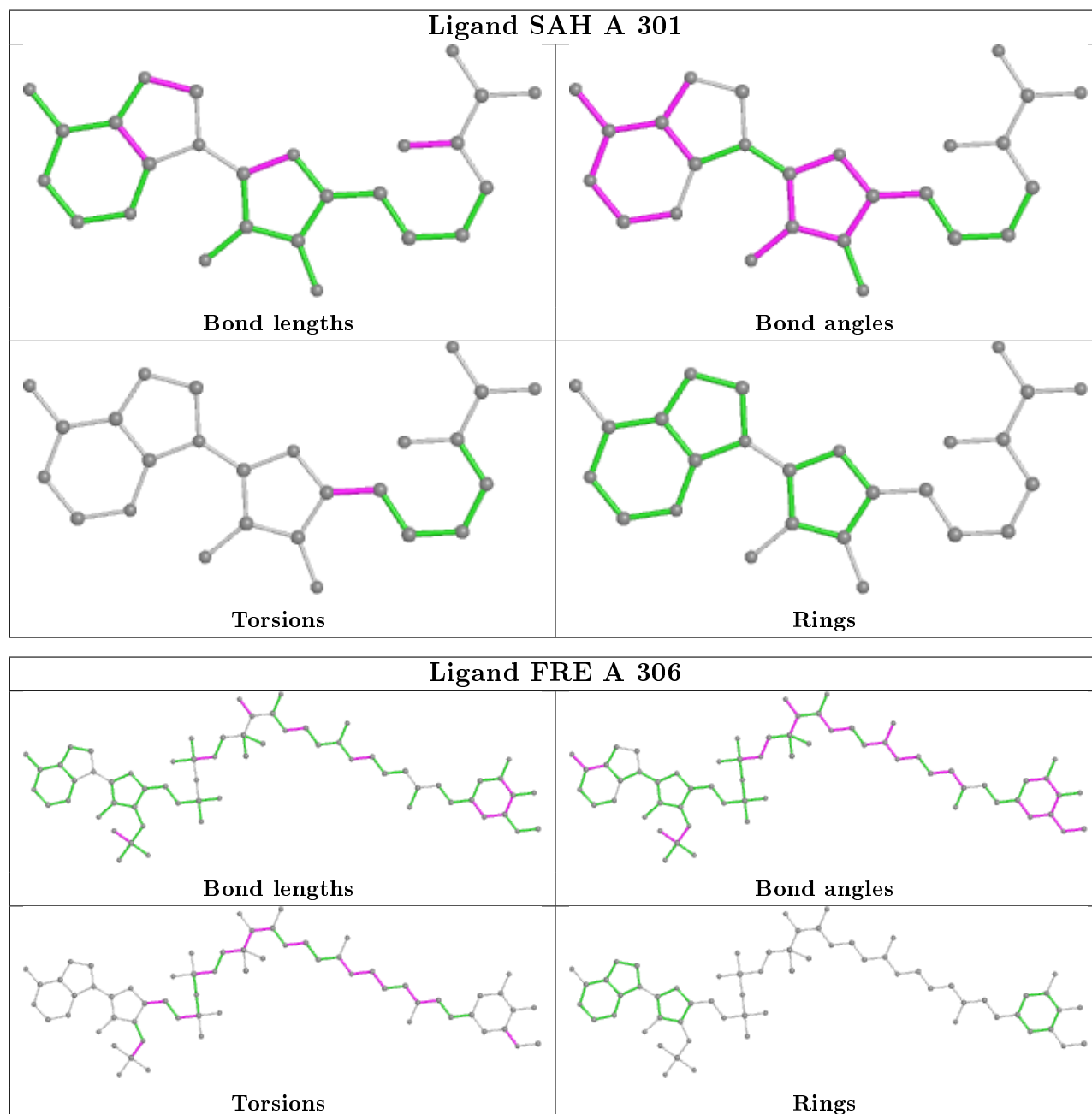
Mol	Chain	Res	Type	Atoms
4	A	306	FRE	C2P-C3P-N4P-C5P
4	A	306	FRE	S1P-C2P-C3P-N4P
4	A	306	FRE	C8-C9-S1P-C2P
4	A	306	FRE	O10-C9-S1P-C2P
3	A	301	SAH	O4'-C4'-C5'-SD
3	A	301	SAH	C3'-C4'-C5'-SD
3	B	302	SAH	CA-CB-CG-SD
3	B	302	SAH	O4'-C4'-C5'-SD
3	B	302	SAH	C3'-C4'-C5'-SD
3	C	303	SAH	O4'-C4'-C5'-SD
3	C	303	SAH	C3'-C4'-C5'-SD
3	D	304	SAH	CA-CB-CG-SD
4	A	306	FRE	C6P-C7P-N8P-C9P
4	A	306	FRE	O5P-C5P-N4P-C3P
3	C	303	SAH	CA-CB-CG-SD
4	A	306	FRE	C5-C6-O13-C13
4	A	306	FRE	CDP-CBP-CCP-O6A
4	A	306	FRE	C7-C8-C9-O10
4	A	306	FRE	C1-C6-O13-C13
4	A	306	FRE	OAP-CAP-CBP-CDP
3	D	304	SAH	CB-CG-SD-C5'
4	A	306	FRE	C3B-O3B-P3B-O7A
4	A	306	FRE	C5B-O5B-P1A-O3A
4	A	306	FRE	CCP-O6A-P2A-O3A
3	D	304	SAH	C3'-C4'-C5'-SD
4	A	306	FRE	C5B-O5B-P1A-O1A
4	A	306	FRE	CCP-O6A-P2A-O4A
3	B	302	SAH	CB-CG-SD-C5'
3	D	304	SAH	O4'-C4'-C5'-SD
4	A	306	FRE	O9P-C9P-CAP-OAP
4	A	306	FRE	N8P-C9P-CAP-OAP
4	A	306	FRE	O9P-C9P-CAP-CBP

There are no ring outliers.

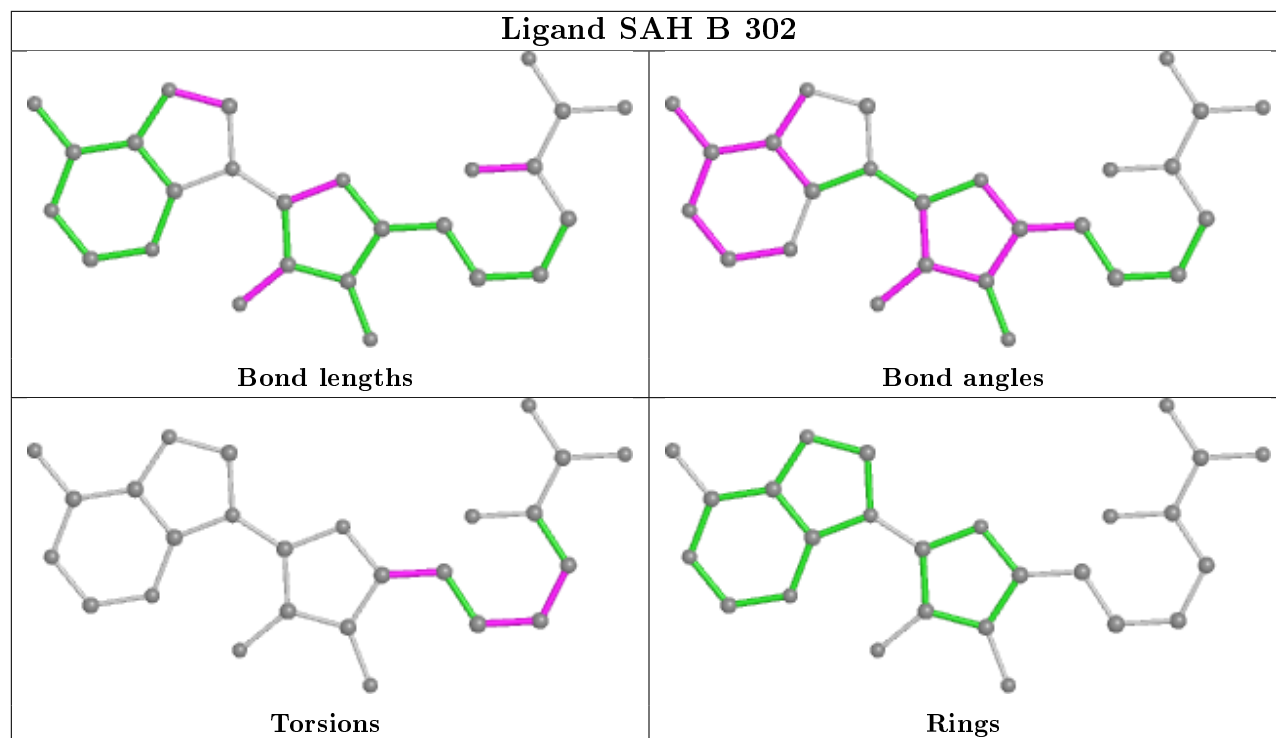
5 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	301	SAH	3	0
4	A	306	FRE	6	0
3	B	302	SAH	2	0
3	C	303	SAH	6	0
3	D	304	SAH	4	0

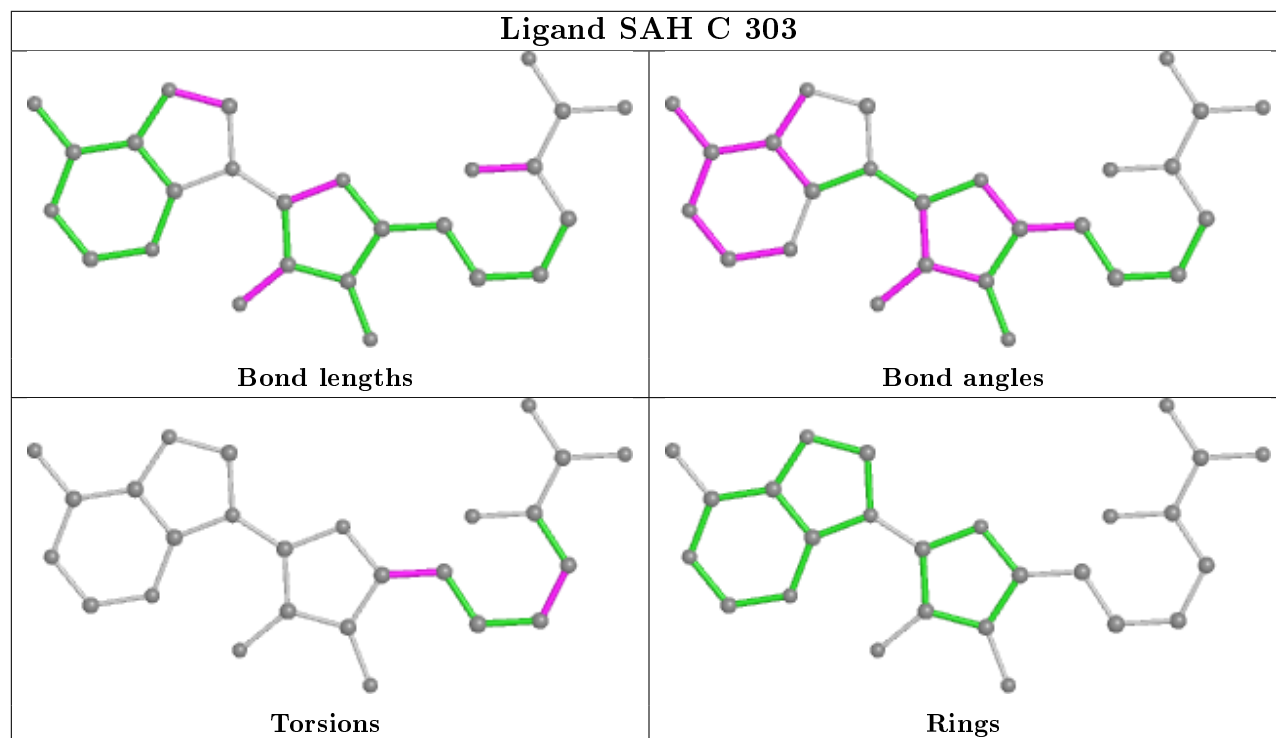
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

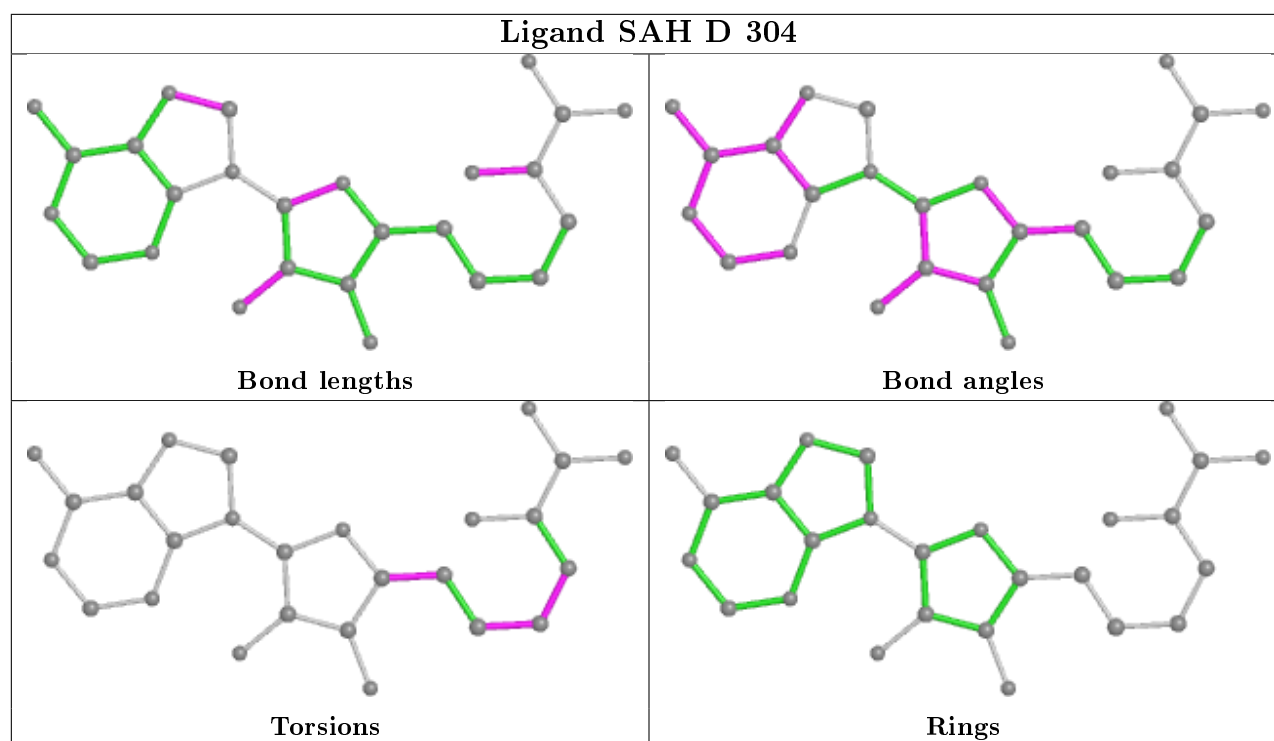


## Ligand SAH B 302



## Ligand SAH C 303





## 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	227/247 (91%)	-0.13	4 (1%) 68 70	37, 54, 83, 98	0
1	B	227/247 (91%)	-0.02	10 (4%) 34 33	41, 56, 87, 103	0
1	C	227/247 (91%)	0.39	19 (8%) 11 9	53, 84, 117, 130	0
1	D	227/247 (91%)	0.95	37 (16%) 1 1	89, 122, 140, 147	0
All	All	908/988 (91%)	0.30	70 (7%) 13 11	37, 72, 134, 147	0

All (70) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	41	ARG	6.2
1	B	203	ALA	5.5
1	C	201	PRO	5.2
1	D	201	PRO	5.1
1	D	161	PHE	4.9
1	D	162	VAL	4.4
1	D	246	ILE	4.4
1	D	175	ARG	4.2
1	D	104	ASP	4.2
1	C	84	MET	4.0
1	B	62	THR	3.9
1	D	102	PRO	3.8
1	C	162	VAL	3.8
1	D	247	LYS	3.7
1	C	202	ASP	3.7
1	B	201	PRO	3.6
1	C	111	ASP	3.5
1	C	161	PHE	3.5
1	B	202	ASP	3.5
1	B	187	GLY	3.4
1	C	247	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	C	200	PRO	3.3
1	D	85	GLU	3.2
1	C	85	GLU	3.1
1	D	86	ILE	3.0
1	D	187	GLY	3.0
1	D	48	GLU	3.0
1	D	152	LYS	2.9
1	C	86	ILE	2.9
1	D	160	ILE	2.9
1	D	93	SER	2.9
1	D	80	ALA	2.9
1	C	93	SER	2.8
1	C	203	ALA	2.8
1	D	27	ASP	2.7
1	D	188	TYR	2.6
1	C	83	THR	2.6
1	C	204	PRO	2.5
1	D	84	MET	2.5
1	D	163	ASP	2.5
1	D	181	LYS	2.5
1	D	151	GLU	2.4
1	D	103	GLU	2.4
1	C	188	TYR	2.4
1	B	161	PHE	2.4
1	B	204	PRO	2.4
1	D	105	GLY	2.4
1	B	152	LYS	2.4
1	D	125	LYS	2.4
1	D	87	GLY	2.3
1	C	110	MET	2.3
1	D	79	ASN	2.3
1	C	61	MET	2.3
1	D	166	LYS	2.3
1	A	161	PHE	2.3
1	C	60	ILE	2.3
1	D	241	THR	2.3
1	D	95	LEU	2.2
1	B	195	GLY	2.2
1	A	86	ILE	2.1
1	D	132	LYS	2.1
1	A	240	ILE	2.1
1	C	187	GLY	2.1

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Mol	Chain	Res	Type	RSRZ
1	D	81	LYS	2.1
1	B	115	GLU	2.1
1	D	129	VAL	2.1
1	D	115	GLU	2.1
1	D	112	ILE	2.0
1	A	85	GLU	2.0
1	D	42	GLU	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 carbohydrates 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<sup>th</sup> 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.

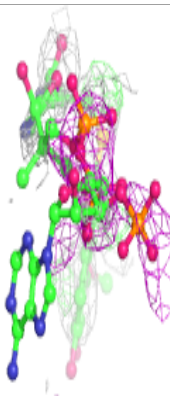
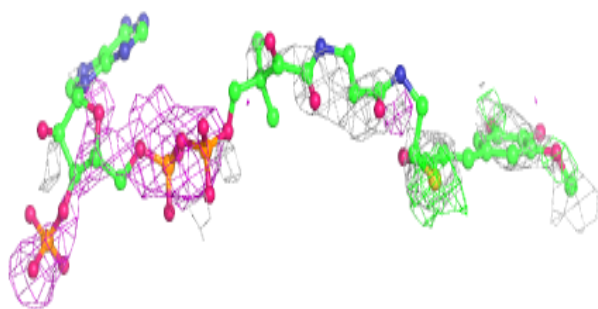
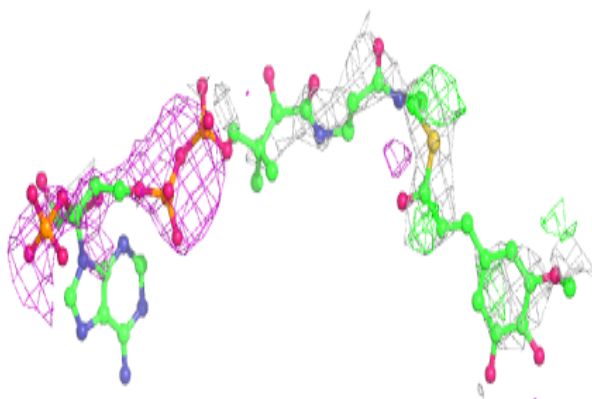
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
4	FRE	A	306	62/62	0.26	0.78	158,178,190,190	1
3	SAH	C	303	26/26	0.29	0.69	167,180,181,181	0
3	SAH	B	302	26/26	0.46	0.49	116,133,134,135	0
3	SAH	D	304	26/26	0.74	0.29	139,142,144,145	0
2	CA	C	307	1/1	0.86	0.16	90,90,90,90	0
3	SAH	A	301	26/26	0.91	0.24	41,54,65,69	0
2	CA	B	306	1/1	0.92	0.17	63,63,63,63	0
2	CA	A	305	1/1	0.92	0.26	59,59,59,59	0
2	CA	D	308	1/1	0.97	0.24	88,88,88,88	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.

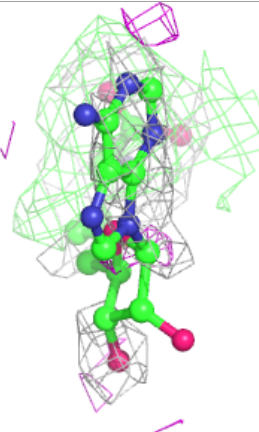
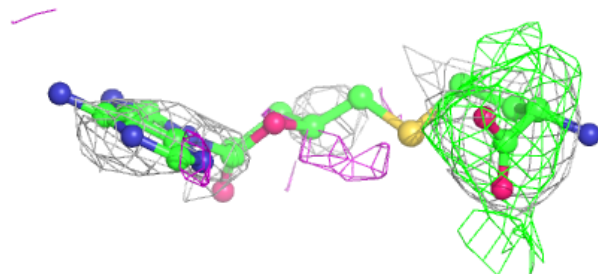
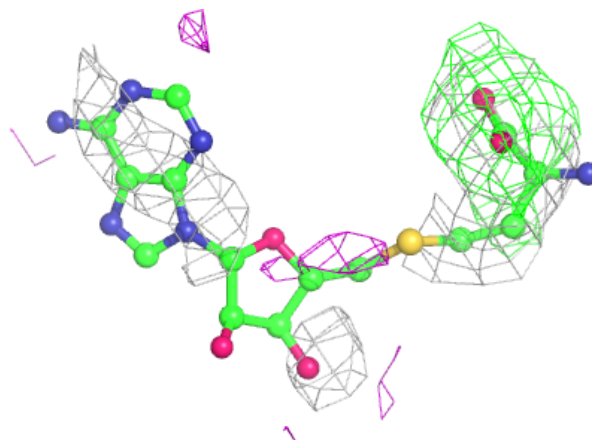


**Electron density around FRE A 306:**

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

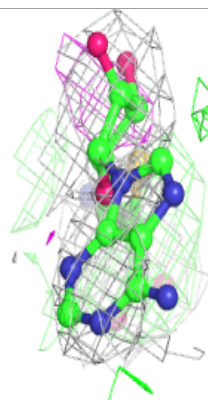
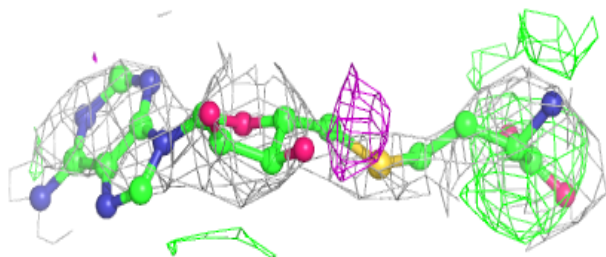
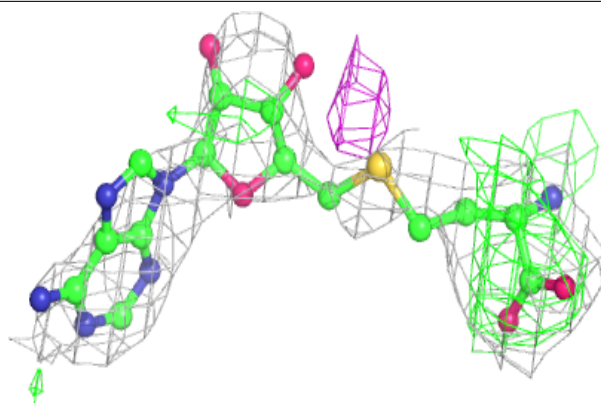
**Electron density around SAH C 303:**

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

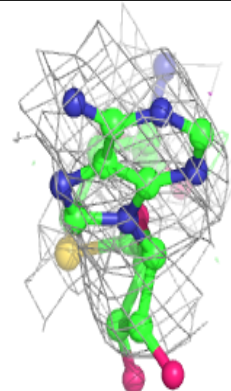
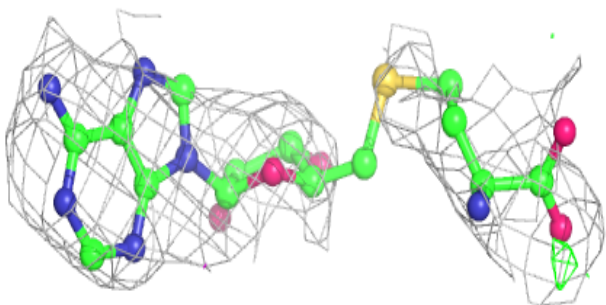
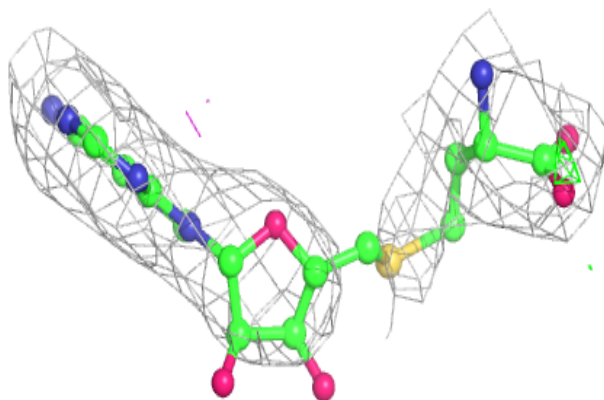


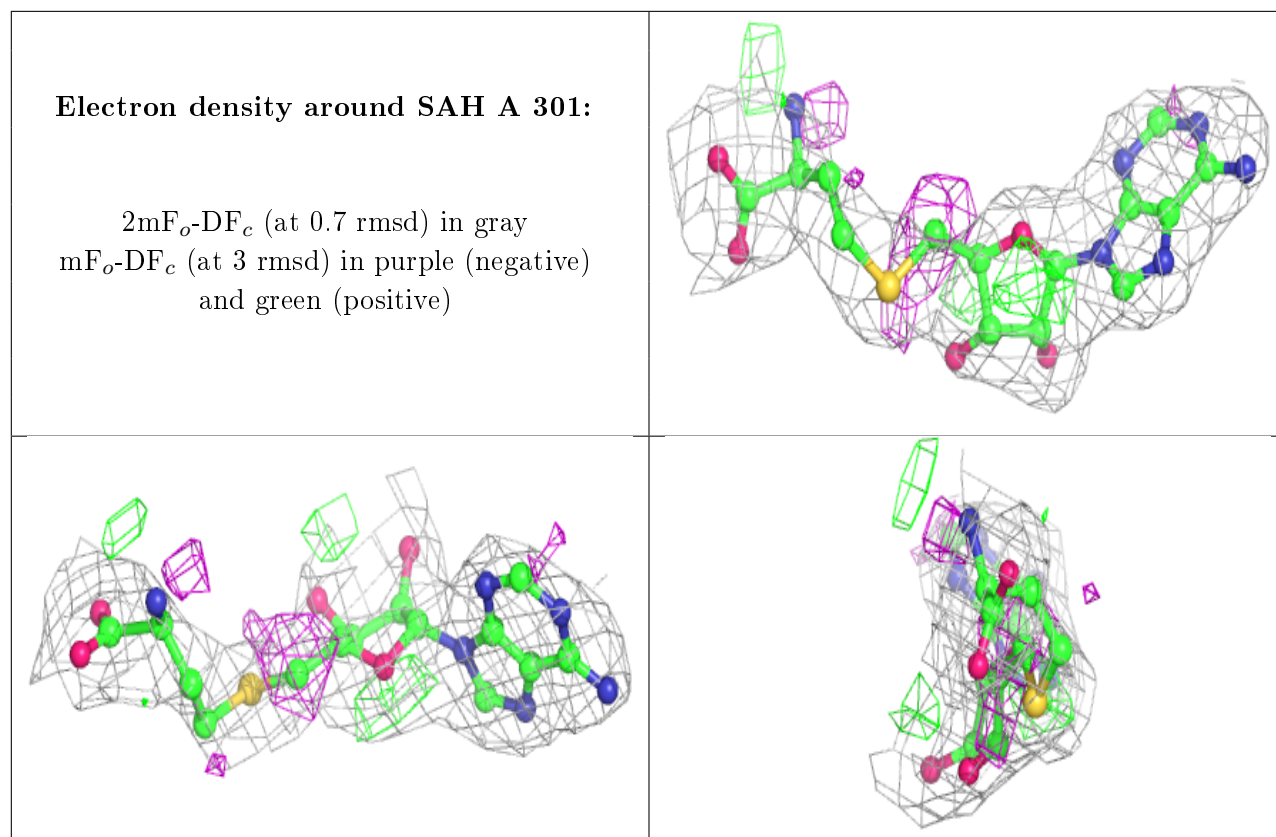
**Electron density around SAH B 302:**

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

**Electron density around SAH D 304:**

$2mF_o-DF_c$  (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.