



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 18, 2026 – 12:07 AM UTC

PDB ID : 1KYZ / pdb_00001kyz
Title : Crystal Structure Analysis of Caffeic acid/5-hydroxyferulic acid 3/5-O-methyltransferase Ferulic Acid Complex
Authors : Zubietta, C.; Kota, P.; Ferrer, J.-L.; Dixon, R.A.; Noel, J.P.
Deposited on : 2002-02-06
Resolution : 2.20 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

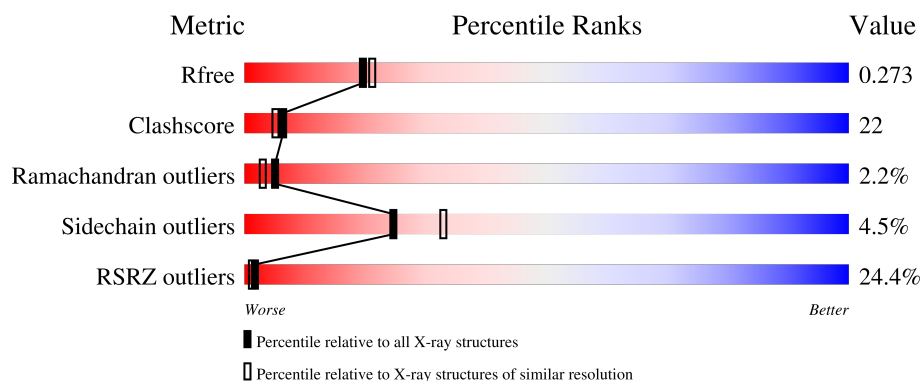
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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	6164 (2.20-2.20)
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	A	365	
1	C	365	
1	E	365	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	SAH	A	1698	X	-	X	-
3	SAH	C	1699	X	-	X	-
3	SAH	E	1697	X	-	-	-

2 Entry composition [i](#)

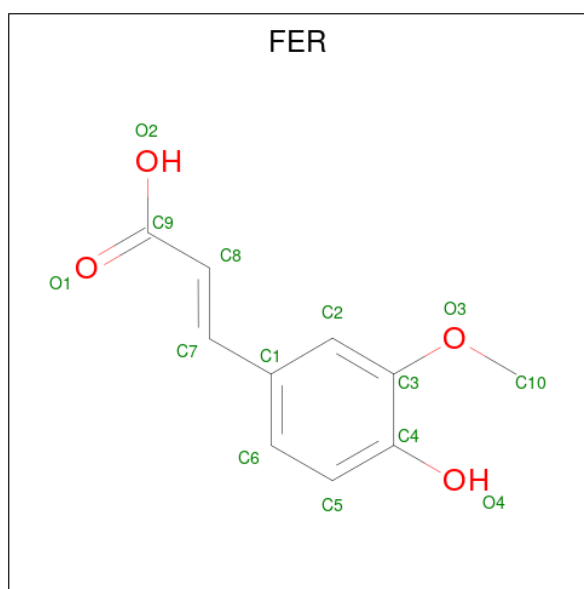
There are 4 unique types of molecules in this entry. The entry contains 8594 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Caffeic acid 3-O-methyltransferase.

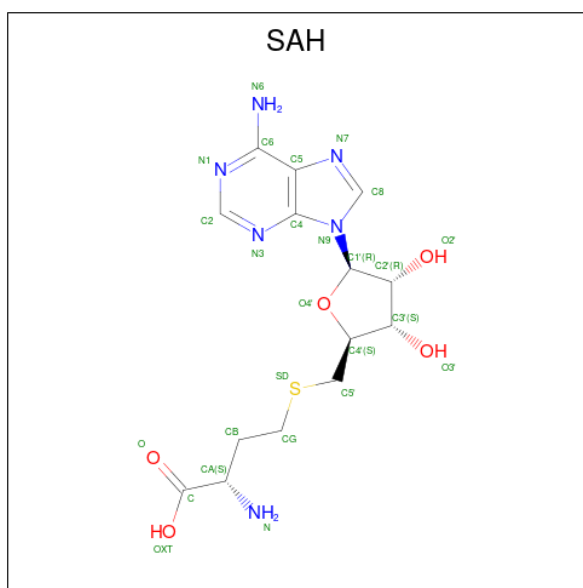
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	0	0
			2693	1728	442	503	20			
1	C	356	Total	C	N	O	S	0	0	0
			2740	1758	450	512	20			
1	E	361	Total	C	N	O	S	0	0	0
			2777	1780	456	521	20			

- Molecule 2 is 3-(4-HYDROXY-3-METHOXYPHENYL)-2-PROPENOIC ACID (CCD ID: FER) (formula: C₁₀H₁₀O₄).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	C	O	0	0
			14	10	4		
2	C	1	Total	C	O	0	0
			14	10	4		
2	E	1	Total	C	O	0	0
			14	10	4		

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



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

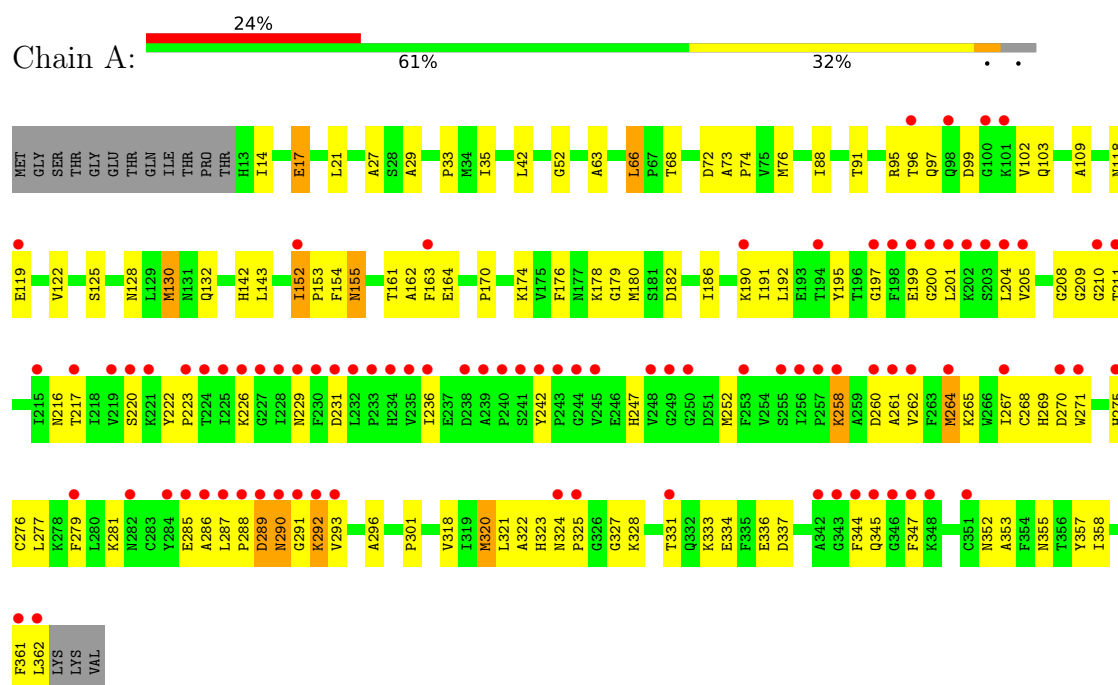
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	91	Total	O	0	0
			91	91		
4	C	55	Total	O	0	0
			55	55		
4	E	118	Total	O	0	0
			118	118		

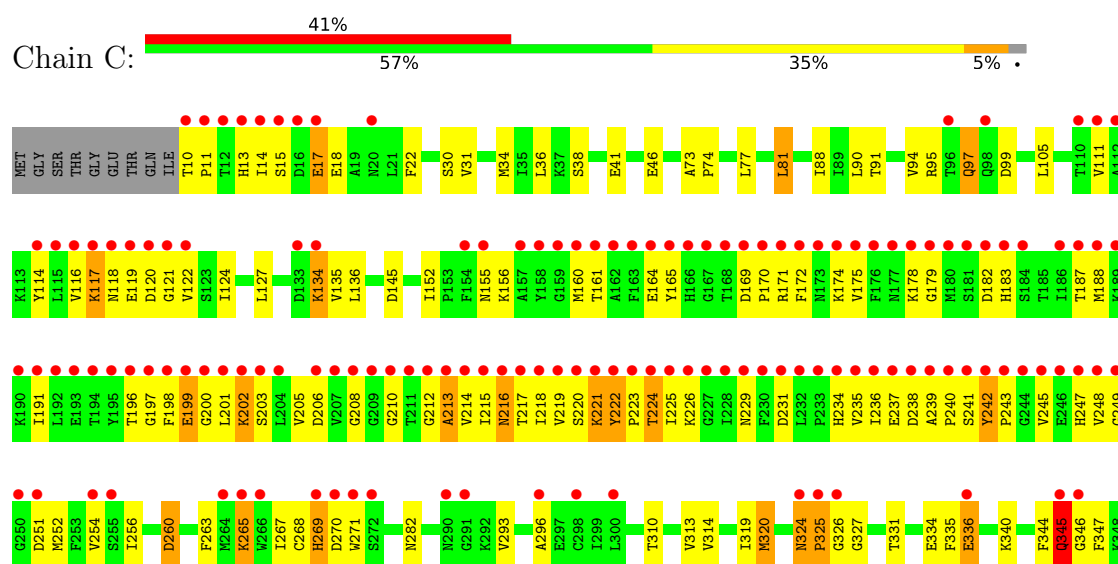
3 Residue-property plots [i](#)

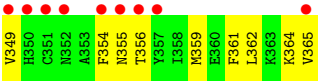
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Caffeic acid 3-O-methyltransferase

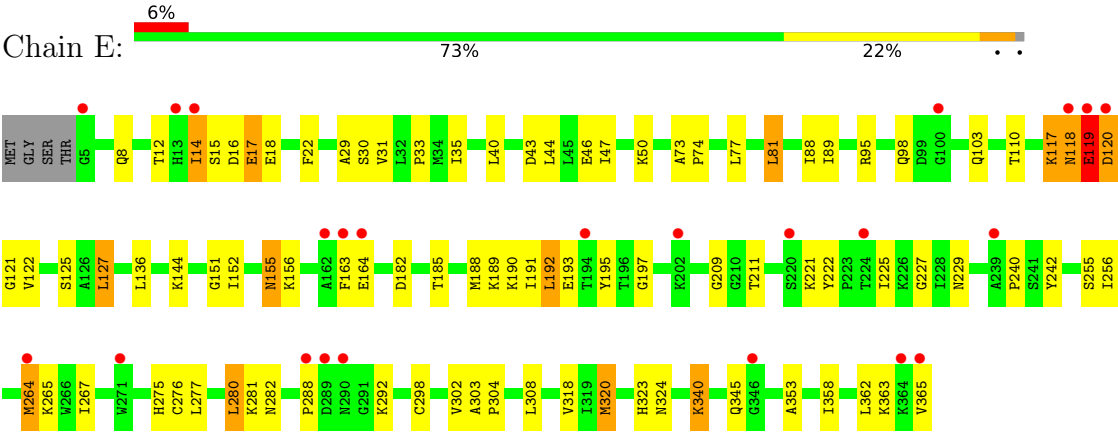


• Molecule 1: Caffeic acid 3-O-methyltransferase





● Molecule 1: Caffeic acid 3-O-methyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	103.73Å 61.87Å 111.23Å 90.00° 112.18° 90.00°	Depositor
Resolution (Å)	61.87 – 2.20 61.87 – 2.20	Depositor EDS
% Data completeness (in resolution range)	97.9 (61.87-2.20) 97.9 (61.87-2.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.83 (at 2.00Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.236 , 0.274 0.235 , 0.273	Depositor DCC
R_{free} test set	3779 reflections (4.36%)	wwPDB-VP
Wilson B-factor (Å ²)	26.8	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 42.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8594	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.52% 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: FER, SAH

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.39	1/2752 (0.0%)	0.88	6/3730 (0.2%)
1	C	0.37	0/2800	0.87	5/3794 (0.1%)
1	E	0.41	0/2837	0.90	8/3844 (0.2%)
All	All	0.39	1/8389 (0.0%)	0.88	19/11368 (0.2%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	130	MET	SD-CE	-5.90	1.64	1.79

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	119	GLU	N-CA-C	-8.75	92.16	110.80
1	A	301	PRO	N-CA-C	-7.76	99.78	111.57
1	C	222	TYR	N-CA-C	-6.62	96.92	108.97
1	E	117	LYS	N-CA-C	6.39	118.11	110.19
1	C	91	THR	N-CA-C	-6.02	101.09	110.42
1	C	222	TYR	CA-C-N	5.82	127.11	119.84
1	C	222	TYR	C-N-CA	5.82	127.11	119.84
1	E	298	CYS	N-CA-C	-5.76	102.92	110.53
1	E	89	ILE	N-CA-C	-5.74	105.50	111.58
1	A	290	ASN	N-CA-C	-5.45	106.63	113.28
1	A	109	ALA	N-CA-C	-5.41	102.74	110.59
1	E	16	ASP	N-CA-C	5.26	118.48	111.75
1	E	44	LEU	N-CA-C	5.24	116.99	111.28
1	A	91	THR	N-CA-C	-5.21	102.35	110.42
1	E	227	GLY	N-CA-C	5.16	118.56	111.54
1	C	319	ILE	N-CA-C	-5.13	105.38	110.62
1	A	52	GLY	CA-C-N	5.10	125.38	119.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	52	GLY	C-N-CA	5.10	125.38	119.93
1	E	225	ILE	N-CA-C	5.04	115.55	108.89

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2693	0	2701	115	0
1	C	2740	0	2757	167	1
1	E	2777	0	2792	77	0
2	A	14	0	8	0	0
2	C	14	0	9	1	0
2	E	14	0	8	2	0
3	A	26	0	17	9	0
3	C	26	0	17	9	0
3	E	26	0	17	8	0
4	A	91	0	0	1	0
4	C	55	0	0	3	0
4	E	118	0	0	3	0
All	All	8594	0	8326	366	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (366) 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)
3:A:1698:SAH:C5'	3:A:1698:SAH:O4'	1.91	1.17
3:C:1699:SAH:C5'	3:C:1699:SAH:O4'	1.92	1.17
3:E:1697:SAH:C5'	3:E:1697:SAH:O4'	1.92	1.16
3:C:1699:SAH:C4'	3:C:1699:SAH:SD	2.35	1.14
3:E:1697:SAH:C4'	3:E:1697:SAH:SD	2.35	1.14
3:C:1699:SAH:C5'	3:C:1699:SAH:C3'	2.25	1.13

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:E:1697:SAH:C5'	3:E:1697:SAH:C3'	2.25	1.13
3:A:1698:SAH:C4'	3:A:1698:SAH:SD	2.37	1.12
3:A:1698:SAH:C5'	3:A:1698:SAH:C3'	2.26	1.11
1:E:320:MET:HE3	1:E:320:MET:HA	1.34	1.06
1:C:202:LYS:HA	1:C:225:ILE:HA	1.43	1.00
1:A:216:ASN:HD22	1:A:242:TYR:HB3	1.24	0.98
3:E:1697:SAH:C4'	3:E:1697:SAH:H5'2	1.46	0.98
3:A:1698:SAH:C4'	3:A:1698:SAH:H5'1	1.46	0.98
3:C:1699:SAH:C4'	3:C:1699:SAH:H5'2	1.47	0.97
3:E:1697:SAH:C4'	3:E:1697:SAH:H5'1	1.46	0.97
3:C:1699:SAH:C4'	3:C:1699:SAH:H5'1	1.47	0.96
3:A:1698:SAH:C4'	3:A:1698:SAH:H5'2	1.46	0.95
1:C:212:GLY:C	1:C:216:ASN:HB2	1.92	0.95
1:E:320:MET:HE2	1:E:324:ASN:HB2	1.49	0.93
1:A:130:MET:HE3	1:A:179:GLY:HA3	1.47	0.93
1:C:11:PRO:HG3	1:C:14:ILE:HD11	1.55	0.88
1:C:222:TYR:HB3	1:C:225:ILE:HD13	1.56	0.88
1:C:134:LYS:HE2	1:C:134:LYS:H	1.38	0.87
1:C:320:MET:HA	1:C:320:MET:HE3	1.57	0.86
1:A:331:THR:HG22	1:A:334:GLU:HG3	1.58	0.85
1:C:134:LYS:H	1:C:134:LYS:CE	1.88	0.85
3:A:1698:SAH:C5'	3:A:1698:SAH:C4'	0.84	0.84
3:C:1699:SAH:C5'	3:C:1699:SAH:C4'	0.84	0.83
3:E:1697:SAH:C5'	3:E:1697:SAH:C4'	0.83	0.83
1:A:344:PHE:HD2	1:A:362:LEU:HB2	1.43	0.82
1:A:260:ASP:O	1:A:291:GLY:HA3	1.77	0.82
1:A:293:VAL:HB	1:A:361:PHE:HB2	1.62	0.82
1:A:216:ASN:ND2	1:A:242:TYR:HB3	1.97	0.79
1:C:345:GLN:NE2	1:C:364:LYS:H	1.81	0.79
1:A:292:LYS:HB2	1:A:361:PHE:O	1.82	0.77
1:E:95:ARG:HH21	1:E:103:GLN:NE2	1.83	0.77
1:C:145:ASP:HB3	1:C:156:LYS:HZ3	1.50	0.77
1:E:320:MET:HA	1:E:320:MET:CE	2.14	0.76
1:E:190:LYS:HG3	1:E:353:ALA:HB1	1.69	0.75
1:A:320:MET:HE3	1:A:320:MET:HA	1.69	0.74
1:C:220:SER:C	1:C:222:TYR:H	1.94	0.74
1:E:118:ASN:HA	1:E:121:GLY:H	1.53	0.74
1:C:331:THR:HG22	1:C:334:GLU:HG3	1.70	0.73
1:E:320:MET:HE2	1:E:324:ASN:CB	2.18	0.73
1:C:14:ILE:HG23	1:C:18:GLU:HG3	1.70	0.73
1:E:15:SER:HB2	1:E:17:GLU:OE2	1.88	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:136:LEU:HD21	2:E:1698:FER:H103	1.71	0.72
1:C:325:PRO:HG2	1:C:326:GLY:H	1.54	0.71
1:A:277:LEU:O	1:A:281:LYS:HG3	1.89	0.71
1:C:212:GLY:HA2	1:C:229:ASN:ND2	2.05	0.70
1:C:202:LYS:HG3	1:C:226:LYS:HB2	1.73	0.70
1:C:216:ASN:OD1	1:C:242:TYR:HD1	1.73	0.70
1:E:276:CYS:O	1:E:280:LEU:HB2	1.91	0.69
1:C:215:ILE:HG22	4:C:1703:HOH:O	1.92	0.69
1:C:160:MET:HE3	1:C:164:GLU:HB3	1.75	0.69
1:E:320:MET:HE1	2:E:1698:FER:C6	2.23	0.69
3:E:1697:SAH:O4'	3:E:1697:SAH:H5'1	1.75	0.69
1:C:320:MET:HE2	1:C:324:ASN:HB3	1.75	0.69
1:C:242:TYR:HB3	1:C:243:PRO:HD2	1.74	0.68
1:E:345:GLN:HG2	1:E:365:VAL:HG23	1.76	0.68
1:A:318:VAL:HG13	1:E:35:ILE:HD11	1.76	0.68
1:E:195:TYR:CZ	1:E:197:GLY:HA3	2.28	0.68
1:A:161:THR:OG1	1:A:164:GLU:HB2	1.92	0.68
1:A:252:MET:HE2	1:A:279:PHE:CD2	2.28	0.67
1:A:155:ASN:N	1:A:155:ASN:HD22	1.93	0.66
1:A:344:PHE:O	1:A:362:LEU:HA	1.96	0.66
1:A:170:PRO:O	1:A:174:LYS:HG2	1.95	0.66
1:A:320:MET:HE2	1:A:324:ASN:HB2	1.76	0.66
1:C:160:MET:HE2	1:C:165:TYR:N	2.11	0.66
1:C:170:PRO:O	1:C:174:LYS:HG3	1.95	0.65
1:C:242:TYR:CB	1:C:243:PRO:HD2	2.27	0.65
1:C:11:PRO:CG	1:C:14:ILE:HD11	2.25	0.65
1:C:169:ASP:OD2	1:C:172:PHE:HB2	1.97	0.65
1:C:251:ASP:OD2	1:C:254:VAL:HG23	1.97	0.65
1:A:152:ILE:HD11	1:A:323:HIS:C	2.21	0.64
1:C:218:ILE:O	1:C:221:LYS:HG2	1.96	0.64
1:A:130:MET:HE2	1:A:176:PHE:HA	1.80	0.64
1:E:255:SER:C	1:E:256:ILE:HD12	2.22	0.63
1:A:14:ILE:HD12	1:E:110:THR:OG1	1.98	0.63
1:C:320:MET:HG3	1:C:324:ASN:ND2	2.14	0.63
1:E:95:ARG:HH21	1:E:103:GLN:HE22	1.46	0.63
1:C:117:LYS:HB3	1:C:121:GLY:HA2	1.79	0.62
1:C:145:ASP:HB3	1:C:156:LYS:NZ	2.13	0.62
1:E:77:LEU:O	1:E:81:LEU:HD22	1.99	0.62
1:A:344:PHE:CD2	1:A:362:LEU:HB2	2.29	0.62
3:C:1699:SAH:O4'	3:C:1699:SAH:H5'1	1.79	0.62
1:E:117:LYS:O	1:E:118:ASN:HB2	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:152:ILE:N	1:E:152:ILE:HD12	2.15	0.62
1:E:122:VAL:HG13	1:E:182:ASP:CG	2.25	0.61
1:E:345:GLN:OE1	1:E:363:LYS:HA	2.00	0.61
1:C:202:LYS:CA	1:C:225:ILE:HA	2.25	0.61
1:C:344:PHE:O	1:C:362:LEU:O	2.19	0.61
1:A:331:THR:HG22	1:A:334:GLU:CG	2.28	0.61
1:C:320:MET:C	1:C:324:ASN:HD22	2.09	0.61
1:C:336:GLU:OE1	1:C:340:LYS:HG3	2.00	0.61
1:C:234:HIS:O	1:C:237:GLU:HG2	2.01	0.60
1:A:27:ALA:HB1	1:E:127:LEU:HB3	1.83	0.60
1:E:340:LYS:NZ	1:E:340:LYS:HB3	2.17	0.60
1:A:252:MET:HE2	1:A:279:PHE:CG	2.36	0.60
1:C:203:SER:HB3	1:C:260:ASP:H	1.66	0.60
1:E:15:SER:O	1:E:18:GLU:HG2	2.01	0.60
1:C:88:ILE:O	1:C:88:ILE:HG22	2.00	0.60
1:C:237:GLU:HG3	1:C:238:ASP:N	2.17	0.60
1:E:264:MET:HG2	1:E:267:ILE:HB	1.84	0.60
1:A:88:ILE:O	1:A:88:ILE:HG22	2.02	0.59
1:A:361:PHE:O	1:A:362:LEU:HB3	2.02	0.59
1:E:191:ILE:HD13	1:E:358:ILE:HD11	1.84	0.59
1:C:336:GLU:HG2	1:C:347:PHE:CG	2.37	0.59
1:C:77:LEU:O	1:C:81:LEU:HD22	2.02	0.59
1:C:212:GLY:O	1:C:216:ASN:N	2.31	0.59
1:C:331:THR:HG22	1:C:334:GLU:CG	2.32	0.59
1:C:220:SER:C	1:C:222:TYR:N	2.61	0.59
1:C:188:MET:HE3	1:C:191:ILE:HB	1.84	0.59
1:C:320:MET:HG3	1:C:324:ASN:HD22	1.68	0.58
1:C:122:VAL:HG13	1:C:182:ASP:HA	1.85	0.58
1:C:122:VAL:HA	1:C:182:ASP:OD2	2.02	0.58
1:C:38:SER:HA	1:C:41:GLU:OE1	2.02	0.58
1:C:331:THR:HG23	1:C:334:GLU:H	1.69	0.58
1:C:14:ILE:HG23	1:C:18:GLU:CG	2.34	0.58
1:C:268:CYS:C	1:C:270:ASP:H	2.12	0.58
1:C:364:LYS:HE2	1:C:364:LYS:O	2.03	0.58
1:A:182:ASP:O	1:A:186:ILE:HG12	2.03	0.58
1:C:216:ASN:OD1	1:C:242:TYR:CD1	2.56	0.58
1:E:88:ILE:O	1:E:88:ILE:HG22	2.04	0.58
1:E:119:GLU:OE1	1:E:185:THR:HG22	2.04	0.58
1:A:97:GLN:HB3	1:A:99:ASP:OD1	2.04	0.58
1:E:188:MET:HE3	1:E:192:LEU:HD13	1.86	0.58
3:A:1698:SAH:O4'	3:A:1698:SAH:H5'1	1.75	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:310:THR:O	1:C:313:VAL:HG12	2.05	0.57
1:E:155:ASN:N	1:E:155:ASN:HD22	2.01	0.57
1:C:331:THR:CG2	1:C:334:GLU:HG3	2.34	0.57
1:A:17:GLU:CD	1:A:17:GLU:H	2.13	0.57
1:A:287:LEU:C	1:A:289:ASP:H	2.14	0.56
1:C:344:PHE:O	1:C:346:GLY:N	2.38	0.56
1:A:119:GLU:OE1	1:A:119:GLU:N	2.34	0.56
1:C:46:GLU:OE2	1:C:116:VAL:HG13	2.05	0.56
1:A:320:MET:HE2	1:A:324:ASN:CB	2.34	0.56
1:A:130:MET:HE2	1:A:176:PHE:O	2.05	0.56
1:A:211:THR:HG22	1:A:242:TYR:OH	2.06	0.56
1:A:258:LYS:H	1:A:258:LYS:HD3	1.71	0.56
1:A:333:LYS:HE2	1:A:337:ASP:OD1	2.06	0.56
1:A:88:ILE:HG13	1:E:12:THR:O	2.06	0.55
1:A:336:GLU:HG2	1:A:347:PHE:CD2	2.41	0.55
1:A:318:VAL:HG11	1:E:31:VAL:HG13	1.89	0.55
1:C:252:MET:HG2	3:C:1699:SAH:N1	2.21	0.55
1:E:211:THR:HG23	1:E:240:PRO:HD2	1.89	0.55
1:C:160:MET:HE2	1:C:165:TYR:HA	1.89	0.55
1:A:216:ASN:HD22	1:A:242:TYR:CB	2.10	0.55
1:A:264:MET:HG2	1:A:267:ILE:HB	1.89	0.55
1:E:163:PHE:CE1	1:E:164:GLU:HG3	2.42	0.55
1:C:145:ASP:CB	1:C:156:LYS:HZ3	2.19	0.55
1:C:212:GLY:O	1:C:213:ALA:C	2.50	0.55
1:C:213:ALA:N	1:C:216:ASN:HB2	2.21	0.55
1:C:119:GLU:O	1:C:122:VAL:HB	2.07	0.54
1:C:196:THR:O	1:C:199:GLU:HG2	2.06	0.54
1:C:97:GLN:HA	1:C:97:GLN:OE1	2.06	0.54
1:C:324:ASN:OD1	1:C:327:GLY:N	2.41	0.54
1:C:171:ARG:O	1:C:175:VAL:HG23	2.07	0.54
1:C:320:MET:HE2	1:C:324:ASN:CB	2.36	0.54
1:A:152:ILE:HD11	1:A:323:HIS:O	2.07	0.53
1:A:292:LYS:HG2	1:A:293:VAL:N	2.22	0.53
1:C:135:VAL:HB	1:C:172:PHE:CE1	2.43	0.53
1:A:271:TRP:HB3	1:A:275:HIS:HB2	1.89	0.53
1:C:15:SER:OG	1:C:17:GLU:HG3	2.09	0.53
1:C:324:ASN:OD1	1:C:324:ASN:C	2.52	0.53
1:E:189:LYS:O	1:E:193:GLU:HG3	2.08	0.53
1:C:134:LYS:H	1:C:134:LYS:HE3	1.74	0.53
1:E:256:ILE:HD13	1:E:282:ASN:HB3	1.91	0.53
1:C:160:MET:HE2	1:C:164:GLU:C	2.34	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:ASP:OD1	1:A:324:ASN:ND2	2.42	0.52
1:C:221:LYS:C	1:C:223:PRO:HD3	2.34	0.52
1:C:10:THR:HG23	1:C:22:PHE:CE2	2.45	0.52
1:A:142:HIS:HD2	4:A:1751:HOH:O	1.90	0.52
1:A:292:LYS:N	1:A:292:LYS:HD2	2.25	0.52
1:C:152:ILE:CD1	1:C:325:PRO:HA	2.39	0.52
1:C:13:HIS:HB2	4:C:1735:HOH:O	2.10	0.52
1:A:331:THR:CG2	1:A:334:GLU:HG3	2.36	0.52
1:C:320:MET:O	1:C:324:ASN:ND2	2.42	0.52
1:A:195:TYR:CZ	1:A:197:GLY:HA3	2.45	0.52
1:C:214:VAL:O	1:C:218:ILE:HB	2.10	0.52
1:C:215:ILE:O	1:C:217:THR:N	2.43	0.51
1:C:320:MET:HA	1:C:320:MET:CE	2.34	0.51
1:C:214:VAL:O	1:C:219:VAL:HG23	2.10	0.51
1:C:187:THR:O	1:C:191:ILE:HG13	2.09	0.51
1:A:265:LYS:HG2	3:A:1698:SAH:OXT	2.11	0.51
1:C:336:GLU:OE2	1:C:340:LYS:HE3	2.10	0.51
1:A:191:ILE:HD13	1:A:358:ILE:HD11	1.93	0.51
1:C:206:ASP:OD1	1:C:263:PHE:HD2	1.93	0.51
1:C:320:MET:CE	1:C:324:ASN:HB3	2.39	0.51
1:C:97:GLN:HB3	1:C:99:ASP:OD1	2.11	0.51
1:A:95:ARG:HD3	1:A:103:GLN:OE1	2.11	0.50
1:C:325:PRO:HG2	1:C:326:GLY:N	2.26	0.50
1:A:204:LEU:HD12	1:A:261:ALA:O	2.11	0.50
1:C:236:ILE:CG2	1:C:247:HIS:HB3	2.41	0.50
1:C:216:ASN:O	1:C:245:VAL:HG21	2.12	0.50
1:C:73:ALA:HB3	1:C:74:PRO:HD3	1.93	0.50
1:C:248:VAL:HG12	1:C:249:GLY:N	2.26	0.50
1:A:29:ALA:HB3	1:E:33:PRO:HB3	1.93	0.50
1:A:236:ILE:HG23	1:A:247:HIS:HB3	1.94	0.50
1:A:265:LYS:HA	1:A:296:ALA:HB3	1.94	0.50
1:C:320:MET:CB	1:C:324:ASN:HD22	2.25	0.50
1:A:154:PHE:CE2	1:A:162:ALA:HA	2.47	0.49
1:A:205:VAL:CG1	1:A:262:VAL:HG22	2.42	0.49
1:C:136:LEU:HG	1:C:172:PHE:HZ	1.76	0.49
1:E:190:LYS:HG3	1:E:353:ALA:CB	2.40	0.49
1:C:111:VAL:HG22	1:C:111:VAL:O	2.12	0.49
1:C:171:ARG:HG2	1:C:171:ARG:HH11	1.78	0.49
1:A:192:LEU:HD11	1:A:217:THR:HG22	1.94	0.49
1:A:320:MET:HG2	1:A:327:GLY:C	2.37	0.49
1:C:347:PHE:CE2	1:C:349:VAL:HG23	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:277:LEU:O	1:E:281:LYS:HG3	2.12	0.49
1:A:118:ASN:HD21	1:A:122:VAL:HB	1.77	0.49
1:A:209:GLY:HA3	1:A:229:ASN:ND2	2.28	0.49
1:C:223:PRO:C	1:C:225:ILE:H	2.21	0.49
1:C:119:GLU:HB3	1:C:122:VAL:O	2.12	0.48
1:C:160:MET:HE2	1:C:165:TYR:CA	2.42	0.48
1:A:288:PRO:C	1:A:290:ASN:N	2.71	0.48
1:A:102:VAL:HG11	1:E:302:VAL:CG1	2.43	0.48
1:A:125:SER:HA	1:A:128:ASN:ND2	2.28	0.48
1:E:323:HIS:HE1	4:E:1788:HOH:O	1.96	0.48
1:E:8:GLN:HG2	1:E:308:LEU:HD21	1.95	0.48
1:E:119:GLU:O	1:E:120:ASP:HB2	2.13	0.48
1:C:160:MET:CE	1:C:164:GLU:HB3	2.43	0.48
1:A:276:CYS:HA	1:A:279:PHE:CZ	2.48	0.48
1:A:281:LYS:O	1:A:285:GLU:HG3	2.13	0.48
1:C:241:SER:O	1:C:242:TYR:CD2	2.66	0.48
1:C:171:ARG:HG2	1:C:171:ARG:NH1	2.28	0.48
1:C:94:VAL:HG12	1:C:95:ARG:N	2.29	0.48
1:C:116:VAL:C	1:C:118:ASN:H	2.22	0.48
1:C:212:GLY:O	1:C:216:ASN:HB2	2.12	0.48
1:C:134:LYS:HE2	1:C:134:LYS:N	2.19	0.47
1:E:14:ILE:HD13	1:E:22:PHE:HB2	1.96	0.47
1:C:14:ILE:HG22	1:C:15:SER:O	2.14	0.47
1:C:197:GLY:C	1:C:199:GLU:H	2.21	0.47
1:C:210:GLY:HA2	1:C:235:VAL:HG11	1.96	0.47
1:C:320:MET:C	1:C:324:ASN:ND2	2.72	0.47
1:A:130:MET:CE	1:A:176:PHE:O	2.62	0.47
1:C:122:VAL:HG13	1:C:182:ASP:CA	2.44	0.47
1:E:46:GLU:O	1:E:50:LYS:HG3	2.14	0.47
1:A:130:MET:HE3	1:A:179:GLY:CA	2.33	0.47
1:C:336:GLU:HG2	1:C:347:PHE:CD2	2.49	0.47
1:C:136:LEU:HG	1:C:172:PHE:CZ	2.50	0.47
1:C:155:ASN:N	1:C:155:ASN:HD22	2.11	0.47
1:A:318:VAL:HG11	1:E:35:ILE:HG13	1.97	0.47
1:C:225:ILE:N	1:C:225:ILE:HD12	2.30	0.47
1:E:122:VAL:HG13	1:E:182:ASP:CB	2.45	0.47
1:E:256:ILE:HD13	1:E:282:ASN:CB	2.44	0.47
1:A:42:LEU:CD2	1:E:144:LYS:HG2	2.45	0.47
1:C:152:ILE:HD13	1:C:325:PRO:HA	1.96	0.46
1:C:293:VAL:HB	1:C:361:PHE:HB2	1.97	0.46
1:E:211:THR:HG23	1:E:240:PRO:CD	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:LEU:HD12	1:C:179:GLY:CA	2.45	0.46
1:E:240:PRO:HG2	1:E:242:TYR:CZ	2.50	0.46
1:A:63:ALA:O	1:A:66:LEU:HB2	2.16	0.46
1:E:95:ARG:NH2	1:E:103:GLN:NE2	2.59	0.46
1:E:119:GLU:O	1:E:120:ASP:CB	2.64	0.46
1:A:130:MET:CE	1:A:179:GLY:HA3	2.31	0.46
1:A:320:MET:HA	1:A:320:MET:CE	2.43	0.46
1:C:30:SER:O	1:C:34:MET:HG2	2.15	0.46
1:C:81:LEU:HD12	1:C:90:LEU:HD11	1.97	0.46
1:C:127:LEU:HD11	1:C:183:HIS:HB2	1.98	0.46
1:C:145:ASP:C	1:C:156:LYS:HZ3	2.24	0.46
1:C:320:MET:HE1	2:C:366:FER:C6	2.46	0.45
1:E:40:LEU:HD13	1:E:125:SER:HB3	1.97	0.45
1:C:202:LYS:H	1:C:225:ILE:HG13	1.82	0.45
1:C:208:GLY:O	3:C:1699:SAH:HB2	2.17	0.45
1:C:344:PHE:C	1:C:346:GLY:H	2.24	0.45
1:A:216:ASN:O	1:A:220:SER:HB2	2.17	0.45
1:C:178:LYS:O	1:C:182:ASP:OD1	2.34	0.45
1:C:212:GLY:O	1:C:214:VAL:N	2.49	0.45
1:A:122:VAL:HG12	1:A:186:ILE:HD11	1.99	0.45
1:A:288:PRO:O	1:A:289:ASP:OD1	2.35	0.45
1:A:352:ASN:HB3	1:A:357:TYR:CE2	2.52	0.45
1:C:320:MET:CG	1:C:324:ASN:HD22	2.29	0.45
1:E:275:HIS:HD2	4:E:1726:HOH:O	2.00	0.45
1:A:125:SER:HA	1:A:128:ASN:HD22	1.81	0.45
1:C:215:ILE:O	1:C:216:ASN:C	2.59	0.45
1:C:10:THR:N	4:C:1722:HOH:O	2.49	0.45
1:C:122:VAL:HG13	1:C:182:ASP:CB	2.47	0.45
1:C:205:VAL:O	1:C:205:VAL:HG13	2.16	0.45
1:C:216:ASN:HD21	1:C:240:PRO:HG2	1.82	0.45
1:C:344:PHE:C	1:C:346:GLY:N	2.75	0.45
1:C:256:ILE:HG12	1:C:282:ASN:HB3	1.99	0.44
1:C:202:LYS:HE3	1:C:226:LYS:HG3	1.98	0.44
1:C:265:LYS:HA	1:C:296:ALA:O	2.16	0.44
1:E:209:GLY:HA3	1:E:229:ASN:ND2	2.32	0.44
1:A:258:LYS:HD3	1:A:258:LYS:N	2.32	0.44
1:C:236:ILE:HG23	1:C:247:HIS:HB3	1.99	0.44
1:C:202:LYS:O	1:C:203:SER:HB2	2.17	0.44
1:C:354:PHE:C	1:C:356:THR:H	2.26	0.44
1:A:331:THR:CG2	1:A:334:GLU:H	2.30	0.44
1:C:212:GLY:HA2	1:C:229:ASN:HD22	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:313:VAL:HG13	1:C:314:VAL:N	2.32	0.44
1:E:14:ILE:CD1	1:E:22:PHE:HB2	2.47	0.44
1:A:286:ALA:O	1:A:288:PRO:HD3	2.18	0.44
1:A:333:LYS:HE2	1:A:337:ASP:CG	2.43	0.44
1:C:220:SER:O	1:C:222:TYR:N	2.51	0.44
1:A:226:LYS:HE2	1:A:226:LYS:HA	1.99	0.43
1:A:190:LYS:HB3	1:A:353:ALA:HB1	2.00	0.43
1:A:231:ASP:HB3	1:A:236:ILE:HG12	2.00	0.43
1:C:202:LYS:HB2	1:C:224:THR:O	2.17	0.43
1:C:114:TYR:HB3	1:C:124:ILE:HD12	1.99	0.43
1:E:110:THR:HG23	4:E:1802:HOH:O	2.17	0.43
1:C:320:MET:HG3	1:C:324:ASN:CB	2.49	0.43
1:A:153:PRO:HB2	1:A:322:ALA:O	2.18	0.43
1:E:151:GLY:C	1:E:152:ILE:HD12	2.43	0.43
1:C:267:ILE:O	1:C:271:TRP:HE3	2.01	0.43
1:E:14:ILE:HG23	1:E:15:SER:O	2.19	0.43
1:C:120:ASP:C	1:C:122:VAL:N	2.77	0.43
1:A:73:ALA:HB3	1:A:74:PRO:HD3	2.00	0.42
1:A:130:MET:HE1	1:A:180:MET:N	2.34	0.42
1:A:209:GLY:C	1:A:229:ASN:HD21	2.27	0.42
1:A:252:MET:HG2	3:A:1698:SAH:N1	2.34	0.42
1:A:264:MET:O	1:A:265:LYS:HB3	2.19	0.42
1:A:33:PRO:HB3	1:E:29:ALA:HB3	2.00	0.42
1:A:324:ASN:HA	1:A:325:PRO:HD3	1.72	0.42
1:E:152:ILE:O	1:E:156:LYS:HG3	2.19	0.42
1:C:203:SER:HB2	1:C:260:ASP:HB2	2.00	0.42
1:C:320:MET:HG3	1:C:324:ASN:HB3	2.00	0.42
1:E:292:LYS:HB3	1:E:362:LEU:HD23	2.00	0.42
1:C:155:ASN:N	1:C:155:ASN:ND2	2.68	0.42
1:C:268:CYS:O	1:C:270:ASP:N	2.50	0.42
1:A:35:ILE:HG13	1:E:318:VAL:HG11	2.00	0.42
1:A:331:THR:HG23	1:A:334:GLU:H	1.84	0.42
1:E:265:LYS:HG2	3:E:1697:SAH:OXT	2.20	0.42
1:C:210:GLY:N	1:C:231:ASP:OD2	2.47	0.42
1:E:221:LYS:HD3	1:E:222:TYR:CE1	2.54	0.42
1:A:72:ASP:O	1:A:76:MET:HG3	2.20	0.42
1:A:344:PHE:O	1:A:362:LEU:HD12	2.20	0.42
1:A:66:LEU:HB3	1:A:68:THR:HG22	2.01	0.42
1:A:152:ILE:HA	1:A:153:PRO:HD3	1.89	0.42
1:A:132:GLN:HE21	1:E:30:SER:CB	2.33	0.41
1:A:208:GLY:HA2	1:A:231:ASP:OD1	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:21:LEU:HB3	1:E:308:LEU:HB3	2.01	0.41
1:A:200:GLY:O	1:A:201:LEU:HG	2.20	0.41
1:C:325:PRO:CG	1:C:326:GLY:H	2.25	0.41
1:E:43:ASP:O	1:E:47:ILE:HG13	2.20	0.41
1:A:192:LEU:CD1	1:A:217:THR:HG22	2.49	0.41
1:E:73:ALA:HB3	1:E:74:PRO:HD3	2.01	0.41
1:A:118:ASN:ND2	1:A:122:VAL:HB	2.35	0.41
1:A:155:ASN:N	1:A:155:ASN:ND2	2.60	0.41
1:A:265:LYS:O	1:A:267:ILE:HG12	2.20	0.41
1:C:269:HIS:CD2	1:C:269:HIS:C	2.98	0.41
1:A:178:LYS:HE3	1:A:178:LYS:HB2	1.85	0.41
1:A:236:ILE:CG2	1:A:247:HIS:HB3	2.49	0.41
1:C:111:VAL:O	1:C:111:VAL:CG2	2.68	0.41
1:C:238:ASP:O	1:C:239:ALA:C	2.63	0.41
1:E:303:ALA:HA	1:E:304:PRO:HD3	1.90	0.41
1:C:210:GLY:HA2	1:C:235:VAL:CG1	2.50	0.41
1:C:335:PHE:CE1	1:C:359:MET:HE1	2.56	0.41
1:E:152:ILE:N	1:E:152:ILE:CD1	2.83	0.41
1:C:324:ASN:ND2	1:C:327:GLY:O	2.53	0.41
1:A:42:LEU:HD21	1:E:144:LYS:HG2	2.03	0.41
1:E:363:LYS:O	1:E:363:LYS:HG3	2.21	0.41
1:A:130:MET:HE1	1:A:180:MET:HG2	2.03	0.40
1:C:237:GLU:CG	1:C:238:ASP:N	2.83	0.40
1:E:163:PHE:CD1	1:E:164:GLU:HG3	2.56	0.40
1:A:288:PRO:C	1:A:290:ASN:H	2.28	0.40
1:C:95:ARG:HD3	1:C:105:LEU:HD11	2.04	0.40
1:A:344:PHE:HB3	1:A:362:LEU:N	2.35	0.40
1:C:365:VAL:HG13	1:C:365:VAL:OXT	2.20	0.40
1:E:14:ILE:HG12	1:E:18:GLU:CD	2.46	0.40
1:A:222:TYR:N	1:A:223:PRO:HD3	2.36	0.40
1:C:73:ALA:O	1:C:77:LEU:HG	2.22	0.40
1:C:202:LYS:HG2	1:C:203:SER:N	2.37	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:10:THR:N	1:C:10:THR:N[2_556]	2.18	0.02

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	348/365 (95%)	326 (94%)	18 (5%)	4 (1%)	11	10
1	C	354/365 (97%)	311 (88%)	29 (8%)	14 (4%)	2	1
1	E	359/365 (98%)	344 (96%)	10 (3%)	5 (1%)	9	7
All	All	1061/1095 (97%)	981 (92%)	57 (5%)	23 (2%)	5	3

All (23) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	199	GLU
1	C	216	ASN
1	C	345	GLN
1	E	119	GLU
1	E	120	ASP
1	A	268	CYS
1	C	161	THR
1	C	200	GLY
1	C	202	LYS
1	C	213	ALA
1	C	265	LYS
1	C	269	HIS
1	A	289	ASP
1	C	201	LEU
1	E	118	ASN
1	C	117	LYS
1	C	221	LYS
1	C	325	PRO
1	E	288	PRO
1	C	199	GLU
1	C	224	THR
1	E	98	GLN
1	A	210	GLY

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	294/307 (96%)	278 (95%)	16 (5%)	20	25
1	C	300/307 (98%)	286 (95%)	14 (5%)	23	31
1	E	304/307 (99%)	294 (97%)	10 (3%)	33	45
All	All	898/921 (98%)	858 (96%)	40 (4%)	24	33

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	17	GLU
1	A	66	LEU
1	A	96	THR
1	A	143	LEU
1	A	152	ILE
1	A	155	ASN
1	A	163	PHE
1	A	258	LYS
1	A	264	MET
1	A	269	HIS
1	A	292	LYS
1	A	320	MET
1	A	321	LEU
1	A	328	LYS
1	A	345	GLN
1	A	355	ASN
1	C	17	GLU
1	C	31	VAL
1	C	36	LEU
1	C	81	LEU
1	C	97	GLN
1	C	134	LYS
1	C	198	PHE
1	C	242	TYR
1	C	260	ASP
1	C	320	MET

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Mol	Chain	Res	Type
1	C	324	ASN
1	C	336	GLU
1	C	345	GLN
1	C	355	ASN
1	E	14	ILE
1	E	17	GLU
1	E	81	LEU
1	E	127	LEU
1	E	155	ASN
1	E	192	LEU
1	E	264	MET
1	E	280	LEU
1	E	320	MET
1	E	340	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (27) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	131	ASN
1	A	132	GLN
1	A	142	HIS
1	A	155	ASN
1	A	216	ASN
1	A	229	ASN
1	A	275	HIS
1	A	282	ASN
1	A	355	ASN
1	C	13	HIS
1	C	25	GLN
1	C	118	ASN
1	C	177	ASN
1	C	216	ASN
1	C	247	HIS
1	C	332	GLN
1	C	345	GLN
1	C	355	ASN
1	E	13	HIS
1	E	25	GLN
1	E	103	GLN
1	E	155	ASN
1	E	229	ASN
1	E	275	HIS

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Mol	Chain	Res	Type
1	E	323	HIS
1	E	332	GLN
1	E	350	HIS

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	SAH	C	1699	-	27,28,28	3.73	6 (22%)	36,40,40	3.27	12 (33%)
2	FER	A	366	-	14,14,14	1.82	5 (35%)	18,18,18	1.42	3 (16%)
3	SAH	A	1698	-	27,28,28	3.73	6 (22%)	36,40,40	3.26	12 (33%)
3	SAH	E	1697	-	27,28,28	3.76	6 (22%)	36,40,40	3.28	12 (33%)
2	FER	E	1698	-	14,14,14	1.99	5 (35%)	18,18,18	1.71	4 (22%)
2	FER	C	366	-	14,14,14	1.80	6 (42%)	18,18,18	1.41	3 (16%)

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	C	1699	-	2/2/6/6	1/15/31/31	0/3/3/3
2	FER	A	366	-	-	0/7/7/7	0/1/1/1
3	SAH	A	1698	-	2/2/6/6	2/15/31/31	0/3/3/3
3	SAH	E	1697	-	2/2/6/6	3/15/31/31	0/3/3/3
2	FER	E	1698	-	-	0/7/7/7	0/1/1/1
2	FER	C	366	-	-	0/7/7/7	0/1/1/1

All (34) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	1697	SAH	C5'-C4'	-17.70	0.83	1.52
3	C	1699	SAH	C5'-C4'	-17.58	0.84	1.52
3	A	1698	SAH	C5'-C4'	-17.54	0.84	1.52
2	E	1698	FER	C2-C3	4.62	1.46	1.38
3	E	1697	SAH	C2-N1	3.74	1.40	1.33
2	A	366	FER	C2-C3	3.53	1.44	1.38
3	A	1698	SAH	C5-C6	3.51	1.50	1.41
3	C	1699	SAH	C5-C6	3.49	1.50	1.41
2	C	366	FER	C2-C3	3.47	1.44	1.38
3	A	1698	SAH	C2-N1	3.43	1.40	1.33
3	C	1699	SAH	C2-N1	3.41	1.40	1.33
3	E	1697	SAH	C5-C6	3.28	1.50	1.41
3	C	1699	SAH	C4-N3	3.23	1.40	1.34
3	A	1698	SAH	C4-N3	3.20	1.40	1.34
2	E	1698	FER	C2-C1	2.99	1.45	1.39
3	E	1697	SAH	C4-N3	2.99	1.40	1.34
2	E	1698	FER	C4-C3	2.58	1.44	1.40
2	A	366	FER	C2-C1	2.56	1.44	1.39
2	C	366	FER	C4-C3	2.48	1.44	1.40
2	C	366	FER	C2-C1	2.46	1.44	1.39
2	A	366	FER	C4-C3	2.38	1.44	1.40
3	E	1697	SAH	C2-N3	2.33	1.38	1.33
3	E	1697	SAH	O-C	2.29	1.28	1.22
2	A	366	FER	O2-C9	2.24	1.36	1.30
3	C	1699	SAH	C2-N3	2.20	1.37	1.33
3	A	1698	SAH	O-C	2.18	1.28	1.22
3	C	1699	SAH	O-C	2.16	1.28	1.22
3	A	1698	SAH	C2-N3	2.15	1.37	1.33
2	E	1698	FER	O3-C3	2.14	1.40	1.37
2	C	366	FER	O2-C9	2.12	1.35	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	366	FER	C6-C5	2.07	1.42	1.38
2	C	366	FER	C5-C4	2.06	1.43	1.39
2	E	1698	FER	O2-C9	2.04	1.35	1.30
2	C	366	FER	C6-C5	2.02	1.42	1.38

All (46) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1699	SAH	O4'-C1'-N9	11.12	129.45	108.09
3	E	1697	SAH	O4'-C1'-N9	11.07	129.36	108.09
3	A	1698	SAH	O4'-C1'-N9	10.75	128.73	108.09
3	A	1698	SAH	C5'-C4'-C3'	9.39	138.53	115.06
3	C	1699	SAH	C5'-C4'-C3'	9.22	138.11	115.06
3	E	1697	SAH	C5'-C4'-C3'	9.09	137.77	115.06
3	C	1699	SAH	C3'-C2'-C1'	5.85	112.53	101.46
3	E	1697	SAH	C3'-C2'-C1'	5.78	112.40	101.46
3	A	1698	SAH	C3'-C2'-C1'	5.70	112.24	101.46
3	A	1698	SAH	C2'-C1'-N9	5.45	126.84	113.30
3	E	1697	SAH	C2'-C1'-N9	5.24	126.33	113.30
3	C	1699	SAH	C2'-C1'-N9	5.19	126.21	113.30
3	A	1698	SAH	N3-C2-N1	-5.03	120.97	128.58
3	C	1699	SAH	N3-C2-N1	-5.01	120.99	128.58
3	E	1697	SAH	N3-C2-N1	-4.95	121.09	128.58
3	A	1698	SAH	C2-N1-C6	3.95	125.22	118.73
3	C	1699	SAH	C2-N1-C6	3.94	125.21	118.73
3	E	1697	SAH	C2-N1-C6	3.88	125.10	118.73
3	E	1697	SAH	C5-C4-N9	-3.81	101.66	105.81
3	E	1697	SAH	C1'-N9-C8	-3.80	118.66	127.09
3	A	1698	SAH	C5-C4-N9	-3.67	101.81	105.81
3	C	1699	SAH	C5-C4-N9	-3.63	101.85	105.81
3	C	1699	SAH	C1'-N9-C8	-3.50	119.32	127.09
3	A	1698	SAH	C1'-N9-C8	-3.42	119.50	127.09
2	E	1698	FER	C10-O3-C3	3.31	122.36	117.51
2	E	1698	FER	C2-C3-C4	-2.94	117.08	120.04
2	C	366	FER	C2-C3-C4	-2.91	117.11	120.04
3	E	1697	SAH	N6-C6-N1	2.86	124.74	118.38
2	A	366	FER	C2-C3-C4	-2.85	117.17	120.04
3	E	1697	SAH	C4-N9-C1'	2.77	133.11	126.63
3	A	1698	SAH	N6-C6-N1	2.70	124.39	118.38
2	A	366	FER	C10-O3-C3	2.61	121.34	117.51
3	C	1699	SAH	N6-C6-N1	2.60	124.18	118.38
2	C	366	FER	C10-O3-C3	2.57	121.28	117.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	1699	SAH	C4-N9-C1'	2.51	132.49	126.63
2	E	1698	FER	C2-C1-C7	2.50	128.09	120.61
3	A	1698	SAH	C4-N9-C8	2.45	108.31	105.74
3	A	1698	SAH	C4-N9-C1'	2.38	132.19	126.63
3	E	1697	SAH	C4-N9-C8	2.38	108.23	105.74
3	C	1699	SAH	C4-N9-C8	2.33	108.18	105.74
2	C	366	FER	C1-C2-C3	2.24	123.16	120.15
2	A	366	FER	C1-C2-C3	2.22	123.14	120.15
2	E	1698	FER	C1-C7-C8	2.19	131.70	126.92
3	E	1697	SAH	N3-C4-N9	2.14	130.80	127.17
3	C	1699	SAH	N3-C4-N9	2.12	130.77	127.17
3	A	1698	SAH	N3-C4-N9	2.05	130.66	127.17

All (6) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	1698	SAH	C1'
3	A	1698	SAH	C4'
3	C	1699	SAH	C1'
3	C	1699	SAH	C4'
3	E	1697	SAH	C1'
3	E	1697	SAH	C4'

All (6) torsion outliers are listed below:

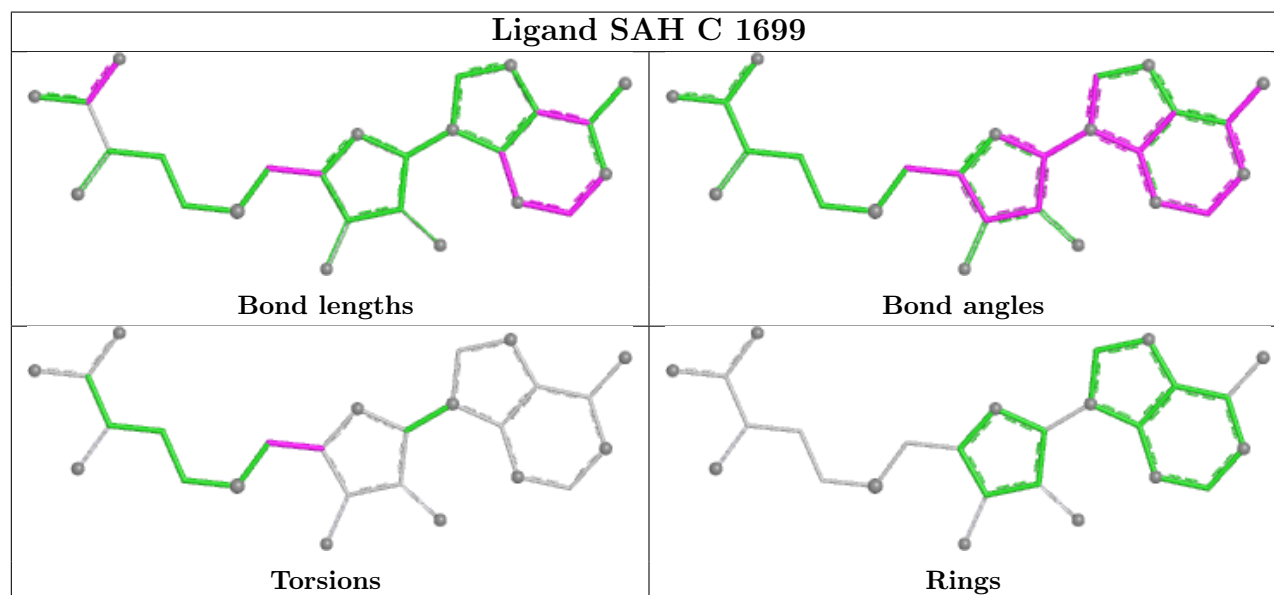
Mol	Chain	Res	Type	Atoms
3	A	1698	SAH	O4'-C4'-C5'-SD
3	C	1699	SAH	O4'-C4'-C5'-SD
3	E	1697	SAH	O4'-C4'-C5'-SD
3	E	1697	SAH	CB-CG-SD-C5'
3	A	1698	SAH	CB-CG-SD-C5'
3	E	1697	SAH	CA-CB-CG-SD

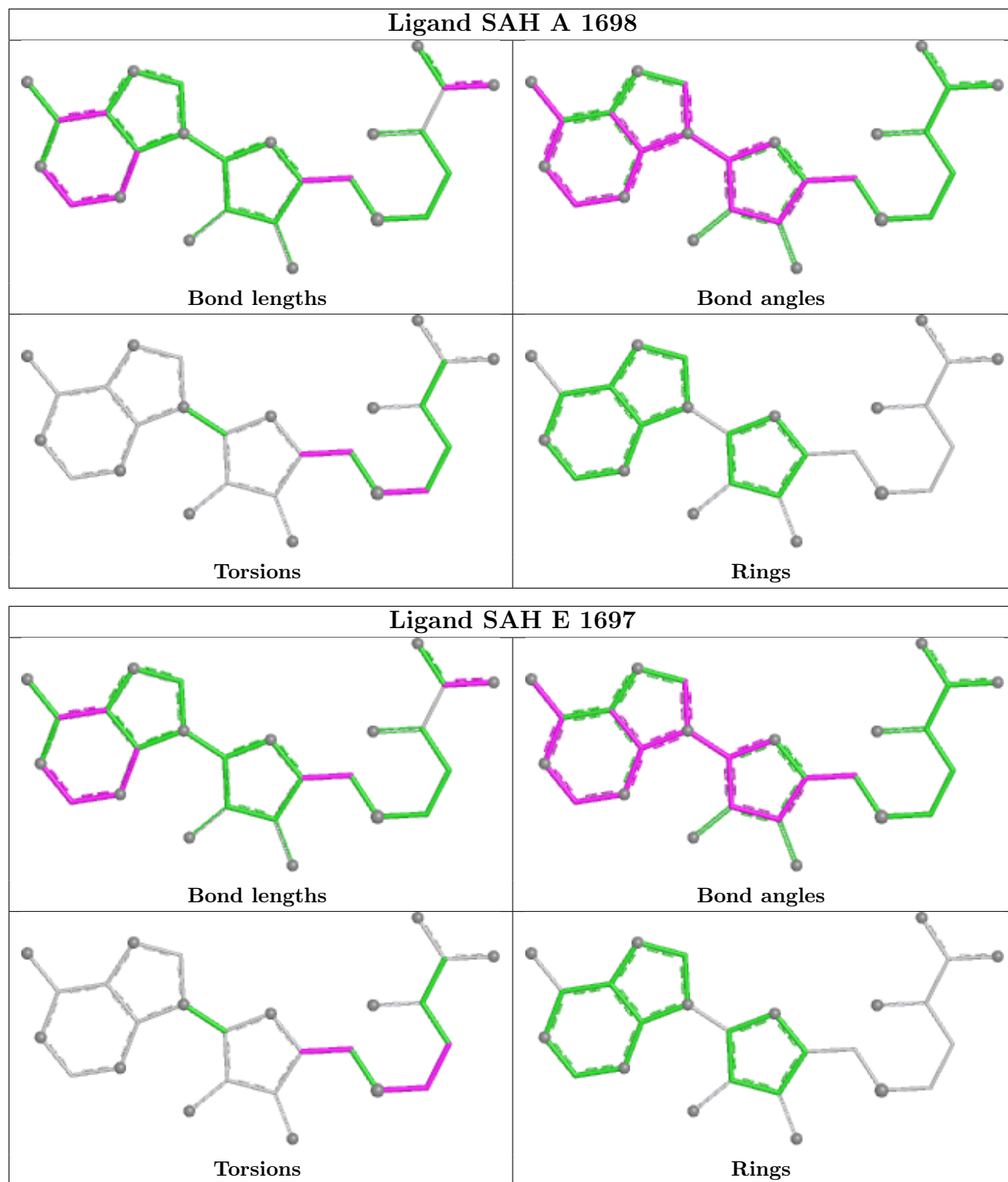
There are no ring outliers.

5 monomers are involved in 29 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	1699	SAH	9	0
3	A	1698	SAH	9	0
3	E	1697	SAH	8	0
2	E	1698	FER	2	0
2	C	366	FER	1	0

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

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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	350/365 (95%)	0.98	88 (25%) 1 1	12, 32, 70, 86	0
1	C	356/365 (97%)	1.83	149 (41%) 0 0	17, 41, 71, 89	0
1	E	361/365 (98%)	0.26	23 (6%) 25 22	13, 27, 47, 72	0
All	All	1067/1095 (97%)	1.02	260 (24%) 2 1	12, 32, 67, 89	0

All (260) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	201	LEU	8.9
1	C	200	GLY	8.0
1	C	163	PHE	7.5
1	C	216	ASN	7.2
1	C	242	TYR	7.2
1	A	163	PHE	6.9
1	C	215	ILE	6.6
1	A	362	LEU	6.5
1	E	118	ASN	6.3
1	A	234	HIS	6.1
1	E	119	GLU	6.0
1	C	217	THR	6.0
1	C	236	ILE	6.0
1	C	324	ASN	5.9
1	A	290	ASN	5.7
1	C	220	SER	5.7
1	C	169	ASP	5.7
1	C	235	VAL	5.7
1	C	218	ILE	5.6
1	C	111	VAL	5.5
1	C	14	ILE	5.5
1	C	232	LEU	5.4
1	C	356	THR	5.3

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Mol	Chain	Res	Type	RSRZ
1	C	167	GLY	5.2
1	C	119	GLU	5.2
1	C	243	PRO	5.2
1	A	224	THR	5.1
1	C	219	VAL	5.1
1	C	157	ALA	5.0
1	C	291	GLY	4.9
1	E	163	PHE	4.9
1	C	202	LYS	4.9
1	C	208	GLY	4.9
1	C	13	HIS	4.8
1	A	236	ILE	4.8
1	C	186	ILE	4.8
1	A	291	GLY	4.8
1	A	228	ILE	4.8
1	C	351	CYS	4.8
1	C	239	ALA	4.7
1	C	214	VAL	4.7
1	C	187	THR	4.7
1	A	325	PRO	4.7
1	A	100	GLY	4.6
1	C	244	GLY	4.6
1	C	172	PHE	4.6
1	C	168	THR	4.5
1	C	365	VAL	4.5
1	C	250	GLY	4.5
1	C	184	SER	4.5
1	C	161	THR	4.5
1	A	288	PRO	4.3
1	E	5	GLY	4.3
1	C	170	PRO	4.3
1	C	192	LEU	4.3
1	C	248	VAL	4.3
1	A	202	LYS	4.3
1	C	325	PRO	4.3
1	C	221	LYS	4.3
1	C	162	ALA	4.2
1	C	196	THR	4.2
1	C	198	PHE	4.2
1	C	357	TYR	4.2
1	C	224	THR	4.2
1	C	120	ASP	4.2

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Mol	Chain	Res	Type	RSRZ
1	C	158	TYR	4.2
1	C	225	ILE	4.1
1	A	238	ASP	4.1
1	C	247	HIS	4.1
1	E	120	ASP	4.1
1	A	219	VAL	4.1
1	C	116	VAL	4.0
1	C	249	GLY	4.0
1	A	351	CYS	4.0
1	C	159	GLY	3.9
1	A	221	LYS	3.9
1	C	222	TYR	3.9
1	C	171	ARG	3.9
1	A	201	LEU	3.9
1	C	188	MET	3.9
1	C	271	TRP	3.9
1	C	10	THR	3.9
1	A	344	PHE	3.9
1	A	242	TYR	3.9
1	C	199	GLU	3.9
1	C	173	ASN	3.8
1	A	244	GLY	3.8
1	C	112	ALA	3.8
1	C	233	PRO	3.8
1	A	229	ASN	3.8
1	A	256	ILE	3.8
1	C	234	HIS	3.8
1	C	245	VAL	3.8
1	C	228	ILE	3.7
1	A	289	ASP	3.7
1	C	350	HIS	3.7
1	A	267	ILE	3.7
1	C	118	ASN	3.7
1	C	290	ASN	3.7
1	C	179	GLY	3.6
1	C	211	THR	3.6
1	C	210	GLY	3.6
1	C	352	ASN	3.6
1	C	175	VAL	3.6
1	C	176	PHE	3.6
1	A	343	GLY	3.6
1	A	258	LYS	3.6

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Mol	Chain	Res	Type	RSRZ
1	A	293	VAL	3.6
1	E	365	VAL	3.6
1	C	240	PRO	3.6
1	A	239	ALA	3.5
1	C	213	ALA	3.5
1	C	183	HIS	3.5
1	A	248	VAL	3.5
1	C	355	ASN	3.5
1	C	241	SER	3.4
1	A	197	GLY	3.4
1	C	346	GLY	3.4
1	C	231	ASP	3.4
1	C	121	GLY	3.4
1	C	238	ASP	3.4
1	C	160	MET	3.3
1	C	206	ASP	3.3
1	A	223	PRO	3.3
1	A	199	GLU	3.3
1	C	155	ASN	3.2
1	A	262	VAL	3.2
1	C	11	PRO	3.2
1	A	203	SER	3.2
1	C	166	HIS	3.2
1	C	195	TYR	3.2
1	C	207	VAL	3.2
1	A	271	TRP	3.2
1	C	12	THR	3.2
1	C	174	LYS	3.1
1	C	182	ASP	3.1
1	C	229	ASN	3.1
1	A	194	THR	3.1
1	A	232	LEU	3.1
1	C	165	TYR	3.1
1	C	223	PRO	3.1
1	C	98	GLN	3.1
1	C	212	GLY	3.1
1	A	287	LEU	3.1
1	C	190	LYS	3.0
1	E	13	HIS	3.0
1	C	266	TRP	3.0
1	C	15	SER	3.0
1	C	193	GLU	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	117	LYS	3.0
1	A	255	SER	3.0
1	A	243	PRO	3.0
1	C	134	LYS	3.0
1	C	96	THR	3.0
1	C	197	GLY	3.0
1	A	292	LYS	2.9
1	A	284	TYR	2.9
1	C	164	GLU	2.9
1	A	204	LEU	2.9
1	A	286	ALA	2.9
1	C	191	ILE	2.9
1	C	154	PHE	2.9
1	C	180	MET	2.9
1	A	227	GLY	2.9
1	A	253	PHE	2.9
1	A	261	ALA	2.9
1	A	279	PHE	2.9
1	C	17	GLU	2.8
1	E	271	TRP	2.8
1	A	264	MET	2.8
1	A	200	GLY	2.8
1	A	241	SER	2.8
1	A	250	GLY	2.8
1	C	189	LYS	2.8
1	C	265	LYS	2.8
1	C	110	THR	2.8
1	A	220	SER	2.7
1	A	233	PRO	2.7
1	C	296	ALA	2.7
1	E	289	ASP	2.7
1	A	198	PHE	2.7
1	A	345	GLN	2.7
1	C	349	VAL	2.7
1	C	194	THR	2.7
1	C	264	MET	2.7
1	A	119	GLU	2.7
1	E	224	THR	2.7
1	C	181	SER	2.7
1	A	98	GLN	2.6
1	C	237	GLU	2.6
1	A	96	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	264	MET	2.6
1	A	235	VAL	2.6
1	E	364	LYS	2.6
1	A	205	VAL	2.6
1	A	210	GLY	2.6
1	C	203	SER	2.6
1	A	249	GLY	2.6
1	C	114	TYR	2.6
1	C	255	SER	2.6
1	C	178	LYS	2.6
1	A	282	ASN	2.5
1	A	347	PHE	2.5
1	A	361	PHE	2.5
1	A	152	ILE	2.5
1	A	190	LYS	2.5
1	A	240	PRO	2.5
1	C	209	GLY	2.5
1	A	211	THR	2.4
1	C	336	GLU	2.4
1	E	14	ILE	2.4
1	E	202	LYS	2.4
1	A	231	ASP	2.4
1	C	177	ASN	2.4
1	E	288	PRO	2.4
1	C	272	SER	2.4
1	C	298	CYS	2.4
1	A	225	ILE	2.4
1	A	245	VAL	2.4
1	C	326	GLY	2.4
1	C	269	HIS	2.4
1	C	345	GLN	2.4
1	A	324	ASN	2.4
1	E	290	ASN	2.4
1	E	346	GLY	2.4
1	A	226	LYS	2.4
1	C	354	PHE	2.4
1	C	226	LYS	2.3
1	A	275	HIS	2.3
1	E	164	GLU	2.3
1	A	215	ILE	2.3
1	A	230	PHE	2.3
1	C	254	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	257	PRO	2.3
1	C	246	GLU	2.3
1	C	122	VAL	2.3
1	A	101	LYS	2.2
1	E	239	ALA	2.2
1	C	16	ASP	2.2
1	C	20	ASN	2.2
1	C	270	ASP	2.2
1	A	346	GLY	2.2
1	A	217	THR	2.2
1	A	342	ALA	2.2
1	E	162	ALA	2.2
1	C	115	LEU	2.1
1	A	270	ASP	2.1
1	A	331	THR	2.1
1	E	194	THR	2.1
1	E	220	SER	2.1
1	A	348	LYS	2.1
1	C	204	LEU	2.1
1	C	133	ASP	2.1
1	C	227	GLY	2.1
1	C	251	ASP	2.0
1	E	100	GLY	2.0
1	C	230	PHE	2.0
1	A	285	GLU	2.0
1	A	260	ASP	2.0
1	C	300	LEU	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,

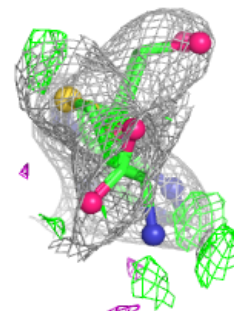
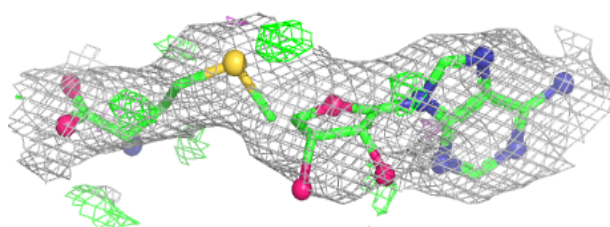
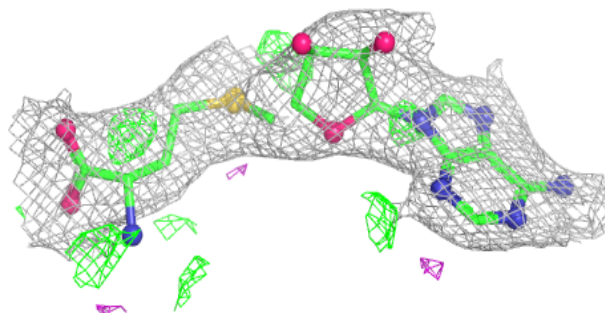
median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	FER	C	366	14/14	0.59	0.31	83,88,90,91	0
2	FER	A	366	14/14	0.62	0.30	74,80,81,82	0
2	FER	E	1698	14/14	0.62	0.23	39,46,49,54	0
3	SAH	C	1699	26/26	0.81	0.20	54,61,71,72	0
3	SAH	A	1698	26/26	0.83	0.15	56,66,68,69	0
3	SAH	E	1697	26/26	0.90	0.11	27,39,46,48	0

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

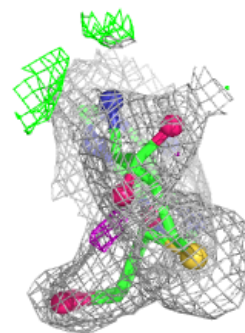
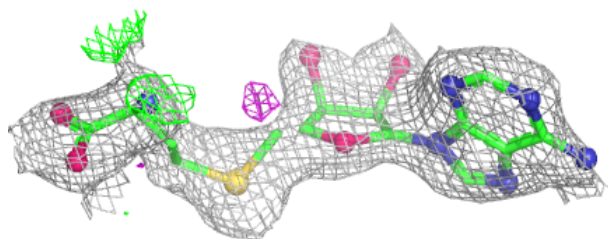
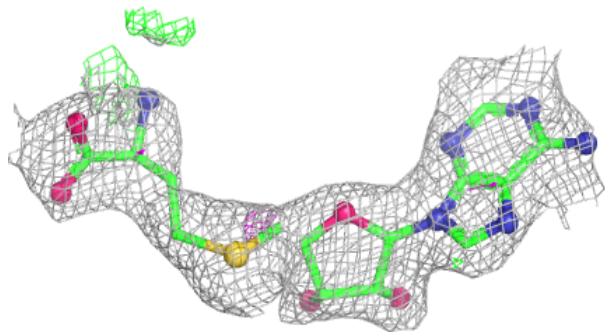
Electron density around SAH C 1699:

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

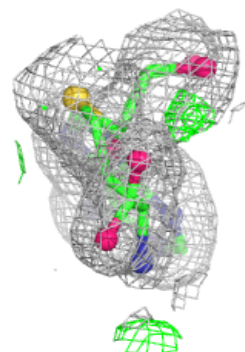
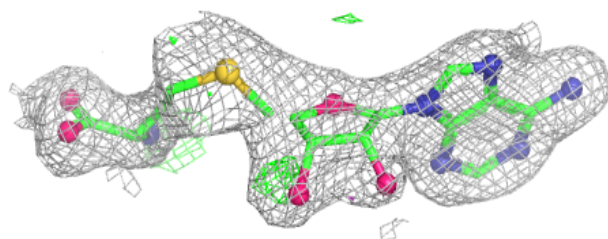
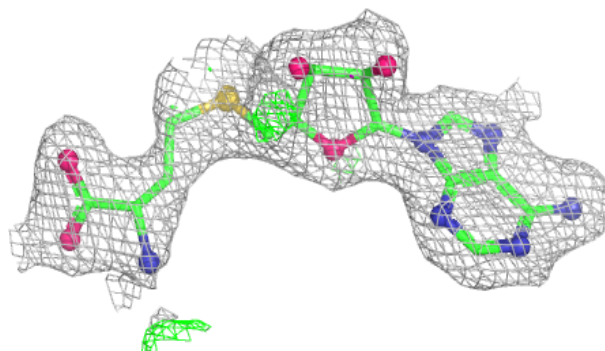


Electron density around SAH A 1698:

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

**Electron density around SAH E 1697:**

$2mF_o-DF_c$ (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.