



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 31, 2016 – 08:35 PM GMT

PDB ID : 1KYZ  
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](mailto:validation@mail.wwpdb.org)  
A user guide is available at  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

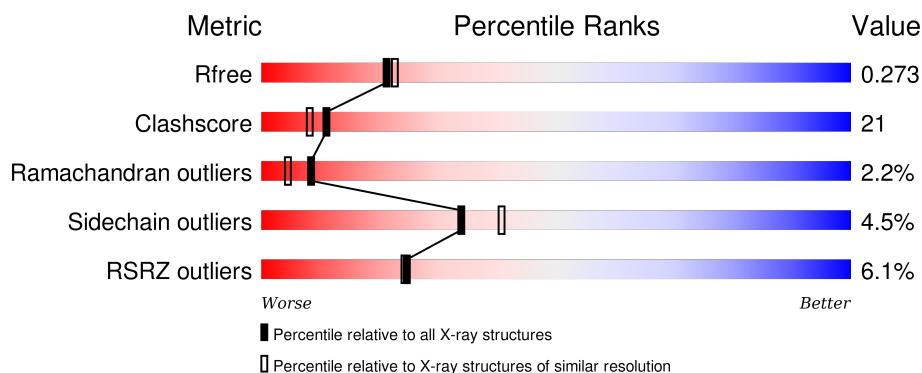
# 1 Overall quality at a glance

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))
$R_{free}$	91344	3774 (2.20-2.20)
Clashscore	102246	4477 (2.20-2.20)
Ramachandran outliers	100387	4404 (2.20-2.20)
Sidechain outliers	100360	4405 (2.20-2.20)
RSRZ outliers	91569	3781 (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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	<div> <div>4%</div> <div>62%</div> <div>32%</div> <div>• •</div> </div>
1	C	365	<div> <div>13%</div> <div>60%</div> <div>32%</div> <div>6%</div> <div>•</div> </div>
1	E	365	<div> <div>%</div> <div>75%</div> <div>21%</div> <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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	SAH	A	1698	X	-	X	-
2	SAH	C	1699	X	-	X	-
2	SAH	E	1697	X	-	-	-
3	FER	A	366	-	-	-	X

## 2 Entry composition [i](#)

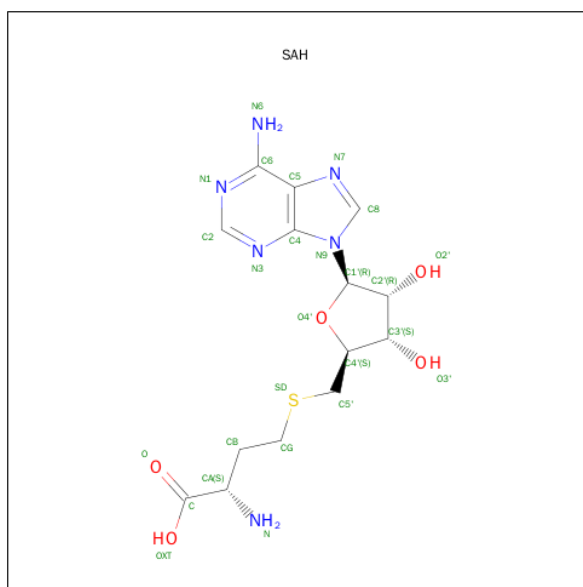
There are 4 unique types of molecules in this entry. The entry contains 8594 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

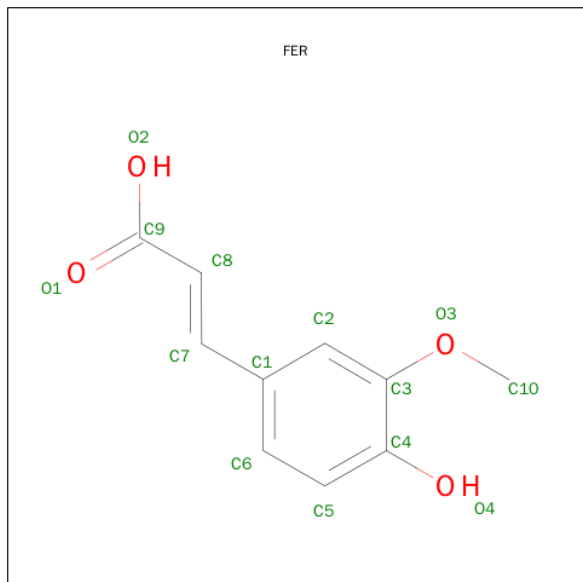
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	350	Total	C	N	O	S	0	0	0
			2693	1728	442	503	20			
1	C	356	Total	C	N	O	S	0	0	0
			2740	1758	450	512	20			
1	E	361	Total	C	N	O	S	0	0	0
			2777	1780	456	521	20			

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



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

- Molecule 3 is 3-(4-HYDROXY-3-METHOXYPHENYL)-2-PROPENOIC ACID (three-letter code: FER) (formula: C<sub>10</sub>H<sub>10</sub>O<sub>4</sub>).

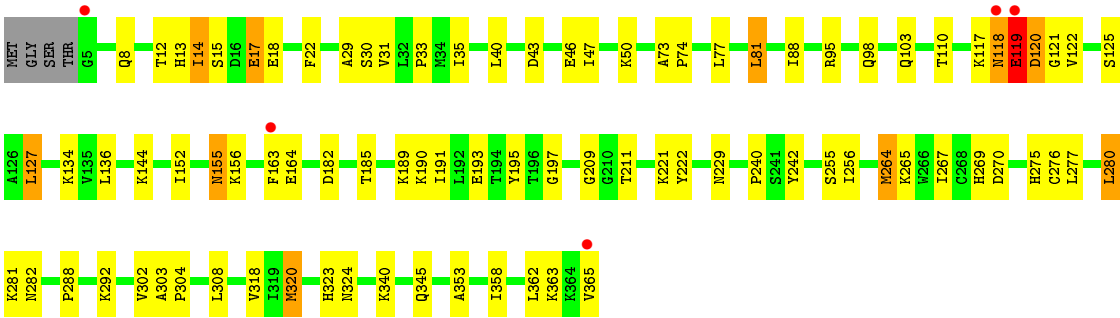


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	E	1	Total	C	O	0	0
			14	10	4		
3	C	1	Total	C	O	0	0
			14	10	4		
3	A	1	Total	C	O	0	0
			14	10	4		

- 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		





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 2 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.73Å 61.87Å 111.23Å 90.00° 112.18° 90.00°	Depositor
Resolution (Å)	61.87 – 2.20 61.86 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.9 (61.87-2.20) 97.9 (61.86-2.00)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.83 (at 2.00Å)	Xtriage
Refinement program	CNS 1.0	Depositor
R, $R_{free}$	0.236 , 0.274 0.235 , 0.273	Depositor DCC
$R_{free}$ test set	3295 reflections (5.04%)	DCC
Wilson B-factor (Å <sup>2</sup> )	26.8	Xtriage
Anisotropy	0.042	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 53.6	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Outliers	1 of 86619 reflections (0.001%)	Xtriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	8594	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	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.*

<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, 0.375 respectively for untwinned datasets, and 0.333, 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: SAH, FER

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	0.33	0/2752	0.56	0/3730
1	C	0.31	0/2800	0.56	1/3794 (0.0%)
1	E	0.35	0/2837	0.60	1/3844 (0.0%)
All	All	0.33	0/8389	0.57	2/11368 (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	E	119	GLU	N-CA-C	-6.98	92.16	111.00
1	C	222	TYR	N-CA-C	-5.22	96.92	111.00

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	2693	0	2701	110	0
1	C	2740	0	2757	157	1
1	E	2777	0	2792	74	0
2	A	26	0	17	9	0
2	C	26	0	17	9	0
2	E	26	0	17	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	14	0	8	0	0
3	C	14	0	9	0	0
3	E	14	0	8	1	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	348	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 21.

All (348) 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)
2:A:1698:SAH:O4'	2:A:1698:SAH:C5'	1.91	1.17
2:C:1699:SAH:O4'	2:C:1699:SAH:C5'	1.92	1.17
2:E:1697:SAH:O4'	2:E:1697:SAH:C5'	1.92	1.16
2:C:1699:SAH:C4'	2:C:1699:SAH:SD	2.35	1.14
2:E:1697:SAH:C4'	2:E:1697:SAH:SD	2.35	1.14
2:C:1699:SAH:C3'	2:C:1699:SAH:C5'	2.25	1.13
2:E:1697:SAH:C3'	2:E:1697:SAH:C5'	2.25	1.13
2:A:1698:SAH:SD	2:A:1698:SAH:C4'	2.37	1.12
2:A:1698:SAH:C5'	2:A:1698:SAH:C3'	2.26	1.11
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
2:E:1697:SAH:C4'	2:E:1697:SAH:H5'2	1.46	0.98
2:A:1698:SAH:C4'	2:A:1698:SAH:H5'1	1.46	0.98
2:C:1699:SAH:C4'	2:C:1699:SAH:H5'2	1.47	0.97
2:E:1697:SAH:C4'	2:E:1697:SAH:H5'1	1.46	0.97
2:C:1699:SAH:C4'	2:C:1699:SAH:H5'1	1.47	0.96
2:A:1698:SAH:C4'	2:A:1698:SAH:H5'2	1.46	0.95
1:C:212:GLY:C	1:C:216:ASN:HB2	1.92	0.90
1:C:222:TYR:HB3	1:C:225:ILE:HD13	1.56	0.88
1:C:11:PRO:HG3	1:C:14:ILE:HD11	1.55	0.88
1:C:134:LYS:HE2	1:C:134:LYS:H	1.38	0.87
1:A:331:THR:HG22	1:A:334:GLU:HG3	1.58	0.85
1:C:134:LYS:CE	1:C:134:LYS:H	1.88	0.85
2:A:1698:SAH:C5'	2:A:1698:SAH:C4'	0.84	0.84
2:C:1699:SAH:C4'	2:C:1699:SAH:C5'	0.84	0.83
2:E:1697:SAH:C4'	2:E:1697:SAH:C5'	0.83	0.83
1:A:344:PHE:HD2	1:A:362:LEU:HB2	1.43	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:E:320:MET:HE2	1:E:320:MET:HA	1.61	0.81
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:C:320:MET:HA	1:C:320:MET:HE2	1.64	0.78
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:320:MET:HE2	1:C:324:ASN:HB3	1.67	0.76
1:E:320:MET:CE	1:E:320:MET:HA	2.14	0.76
1:E:190:LYS:HG3	1:E:353:ALA:HB1	1.69	0.75
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: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
1:E:136:LEU:HD21	3: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:A:130:MET:HE2	1:A:176:PHE:O	1.92	0.70
1:C:216:ASN:OD1	1:C:242:TYR:HD1	1.73	0.70
1:C:220:SER:C	1:C:222:TYR:H	1.94	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
2:E:1697:SAH:O4'	2:E:1697:SAH:H5'1	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:155:ASN:HD22	1:A:155:ASN:N	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:C:242:TYR:CB	1:C:243:PRO:HD2	2.27	0.65
1:C:170:PRO:O	1:C:174:LYS:HG3	1.95	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:320:MET:HE2	1:A:320:MET:HA	1.78	0.65
1:C:218:ILE:O	1:C:221:LYS:HG2	1.96	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
2:C:1699:SAH:H5'1	2:C:1699:SAH:O4'	1.79	0.62
1:A:344:PHE:CD2	1:A:362:LEU:HB2	2.29	0.62
1:E:117:LYS:O	1:E:118:ASN:HB2	1.99	0.62
1:E:152:ILE:HD12	1:E:152:ILE:N	2.15	0.62
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: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:HB3	1:E:340:LYS:NZ	2.17	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:A:130:MET:HE1	1:A:179:GLY:HA3	1.83	0.60
1:A:152:ILE:HD11	1:A:323:HIS:C	2.21	0.60
1:E:264:MET:HG2	1:E:267:ILE:HB	1.84	0.60
1:A:88:ILE:HG22	1:A:88:ILE:O	2.02	0.59
1:A:361:PHE:O	1:A:362:LEU:HB3	2.02	0.59
1:E:255:SER:C	1:E:256:ILE:HD12	2.22	0.59
1:E:191:ILE:HD13	1:E:358:ILE:HD11	1.84	0.59
1:A:130:MET:CE	1:A:179:GLY:HA3	2.31	0.59
1:C:336:GLU:HG2	1:C:347:PHE:CG	2.37	0.59
1:C:212:GLY:O	1:C:216:ASN:N	2.31	0.59
1:C:77:LEU:O	1:C:81:LEU:HD22	2.02	0.59
1:C:331:THR:HG22	1:C:334:GLU:CG	2.32	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:160:MET:HE2	1:C:164:GLU:HB3	1.85	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:364:LYS:O	1:C:364:LYS:HE2	2.03	0.58
1:C:216:ASN:OD1	1:C:242:TYR:CD1	2.56	0.58
1:E:88:ILE:HG22	1:E:88:ILE:O	2.04	0.58
1:A:182:ASP:O	1:A:186:ILE:HG12	2.03	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
2:A:1698:SAH:O4'	2:A:1698:SAH:H5'1	1.75	0.57
1:E:155:ASN:N	1:E:155:ASN:HD22	2.01	0.57
1:C:310:THR:O	1:C:313:VAL:HG12	2.05	0.57
1:C:320:MET:CE	1:C:320:MET:HA	2.34	0.57
1:C:331:THR:CG2	1:C:334:GLU:HG3	2.34	0.57
1:E:122:VAL:HG13	1:E:182:ASP:CG	2.25	0.57
1:C:344:PHE:O	1:C:346:GLY:N	2.38	0.56
1:C:320:MET:C	1:C:324:ASN:HD22	2.09	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:211:THR:HG22	1:A:242:TYR:OH	2.06	0.56
1:A:258:LYS:HD3	1:A:258:LYS:H	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	2:C:1699:SAH:N1	2.21	0.55
1:E:211:THR:HG23	1:E:240:PRO:HD2	1.89	0.55
1:A:264:MET:HG2	1:A:267:ILE:HB	1.89	0.55
1:A:216:ASN:HD22	1:A:242:TYR:CB	2.10	0.55
1:E:163:PHE:CE1	1:E:164:GLU:HG3	2.42	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:OE1	1:C:97:GLN:HA	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:220:SER:C	1:C:222:TYR:N	2.61	0.54
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:152:ILE:HD11	1:A:323:HIS:O	2.07	0.53
1:C:268:CYS:C	1:C:270:ASP:H	2.12	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:E:189:LYS:O	1:E:193:GLU:HG3	2.08	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:270:ASP:OD1	1:A:324:ASN:ND2	2.42	0.52
1:C:10:THR:HG23	1:C:22:PHE:CE2	2.45	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:A:142:HIS:HD2	4:A:1751:HOH:O	1.90	0.52
1:A:17:GLU:CD	1:A:17:GLU:H	2.13	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:145:ASP:HB3	1:C:156:LYS:HZ3	1.74	0.51
1:C:214:VAL:O	1:C:219:VAL:HG23	2.10	0.51
1:C:320:MET:CE	1:C:324:ASN:HB3	2.39	0.51
1:C:187:THR:O	1:C:191:ILE:HG13	2.09	0.51
1:C:160:MET:HE2	1:C:165:TYR:N	2.25	0.51
1:A:265:LYS:HG2	2: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:A:287:LEU:C	1:A:289:ASP:H	2.14	0.51
1:C:206:ASP:OD1	1:C:263:PHE:HD2	1.93	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:212:GLY:O	1:C:213:ALA:C	2.50	0.50
1:E:320:MET:CE	1:E:324:ASN:HB2	2.42	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: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:C:145:ASP:C	1:C:156:LYS:HZ3	2.15	0.50
1:A:236:ILE:HG23	1:A:247:HIS:HB3	1.94	0.50
1:A:29:ALA:HB3	1:E:33:PRO:HB3	1.93	0.50
1:C:136:LEU:HG	1:C:172:PHE:HZ	1.76	0.49
1:A:154:PHE:CE2	1:A:162:ALA:HA	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:205:VAL:CG1	1:A:262:VAL:HG22	2.42	0.49
1:E:190:LYS:HG3	1:E:353:ALA:CB	2.40	0.49
1:A:252:MET:HE1	1:A:279:PHE:CD2	2.47	0.49
1:C:171:ARG:HG2	1:C:171:ARG:HH11	1.78	0.49
1:C:111:VAL:HG22	1:C:111:VAL:O	2.12	0.49
1:C:347:PHE:CE2	1:C:349:VAL:HG23	2.48	0.49
1:E:277:LEU:O	1:E:281:LYS:HG3	2.12	0.49
1:A:192:LEU:HD11	1:A:217:THR:HG22	1.94	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:119:GLU:HB3	1:C:122:VAL:O	2.12	0.48
1:A:125:SER:HA	1:A:128:ASN:ND2	2.28	0.48
1:A:102:VAL:HG11	1:E:302:VAL:CG1	2.43	0.48
1:E:323:HIS:HE1	4:E:1788:HOH:O	1.96	0.48
1:C:324:ASN:C	1:C:324:ASN:OD1	2.52	0.48
1:E:119:GLU:O	1:E:120:ASP:HB2	2.13	0.48
1:E:8:GLN:HG2	1:E:308:LEU:HD21	1.95	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:C:241:SER:O	1:C:242:TYR:CD2	2.66	0.48
1:A:281:LYS:O	1:A:285:GLU:HG3	2.13	0.48
1:C:171:ARG:NH1	1:C:171:ARG:HG2	2.28	0.48
1:C:212:GLY:O	1:C:216:ASN:HB2	2.12	0.48
1:C:221:LYS:C	1:C:223:PRO:HD3	2.34	0.48
1:C:94:VAL:HG12	1:C:95:ARG:N	2.29	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:A:130:MET:HE1	1:A:179:GLY:CA	2.44	0.47
1:C:210:GLY:HA2	1:C:235:VAL:HG11	1.96	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:A:155:ASN:ND2	1:A:155:ASN:N	2.60	0.47
1:E:46:GLU:O	1:E:50:LYS:HG3	2.14	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:HD22	1:C:155:ASN:N	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:256:ILE:HD13	1:E:282:ASN:CB	2.44	0.47
1:E:122:VAL:HG13	1:E:182:ASP:CB	2.45	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
1:E:240:PRO:HG2	1:E:242:TYR:CZ	2.50	0.46
1:C:127:LEU:HD12	1:C:179:GLY:CA	2.45	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:63:ALA:O	1:A:66:LEU:HB2	2.16	0.46
1:A:320:MET:CE	1:A:320:MET:HA	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:E:40:LEU:HD13	1:E:125:SER:HB3	1.97	0.45
1:C:208:GLY:O	2:C:1699:SAH:HB2	2.17	0.45
1:C:202:LYS:H	1:C:225:ILE:HG13	1.82	0.45
1:C:212:GLY:O	1:C:214:VAL:N	2.49	0.45
1:A:211:THR:HG22	1:A:242:TYR:HH	1.81	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: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:216:ASN:HD21	1:C:240:PRO:HG2	1.82	0.45
1:C:122:VAL:HG13	1:C:182:ASP:CB	2.47	0.45
1:C:10:THR:N	4:C:1722:HOH:O	2.49	0.45
1:C:205:VAL:HG13	1:C:205:VAL:O	2.16	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:A:320:MET:HG2	1:A:327:GLY:C	2.37	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:N	1:A:258:LYS:HD3	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:212:GLY:HA2	1:C:229:ASN:HD22	1.82	0.44
1:C:223:PRO:C	1:C:225:ILE:H	2.21	0.44
1:A:331:THR:CG2	1:A:334:GLU:H	2.30	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:14:ILE:CD1	1:E:22:PHE:HB2	2.47	0.44
1:C:313:VAL:HG13	1:C:314:VAL:N	2.32	0.44
1:C:188:MET:HE3	1:C:191:ILE:HB	1.99	0.44
1:A:286:ALA:O	1:A:288:PRO:HD3	2.18	0.44
1:A:288:PRO:C	1:A:290:ASN:N	2.71	0.44
1:C:220:SER:O	1:C:222:TYR:N	2.51	0.44
1:A:226:LYS:HA	1:A:226:LYS:HE2	1.99	0.43
1:C:202:LYS:HB2	1:C:224:THR:O	2.17	0.43
1:A:231:ASP:HB3	1:A:236:ILE:HG12	2.00	0.43
1:A:190:LYS:HB3	1:A:353:ALA:HB1	2.00	0.43
1:C:160:MET:HE2	1:C:164:GLU:C	2.38	0.43
1:E:110:THR:HG23	4:E:1802:HOH:O	2.17	0.43
1:C:114:TYR:HB3	1:C:124:ILE:HD12	1.99	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:C:116:VAL:C	1:C:118:ASN:H	2.22	0.43
1:C:197:GLY:C	1:C:199:GLU:H	2.21	0.43
1:E:320:MET:HE2	1:E:324:ASN:HB2	2.01	0.43
1:E:14:ILE:HG23	1:E:15:SER:O	2.19	0.43
1:C:267:ILE:O	1:C:271:TRP:HE3	2.01	0.43
1:C:320:MET:C	1:C:324:ASN:ND2	2.72	0.43
1:A:252:MET:HG2	2:A:1698:SAH:N1	2.34	0.42
1:A:264:MET:O	1:A:265:LYS:HB3	2.19	0.42
1:A:73:ALA:HB3	1:A:74:PRO:HD3	2.00	0.42
1:C:145:ASP:HB3	1:C:156:LYS:HZ1	1.83	0.42
1:E:152:ILE:O	1:E:156:LYS:HG3	2.19	0.42
1:A:324:ASN:HA	1:A:325:PRO:HD3	1.72	0.42
1:A:33:PRO:HB3	1:E:29:ALA:HB3	2.00	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:268:CYS:O	1:C:270:ASP:N	2.50	0.42
1:C:155:ASN:ND2	1:C:155:ASN:N	2.68	0.42
1:E:265:LYS:HG2	2:E:1697:SAH:OXT	2.20	0.42
1:A:331:THR:HG23	1:A:334:GLU:H	1.84	0.42
1:A:130:MET:HE1	1:A:180:MET:N	2.34	0.42
1:A:35:ILE:HG13	1:E:318:VAL:HG11	2.00	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:344:PHE:O	1:A:362:LEU:HD12	2.20	0.42
1:A:72:ASP:O	1:A:76:MET:HG3	2.20	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:152:ILE:HA	1:A:153:PRO:HD3	1.89	0.42
1:A:66:LEU:HB3	1:A:68:THR:HG22	2.01	0.42
1:A:208:GLY:HA2	1:A:231:ASP:OD1	2.20	0.41
1:A:132:GLN:HE21	1:E:30:SER:CB	2.33	0.41
1:C:325:PRO:CG	1:C:326:GLY:H	2.25	0.41
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: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:265:LYS:O	1:A:267:ILE:HG12	2.20	0.41
1:A:118:ASN:ND2	1:A:122:VAL:HB	2.35	0.41
1:A:130:MET:HE3	1:A:179:GLY:HA3	2.02	0.41
1:A:236:ILE:CG2	1:A:247:HIS:HB3	2.49	0.41
1:C:111:VAL:CG2	1:C:111:VAL:O	2.68	0.41
1:A:178:LYS:HB2	1:A:178:LYS:HE3	1.85	0.41
1:E:303:ALA:HA	1:E:304:PRO:HD3	1.90	0.41
1:E:152:ILE:CD1	1:E:152:ILE:N	2.83	0.41
1:E:211:THR:O	1:E:211:THR:HG22	2.21	0.41
1:C:210:GLY:HA2	1:C:235:VAL:CG1	2.50	0.41
1:C:324:ASN:ND2	1:C:327:GLY:O	2.53	0.41
1:E:363:LYS:HG3	1:E:363:LYS:O	2.21	0.41
1:C:344:PHE:C	1:C:346:GLY:H	2.24	0.41
1:A:42:LEU:HD21	1:E:144:LYS:HG2	2.03	0.41
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:83:LEU:O	1:A:83:LEU:HG	2.21	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:160:MET:HE2	1:C:164:GLU:CB	2.51	0.40
1:C:365:VAL:OXT	1:C:365:VAL:HG13	2.20	0.40
1:C:202:LYS:HG2	1:C:203:SER:N	2.37	0.40
1:C:73:ALA:O	1:C:77:LEU:HG	2.22	0.40
1:A:222:TYR:N	1:A:223:PRO:HD3	2.36	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%)	17	14
1	C	354/365 (97%)	311 (88%)	29 (8%)	14 (4%)	4	1
1	E	359/365 (98%)	344 (96%)	10 (3%)	5 (1%)	14	10
All	All	1061/1095 (97%)	981 (92%)	57 (5%)	23 (2%)	8	4

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%)	281 (96%)	13 (4%)	35	42
1	C	300/307 (98%)	285 (95%)	15 (5%)	30	35
1	E	304/307 (99%)	292 (96%)	12 (4%)	39	48
All	All	898/921 (98%)	858 (96%)	40 (4%)	34	41

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

Mol	Chain	Res	Type
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	269	HIS
1	A	292	LYS
1	A	320	MET
1	A	321	LEU
1	A	328	LYS
1	A	355	ASN
1	C	13	HIS
1	C	17	GLU
1	C	36	LEU
1	C	81	LEU
1	C	134	LYS
1	C	182	ASP
1	C	198	PHE
1	C	242	TYR
1	C	260	ASP
1	C	269	HIS
1	C	320	MET
1	C	324	ASN
1	C	336	GLU

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Mol	Chain	Res	Type
1	C	345	GLN
1	C	355	ASN
1	E	13	HIS
1	E	14	ILE
1	E	17	GLU
1	E	81	LEU
1	E	127	LEU
1	E	134	LYS
1	E	155	ASN
1	E	264	MET
1	E	269	HIS
1	E	270	ASP
1	E	280	LEU
1	E	320	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (22) 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	118	ASN
1	C	155	ASN
1	C	177	ASN
1	C	216	ASN
1	C	345	GLN
1	C	355	ASN
1	E	13	HIS
1	E	103	GLN
1	E	155	ASN
1	E	229	ASN
1	E	275	HIS
1	E	323	HIS
1	E	352	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

6 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z  > 2$	Counts	RMSZ	# $ Z  > 2$
2	SAH	A	1698	-	20,28,28	5.55	7 (35%)	19,40,40	4.69	9 (47%)
3	FER	A	366	-	11,14,14	1.90	4 (36%)	14,18,18	1.41	3 (21%)
2	SAH	C	1699	-	20,28,28	5.56	7 (35%)	19,40,40	4.66	9 (47%)
3	FER	C	366	-	11,14,14	1.89	4 (36%)	14,18,18	1.41	3 (21%)
2	SAH	E	1697	-	20,28,28	5.62	7 (35%)	19,40,40	4.67	9 (47%)
3	FER	E	1698	-	11,14,14	2.08	4 (36%)	14,18,18	1.67	3 (21%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SAH	A	1698	-	2/2/6/6	0/7/31/31	0/3/3/3
3	FER	A	366	-	-	0/5/7/7	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	SAH	C	1699	-	2/2/6/6	0/7/31/31	0/3/3/3
3	FER	C	366	-	-	0/5/7/7	0/1/1/1
2	SAH	E	1697	-	2/2/6/6	0/7/31/31	0/3/3/3
3	FER	E	1698	-	-	0/5/7/7	0/1/1/1

All (33) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	1697	SAH	C5'-C4'	-23.65	0.83	1.52
2	C	1699	SAH	C5'-C4'	-23.49	0.84	1.52
2	A	1698	SAH	C5'-C4'	-23.44	0.84	1.52
2	A	1698	SAH	C8-N7	-3.49	1.27	1.34
2	E	1697	SAH	C8-N7	-3.44	1.28	1.34
2	C	1699	SAH	C8-N7	-3.34	1.28	1.34
3	C	366	FER	C6-C1	2.03	1.43	1.39
3	A	366	FER	C6-C1	2.04	1.43	1.39
3	E	1698	FER	O3-C3	2.18	1.40	1.37
2	C	1699	SAH	C5'-SD	2.48	1.86	1.81
2	A	1698	SAH	C5'-SD	2.50	1.86	1.81
3	C	366	FER	C2-C1	2.55	1.44	1.39
3	A	366	FER	C4-C3	2.60	1.44	1.40
3	A	366	FER	C2-C1	2.66	1.44	1.39
3	C	366	FER	C4-C3	2.72	1.44	1.40
3	E	1698	FER	C4-C3	2.82	1.44	1.40
2	E	1697	SAH	C5'-SD	2.94	1.87	1.81
2	E	1697	SAH	C4-N3	2.98	1.40	1.35
2	A	1698	SAH	O4'-C1'	3.07	1.45	1.41
3	E	1698	FER	C2-C1	3.11	1.45	1.39
2	A	1698	SAH	C2-N3	3.14	1.37	1.32
2	C	1699	SAH	C2-N3	3.20	1.37	1.32
2	C	1699	SAH	C2-N1	3.20	1.40	1.33
3	C	366	FER	C2-C3	3.21	1.44	1.38
2	A	1698	SAH	C2-N1	3.22	1.40	1.33
2	A	1698	SAH	C4-N3	3.24	1.40	1.35
3	A	366	FER	C2-C3	3.26	1.44	1.38
2	C	1699	SAH	O4'-C1'	3.27	1.45	1.41
2	C	1699	SAH	C4-N3	3.28	1.40	1.35
2	E	1697	SAH	C2-N3	3.33	1.38	1.32
2	E	1697	SAH	C2-N1	3.51	1.40	1.33
2	E	1697	SAH	O4'-C1'	3.62	1.45	1.41
3	E	1698	FER	C2-C3	4.25	1.46	1.38

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	1698	SAH	N3-C2-N1	-10.35	120.97	128.89
2	C	1699	SAH	N3-C2-N1	-10.32	120.99	128.89
2	E	1697	SAH	N3-C2-N1	-10.19	121.09	128.89
3	E	1698	FER	C2-C3-C4	-2.75	117.08	120.04
3	C	366	FER	C2-C3-C4	-2.72	117.11	120.04
3	A	366	FER	C2-C3-C4	-2.66	117.17	120.04
3	A	366	FER	C1-C2-C3	2.24	123.14	120.17
3	C	366	FER	C1-C2-C3	2.26	123.16	120.17
2	C	1699	SAH	N6-C6-N1	2.32	124.18	119.20
3	E	1698	FER	C2-C1-C7	2.33	128.09	120.59
2	A	1698	SAH	N6-C6-N1	2.42	124.39	119.20
3	C	366	FER	C10-O3-C3	2.46	121.28	117.54
3	A	366	FER	C10-O3-C3	2.51	121.34	117.54
2	E	1697	SAH	N6-C6-N1	2.58	124.74	119.20
2	E	1697	SAH	C4'-O4'-C1'	2.76	112.75	109.72
2	C	1699	SAH	C4'-O4'-C1'	2.90	112.91	109.72
2	A	1698	SAH	C4'-O4'-C1'	3.16	113.19	109.72
3	E	1698	FER	C10-O3-C3	3.18	122.36	117.54
2	A	1698	SAH	C1'-N9-C4	3.48	132.19	126.94
2	C	1699	SAH	C4-C5-N7	3.51	112.70	109.48
2	A	1698	SAH	C4-C5-N7	3.53	112.73	109.48
2	E	1697	SAH	C2-N1-C6	3.55	125.10	118.77
2	C	1699	SAH	C2-N1-C6	3.60	125.21	118.77
2	A	1698	SAH	C2-N1-C6	3.61	125.22	118.77
2	E	1697	SAH	C4-C5-N7	3.68	112.86	109.48
2	C	1699	SAH	C1'-N9-C4	3.68	132.49	126.94
2	E	1697	SAH	C1'-N9-C4	4.09	133.11	126.94
2	C	1699	SAH	C2'-C1'-N9	7.80	126.21	114.29
2	E	1697	SAH	C2'-C1'-N9	7.88	126.33	114.29
2	A	1698	SAH	C2'-C1'-N9	8.21	126.84	114.29
2	E	1697	SAH	C5'-C4'-C3'	8.79	137.77	114.98
2	C	1699	SAH	C5'-C4'-C3'	8.92	138.11	114.98
2	A	1698	SAH	C5'-C4'-C3'	9.08	138.53	114.98
2	A	1698	SAH	O4'-C1'-N9	9.85	128.73	108.10
2	E	1697	SAH	O4'-C1'-N9	10.16	129.36	108.10
2	C	1699	SAH	O4'-C1'-N9	10.20	129.45	108.10

All (6) chirality outliers are listed below:

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

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Mol	Chain	Res	Type	Atom
2	E	1697	SAH	C4'
2	E	1697	SAH	C1'
2	A	1698	SAH	C4'
2	A	1698	SAH	C1'

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 27 short contacts:

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

## 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	350/365 (95%)	0.04	14 (4%) 42 41	12, 32, 70, 86	0
1	C	356/365 (97%)	0.48	46 (12%) 5 4	17, 41, 71, 89	0
1	E	361/365 (98%)	-0.36	5 (1%) 78 77	13, 27, 47, 72	0
All	All	1067/1095 (97%)	0.05	65 (6%) 25 24	12, 32, 67, 89	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	290	ASN	11.9
1	C	163	PHE	7.8
1	C	242	TYR	6.3
1	C	201	LEU	6.3
1	C	14	ILE	5.9
1	A	234	HIS	4.9
1	C	351	CYS	4.9
1	E	163	PHE	4.8
1	C	162	ALA	4.6
1	C	111	VAL	4.5
1	C	13	HIS	4.3
1	C	202	LYS	4.3
1	E	119	GLU	4.2
1	C	119	GLU	3.9
1	A	325	PRO	3.9
1	A	224	THR	3.9
1	C	167	GLY	3.9
1	C	219	VAL	3.8
1	C	216	ASN	3.8
1	C	324	ASN	3.8
1	C	365	VAL	3.7
1	C	232	LEU	3.6
1	C	200	GLY	3.4

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Mol	Chain	Res	Type	RSRZ
1	C	118	ASN	3.4
1	C	192	LEU	3.4
1	A	287	LEU	3.3
1	A	351	CYS	3.3
1	A	238	ASP	3.3
1	C	243	PRO	3.3
1	A	258	LYS	3.2
1	A	163	PHE	3.2
1	C	224	THR	3.2
1	A	291	GLY	3.2
1	C	170	PRO	3.1
1	E	365	VAL	3.0
1	C	352	ASN	2.9
1	C	235	VAL	2.8
1	C	236	ILE	2.8
1	C	12	THR	2.7
1	A	242	TYR	2.6
1	C	172	PHE	2.6
1	C	199	GLU	2.5
1	C	98	GLN	2.5
1	C	239	ALA	2.5
1	C	356	THR	2.5
1	E	118	ASN	2.5
1	C	186	ILE	2.5
1	C	248	VAL	2.4
1	C	121	GLY	2.4
1	C	120	ASP	2.3
1	C	215	ILE	2.3
1	E	5	GLY	2.2
1	C	234	HIS	2.2
1	A	256	ILE	2.2
1	C	222	TYR	2.2
1	C	217	THR	2.2
1	C	15	SER	2.2
1	C	116	VAL	2.2
1	C	211	THR	2.2
1	C	176	PHE	2.2
1	C	187	THR	2.1
1	C	238	ASP	2.1
1	A	236	ILE	2.1
1	A	232	LEU	2.1
1	C	158	TYR	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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors(Å <sup>2</sup> )	Q<0.9
3	FER	A	366	14/14	0.38	0.30	3.34	74,80,81,82	0
3	FER	C	366	14/14	0.39	0.39	1.53	83,88,90,91	0
3	FER	E	1698	14/14	0.62	0.22	1.33	39,46,49,54	0
2	SAH	E	1697	26/26	0.91	0.13	0.56	27,39,46,48	0
2	SAH	A	1698	26/26	0.84	0.17	0.15	56,66,68,69	0
2	SAH	C	1699	26/26	0.84	0.19	-0.15	54,61,71,72	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.