



Full wwPDB X-ray Structure Validation Report

Feb 27, 2014 – 08:15 PM GMT

PDB ID : 2EG5
Title : The structure of xanthosine methyltransferase
Authors : McCarthy, A.A.; McCarthy, J.G.
Deposited on : 2007-02-28
Resolution : 2.20 Å(reported)

This is a full wwPDB validation report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at <http://wwpdb.org/ValidationPDFNotes.html>

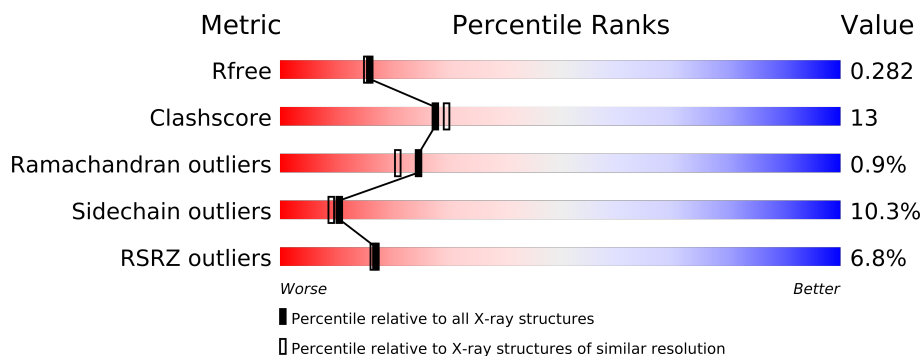
The following versions of software and data (see [references](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.15 2013
Xtriage (Phenix) : dev-1323
EDS : stable22639
Percentile statistics : 21963
Refmac : 5.8.0049
CCP4 : 6.3.0 (Settle)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : stable22683

1 Overall quality at a glance

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}	66092	2938 (2.20-2.20)
Clashscore	79885	3751 (2.20-2.20)
Ramachandran outliers	78287	3681 (2.20-2.20)
Sidechain outliers	78261	3682 (2.20-2.20)
RSRZ outliers	66119	2939 (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 ≥ 3 , 2, 1 and 0 types of geometric quality criteria. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density.

Mol	Chain	Length	Quality of chain
1	A	372	
1	C	372	
1	E	372	
1	G	372	

The following table lists non-polymeric compounds that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Geometry	Electron density
2	SAH	E	2501	-	X
3	XTS	E	2502	-	X
3	XTS	G	3502	-	X

2 Entry composition i

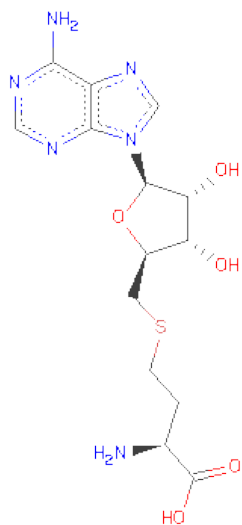
There are 4 unique types of molecules in this entry. The entry contains 11430 atoms, of which 0 are hydrogen and 0 are deuterium.

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 Xanthosine methyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	344	Total	C	N	O	S	0	3	0
			2701	1744	449	495	13			
1	C	344	Total	C	N	O	S	0	3	0
			2681	1734	444	490	13			
1	E	346	Total	C	N	O	S	0	4	0
			2698	1745	444	494	15			
1	G	343	Total	C	N	O	S	0	3	0
			2667	1725	440	489	13			

- Molecule 2 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: C₁₄H₂₀N₆O₅S).



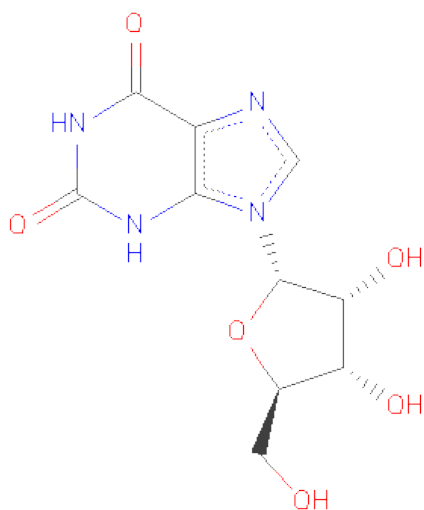
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			26	14	6	5	1		
2	C	1	Total	C	N	O	S	0	0
			26	14	6	5	1		

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

- Molecule 3 is 9-[(2R,3R,4S,5R)-3,4-DIHYDROXY-5-(HYDROXYMETHYL)OXOLAN-2-YL]-3H-PURINE-2,6-DIONE (three-letter code: XTS) (formula: C₁₀H₁₂N₄O₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			20	10	4	6		
3	C	1	Total	C	N	O	0	0
			20	10	4	6		
3	E	1	Total	C	N	O	0	0
			20	10	4	6		
3	G	1	Total	C	N	O	0	0
			20	10	4	6		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	156	Total	O	0	0
			156	156		
4	C	132	Total	O	0	0
			132	132		
4	E	114	Total	O	0	0
			114	114		

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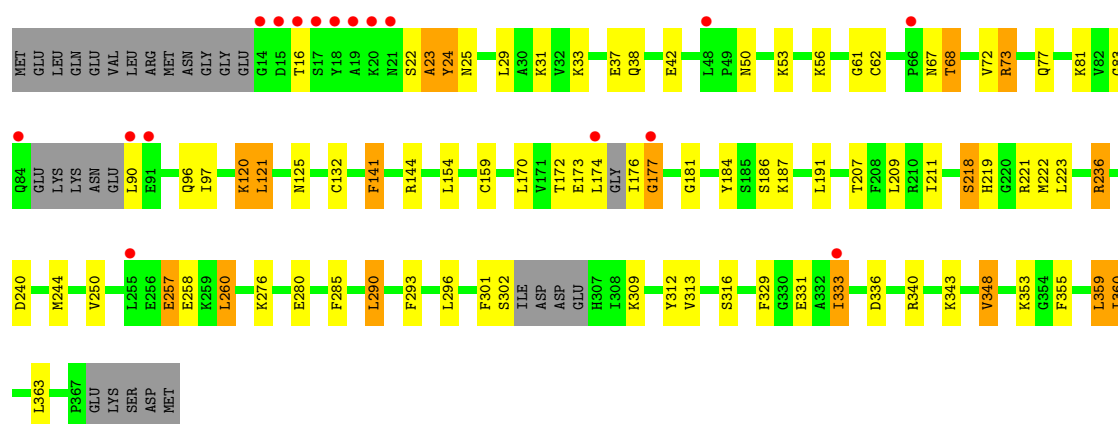
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	G	97	Total	O	0	0
			97	97		

3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

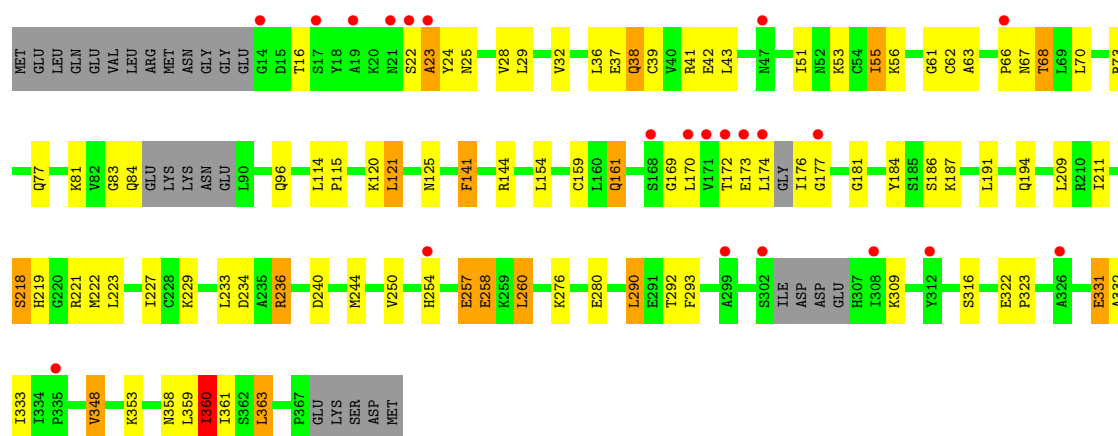
• Molecule 1: Xanthosine methyltransferase

Chain A: 



• Molecule 1: Xanthosine methyltransferase

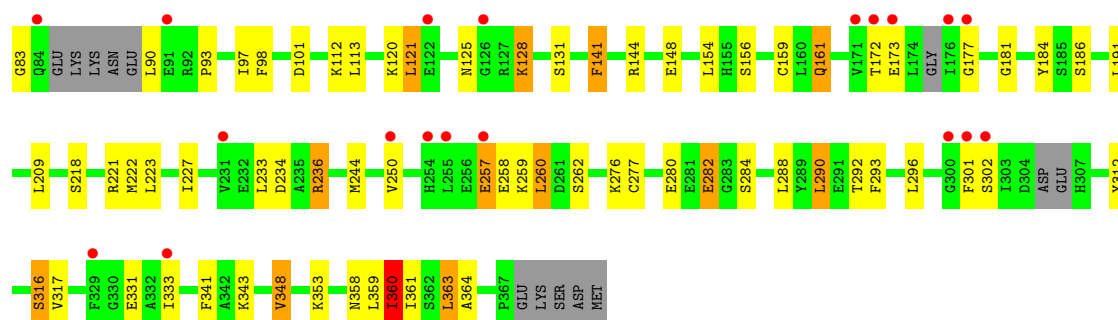
Chain C: 



• Molecule 1: Xanthosine methyltransferase

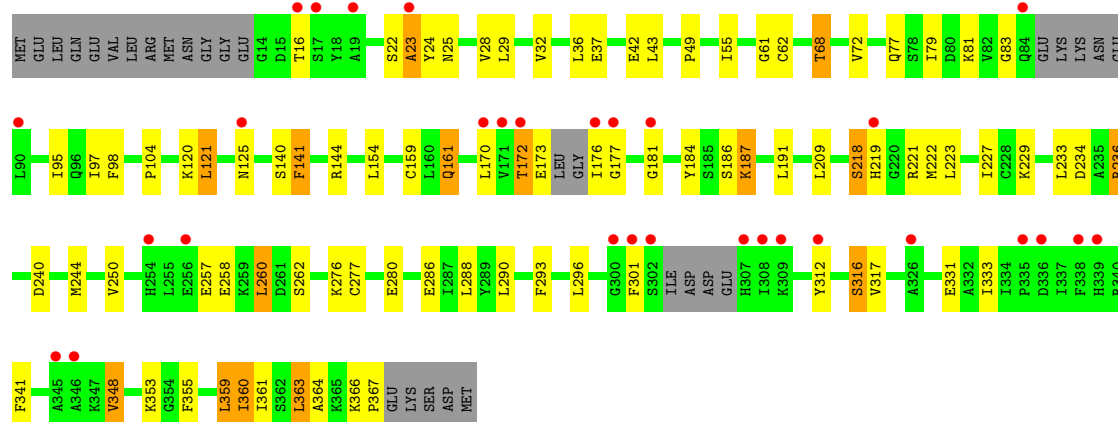
Chain E: 





• Molecule 1: Xanthosine methyltransferase

Chain G: 



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	57.59Å 119.80Å 116.40Å 90.00° 102.16° 90.00°	Depositor
Resolution (Å)	30.00 – 2.20 29.95 – 2.20	Depositor EDS
% Data completeness (in resolution range)	96.7 (30.00-2.20) 86.6 (29.95-2.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.20Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.230 , 0.284 0.231 , 0.282	Depositor DCC
R_{free} test set	3830 reflections (5.33%)	DCC
Wilson B-factor (Å ²)	31.7	Xtriage
Anisotropy	0.155	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 40.2	EDS
Estimated twinning fraction	0.089 for h,-k,-h-l	Xtriage
L-test for twinning	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Outliers	0 of 75624 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	11430	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 26.23 % of the origin peak, indicating pseudo translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo translational symmetry is equal to 2.7398e-03.*

¹Intensities estimated from amplitudes.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0.80	1/2765 (0.0%)	0.80	1/3739 (0.0%)
1	C	0.79	0/2745	0.79	1/3714 (0.0%)
1	E	0.67	0/2765	0.74	3/3740 (0.1%)
1	G	0.73	0/2731	0.76	0/3698
All	All	0.75	1/11006 (0.0%)	0.77	5/14891 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	E	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	132	CYS	CB-SG	-5.60	1.72	1.81

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	101	ASP	CB-CG-OD2	5.55	123.29	118.30
1	E	173	GLU	OE1-CD-OE2	-5.53	116.67	123.30
1	C	360	ILE	CB-CA-C	-5.24	101.13	111.60
1	A	173	GLU	OE1-CD-OE2	-5.11	117.17	123.30
1	E	360	ILE	CB-CA-C	-5.03	101.55	111.60

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	302	SER	Peptide

5.2 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 hydrogens added by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, and the number in parentheses is this value normalized per 1000 atoms of the molecule in the chain. The Symm-Clashes column gives symmetry related clashes, in the same way as for the Clashes column.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2701	0	2702	69	0
1	C	2681	0	2667	71	0
1	E	2698	0	2686	73	0
1	G	2667	0	2634	66	0
2	A	26	0	19	2	0
2	C	26	0	19	3	0
2	E	26	0	19	2	0
2	G	26	0	19	2	0
3	A	20	0	12	9	0
3	C	20	0	12	6	0
3	E	20	0	12	8	0
3	G	20	0	12	7	0
4	A	156	0	0	9	0
4	C	132	0	0	11	0
4	E	114	0	0	11	0
4	G	97	0	0	6	0
All	All	11430	0	10813	278	0

Clashscore is defined as the number of clashes calculated for the entry per 1000 atoms (including hydrogens) of the entry. The overall clashscore for this entry is 13.

All (278) close contacts within the same asymmetric unit are listed below.

Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:24:TYR:HB3	3:E:2502:XTS:H5'2	1.21	1.17
1:A:24:TYR:HB3	3:A:502:XTS:H5'2	1.26	1.16
1:C:290:LEU:CD2	1:C:359:LEU:HD11	1.74	1.16
1:E:236:ARG:HD3	1:E:244:MET:HE1	1.28	1.14
1:G:236:ARG:HD3	1:G:244:MET:HE1	1.28	1.09
1:A:236:ARG:HD3	1:A:244:MET:HE1	1.26	1.08
1:E:290:LEU:HD21	1:E:359:LEU:HD11	1.34	1.07

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:C:24:TYR:HB3	3:C:1502:XTS:H5'2	1.38	1.06
1:C:236:ARG:HD3	1:C:244:MET:HE1	1.31	1.06
1:C:290:LEU:HD21	1:C:359:LEU:HD11	1.34	1.04
1:G:24:TYR:HB3	3:G:3502:XTS:H5'2	1.45	0.97
1:G:316:SER:HB3	3:G:3502:XTS:H4'	1.51	0.92
1:G:61:GLY:HA3	1:G:159:CYS:SG	2.10	0.92
1:C:316:SER:HB3	3:C:1502:XTS:H4'	1.52	0.89
1:E:290:LEU:CD2	1:E:359:LEU:HD11	2.02	0.89
1:C:290:LEU:HD23	1:C:359:LEU:HD11	1.55	0.88
1:E:290:LEU:HD21	1:E:359:LEU:CD1	2.02	0.88
1:A:236:ARG:CD	1:A:244:MET:HE1	2.04	0.88
1:A:177:GLY:HA3	4:A:619:HOH:O	1.72	0.88
1:A:25:ASN:HD21	3:A:502:XTS:H8	1.37	0.87
1:G:236:ARG:CD	1:G:244:MET:HE1	2.06	0.86
1:A:316:SER:HB3	3:A:502:XTS:H4'	1.56	0.84
1:E:25:ASN:HD21	3:E:2502:XTS:H8	1.43	0.84
1:E:24:TYR:HB3	3:E:2502:XTS:C5'	2.08	0.82
1:E:24:TYR:CB	3:E:2502:XTS:H5'2	2.09	0.82
1:E:156:SER:OG	1:E:159[B]:CYS:SG	2.38	0.80
1:E:316:SER:HB3	3:E:2502:XTS:H4'	1.61	0.80
1:E:290:LEU:CD2	1:E:359:LEU:CD1	2.59	0.79
1:C:290:LEU:CD2	1:C:359:LEU:CD1	2.61	0.76
1:A:73:ARG:NH2	1:A:120:LYS:HB3	2.01	0.76
1:E:236:ARG:CD	1:E:244:MET:HE1	2.13	0.76
1:A:29:LEU:HD11	4:A:631:HOH:O	1.85	0.75
1:C:236:ARG:CD	1:C:244:MET:HE1	2.14	0.75
1:C:161:GLN:HG2	1:C:227:ILE:HD12	1.70	0.72
1:C:41:ARG:NH1	4:C:1634:HOH:O	2.22	0.71
1:E:53:LYS:HD2	1:E:53:LYS:N	2.06	0.71
1:C:25:ASN:HD21	3:C:1502:XTS:H8	1.55	0.70
1:E:277[B]:CYS:SG	4:E:2590:HOH:O	2.51	0.68
1:A:33:LYS:HE2	4:A:569:HOH:O	1.93	0.68
1:E:161:GLN:HG2	1:E:227:ILE:HD12	1.75	0.68
1:A:53:LYS:N	1:A:53:LYS:HD2	2.08	0.68
1:E:62:CYS:O	1:E:68:THR:HB	1.93	0.67
1:C:290:LEU:HD23	1:C:359:LEU:CD1	2.25	0.67
1:A:257:GLU:CG	1:A:257:GLU:O	2.42	0.67
1:C:84:GLN:NE2	4:C:1550:HOH:O	2.26	0.67
1:A:67:ASN:HB3	4:A:631:HOH:O	1.94	0.67
1:G:62:CYS:O	1:G:68:THR:HB	1.95	0.66
1:A:62:CYS:O	1:A:68:THR:HB	1.95	0.66
1:A:257:GLU:HG3	1:A:257:GLU:O	1.95	0.66

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:161:GLN:HG2	1:G:227:ILE:HD12	1.76	0.66
1:A:25:ASN:HD21	3:A:502:XTS:C8	2.07	0.66
1:G:25:ASN:HD21	3:G:3502:XTS:H8	1.60	0.66
1:A:290:LEU:HD21	1:A:359:LEU:HD11	1.76	0.66
1:C:348:VAL:HG22	1:C:353:LYS:HB2	1.78	0.64
1:C:236:ARG:HD3	1:C:244:MET:CE	2.18	0.64
1:A:61:GLY:HA3	1:A:159:CYS:SG	2.36	0.64
1:C:181:GLY:HA2	1:C:260:LEU:HD13	1.79	0.64
1:C:61:GLY:HA3	1:C:159:CYS:SG	2.37	0.64
1:G:77:GLN:HG2	1:G:125:ASN:HD21	1.62	0.64
1:A:348:VAL:HG22	1:A:353:LYS:HB2	1.79	0.63
1:E:348:VAL:HG22	1:E:353:LYS:HB2	1.79	0.63
1:C:62:CYS:O	1:C:68:THR:HB	1.99	0.63
1:C:24:TYR:HB3	3:C:1502:XTS:C5'	2.23	0.62
1:E:77:GLN:HG2	1:E:125:ASN:HD21	1.65	0.62
1:E:259:LYS:HD2	4:E:2576:HOH:O	1.99	0.62
1:C:22:SER:O	1:C:23:ALA:HB3	1.99	0.61
1:C:229:LYS:NZ	4:C:1630:HOH:O	2.33	0.61
1:E:22:SER:O	1:E:23:ALA:HB3	1.99	0.61
1:E:33:LYS:HE2	4:E:2569:HOH:O	2.01	0.61
1:E:22:SER:O	1:E:23:ALA:CB	2.49	0.61
1:G:348:VAL:HG22	1:G:353:LYS:HB2	1.81	0.61
1:C:77:GLN:HG2	1:C:125:ASN:HD21	1.66	0.60
1:E:262:SER:HB3	4:E:2599:HOH:O	2.00	0.60
1:A:24:TYR:HB3	3:A:502:XTS:C5'	2.19	0.60
1:A:25:ASN:ND2	3:A:502:XTS:H8	2.15	0.60
1:G:229:LYS:NZ	4:G:3586:HOH:O	2.30	0.59
1:A:29:LEU:CD1	4:A:631:HOH:O	2.44	0.59
1:C:22:SER:O	1:C:23:ALA:CB	2.49	0.59
1:E:236:ARG:HD3	1:E:244:MET:CE	2.17	0.59
1:A:290:LEU:HD21	1:A:359:LEU:CD1	2.31	0.59
1:G:24:TYR:HB3	3:G:3502:XTS:C5'	2.29	0.59
1:G:22:SER:O	1:G:23:ALA:HB3	2.03	0.58
1:G:181:GLY:HA2	1:G:260:LEU:HD13	1.86	0.58
1:A:181:GLY:HA2	1:A:260:LEU:HD13	1.86	0.58
1:A:50:ASN:HA	1:A:53:LYS:HD3	1.85	0.58
1:E:66:PRO:HD2	4:E:2609:HOH:O	2.03	0.57
1:A:22:SER:O	1:A:23:ALA:HB3	2.03	0.57
1:E:25:ASN:HD21	3:E:2502:XTS:C8	2.15	0.57
1:G:257:GLU:CG	1:G:257:GLU:O	2.51	0.57
1:A:62:CYS:HB2	4:A:562:HOH:O	2.03	0.57
1:G:262:SER:HB3	4:G:3550:HOH:O	2.04	0.57

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:G:276:LYS:O	1:G:280:GLU:HG3	2.05	0.57
1:A:22:SER:O	1:A:23:ALA:CB	2.53	0.56
1:A:236:ARG:HD3	1:A:244:MET:CE	2.17	0.56
1:G:22:SER:O	1:G:23:ALA:CB	2.54	0.56
1:A:77:GLN:HG2	1:A:125:ASN:HD21	1.70	0.56
1:A:276:LYS:O	1:A:280:GLU:HG3	2.04	0.56
1:C:293:PHE:CE2	1:C:360:ILE:HD11	2.40	0.56
1:G:257:GLU:HG3	1:G:257:GLU:O	2.04	0.56
1:G:361:ILE:HG12	1:G:363:LEU:HD13	1.86	0.56
1:E:276:LYS:O	1:E:280:GLU:HG3	2.04	0.56
1:C:194:GLN:NE2	4:C:1540:HOH:O	2.38	0.56
1:G:293:PHE:CE2	1:G:360:ILE:HD11	2.40	0.55
1:C:257:GLU:CG	1:C:257:GLU:O	2.54	0.55
1:E:181:GLY:HA2	1:E:260:LEU:HD13	1.88	0.55
1:G:25:ASN:O	1:G:29:LEU:HG	2.06	0.55
1:C:361:ILE:HG12	1:C:363:LEU:HD13	1.89	0.54
1:E:112:LYS:HE3	1:G:104:PRO:HA	1.90	0.54
1:A:218:SER:O	1:A:219:HIS:HB2	2.08	0.54
1:G:236:ARG:CG	1:G:244:MET:HE1	2.37	0.54
1:C:24:TYR:CB	3:C:1502:XTS:H5'2	2.26	0.54
1:E:53:LYS:HD2	1:E:53:LYS:H	1.73	0.54
1:A:25:ASN:O	1:A:29:LEU:HG	2.07	0.53
1:E:37:GLU:OE2	1:E:81:LYS:HE3	2.07	0.53
1:A:236:ARG:CG	1:A:244:MET:HE1	2.38	0.53
1:E:161:GLN:CG	1:E:227:ILE:HD12	2.37	0.53
1:E:257:GLU:O	1:E:257:GLU:CG	2.57	0.53
1:E:50:ASN:HA	1:E:53:LYS:HD3	1.89	0.52
1:E:290:LEU:HD23	1:E:359:LEU:CD1	2.37	0.52
1:G:37:GLU:OE2	1:G:81:LYS:HE3	2.09	0.52
1:C:25:ASN:HD21	3:C:1502:XTS:C8	2.23	0.52
1:C:211:ILE:HD11	4:C:1530:HOH:O	2.09	0.51
1:G:286:GLU:HG3	4:G:3535:HOH:O	2.09	0.51
1:E:141:PHE:CD2	2:E:2501:SAH:C2	2.93	0.51
1:E:233:LEU:O	1:E:234:ASP:HB2	2.10	0.51
1:G:154:LEU:O	1:G:222:MET:HA	2.11	0.51
1:A:67:ASN:CB	4:A:631:HOH:O	2.57	0.51
1:G:42:GLU:HB3	1:G:221[B]:ARG:HH22	1.75	0.51
1:G:296:LEU:HD23	1:G:355:PHE:HB3	1.93	0.50
1:E:128:LYS:HD3	1:E:131:SER:HB3	1.92	0.50
1:E:128:LYS:CD	1:E:131:SER:HB3	2.41	0.50
1:A:285:PHE:HB3	1:A:363:LEU:HB3	1.93	0.50
1:C:73:ARG:NH2	1:C:120:LYS:HB3	2.27	0.50

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:A:293:PHE:CE2	1:A:360:ILE:HD11	2.47	0.50
1:C:257:GLU:HG3	1:C:257:GLU:O	2.12	0.50
1:C:154:LEU:O	1:C:222:MET:HA	2.12	0.50
1:E:61:GLY:HA3	1:E:159[A]:CYS:SG	2.51	0.50
1:C:233:LEU:O	1:C:234:ASP:HB2	2.11	0.50
1:G:72:VAL:HG13	1:G:97:ILE:CD1	2.41	0.49
1:C:276:LYS:O	1:C:280:GLU:HG3	2.12	0.49
1:E:361:ILE:HG12	1:E:363:LEU:HD13	1.94	0.49
1:G:140:SER:HA	2:G:3501:SAH:N1	2.27	0.49
1:E:257:GLU:O	1:E:257:GLU:HG3	2.12	0.49
1:C:331:GLU:HG3	4:C:1560:HOH:O	2.12	0.49
1:A:240:ASP:O	1:A:244:MET:HE2	2.13	0.48
1:G:233:LEU:O	1:G:234:ASP:HB2	2.12	0.48
1:C:293:PHE:HE2	1:C:360:ILE:HD11	1.78	0.48
1:G:301:PHE:CZ	1:G:312:TYR:HB3	2.49	0.48
1:A:316:SER:CB	3:A:502:XTS:H4'	2.38	0.48
1:C:141:PHE:N	2:C:1501:SAH:N1	2.57	0.48
1:G:77:GLN:CG	1:G:125:ASN:HD21	2.27	0.47
1:A:81:LYS:HE3	4:A:550:HOH:O	2.14	0.47
1:E:236:ARG:HG2	1:E:244:MET:HE3	1.97	0.47
1:A:236:ARG:CG	1:A:244:MET:CE	2.91	0.47
1:C:169:GLY:HA3	4:C:1575:HOH:O	2.14	0.47
1:E:293:PHE:CE2	1:E:360:ILE:HD11	2.49	0.47
1:E:348:VAL:HG22	1:E:353:LYS:CB	2.42	0.47
1:E:250:VAL:HB	1:E:257:GLU:HB2	1.96	0.47
1:C:292:THR:HA	1:C:358:ASN:O	2.15	0.47
1:A:154:LEU:O	1:A:222:MET:HA	2.14	0.47
1:E:25:ASN:O	1:E:29:LEU:HG	2.14	0.47
1:G:359:LEU:HD23	1:G:359:LEU:O	2.15	0.47
1:C:51:ILE:O	1:C:55[B]:ILE:HD13	2.14	0.47
1:C:77:GLN:CG	1:C:125:ASN:HD21	2.28	0.46
1:E:128:LYS:HG3	1:E:128:LYS:H	1.56	0.46
1:A:209:LEU:HD23	1:A:222:MET:HE1	1.98	0.46
1:G:173:GLU:HG3	4:G:3570:HOH:O	2.15	0.46
1:C:293:PHE:HE2	1:C:360:ILE:CD1	2.28	0.46
1:G:209:LEU:HD23	1:G:222:MET:HE1	1.98	0.46
1:G:42:GLU:HB2	1:G:221[B]:ARG:HH12	1.81	0.46
1:E:209:LEU:HD23	1:E:222:MET:HE1	1.97	0.46
1:A:250:VAL:HB	1:A:257:GLU:HB2	1.98	0.46
1:G:250:VAL:HB	1:G:257:GLU:HB2	1.98	0.46
1:A:24:TYR:CB	3:A:502:XTS:H5'2	2.19	0.46
1:E:33:LYS:HD2	4:E:2596:HOH:O	2.15	0.46

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:288:LEU:HD11	1:E:364:ALA:HB2	1.98	0.46
1:G:170:LEU:HA	1:G:176:ILE:N	2.31	0.46
1:G:141:PHE:N	2:G:3501:SAH:N1	2.56	0.45
1:G:316:SER:CB	3:G:3502:XTS:H4'	2.34	0.45
1:C:170:LEU:HA	1:C:176:ILE:N	2.31	0.45
1:G:218:SER:O	1:G:219:HIS:HB2	2.16	0.45
1:G:293:PHE:HE2	1:G:360:ILE:CD1	2.29	0.45
1:A:336:ASP:O	1:A:340[B]:ARG:HG2	2.17	0.45
1:E:67:ASN:HA	1:E:70:LEU:HD12	1.97	0.45
1:C:25:ASN:O	1:C:29:LEU:HG	2.16	0.45
1:C:240:ASP:O	1:C:244:MET:HE2	2.16	0.45
1:G:187:LYS:HD3	1:G:187:LYS:N	2.32	0.45
1:C:121:LEU:O	1:C:125:ASN:HB2	2.16	0.45
1:C:194:GLN:HB3	4:C:1509:HOH:O	2.16	0.45
1:C:37:GLU:OE2	1:C:81:LYS:HE3	2.16	0.45
2:A:501:SAH:HG1	2:A:501:SAH:H4'	1.83	0.44
1:G:55:ILE:CG2	1:G:95:ILE:HG23	2.47	0.44
1:A:56:LYS:HE3	1:A:96:GLN:NE2	2.32	0.44
1:C:42:GLU:HB2	1:C:221[B]:ARG:HH12	1.82	0.44
1:G:28:VAL:O	1:G:32:VAL:HG23	2.17	0.44
1:E:154:LEU:O	1:E:222:MET:HA	2.17	0.44
1:C:161:GLN:CG	1:C:227:ILE:HD12	2.45	0.44
1:C:114:LEU:N	1:C:115:PRO:CD	2.80	0.44
1:E:296:LEU:HD13	4:E:2537:HOH:O	2.17	0.44
1:E:42:GLU:HB3	1:E:221[B]:ARG:HH22	1.81	0.44
1:G:43:LEU:HD13	1:G:221[B]:ARG:HG3	2.00	0.44
1:A:53:LYS:HD2	1:A:53:LYS:H	1.82	0.44
1:C:209:LEU:HD23	1:C:222:MET:HE1	2.00	0.44
1:A:37:GLU:HG2	4:A:550:HOH:O	2.17	0.44
1:C:218:SER:O	1:C:219:HIS:HB2	2.17	0.44
1:A:207:THR:HG22	1:A:211:ILE:HD12	2.00	0.43
1:G:43:LEU:HD13	1:G:221[B]:ARG:CG	2.48	0.43
1:A:37:GLU:OE2	1:A:81:LYS:HE3	2.18	0.43
1:G:288:LEU:HD11	1:G:364:ALA:HB2	1.99	0.43
1:G:236:ARG:CG	1:G:244:MET:CE	2.95	0.43
2:C:1501:SAH:H4'	2:C:1501:SAH:HG1	1.84	0.43
1:E:42:GLU:HB2	1:E:221[B]:ARG:HH12	1.83	0.43
1:E:60:LEU:O	1:E:159[B]:CYS:SG	2.76	0.43
1:C:348:VAL:HG22	1:C:353:LYS:CB	2.46	0.43
1:G:121:LEU:O	1:G:125:ASN:HB2	2.18	0.43
1:A:72:VAL:HG13	1:A:97:ILE:CD1	2.49	0.43
1:A:121:LEU:O	1:A:125:ASN:HB2	2.18	0.43

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:282:GLU:OE2	1:E:284:SER:OG	2.22	0.43
1:E:292:THR:HA	1:E:358:ASN:O	2.18	0.43
1:A:22:SER:HB3	1:A:67:ASN:OD1	2.19	0.43
1:G:172:THR:HG23	4:G:3570:HOH:O	2.18	0.43
1:C:332:ALA:HA	1:G:367:PRO:HB3	2.00	0.43
1:G:72:VAL:HG13	1:G:97:ILE:HD13	2.01	0.43
1:E:72:VAL:HG13	1:E:97:ILE:CD1	2.49	0.43
1:C:236:ARG:HG2	1:C:244:MET:HE3	2.01	0.42
1:A:73:ARG:HH22	1:A:120:LYS:HG2	1.83	0.42
1:E:25:ASN:ND2	3:E:2502:XTS:H8	2.23	0.42
1:A:348:VAL:HG22	1:A:353:LYS:CB	2.49	0.42
1:C:56:LYS:HE3	1:C:96:GLN:NE2	2.34	0.42
1:C:38:GLN:HE21	1:C:39:CYS:N	2.17	0.42
1:A:24:TYR:CG	3:A:502:XTS:H3'	2.55	0.42
1:C:63:ALA:HB2	2:C:1501:SAH:HG2	2.02	0.42
1:A:42:GLU:HB3	1:A:221[B]:ARG:HH22	1.85	0.42
1:G:366:LYS:NZ	4:G:3527:HOH:O	2.50	0.42
1:C:250:VAL:HB	1:C:257:GLU:HB2	2.00	0.42
1:C:322:GLU:O	1:C:323:PRO:C	2.57	0.42
1:C:254:HIS:HA	1:G:49:PRO:HB3	2.00	0.42
1:C:67:ASN:HA	1:C:70:LEU:HD12	2.02	0.42
1:E:236:ARG:CG	1:E:244:MET:CE	2.98	0.42
1:G:55:ILE:HG23	1:G:95:ILE:HG23	2.02	0.42
1:A:257:GLU:CD	1:A:257:GLU:O	2.58	0.41
1:A:309:LYS:HE2	1:A:309:LYS:HB2	1.74	0.41
1:A:141:PHE:N	2:A:501:SAH:N1	2.56	0.41
1:C:66:PRO:O	1:C:70:LEU:HG	2.20	0.41
1:E:316:SER:CB	3:E:2502:XTS:H4'	2.42	0.41
1:G:240:ASP:O	1:G:244:MET:HE2	2.20	0.41
1:C:236:ARG:CG	1:C:244:MET:CE	2.99	0.41
1:G:25:ASN:HD21	3:G:3502:XTS:C8	2.32	0.41
1:G:55:ILE:HG21	1:G:79:ILE:HD13	2.02	0.41
1:A:296:LEU:HD23	1:A:355:PHE:HB3	2.02	0.41
1:C:258:GLU:HB3	4:C:1542:HOH:O	2.21	0.41
1:A:31:LYS:HE3	1:A:31:LYS:HB3	1.76	0.41
1:A:301:PHE:CZ	1:A:312:TYR:HB3	2.55	0.41
1:E:45:ARG:NH2	4:E:2582:HOH:O	2.52	0.41
1:A:309:LYS:O	1:A:313:VAL:HG23	2.21	0.41
1:G:24:TYR:CB	3:G:3502:XTS:H5'2	2.33	0.41
1:E:90:LEU:N	4:E:2581:HOH:O	2.53	0.41
1:E:148:GLU:HG3	1:E:148:GLU:H	1.61	0.41
1:A:170:LEU:HA	1:A:176:ILE:N	2.36	0.41

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Atom-1	Atom-2	Distance(Å)	Clash(Å)
1:E:73:ARG:HH21	1:E:120:LYS:HB3	1.85	0.41
1:A:141:PHE:CE2	1:A:159:CYS:HB3	2.56	0.41
1:A:77:GLN:CG	1:A:125:ASN:HD21	2.34	0.41
1:E:93:PRO:HD2	4:E:2548:HOH:O	2.20	0.41
1:G:317:VAL:HG21	1:G:341:PHE:CZ	2.56	0.41
1:E:301:PHE:CZ	1:E:312:TYR:HB3	2.56	0.41
1:A:329:PHE:HB3	1:A:333:ILE:HD11	2.02	0.41
1:G:348:VAL:HG22	1:G:353:LYS:CB	2.48	0.41
1:E:317:VAL:HG21	1:E:341:PHE:CZ	2.56	0.41
1:E:98:PHE:HE1	1:G:98:PHE:HE1	1.69	0.40
1:E:121:LEU:O	1:E:125:ASN:HB2	2.22	0.40
2:E:2501:SAH:HG1	2:E:2501:SAH:H4'	1.88	0.40
1:C:169:GLY:CA	4:C:1575:HOH:O	2.70	0.40
1:A:42:GLU:HB2	1:A:221[B]:ARG:HH12	1.86	0.40
1:C:81:LYS:NZ	4:C:1563:HOH:O	2.43	0.40
1:C:28:VAL:O	1:C:32:VAL:HG23	2.21	0.40
1:G:161:GLN:CG	1:G:227:ILE:HD12	2.48	0.40
1:E:113:LEU:HA	4:E:2512:HOH:O	2.20	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	339/372 (91%)	323 (95%)	13 (4%)	3 (1%)	25	21
1	C	339/372 (91%)	324 (96%)	12 (4%)	3 (1%)	25	21
1	E	342/372 (92%)	328 (96%)	11 (3%)	3 (1%)	25	21
1	G	338/372 (91%)	324 (96%)	11 (3%)	3 (1%)	25	21
All	All	1358/1488 (91%)	1299 (96%)	47 (4%)	12 (1%)	25	21

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	177	GLY
1	C	177	GLY
1	E	177	GLY
1	G	177	GLY
1	A	23	ALA
1	C	23	ALA
1	E	23	ALA
1	G	23	ALA
1	G	83	GLY
1	C	83	GLY
1	E	83	GLY
1	A	83	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	293/327 (90%)	263 (90%)	30 (10%)	11	9
1	C	287/327 (88%)	255 (89%)	32 (11%)	9	7
1	E	290/327 (89%)	261 (90%)	29 (10%)	11	10
1	G	283/327 (86%)	256 (90%)	27 (10%)	12	11
All	All	1153/1308 (88%)	1035 (90%)	118 (10%)	10	9

All (118) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	THR
1	A	24	TYR
1	A	38	GLN
1	A	68	THR
1	A	73	ARG
1	A	90	LEU
1	A	120	LYS
1	A	121	LEU
1	A	141	PHE
1	A	144	ARG
1	A	172	THR

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Mol	Chain	Res	Type
1	A	174	LEU
1	A	184	TYR
1	A	186	SER
1	A	187	LYS
1	A	191	LEU
1	A	218	SER
1	A	223	LEU
1	A	236	ARG
1	A	257	GLU
1	A	258	GLU
1	A	260	LEU
1	A	290	LEU
1	A	302	SER
1	A	331	GLU
1	A	333	ILE
1	A	343	LYS
1	A	348	VAL
1	A	359	LEU
1	A	360	ILE
1	C	16	THR
1	C	36	LEU
1	C	38	GLN
1	C	43	LEU
1	C	53	LYS
1	C	55[A]	ILE
1	C	55[B]	ILE
1	C	68	THR
1	C	121	LEU
1	C	141	PHE
1	C	144	ARG
1	C	161	GLN
1	C	172	THR
1	C	173	GLU
1	C	174	LEU
1	C	184	TYR
1	C	186	SER
1	C	187	LYS
1	C	191	LEU
1	C	218	SER
1	C	223	LEU
1	C	236	ARG
1	C	257	GLU

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Mol	Chain	Res	Type
1	C	258	GLU
1	C	260	LEU
1	C	290	LEU
1	C	309	LYS
1	C	331	GLU
1	C	333	ILE
1	C	348	VAL
1	C	360	ILE
1	C	363	LEU
1	E	16	THR
1	E	31	LYS
1	E	43	LEU
1	E	55	ILE
1	E	68	THR
1	E	121	LEU
1	E	128	LYS
1	E	141	PHE
1	E	144	ARG
1	E	161	GLN
1	E	172	THR
1	E	184	TYR
1	E	186	SER
1	E	191	LEU
1	E	218	SER
1	E	223	LEU
1	E	236	ARG
1	E	257	GLU
1	E	258	GLU
1	E	260	LEU
1	E	282	GLU
1	E	290	LEU
1	E	316	SER
1	E	331	GLU
1	E	333	ILE
1	E	343	LYS
1	E	348	VAL
1	E	360	ILE
1	E	363	LEU
1	G	16	THR
1	G	36	LEU
1	G	68	THR
1	G	120	LYS

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Mol	Chain	Res	Type
1	G	121	LEU
1	G	141	PHE
1	G	144	ARG
1	G	161	GLN
1	G	172	THR
1	G	184	TYR
1	G	186	SER
1	G	187	LYS
1	G	191	LEU
1	G	218	SER
1	G	223	LEU
1	G	236	ARG
1	G	258	GLU
1	G	260	LEU
1	G	277	CYS
1	G	290	LEU
1	G	316	SER
1	G	331	GLU
1	G	333	ILE
1	G	348	VAL
1	G	359	LEU
1	G	360	ILE
1	G	363	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	25	ASN
1	A	77	GLN
1	A	96	GLN
1	A	125	ASN
1	C	25	ASN
1	C	38	GLN
1	C	96	GLN
1	E	25	ASN
1	E	77	GLN
1	E	96	GLN
1	E	125	ASN
1	G	25	ASN
1	G	96	GLN
1	G	125	ASN

5.3.3 RNA ⓘ

There are no RNA chains 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 ⓘ

8 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	501	-	28,28,28	1.32	3 (10%)	40,40,40	2.54	9 (22%)
3	XTS	A	502	-	22,22,22	1.74	6 (27%)	27,33,33	4.99	8 (29%)
2	SAH	C	1501	-	28,28,28	1.11	2 (7%)	40,40,40	2.55	11 (27%)
3	XTS	C	1502	-	22,22,22	1.56	6 (27%)	27,33,33	5.02	7 (25%)
2	SAH	E	2501	-	28,28,28	1.05	2 (7%)	40,40,40	2.64	10 (25%)
3	XTS	E	2502	-	22,22,22	1.56	5 (22%)	27,33,33	5.37	7 (25%)
2	SAH	G	3501	-	28,28,28	1.24	3 (10%)	40,40,40	2.69	9 (22%)
3	XTS	G	3502	-	22,22,22	1.57	5 (22%)	27,33,33	5.74	7 (25%)

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	501	-	-	0/15/31/31	0/1/3/3
3	XTS	A	502	-	-	0/6/22/22	0/1/3/3
2	SAH	C	1501	-	-	0/15/31/31	0/1/3/3
3	XTS	C	1502	-	-	0/6/22/22	0/1/3/3
2	SAH	E	2501	-	-	0/15/31/31	0/1/3/3
3	XTS	E	2502	-	-	0/6/22/22	0/1/3/3
2	SAH	G	3501	-	-	0/15/31/31	0/1/3/3
3	XTS	G	3502	-	-	0/6/22/22	0/1/3/3

All (32) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	502	XTS	O4'-C1'	4.83	1.48	1.41
2	A	501	SAH	C2-N1	4.13	1.42	1.33
3	E	2502	XTS	O4'-C1'	4.07	1.47	1.41
2	A	501	SAH	C2-N3	3.88	1.39	1.32
2	G	3501	SAH	C2-N3	3.79	1.39	1.32
3	C	1502	XTS	O4'-C1'	3.76	1.47	1.41
3	G	3502	XTS	O4'-C1'	3.71	1.47	1.41
2	E	2501	SAH	C2-N3	3.51	1.39	1.32
2	G	3501	SAH	C2-N1	3.37	1.40	1.33
2	C	1501	SAH	C2-N1	3.23	1.40	1.33
3	A	502	XTS	C4-N9	-3.12	1.32	1.38
2	C	1501	SAH	C2-N3	3.08	1.38	1.32
3	G	3502	XTS	C6-N1	3.06	1.42	1.37
2	E	2501	SAH	C2-N1	2.83	1.39	1.33
3	C	1502	XTS	C4-N9	-2.82	1.33	1.38
3	C	1502	XTS	C6-N1	2.73	1.41	1.37
3	A	502	XTS	C2-N1	2.71	1.42	1.37
3	E	2502	XTS	C4-N3	2.70	1.41	1.37
2	A	501	SAH	C4-N3	2.65	1.39	1.35
3	A	502	XTS	C6-N1	2.64	1.41	1.37
3	E	2502	XTS	C4-N9	-2.62	1.33	1.38
3	C	1502	XTS	C4-N3	2.43	1.40	1.37
3	C	1502	XTS	C2-N1	2.39	1.42	1.37
3	G	3502	XTS	C4-N9	-2.35	1.34	1.38
3	G	3502	XTS	C4-N3	2.33	1.40	1.37
3	E	2502	XTS	C2-N1	2.29	1.41	1.37
3	A	502	XTS	C2'-C1'	2.22	1.56	1.53
2	G	3501	SAH	OXT-C	-2.19	1.22	1.30
3	A	502	XTS	C4-N3	2.17	1.40	1.37
3	C	1502	XTS	C2-N3	2.14	1.41	1.37
3	G	3502	XTS	C2-N1	2.11	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	2502	XTS	C6-N1	2.09	1.40	1.37

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	3502	XTS	C6-C5-N7	-19.74	131.48	134.14
3	G	3502	XTS	N3-C4-N9	17.95	132.77	126.41
3	C	1502	XTS	N3-C4-N9	17.94	132.77	126.41
3	E	2502	XTS	N3-C4-N9	17.61	132.65	126.41
3	E	2502	XTS	C6-C5-N7	-17.31	131.81	134.14
3	A	502	XTS	C6-C5-N7	-16.27	131.95	134.14
3	A	502	XTS	N3-C4-N9	15.39	131.87	126.41
2	E	2501	SAH	N3-C2-N1	-13.75	117.22	128.71
3	C	1502	XTS	C6-C5-N7	-13.75	132.29	134.14
2	G	3501	SAH	N3-C2-N1	-13.60	117.34	128.71
2	C	1501	SAH	N3-C2-N1	-12.93	117.90	128.71
2	A	501	SAH	N3-C2-N1	-12.45	118.30	128.71
3	G	3502	XTS	O4'-C1'-N9	-8.94	100.12	108.44
3	E	2502	XTS	O4'-C1'-N9	-8.16	100.85	108.44
3	C	1502	XTS	O4'-C1'-N9	-8.14	100.87	108.44
3	A	502	XTS	O4'-C1'-N9	-8.13	100.88	108.44
3	A	502	XTS	C2'-C1'-N9	6.89	130.95	113.27
3	E	2502	XTS	C2'-C1'-N9	6.21	129.22	113.27
3	C	1502	XTS	C2'-C1'-N9	5.82	128.21	113.27
3	G	3502	XTS	C2'-C1'-N9	5.81	128.18	113.27
3	E	2502	XTS	C4'-O4'-C1'	-5.09	104.22	109.75
3	G	3502	XTS	C4'-O4'-C1'	-5.02	104.30	109.75
3	C	1502	XTS	C4'-O4'-C1'	-4.92	104.41	109.75
2	G	3501	SAH	N3-C4-N9	4.24	133.09	125.43
3	A	502	XTS	C4'-O4'-C1'	-4.11	105.28	109.75
2	A	501	SAH	N3-C4-N9	3.90	132.47	125.43
2	C	1501	SAH	N3-C4-N9	3.85	132.39	125.43
2	E	2501	SAH	N3-C4-N9	3.77	132.23	125.43
3	E	2502	XTS	O4'-C1'-C2'	-3.65	101.18	106.77
2	A	501	SAH	C-CA-N	3.57	115.28	109.36
3	C	1502	XTS	O4'-C1'-C2'	-3.36	101.62	106.77
3	G	3502	XTS	C6-N1-C2	-3.26	118.74	125.36
2	A	501	SAH	O4'-C1'-C2'	-3.23	101.83	106.77
3	C	1502	XTS	C6-N1-C2	-3.02	119.24	125.36
2	C	1501	SAH	O4'-C1'-C2'	-3.01	102.15	106.77
3	A	502	XTS	O4'-C1'-C2'	-2.95	102.26	106.77
2	G	3501	SAH	OXT-C-O	-2.94	117.43	124.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2501	SAH	C5'-SD-CG	-2.92	93.69	102.42
2	C	1501	SAH	OXT-C-O	-2.79	117.76	124.07
2	E	2501	SAH	C2-N3-C4	2.72	121.76	114.01
2	C	1501	SAH	C5'-SD-CG	-2.68	94.42	102.42
2	G	3501	SAH	C2-N3-C4	2.60	121.43	114.01
2	A	501	SAH	OXT-C-O	-2.59	118.21	124.07
2	C	1501	SAH	C-CA-N	2.58	113.64	109.36
2	E	2501	SAH	O4'-C1'-C2'	-2.50	102.94	106.77
2	C	1501	SAH	C2-N3-C4	2.47	121.05	114.01
2	G	3501	SAH	CG-CB-CA	-2.43	109.15	113.22
2	A	501	SAH	C2-N3-C4	2.40	120.84	114.01
2	E	2501	SAH	C-CA-N	2.39	113.32	109.36
2	C	1501	SAH	O4'-C1'-N9	2.36	110.63	108.44
2	C	1501	SAH	C2-N1-C6	2.32	122.95	118.77
2	G	3501	SAH	C4'-O4'-C1'	-2.31	107.24	109.75
2	G	3501	SAH	O4'-C1'-N9	2.29	110.57	108.44
3	G	3502	XTS	O4'-C1'-C2'	-2.28	103.28	106.77
3	A	502	XTS	C2'-C3'-C4'	2.27	107.18	102.65
2	E	2501	SAH	C5-C4-N3	-2.26	120.78	125.70
2	C	1501	SAH	OXT-C-CA	2.24	121.91	116.88
2	G	3501	SAH	C8-N9-C4	2.23	108.61	106.90
2	A	501	SAH	CB-CG-SD	-2.22	109.28	113.57
3	A	502	XTS	C6-N1-C2	-2.22	120.85	125.36
2	E	2501	SAH	C2-N1-C6	2.17	122.69	118.77
2	G	3501	SAH	C5-C4-N3	-2.17	120.97	125.70
2	C	1501	SAH	C5-C4-N3	-2.15	121.01	125.70
2	E	2501	SAH	OXT-C-O	-2.13	119.25	124.07
3	E	2502	XTS	C6-N1-C2	-2.11	121.08	125.36
2	E	2501	SAH	CG-CB-CA	-2.08	109.74	113.22
2	A	501	SAH	C5-C4-N3	-2.04	121.26	125.70
2	A	501	SAH	CG-CB-CA	-2.00	109.87	113.22

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

5.7 Other polymers ⓘ

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	344/372 (92%)	0.35	17 (4%) 28 28	30, 43, 65, 79	12 (3%)
1	C	344/372 (92%)	0.44	22 (6%) 19 18	31, 43, 65, 79	15 (4%)
1	E	346/372 (93%)	0.43	25 (7%) 15 15	31, 43, 65, 79	5 (1%)
1	G	343/372 (92%)	0.54	30 (8%) 10 10	31, 43, 65, 79	11 (3%)
All	All	1377/1488 (92%)	0.44	94 (6%) 17 16	30, 43, 66, 79	43 (3%)

All (94) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	174	LEU	12.1
1	E	176	ILE	10.0
1	G	177	GLY	8.8
1	C	170	LEU	8.1
1	G	176	ILE	8.0
1	G	84	GLN	8.0
1	C	172	THR	6.9
1	A	14	GLY	6.7
1	G	16	THR	6.4
1	A	15	ASP	5.9
1	E	255	LEU	5.8
1	C	171	VAL	5.4
1	E	302	SER	5.2
1	G	300	GLY	4.8
1	C	312	TYR	4.6
1	E	257	GLU	4.4
1	G	171	VAL	4.4
1	E	84	GLN	4.3
1	C	302	SER	4.3
1	C	173	GLU	4.2
1	A	17	SER	4.1

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Mol	Chain	Res	Type	RSRZ
1	G	170	LEU	4.0
1	E	16	THR	4.0
1	G	254	HIS	3.8
1	C	19	ALA	3.7
1	C	23	ALA	3.7
1	E	301	PHE	3.7
1	E	66	PRO	3.7
1	E	91	GLU	3.7
1	E	333	ILE	3.7
1	G	312	TYR	3.5
1	A	18	TYR	3.5
1	E	254	HIS	3.5
1	G	338	PHE	3.4
1	A	84	GLN	3.4
1	C	66	PRO	3.3
1	A	16	THR	3.3
1	G	301	PHE	3.2
1	E	172	THR	3.1
1	G	172	THR	3.1
1	G	302	SER	3.1
1	C	254	HIS	3.1
1	E	177	GLY	3.1
1	E	231	VAL	3.0
1	A	21	ASN	3.0
1	G	346	ALA	3.0
1	E	122	GLU	2.9
1	E	126	GLY	2.9
1	E	329	PHE	2.9
1	G	308	ILE	2.8
1	E	173	GLU	2.8
1	A	19	ALA	2.8
1	E	250	VAL	2.8
1	G	256	GLU	2.8
1	C	17	SER	2.7
1	C	326	ALA	2.7
1	C	335	PRO	2.7
1	G	326	ALA	2.7
1	G	339	HIS	2.6
1	C	47	ASN	2.6
1	C	177	GLY	2.6
1	G	219	HIS	2.6
1	E	17	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	333	ILE	2.5
1	A	91	GLU	2.5
1	G	17	SER	2.5
1	G	309	LYS	2.5
1	A	90	LEU	2.5
1	A	255	LEU	2.5
1	C	14	GLY	2.4
1	C	21	ASN	2.4
1	G	125	ASN	2.4
1	E	82	VAL	2.4
1	G	23	ALA	2.4
1	G	181	GLY	2.3
1	C	308	ILE	2.3
1	G	345	ALA	2.3
1	G	336	ASP	2.3
1	A	20	LYS	2.3
1	E	171	VAL	2.3
1	G	19	ALA	2.3
1	A	174	LEU	2.2
1	A	66	PRO	2.2
1	E	300	GLY	2.2
1	C	22	SER	2.2
1	G	307	HIS	2.1
1	C	299	ALA	2.1
1	A	177	GLY	2.1
1	G	335	PRO	2.1
1	G	90	LEU	2.1
1	C	168	SER	2.1
1	E	52	ASN	2.1
1	E	15	ASP	2.0
1	A	48	LEU	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

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

6.3 Carbohydrates ⓘ

There are no carbohydrates in this entry.

6.4 Ligands

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, 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	RSR	LLDF	B-factors(Å ²)	Q<0.9
2	SAH	E	2501	26/26	0.21	4.88	53,57,67,68	0
3	XTS	G	3502	20/20	0.29	3.50	64,65,67,67	2
3	XTS	E	2502	20/20	0.24	3.25	64,65,67,67	2
2	SAH	A	501	26/26	0.20	1.37	53,56,67,68	0
3	XTS	C	1502	20/20	0.24	1.28	64,65,67,67	2
2	SAH	C	1501	26/26	0.17	0.96	53,56,67,68	0
2	SAH	G	3501	26/26	0.16	0.83	53,56,67,68	0
3	XTS	A	502	20/20	0.19	0.40	64,65,67,67	2

6.5 Other polymers

There are no such residues in this entry.