



Full wwPDB X-ray Structure Validation Report ⓘ

Nov 28, 2016 – 03:14 PM EST

PDB ID : 5GP1
Title : Crystal structure of ZIKV NS5 Methyltransferase in complex with GTP and SAH
Authors : Zhang, C.; Jin, T.
Deposited on : 2016-07-30
Resolution : 2.44 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

<http://wwpdb.org/validation/2016/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467
Mogul : 1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20028320
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) : rb-20028320

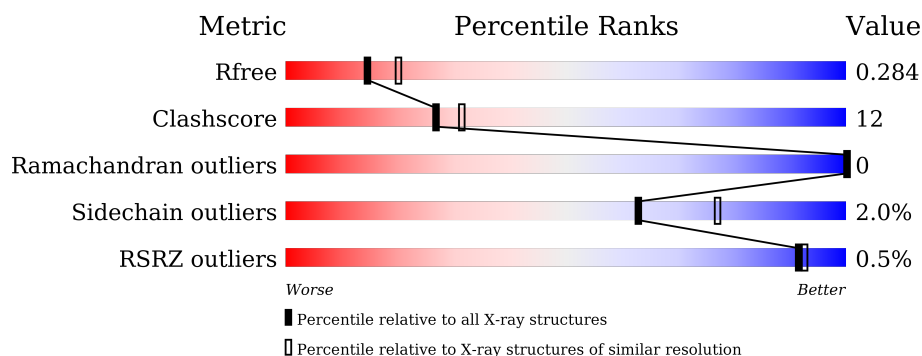
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.44 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	1003 (2.46-2.42)
Clashscore	102246	1071 (2.46-2.42)
Ramachandran outliers	100387	1065 (2.46-2.42)
Sidechain outliers	100360	1065 (2.46-2.42)
RSRZ outliers	91569	1005 (2.46-2.42)

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. 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	269	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red 1%, orange 1%, yellow 70%, green 27%, grey 4%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> % 70% 27% .. </div> </div>
1	B	269	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 72%, green 24%, grey 4%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 72% 24% . </div> </div>
1	C	269	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, yellow 74%, green 22%, orange 3%, grey 1%);"></div> <div style="display: flex; justify-content: space-between; width: 90%; margin: 0 auto;"> 74% 22% .. </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	SO4	A	303	-	-	-	X

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 6440 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 RNA-directed RNA polymerase NS5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	0	0
			2038	1274	369	381	14			
1	B	260	Total	C	N	O	S	0	0	0
			2027	1268	367	378	14			
1	C	261	Total	C	N	O	S	0	0	0
			2033	1271	368	380	14			

There are 21 discrepancies between the modelled and reference sequences:

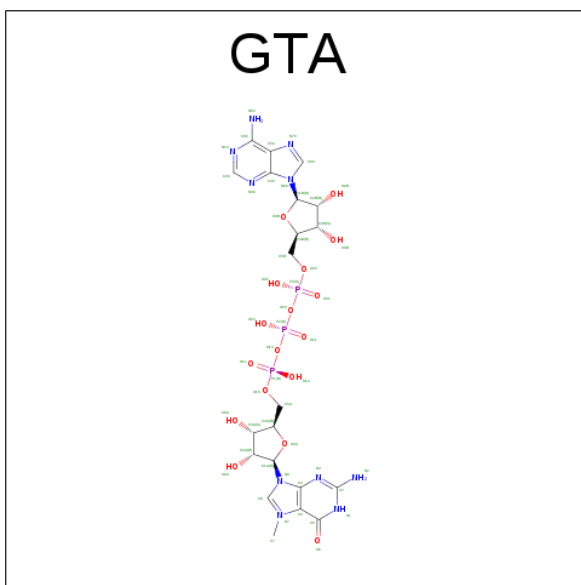
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	GLY	-	expression tag	UNP H9A910
A	1	SER	-	expression tag	UNP H9A910
A	2	VAL	-	expression tag	UNP H9A910
A	3	ASP	-	expression tag	UNP H9A910
A	266	ALA	-	expression tag	UNP H9A910
A	267	ALA	-	expression tag	UNP H9A910
A	268	SER	-	expression tag	UNP H9A910
B	0	GLY	-	expression tag	UNP H9A910
B	1	SER	-	expression tag	UNP H9A910
B	2	VAL	-	expression tag	UNP H9A910
B	3	ASP	-	expression tag	UNP H9A910
B	266	ALA	-	expression tag	UNP H9A910
B	267	ALA	-	expression tag	UNP H9A910
B	268	SER	-	expression tag	UNP H9A910
C	0	GLY	-	expression tag	UNP H9A910
C	1	SER	-	expression tag	UNP H9A910
C	2	VAL	-	expression tag	UNP H9A910
C	3	ASP	-	expression tag	UNP H9A910
C	266	ALA	-	expression tag	UNP H9A910
C	267	ALA	-	expression tag	UNP H9A910
C	268	SER	-	expression tag	UNP H9A910

- Molecule 2 is SULFATE ION (three-letter code: SO4) (formula: O₄S).



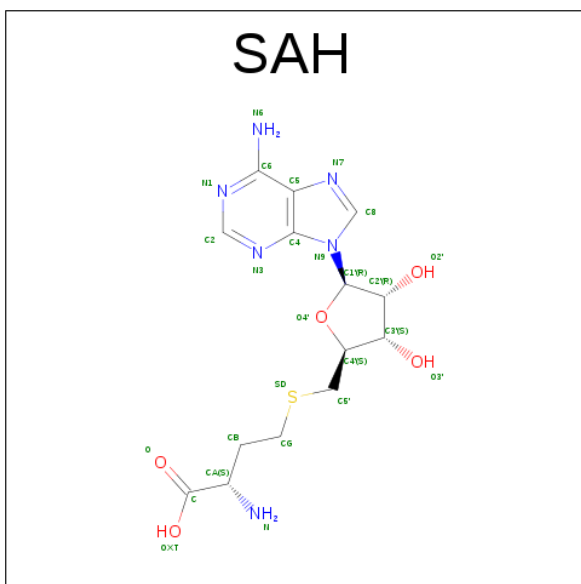
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	A	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	B	1	Total	O	S	0	0
			5	4	1		
2	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 3 is P1-7-METHYLGUANOSINE-P3-ADENOSINE-5',5'-TRIPHOSPHATE (three-letter code: GTA) (formula: C₂₁H₃₀N₁₀O₁₇P₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	A	1	Total	C	N	O	P	0	0
			51	21	10	17	3		
3	B	1	Total	C	N	O	P	0	0
			51	21	10	17	3		
3	C	1	Total	C	N	O	P	0	0
			51	21	10	17	3		

- Molecule 4 is S-ADENOSYL-L-HOMOCYSTEINE (three-letter code: SAH) (formula: $C_{14}H_{20}N_6O_5S$).



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

- Molecule 5 is NICKEL (II) ION (three-letter code: NI) (formula: Ni).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	C	1	Total	Ni	0	0
			1	1		

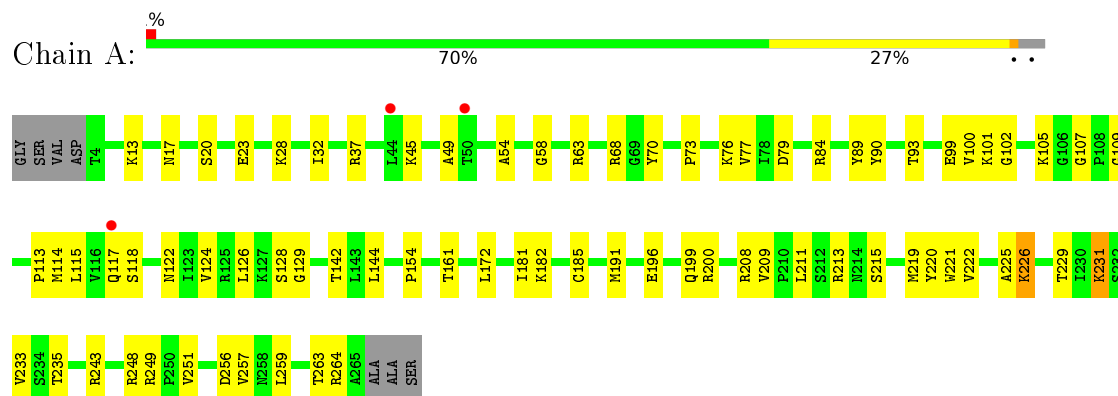
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	31	Total	O	0	0
			31	31		
6	B	19	Total	O	0	0
			19	19		
6	C	20	Total	O	0	0
			20	20		

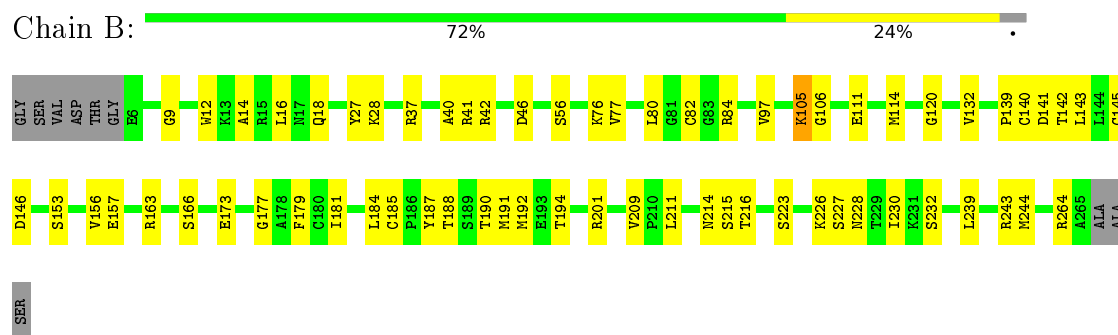
3 Residue-property plots [i](#)

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

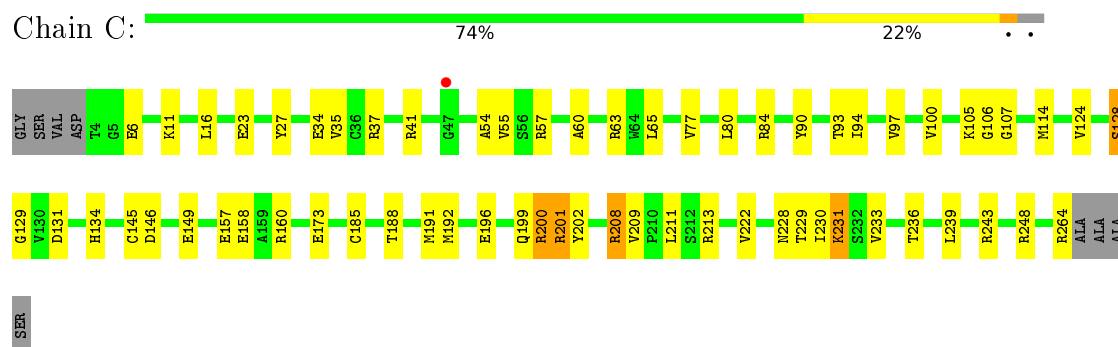
- Molecule 1: RNA-directed RNA polymerase NS5



- Molecule 1: RNA-directed RNA polymerase NS5



- Molecule 1: RNA-directed RNA polymerase NS5



4 Data and refinement statistics

Property	Value	Source
Space group	P 61	Depositor
Cell constants a, b, c, α , β , γ	123.77Å 123.77Å 119.36Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	48.89 – 2.44 48.89 – 2.45	Depositor EDS
% Data completeness (in resolution range)	98.7 (48.89-2.44) 91.3 (48.89-2.45)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.62 (at 2.45Å)	Xtriage
Refinement program	PHENIX (dev_2481: ???)	Depositor
R, R_{free}	0.237 , 0.280 0.239 , 0.284	Depositor DCC
R_{free} test set	2005 reflections (5.26%)	DCC
Wilson B-factor (Å ²)	35.1	Xtriage
Anisotropy	0.578	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 21.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	0.468 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	6440	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 49.53 % 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 7.3603e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹ Intensities estimated from amplitudes.

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

5 Model quality [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: GTA, SAH, SO4, NI

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	0.26	0/2078	0.44	0/2800
1	B	0.24	0/2067	0.43	0/2785
1	C	0.25	0/2073	0.43	0/2793
All	All	0.25	0/6218	0.43	0/8378

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	C	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	107	GLY	Peptide

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	2038	0	2039	51	0
1	B	2027	0	2031	46	0
1	C	2033	0	2036	45	0
2	A	25	0	0	1	0
2	B	10	0	0	1	0
2	C	5	0	0	1	0
3	A	51	0	26	4	0
3	B	51	0	26	6	0
3	C	51	0	26	4	0
4	A	26	0	19	1	0
4	B	26	0	19	4	0
4	C	26	0	19	1	0
5	C	1	0	0	0	0
6	A	31	0	0	1	0
6	B	19	0	0	1	0
6	C	20	0	0	3	0
All	All	6440	0	6241	152	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (152) 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:B:303:GTA:C1A	3:B:303:GTA:O4A	1.66	1.25
3:C:303:GTA:O4A	3:C:303:GTA:C1A	1.66	1.24
3:A:306:GTA:O4A	3:A:306:GTA:C1A	1.66	1.23
1:C:199:GLN:HE21	1:C:200:ARG:HH22	1.15	0.90
1:C:208:ARG:NH1	6:C:401:HOH:O	2.03	0.90
1:B:173:GLU:OE2	1:B:201:ARG:NH1	2.11	0.83
1:A:256:ASP:OD2	6:A:401:HOH:O	2.01	0.78
3:B:303:GTA:O3B	3:B:303:GTA:O22	2.01	0.78
1:C:23:GLU:O	1:C:248:ARG:NH1	2.18	0.76
1:C:63:ARG:NH2	6:C:402:HOH:O	2.22	0.71
1:A:77:VAL:HG12	1:A:142:THR:HB	1.72	0.70
1:B:41:ARG:NH1	2:B:302:SO4:O4	2.25	0.70
1:B:214:ASN:HD21	1:B:243:ARG:HH21	1.39	0.68
1:B:97:VAL:O	1:B:264:ARG:NH2	2.26	0.68
1:A:243:ARG:HE	1:A:249:ARG:HH12	1.42	0.68
1:C:173:GLU:OE1	1:C:201:ARG:NH1	2.28	0.67
1:A:196:GLU:HA	1:A:199:GLN:HG2	1.78	0.66
1:C:97:VAL:O	1:C:264:ARG:NH2	2.29	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:60:ALA:O	6:C:402:HOH:O	2.15	0.65
1:C:77:VAL:HB	1:C:100:VAL:HG12	1.77	0.65
1:A:79:ASP:HA	1:A:144:LEU:HB2	1.79	0.65
1:A:231:LYS:O	1:A:235:THR:OG1	2.15	0.64
1:B:42:ARG:NH2	1:B:46:ASP:OD2	2.31	0.64
1:C:84:ARG:HB3	1:C:114:MET:HG3	1.80	0.64
1:A:122:ASN:HD21	1:A:263:THR:HA	1.63	0.63
1:B:146:ASP:OD2	4:B:304:SAH:HB2	1.99	0.63
1:C:37:ARG:NH1	1:C:54:ALA:O	2.31	0.61
3:B:303:GTA:H8	3:B:303:GTA:O33	2.02	0.59
1:A:229:THR:O	1:A:233:VAL:HG23	2.04	0.58
1:B:111:GLU:OE1	4:B:304:SAH:O3'	2.22	0.57
1:C:100:VAL:HG23	1:C:124:VAL:HA	1.87	0.57
1:B:179:PHE:N	1:B:223:SER:OG	2.36	0.56
1:A:84:ARG:HA	1:A:113:PRO:HA	1.87	0.56
1:A:263:THR:HG22	1:A:264:ARG:H	1.70	0.56
1:A:90:TYR:HA	1:A:259:LEU:CD2	2.35	0.56
1:B:76:LYS:NZ	1:B:139:PRO:O	2.32	0.56
1:B:76:LYS:HD3	1:B:140:CYS:HA	1.88	0.55
1:A:208:ARG:NH1	1:A:213:ARG:O	2.40	0.55
1:B:28:LYS:NZ	3:B:303:GTA:O23	2.39	0.55
1:C:208:ARG:HD3	1:C:236:THR:HG23	1.88	0.55
1:A:89:TYR:OH	1:A:115:LEU:HA	2.07	0.55
1:B:80:LEU:HD22	1:B:132:VAL:HG11	1.88	0.54
1:C:158:GLU:OE2	1:C:188:THR:OG1	2.16	0.54
1:A:105:LYS:HD2	1:A:129:GLY:HA2	1.88	0.54
1:C:105:LYS:O	1:C:129:GLY:N	2.33	0.54
1:A:73:PRO:HB3	1:A:142:THR:HG21	1.89	0.54
1:B:105:LYS:HG3	1:B:106:GLY:O	2.06	0.53
1:A:84:ARG:HG2	1:A:114:MET:N	2.24	0.53
1:C:27:TYR:HB2	1:C:248:ARG:NH1	2.23	0.53
1:A:213:ARG:NH1	2:A:301:SO4:O2	2.41	0.53
1:A:37:ARG:NH2	1:A:54:ALA:O	2.39	0.53
1:A:105:LYS:O	1:A:128:SER:OG	2.27	0.53
1:A:102:GLY:HA3	1:A:126:LEU:HD23	1.91	0.53
1:B:153:SER:HB3	1:B:156:VAL:HB	1.92	0.52
1:C:6:GLU:OE2	1:C:11:LYS:NZ	2.42	0.52
1:B:120:GLY:HA2	1:B:264:ARG:HG3	1.91	0.52
1:B:37:ARG:HH11	1:B:40:ALA:CB	2.22	0.51
1:B:84:ARG:HB3	1:B:114:MET:HG3	1.91	0.51
1:C:34:GLU:HG3	1:C:57:ARG:NH1	2.24	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:63:ARG:CZ	1:A:257:VAL:HG12	2.40	0.51
1:C:188:THR:OG1	1:C:191:MET:HG2	2.11	0.50
3:C:303:GTA:H4B	3:C:303:GTA:H3A	1.93	0.50
1:B:12:TRP:CD1	1:B:244:MET:CE	2.94	0.50
1:B:12:TRP:HD1	1:B:244:MET:CE	2.25	0.50
1:C:16:LEU:O	3:C:303:GTA:N2	2.43	0.50
1:A:17:ASN:OD1	3:A:306:GTA:O2A	2.18	0.49
1:B:145:CYS:HB3	1:B:181:ILE:HG23	1.95	0.49
1:C:188:THR:O	1:C:192:MET:HG2	2.13	0.49
1:B:141:ASP:O	1:B:177:GLY:N	2.46	0.49
1:B:214:ASN:HD21	1:B:243:ARG:NH2	2.07	0.49
1:B:163:ARG:O	1:B:166:SER:OG	2.26	0.48
1:B:56:SER:HB3	1:B:84:ARG:HD3	1.95	0.48
1:C:229:THR:O	1:C:233:VAL:HG12	2.13	0.48
1:A:13:LYS:HD3	1:A:154:PRO:HG3	1.96	0.48
1:B:157:GLU:HB3	1:B:185:CYS:HB2	1.95	0.47
1:B:9:GLY:HA3	1:B:187:TYR:HB2	1.96	0.47
1:B:163:ARG:NH1	6:B:402:HOH:O	2.44	0.47
1:C:199:GLN:HE21	1:C:200:ARG:NH2	1.98	0.47
1:B:239:LEU:O	1:B:243:ARG:HG3	2.15	0.47
1:A:219:MET:HE1	1:A:233:VAL:HG22	1.95	0.47
1:A:100:VAL:CG2	1:A:124:VAL:HA	2.45	0.46
1:A:182:LYS:HB2	1:A:220:TYR:CE2	2.50	0.46
1:A:225:ALA:O	1:A:226:LYS:HD3	2.14	0.46
1:B:209:VAL:HG12	1:B:211:LEU:H	1.80	0.46
1:C:65:LEU:HD22	1:C:222:VAL:HG11	1.97	0.46
1:A:77:VAL:HG22	1:A:100:VAL:HG12	1.97	0.46
1:B:215:SER:OG	3:B:303:GTA:O12	2.29	0.46
1:C:239:LEU:O	1:C:243:ARG:HG3	2.16	0.46
1:A:185:CYS:O	1:A:191:MET:HG3	2.16	0.46
1:A:93:THR:HG21	1:A:259:LEU:HD23	1.97	0.46
1:C:157:GLU:HB3	1:C:185:CYS:HB2	1.98	0.46
1:C:37:ARG:HG3	1:C:37:ARG:O	2.16	0.46
1:C:90:TYR:O	1:C:93:THR:HG22	2.16	0.46
1:C:34:GLU:OE1	1:C:213:ARG:NH1	2.49	0.46
1:A:79:ASP:HB2	1:A:144:LEU:HD12	1.98	0.46
1:C:146:ASP:OD1	4:C:304:SAH:N	2.48	0.46
1:B:27:TYR:CE1	1:B:244:MET:HG2	2.50	0.45
1:C:199:GLN:NE2	1:C:200:ARG:HH22	1.97	0.45
1:C:229:THR:OG1	1:C:230:ILE:N	2.50	0.45
1:A:181:ILE:O	1:A:221:TRP:N	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:20:SER:HB3	1:A:23:GLU:HG3	1.98	0.45
1:A:89:TYR:HD2	1:A:118:SER:OG	2.00	0.45
1:B:228:ASN:O	1:B:232:SER:OG	2.26	0.44
1:C:27:TYR:HB2	1:C:248:ARG:HH12	1.81	0.44
3:A:306:GTA:O32	3:A:306:GTA:O11	2.34	0.44
1:B:190:THR:O	1:B:194:THR:HG23	2.17	0.44
1:C:196:GLU:O	1:C:200:ARG:HD2	2.17	0.44
3:C:303:GTA:H2B	3:C:303:GTA:H8C	1.84	0.44
1:B:192:MET:HE3	1:B:230:ILE:HG12	1.99	0.44
4:B:304:SAH:HG2	4:B:304:SAH:O	2.17	0.44
1:A:76:LYS:HE2	1:A:101:LYS:HE2	2.00	0.43
1:B:192:MET:HE3	1:B:230:ILE:HA	1.99	0.43
1:C:94:ILE:O	1:C:264:ARG:NH1	2.48	0.43
1:A:225:ALA:C	1:A:226:LYS:HD3	2.39	0.43
1:C:35:VAL:H	1:C:57:ARG:HH12	1.66	0.43
1:A:49:ALA:HB1	1:A:117:GLN:N	2.34	0.42
1:A:172:LEU:HD21	1:A:181:ILE:HD11	2.01	0.42
1:A:243:ARG:HE	1:A:249:ARG:NH1	2.14	0.42
1:A:209:VAL:HG12	1:A:211:LEU:H	1.84	0.42
1:A:199:GLN:HG3	1:A:200:ARG:N	2.34	0.42
1:B:80:LEU:HD11	1:B:143:LEU:HD11	2.01	0.42
1:B:188:THR:O	1:B:192:MET:HG2	2.20	0.42
1:B:226:LYS:HA	1:B:226:LYS:HD2	1.81	0.42
3:A:306:GTA:H2A	3:A:306:GTA:N3C	2.34	0.42
1:A:49:ALA:HB1	1:A:117:GLN:H	1.84	0.42
1:A:213:ARG:HG3	1:A:213:ARG:HH21	1.85	0.42
1:C:209:VAL:HG12	1:C:211:LEU:H	1.85	0.42
1:C:55:VAL:HB	1:C:114:MET:SD	2.60	0.42
1:A:70:TYR:O	1:A:222:VAL:HB	2.20	0.41
1:C:106:GLY:HA3	1:C:128:SER:OG	2.20	0.41
1:A:23:GLU:O	1:A:248:ARG:NH1	2.53	0.41
1:A:161:THR:HB	1:A:191:MET:CE	2.50	0.41
1:A:32:ILE:O	1:A:251:VAL:HG23	2.20	0.41
1:C:228:ASN:HD22	1:C:231:LYS:HB2	1.85	0.41
1:A:77:VAL:HA	1:A:142:THR:O	2.21	0.41
1:B:188:THR:OG1	1:B:191:MET:HG2	2.21	0.41
1:C:80:LEU:HD12	1:C:145:CYS:HB2	2.03	0.41
1:A:58:GLY:HA3	4:A:307:SAH:O	2.20	0.41
1:B:14:ALA:O	1:B:18:GLN:HG3	2.21	0.41
1:C:84:ARG:NH2	2:C:301:SO4:O4	2.54	0.41
1:B:77:VAL:HG23	1:B:142:THR:HB	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:149:GLU:HB3	1:C:160:ARG:HD3	2.02	0.41
1:A:107:GLY:C	1:A:109:GLY:H	2.23	0.41
1:A:28:LYS:HE2	1:A:215:SER:OG	2.20	0.41
1:B:132:VAL:HG23	4:B:304:SAH:C2	2.51	0.41
1:B:80:LEU:HD12	1:B:145:CYS:HB2	2.03	0.41
1:B:227:SER:HB2	1:B:232:SER:OG	2.21	0.41
1:C:37:ARG:HG3	1:C:41:ARG:HG3	2.03	0.41
1:B:157:GLU:HG2	1:B:184:LEU:HD21	2.03	0.40
1:B:216:THR:HB	3:B:303:GTA:O11	2.21	0.40
1:C:131:ASP:OD2	1:C:134:HIS:NE2	2.55	0.40
1:C:201:ARG:HG2	1:C:202:TYR:CE2	2.56	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	260/269 (97%)	250 (96%)	10 (4%)	0	100	100
1	B	258/269 (96%)	249 (96%)	9 (4%)	0	100	100
1	C	259/269 (96%)	249 (96%)	10 (4%)	0	100	100
All	All	777/807 (96%)	748 (96%)	29 (4%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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	217/221 (98%)	212 (98%)	5 (2%)	58	73
1	B	216/221 (98%)	213 (99%)	3 (1%)	74	84
1	C	217/221 (98%)	212 (98%)	5 (2%)	58	73
All	All	650/663 (98%)	637 (98%)	13 (2%)	63	77

All (13) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LYS
1	A	68	ARG
1	A	99	GLU
1	A	226	LYS
1	A	231	LYS
1	B	16	LEU
1	B	82	CYS
1	B	105	LYS
1	C	128	SER
1	C	200	ARG
1	C	201	ARG
1	C	208	ARG
1	C	231	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	117	GLN
1	A	122	ASN
1	A	214	ASN
1	B	18	GLN
1	B	199	GLN
1	B	214	ASN
1	C	18	GLN
1	C	117	GLN
1	C	199	GLN
1	C	228	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 ⓘ

Of 15 ligands modelled in this entry, 1 is monoatomic - leaving 14 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	SO4	A	301	1	4,4,4	0.73	0	6,6,6	0.18	0
2	SO4	A	302	1	4,4,4	0.24	0	6,6,6	0.11	0
2	SO4	A	303	-	4,4,4	0.31	0	6,6,6	0.08	0
2	SO4	A	304	-	4,4,4	0.24	0	6,6,6	0.09	0
2	SO4	A	305	-	4,4,4	0.24	0	6,6,6	0.08	0
3	GTA	A	306	-	45,56,56	5.51	23 (51%)	48,88,88	2.57	7 (14%)
4	SAH	A	307	-	22,28,28	1.08	2 (9%)	18,40,40	2.89	2 (11%)
2	SO4	B	301	-	4,4,4	0.26	0	6,6,6	0.08	0
2	SO4	B	302	-	4,4,4	0.25	0	6,6,6	0.05	0
3	GTA	B	303	-	45,56,56	5.54	22 (48%)	48,88,88	2.71	9 (18%)
4	SAH	B	304	-	22,28,28	1.06	2 (9%)	18,40,40	2.93	2 (11%)
2	SO4	C	301	-	4,4,4	0.28	0	6,6,6	0.09	0
3	GTA	C	303	-	45,56,56	5.53	22 (48%)	48,88,88	2.56	7 (14%)
4	SAH	C	304	-	22,28,28	1.05	2 (9%)	18,40,40	2.97	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
2	SO4	A	301	1	-	0/0/0/0	0/0/0/0
2	SO4	A	302	1	-	0/0/0/0	0/0/0/0
2	SO4	A	303	-	-	0/0/0/0	0/0/0/0
2	SO4	A	304	-	-	0/0/0/0	0/0/0/0
2	SO4	A	305	-	-	0/0/0/0	0/0/0/0
3	GTA	A	306	-	-	0/24/64/64	0/6/6/6
4	SAH	A	307	-	-	0/7/31/31	0/3/3/3
2	SO4	B	301	-	-	0/0/0/0	0/0/0/0
2	SO4	B	302	-	-	0/0/0/0	0/0/0/0
3	GTA	B	303	-	-	0/24/64/64	0/6/6/6
4	SAH	B	304	-	-	0/7/31/31	0/3/3/3
2	SO4	C	301	-	-	0/0/0/0	0/0/0/0
3	GTA	C	303	-	-	0/24/64/64	0/6/6/6
4	SAH	C	304	-	-	0/7/31/31	0/3/3/3

All (73) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	303	GTA	C2B-C1B	-15.44	1.29	1.53
3	B	303	GTA	C2B-C1B	-15.27	1.29	1.53
3	A	306	GTA	C2B-C1B	-15.16	1.29	1.53
3	C	303	GTA	C2A-C1A	-12.36	1.34	1.53
3	A	306	GTA	C2A-C1A	-12.26	1.34	1.53
3	B	303	GTA	C2A-C1A	-11.97	1.34	1.53
3	C	303	GTA	O4B-C4B	-6.37	1.30	1.45
3	A	306	GTA	O4B-C4B	-6.34	1.30	1.45
3	B	303	GTA	O4A-C4A	-6.33	1.30	1.45
3	A	306	GTA	O4A-C4A	-6.33	1.30	1.45
3	B	303	GTA	O4B-C4B	-6.30	1.30	1.45
3	C	303	GTA	O4A-C4A	-6.13	1.31	1.45
3	B	303	GTA	O3A-C3A	-4.49	1.32	1.43
3	A	306	GTA	O3A-C3A	-4.47	1.32	1.43
3	C	303	GTA	O3A-C3A	-4.41	1.32	1.43
3	B	303	GTA	O6-C6	-2.80	1.17	1.24
3	C	303	GTA	O6-C6	-2.79	1.17	1.24
3	A	306	GTA	O6-C6	-2.76	1.17	1.24
3	C	303	GTA	C5C-C4C	-2.54	1.34	1.40
3	B	303	GTA	O3B-C3B	-2.52	1.37	1.43
3	C	303	GTA	O3B-C3B	-2.51	1.37	1.43
3	A	306	GTA	C5C-C4C	-2.50	1.34	1.40
3	A	306	GTA	O3B-C3B	-2.47	1.37	1.43
3	B	303	GTA	C5C-C4C	-2.47	1.34	1.40
3	A	306	GTA	P3-O33	2.02	1.67	1.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	306	GTA	C2-N3	2.14	1.46	1.35
3	A	306	GTA	P1-O15	2.21	1.68	1.59
3	B	303	GTA	C2-N3	2.22	1.46	1.35
3	C	303	GTA	C6C-N6C	2.23	1.43	1.34
3	B	303	GTA	C6C-N6C	2.24	1.43	1.34
3	C	303	GTA	C2-N3	2.27	1.47	1.35
3	A	306	GTA	C6C-N6C	2.27	1.43	1.34
4	B	304	SAH	C2-N1	2.27	1.38	1.33
4	C	304	SAH	C2-N1	2.28	1.38	1.33
3	B	303	GTA	C5B-C4B	2.31	1.59	1.51
4	A	307	SAH	C2-N1	2.32	1.38	1.33
3	A	306	GTA	C5B-C4B	2.32	1.59	1.51
3	C	303	GTA	C5B-C4B	2.35	1.59	1.51
3	C	303	GTA	C2C-N3C	2.39	1.36	1.32
3	B	303	GTA	P1-O15	2.41	1.69	1.59
3	C	303	GTA	P1-O15	2.41	1.69	1.59
3	A	306	GTA	C2C-N3C	2.44	1.36	1.32
3	B	303	GTA	C3A-C4A	2.44	1.59	1.53
3	B	303	GTA	C2C-N3C	2.44	1.36	1.32
3	A	306	GTA	C3A-C4A	2.61	1.60	1.53
3	C	303	GTA	C3A-C4A	2.74	1.60	1.53
3	B	303	GTA	O2B-C2B	3.20	1.50	1.43
4	C	304	SAH	C2-N3	3.39	1.38	1.32
4	B	304	SAH	C2-N3	3.42	1.38	1.32
3	C	303	GTA	O2B-C2B	3.51	1.51	1.43
4	A	307	SAH	C2-N3	3.52	1.38	1.32
3	A	306	GTA	O2B-C2B	3.62	1.51	1.43
3	B	303	GTA	C2-N1	4.40	1.43	1.35
3	C	303	GTA	C2-N1	4.44	1.43	1.35
3	A	306	GTA	C2-N1	4.50	1.43	1.35
3	B	303	GTA	C6-C5	6.52	1.54	1.41
3	B	303	GTA	C6-N1	6.53	1.44	1.33
3	C	303	GTA	C6-N1	6.55	1.44	1.33
3	C	303	GTA	C6-C5	6.61	1.54	1.41
3	A	306	GTA	C6-C5	6.70	1.54	1.41
3	A	306	GTA	C6-N1	6.71	1.45	1.33
3	A	306	GTA	C2-N2	7.52	1.50	1.34
3	B	303	GTA	C2-N2	7.54	1.50	1.34
3	C	303	GTA	C2-N2	7.54	1.50	1.34
3	A	306	GTA	C4-N3	9.97	1.51	1.35
3	B	303	GTA	C4-N3	10.07	1.51	1.35
3	C	303	GTA	C4-N3	10.23	1.51	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	303	GTA	O4B-C1B	14.90	1.62	1.41
3	A	306	GTA	O4B-C1B	15.21	1.63	1.41
3	B	303	GTA	O4B-C1B	15.40	1.63	1.41
3	A	306	GTA	O4A-C1A	17.40	1.66	1.41
3	C	303	GTA	O4A-C1A	17.55	1.66	1.41
3	B	303	GTA	O4A-C1A	17.97	1.66	1.41

All (30) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	303	GTA	N3C-C2C-N1C	-11.45	119.88	128.87
3	B	303	GTA	N3C-C2C-N1C	-11.43	119.89	128.87
3	A	306	GTA	N3C-C2C-N1C	-11.43	119.89	128.87
4	B	304	SAH	N3-C2-N1	-11.36	119.94	128.87
4	A	307	SAH	N3-C2-N1	-11.04	120.20	128.87
4	C	304	SAH	N3-C2-N1	-10.89	120.32	128.87
3	C	303	GTA	N6C-C6C-N1C	-7.55	105.85	118.52
3	A	306	GTA	N6C-C6C-N1C	-7.49	105.94	118.52
3	B	303	GTA	N6C-C6C-N1C	-7.43	106.06	118.52
3	A	306	GTA	C1A-N9-C4	-6.68	119.35	126.81
3	B	303	GTA	C4A-O4A-C1A	-6.24	103.03	109.64
3	A	306	GTA	N3-C2-N1	-5.65	119.88	127.56
3	B	303	GTA	N3-C2-N1	-5.50	120.08	127.56
3	C	303	GTA	N3-C2-N1	-5.42	120.19	127.56
3	C	303	GTA	C4B-O4B-C1B	-5.33	104.00	109.64
3	C	303	GTA	C1A-N9-C4	-5.10	121.12	126.81
3	B	303	GTA	C4B-O4B-C1B	-4.77	104.58	109.64
3	B	303	GTA	C1A-N9-C4	-4.40	121.89	126.81
4	A	307	SAH	C5'-SD-CG	-3.79	90.92	102.42
4	C	304	SAH	C5'-SD-CG	-3.67	91.28	102.42
4	B	304	SAH	C5'-SD-CG	-3.35	92.25	102.42
3	A	306	GTA	C5-C6-N1	-2.84	119.81	123.52
3	B	303	GTA	C5-C6-N1	-2.68	120.02	123.52
3	C	303	GTA	C5-C6-N1	-2.57	120.16	123.52
3	A	306	GTA	N2-C2-N1	2.01	120.52	117.20
3	B	303	GTA	O4B-C1B-N9C	2.15	112.17	108.11
4	C	304	SAH	O4'-C1'-N9	3.09	113.94	108.11
3	C	303	GTA	C6-N1-C2	3.12	119.53	115.88
3	B	303	GTA	C6-N1-C2	3.28	119.73	115.88
3	A	306	GTA	C6-N1-C2	3.51	120.00	115.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

9 monomers are involved in 23 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	SO4	1	0
3	A	306	GTA	4	0
4	A	307	SAH	1	0
2	B	302	SO4	1	0
3	B	303	GTA	6	0
4	B	304	SAH	4	0
2	C	301	SO4	1	0
3	C	303	GTA	4	0
4	C	304	SAH	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 [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	262/269 (97%)	0.01	3 (1%) 82 84	34, 50, 78, 110	0
1	B	260/269 (96%)	-0.37	0 100 100	26, 38, 60, 93	0
1	C	261/269 (97%)	-0.28	1 (0%) 93 94	28, 43, 67, 98	0
All	All	783/807 (97%)	-0.21	4 (0%) 91 92	26, 43, 71, 110	0

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	44	LEU	5.2
1	C	47	GLY	2.5
1	A	50	THR	2.4
1	A	117	GLN	2.3

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, 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	LLDF	B-factors(\AA^2)	Q<0.9
2	SO4	A	303	5/5	0.90	0.22	3.28	52,66,72,73	0
3	GTA	B	303	51/51	0.94	0.14	0.85	18,53,74,75	0
3	GTA	C	303	51/51	0.95	0.12	0.37	19,48,76,78	0
4	SAH	A	307	26/26	0.92	0.17	-0.16	30,44,50,52	0
3	GTA	A	306	51/51	0.94	0.12	-0.49	18,35,66,69	0
4	SAH	C	304	26/26	0.95	0.13	-0.64	21,31,40,46	0
2	SO4	A	302	5/5	0.98	0.09	-0.99	29,33,41,50	0
4	SAH	B	304	26/26	0.96	0.12	-1.07	20,32,42,44	0
2	SO4	B	301	5/5	0.99	0.09	-1.96	33,37,52,53	0
2	SO4	C	301	5/5	0.97	0.10	-2.76	48,57,58,64	0
2	SO4	A	305	5/5	0.95	0.13	-	68,68,72,72	0
2	SO4	B	302	5/5	0.96	0.08	-	64,65,68,74	0
2	SO4	A	301	5/5	0.91	0.10	-	41,59,61,62	0
5	NI	C	302	1/1	0.96	0.12	-	77,77,77,77	0
2	SO4	A	304	5/5	0.96	0.11	-	36,46,52,53	0

6.5 Other polymers [i](#)

There are no such residues in this entry.