W O R L D W I D E
wwPDB
PROTEIN DATA BANK

Full wwPDB X-ray Structure Validation Report (i)

Feb 19, 2016 – 08:44 PM GMT

PDB ID : 4YUZ
Title : Crystal structure of Trypanosoma cruzi spermidine synthase in complex with 5-[(4-methylbenzyl)oxy]quinazoline-2,4-diamine
Authors : Amano, Y.; Tateishi, Y.
Deposited on : 2015-03-19
Resolution : 1.97 Å(reported)

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

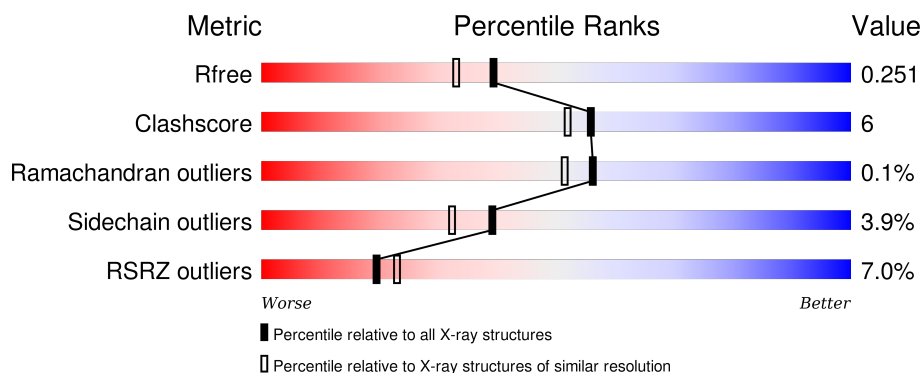|		
MolProbity	:	4.02b-467
Mogul	:	1.7.1 (RC1), CSD as537be (2016)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026982
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	rb-20026982

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	Percentile Ranks	Value
Rfree		0.251
Clashscore		6
Ramachandran outliers		0.1%
Sidechain outliers		3.9%
RSRZ outliers		7.0%

Worse　　　　　　　　　　　　　　　　　　　　　　*Better*

▮ Percentile relative to all X-ray structures

▯ Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	8664 (2.00-1.96)
Clashscore	102246	9905 (2.00-1.96)
Ramachandran outliers	100387	9792 (2.00-1.96)
Sidechain outliers	100360	9791 (2.00-1.96)
RSRZ outliers	91569	8679 (2.00-1.96)

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 <=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	304	6% / 72% / 16% · 10%
1	B	304	6% / 81% / 9% · 9%
1	C	304	8% / 76% / 13% ·· 10%
1	D	304	7% / 76% / 14% · 9%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9047 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 Spermidine synthase, putative.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	273	Total	C	N	O	S	0	0	0
			2163	1374	371	404	14			
1	B	276	Total	C	N	O	S	0	0	0
			2172	1379	371	408	14			
1	C	274	Total	C	N	O	S	0	0	0
			2158	1369	370	405	14			
1	D	277	Total	C	N	O	S	0	0	0
			2181	1383	373	411	14			

There are 32 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-7	MET	-	initiating methionine	UNP Q4DA73
A	-6	ALA	-	expression tag	UNP Q4DA73
A	-5	HIS	-	expression tag	UNP Q4DA73
A	-4	HIS	-	expression tag	UNP Q4DA73
A	-3	HIS	-	expression tag	UNP Q4DA73
A	-2	HIS	-	expression tag	UNP Q4DA73
A	-1	HIS	-	expression tag	UNP Q4DA73
A	0	HIS	-	expression tag	UNP Q4DA73
B	-7	MET	-	initiating methionine	UNP Q4DA73
B	-6	ALA	-	expression tag	UNP Q4DA73
B	-5	HIS	-	expression tag	UNP Q4DA73
B	-4	HIS	-	expression tag	UNP Q4DA73
B	-3	HIS	-	expression tag	UNP Q4DA73
B	-2	HIS	-	expression tag	UNP Q4DA73
B	-1	HIS	-	expression tag	UNP Q4DA73
B	0	HIS	-	expression tag	UNP Q4DA73
C	-7	MET	-	initiating methionine	UNP Q4DA73
C	-6	ALA	-	expression tag	UNP Q4DA73
C	-5	HIS	-	expression tag	UNP Q4DA73
C	-4	HIS	-	expression tag	UNP Q4DA73
C	-3	HIS	-	expression tag	UNP Q4DA73

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Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	HIS	-	expression tag	UNP Q4DA73
C	-1	HIS	-	expression tag	UNP Q4DA73
C	0	HIS	-	expression tag	UNP Q4DA73
D	-7	MET	-	initiating methionine	UNP Q4DA73
D	-6	ALA	-	expression tag	UNP Q4DA73
D	-5	HIS	-	expression tag	UNP Q4DA73
D	-4	HIS	-	expression tag	UNP Q4DA73
D	-3	HIS	-	expression tag	UNP Q4DA73
D	-2	HIS	-	expression tag	UNP Q4DA73
D	-1	HIS	-	expression tag	UNP Q4DA73
D	0	HIS	-	expression tag	UNP Q4DA73

- Molecule 2 is 5'-[(S)-(3-AMINOPROPYL)(METHYL)-LAMBDA 4 -SULFANYL]-5'-DEO XYADENOSINE (three-letter code: S4M) (formula: $C_{14}H_{24}N_6O_3S$).
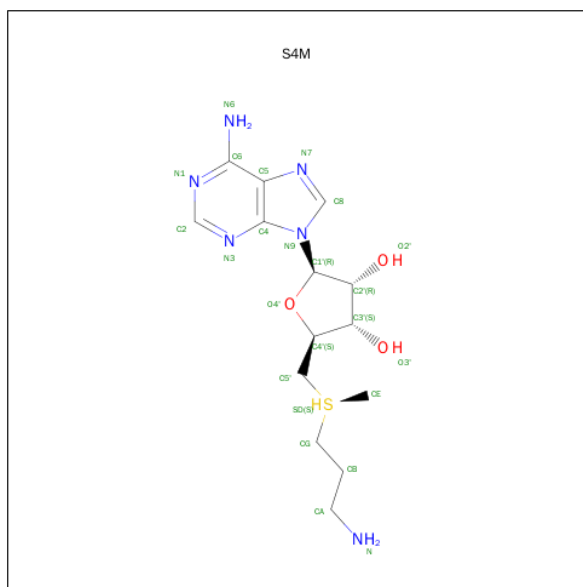
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			24	14	6	3	1		
2	B	1	Total	C	N	O	S	0	0
			24	14	6	3	1		
2	C	1	Total	C	N	O	S	0	0
			24	14	6	3	1		
2	D	1	Total	C	N	O	S	0	0
			24	14	6	3	1		

- Molecule 3 is 5-[(4-methylbenzyl)oxy]quinazoline-2,4-diamine (three-letter code: 4JV) (formula: $C_{16}H_{16}N_4O$).
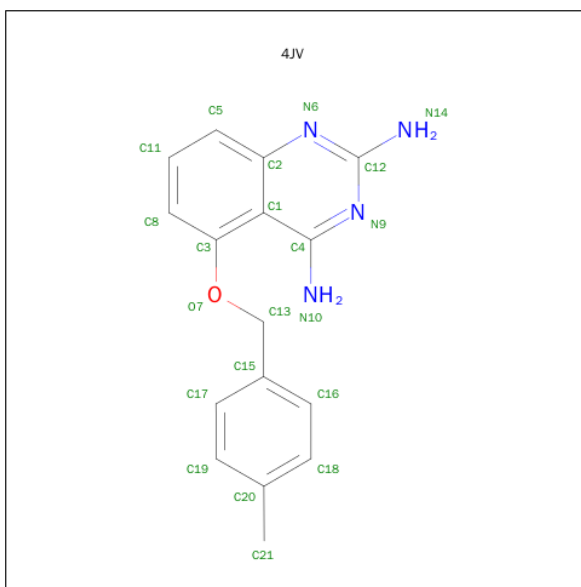
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	B	1	Total 21	C 16	N 4	O 1	0	0
3	D	1	Total 21	C 16	N 4	O 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	61	Total 61	O 61	0	0
4	B	71	Total 71	O 71	0	0
4	C	47	Total 47	O 47	0	0
4	D	56	Total 56	O 56	0	0

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: Spermidine synthase, putative
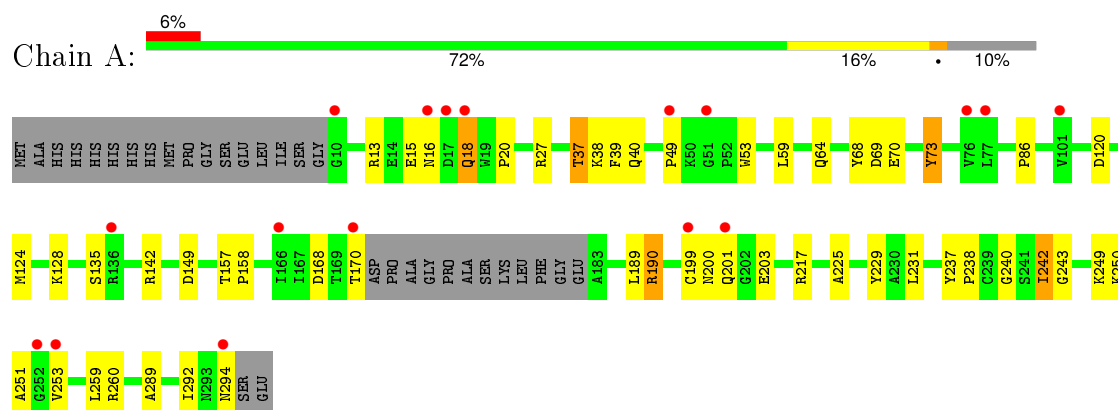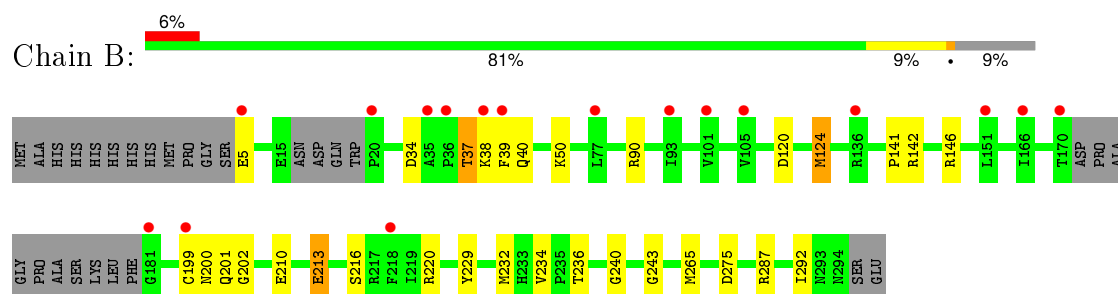
Chain A:

- Molecule 1: Spermidine synthase, putative

Chain B:

- Molecule 1: Spermidine synthase, putative

Chain C:

• Molecule 1: Spermidine synthase, putative

Chain D:

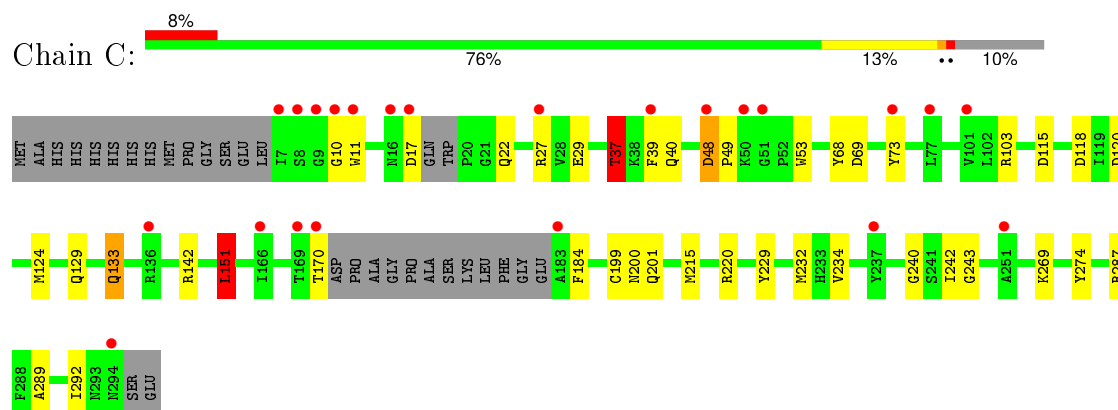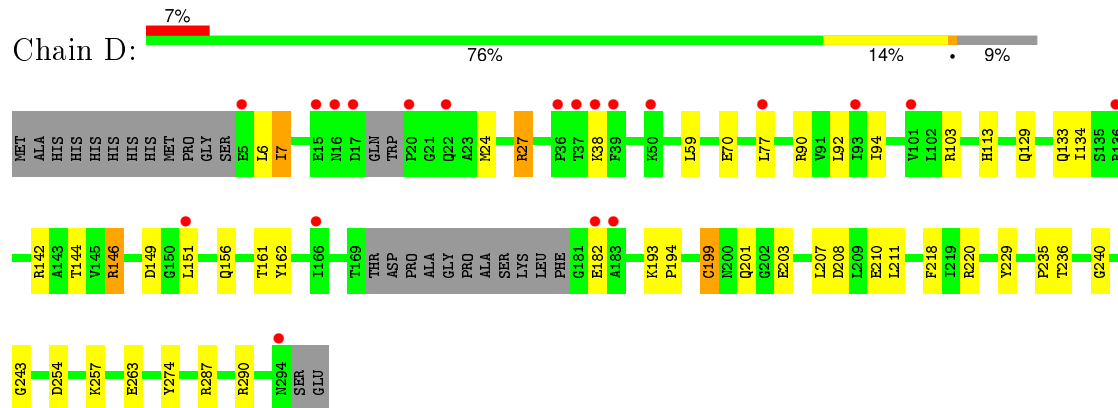# 4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	43.53Å 99.67Å 134.61Å 90.00° 91.70° 90.00°	Depositor
Resolution (Å)	29.73 – 1.97 29.73 – 1.97	Depositor EDS
% Data completeness (in resolution range)	97.6 (29.73-1.97) 97.6 (29.73-1.97)	Depositor EDS
R_{merge}	0.15	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	7.85 (at 1.98Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, R_{free}	0.199 , 0.250 0.200 , 0.251	Depositor DCC
R_{free} test set	3948 reflections (5.27%)	DCC
Wilson B-factor (Å^2)	26.1	Xtriage
Anisotropy	0.059	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.46 , 59.9	EDS
Estimated twinning fraction	0.022 for h,-k,-l	Xtriage
L-test for twinning[2]	$<|L|> = 0.50$, $<L^2> = 0.33$	Xtriage
Outliers	2 of 78844 reflections (0.003%)	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	9047	wwPDB-VP
Average B, all atoms (Å^2)	31.0	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 41.16 % 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 2.4612e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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[1]Intensities estimated from amplitudes.

[2]Theoretical values of $<|L|>$, $<L^2>$ 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: S4M, 4JV

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	1.03	0/2216	1.06	10/3005 (0.3%)
1	B	1.06	0/2222	1.03	8/3008 (0.3%)
1	C	1.01	1/2208 (0.0%)	0.99	10/2990 (0.3%)
1	D	0.97	2/2231 (0.1%)	1.00	9/3020 (0.3%)
All	All	1.02	3/8877 (0.0%)	1.02	37/12023 (0.3%)

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	263	GLU	CD-OE2	6.27	1.32	1.25
1	C	274	TYR	CE1-CZ	5.56	1.45	1.38
1	D	274	TYR	CE1-CZ	5.10	1.45	1.38

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	190	ARG	NE-CZ-NH2	-12.44	114.08	120.30
1	A	190	ARG	NE-CZ-NH1	10.62	125.61	120.30
1	B	142	ARG	NE-CZ-NH2	-10.00	115.30	120.30
1	D	287	ARG	NE-CZ-NH2	-8.29	116.15	120.30
1	C	103	ARG	NE-CZ-NH2	-7.64	116.48	120.30
1	A	142	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	B	142	ARG	NE-CZ-NH1	7.57	124.08	120.30
1	D	142	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	C	103	ARG	NE-CZ-NH1	7.43	124.01	120.30
1	A	217	ARG	NE-CZ-NH2	-7.37	116.62	120.30
1	D	220	ARG	NE-CZ-NH2	6.89	123.75	120.30
1	D	149	ASP	CB-CG-OD1	6.87	124.49	118.30
1	D	146	ARG	NE-CZ-NH2	6.81	123.71	120.30
1	C	287	ARG	NE-CZ-NH2	-6.78	116.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	69	ASP	CB-CG-OD1	6.71	124.34	118.30
1	A	142	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	D	287	ARG	NE-CZ-NH1	6.36	123.48	120.30
1	D	199	CYS	CB-CA-C	6.31	123.02	110.40
1	B	213	GLU	CG-CD-OE2	6.12	130.55	118.30
1	D	220	ARG	NE-CZ-NH1	-5.72	117.44	120.30
1	C	37	THR	N-CA-C	-5.62	95.83	111.00
1	C	115	ASP	CB-CG-OD1	-5.62	113.25	118.30
1	B	275	ASP	CB-CG-OD1	5.61	123.35	118.30
1	A	231	LEU	CA-CB-CG	5.59	128.15	115.30
1	B	199	CYS	CA-CB-SG	5.56	124.00	114.00
1	C	287	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	B	287	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	A	190	ARG	CG-CD-NE	-5.45	100.35	111.80
1	C	151	LEU	CA-CB-CG	5.44	127.81	115.30
1	A	149	ASP	CB-CG-OD1	5.37	123.13	118.30
1	A	217	ARG	NE-CZ-NH1	5.29	122.94	120.30
1	D	103	ARG	NE-CZ-NH2	-5.17	117.71	120.30
1	B	146	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	C	142	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	C	48	ASP	CB-CG-OD1	5.01	122.81	118.30
1	C	69	ASP	CB-CG-OD1	5.01	122.81	118.30
1	B	275	ASP	CB-CG-OD2	-5.00	113.80	118.30

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	2163	0	2115	32	0
1	B	2172	0	2132	24	0
1	C	2158	0	2116	26	0
1	D	2181	0	2135	31	0
2	A	24	0	24	1	0
2	B	24	0	24	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	C	24	0	24	0	0
2	D	24	0	24	0	0
3	B	21	0	16	1	0
3	D	21	0	16	4	0
4	A	61	0	0	0	0
4	B	71	0	0	4	0
4	C	47	0	0	1	0
4	D	56	0	0	0	0
All	All	9047	0	8626	108	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 6.

All (108) 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)
1:D:27:ARG:HH11	1:D:27:ARG:HG3	1.01	1.12
1:B:37:THR:HG21	1:B:120:ASP:OD2	1.54	1.06
1:A:157:THR:O	1:A:190:ARG:NH2	1.89	1.03
1:D:27:ARG:HH11	1:D:27:ARG:CG	1.77	0.98
1:C:37:THR:HG21	1:C:120:ASP:OD2	1.63	0.97
1:A:37:THR:HG21	1:A:120:ASP:OD2	1.70	0.91
1:A:259:LEU:HD11	1:D:146:ARG:HG2	1.51	0.91
1:D:27:ARG:HG3	1:D:27:ARG:NH1	1.84	0.85
1:C:133:GLN:HE21	1:C:133:GLN:H	1.22	0.84
1:D:92:LEU:HD21	1:D:94:ILE:HD11	1.64	0.80
1:C:118:ASP:HB3	1:C:124:MET:CE	2.11	0.80
1:C:151:LEU:HD13	1:C:184:PHE:HB2	1.64	0.80
1:B:37:THR:CG2	1:B:39:PHE:H	1.95	0.80
1:A:37:THR:HG22	1:A:40:GLN:H	1.46	0.79
1:B:37:THR:HG22	1:B:40:GLN:H	1.50	0.76
1:B:37:THR:HG22	1:B:39:PHE:H	1.51	0.76
1:C:37:THR:HG22	1:C:39:PHE:H	1.51	0.75
1:D:203:GLU:HG3	1:D:211:LEU:HD23	1.69	0.74
1:A:37:THR:CG2	1:A:39:PHE:H	2.02	0.73
1:D:182:GLU:HA	1:D:218:PHE:HZ	1.53	0.73
1:A:70:GLU:HA	1:A:73:TYR:CZ	2.24	0.72
1:C:73:TYR:OH	1:C:201:GLN:HB2	1.92	0.69
1:A:200:ASN:O	1:A:200:ASN:OD1	2.11	0.68
1:C:118:ASP:HB3	1:C:124:MET:HE2	1.75	0.68
1:C:200:ASN:O	1:C:200:ASN:OD1	2.11	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:5:GLU:N	1:B:34:ASP:OD2	2.28	0.67
1:D:27:ARG:NH1	1:D:27:ARG:CG	2.45	0.66
1:B:202:GLY:HA2	1:B:243:GLY:O	1.97	0.65
1:D:203:GLU:CG	1:D:211:LEU:HD23	2.27	0.64
1:C:151:LEU:CD1	1:C:184:PHE:HB2	2.28	0.64
1:A:37:THR:HG23	1:A:39:PHE:H	1.64	0.61
1:D:290:ARG:HH11	1:D:290:ARG:HG2	1.64	0.61
1:C:22:GLN:HB3	3:D:302:4JV:H7	1.84	0.60
1:C:118:ASP:HB3	1:C:124:MET:HE3	1.83	0.60
1:C:200:ASN:C	1:C:200:ASN:OD1	2.41	0.59
1:C:37:THR:HG22	1:C:40:GLN:H	1.68	0.58
1:A:59:LEU:HG	1:A:64:GLN:HG3	1.85	0.58
1:A:242:ILE:HG13	1:A:243:GLY:H	1.69	0.57
1:D:210:GLU:CD	1:D:210:GLU:H	2.07	0.57
1:B:37:THR:HG22	1:B:39:PHE:N	2.20	0.57
1:D:203:GLU:HB3	1:D:208:ASP:OD2	2.05	0.56
1:A:237:TYR:CG	1:A:238:PRO:HD2	2.41	0.55
1:A:289:ALA:O	1:A:292:ILE:HG12	2.06	0.55
1:A:37:THR:HG22	1:A:39:PHE:H	1.71	0.55
1:D:235:PRO:O	3:D:302:4JV:N10	2.30	0.55
1:D:236:THR:HA	3:D:302:4JV:N9	2.22	0.55
1:D:254:ASP:OD2	1:D:257:LYS:HE2	2.07	0.54
1:B:37:THR:HG23	1:B:39:PHE:H	1.72	0.54
1:D:203:GLU:HB3	1:D:208:ASP:HB2	1.90	0.53
1:B:232:MET:HG3	1:B:234:VAL:HG23	1.92	0.52
1:A:37:THR:HG23	1:A:38:LYS:N	2.25	0.51
1:B:265:MET:HE1	4:B:464:HOH:O	2.12	0.50
1:D:193:LYS:HB3	1:D:194:PRO:HD2	1.92	0.50
1:C:53:TRP:CZ3	1:C:68:TYR:HD2	2.30	0.50
1:D:203:GLU:CB	1:D:208:ASP:HB2	2.41	0.49
1:B:265:MET:CE	4:B:464:HOH:O	2.59	0.49
1:D:70:GLU:HG2	1:D:134:ILE:HD11	1.95	0.49
1:C:37:THR:CG2	1:C:39:PHE:H	2.23	0.48
1:A:168:ASP:OD1	2:A:301:S4M:HB2	2.14	0.48
1:A:237:TYR:CD1	1:A:238:PRO:HD2	2.49	0.48
1:A:259:LEU:HD11	1:D:146:ARG:CG	2.35	0.47
1:C:48:ASP:HA	1:C:49:PRO:HD2	1.76	0.47
1:A:200:ASN:OD1	1:A:200:ASN:C	2.53	0.47
1:D:7:ILE:H	1:D:7:ILE:HD13	1.80	0.47
1:C:240:GLY:HA3	1:D:240:GLY:HA3	1.95	0.47
1:C:11:TRP:CE2	1:C:27:ARG:HG3	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:ASN:OD1	1:B:200:ASN:C	2.52	0.47
1:A:18:GLN:HA	1:A:18:GLN:HE21	1.79	0.47
1:D:113:HIS:CE1	1:D:144:THR:OG1	2.68	0.46
1:B:37:THR:HG23	1:B:38:LYS:N	2.31	0.46
1:C:133:GLN:H	1:C:133:GLN:NE2	2.00	0.46
1:D:90:ARG:HD3	1:D:161:THR:O	2.16	0.46
1:A:250:LYS:HE2	1:D:156:GLN:O	2.16	0.46
1:A:240:GLY:HA3	1:B:240:GLY:HA3	1.97	0.46
1:A:189:LEU:HD12	1:A:249:LYS:HD2	1.97	0.46
1:B:37:THR:HG22	1:B:40:GLN:N	2.26	0.45
1:C:232:MET:HG3	1:C:234:VAL:HG23	1.99	0.45
1:C:133:GLN:HE21	1:C:133:GLN:N	2.03	0.45
1:D:229:TYR:CZ	1:D:243:GLY:HA3	2.51	0.45
1:B:265:MET:HE2	4:B:456:HOH:O	2.16	0.45
1:B:229:TYR:CZ	1:B:243:GLY:HA3	2.52	0.44
1:A:225:ALA:HB1	1:A:251:ALA:HB2	1.98	0.44
1:D:290:ARG:HH11	1:D:290:ARG:CG	2.30	0.44
1:B:216:SER:OG	1:B:220:ARG:NH1	2.51	0.44
1:A:229:TYR:CZ	1:A:243:GLY:HA3	2.53	0.43
1:D:90:ARG:HG2	1:D:162:TYR:CD1	2.54	0.43
1:B:124:MET:HG2	1:B:124:MET:H	1.38	0.43
1:A:201:GLN:HE21	1:A:203:GLU:H	1.66	0.43
3:D:302:4JV:H7	3:D:302:4JV:C15	2.48	0.43
1:A:53:TRP:CZ3	1:A:68:TYR:CD2	3.07	0.43
1:C:200:ASN:HB2	4:C:440:HOH:O	2.18	0.42
1:C:289:ALA:O	1:C:292:ILE:HG12	2.19	0.42
1:A:128:LYS:HA	1:A:135:SER:OG	2.20	0.42
1:D:59:LEU:HD23	1:D:59:LEU:HA	1.84	0.41
1:B:210:GLU:CD	1:B:210:GLU:H	2.23	0.41
1:B:236:THR:HA	3:B:302:4JV:N9	2.35	0.41
1:A:242:ILE:HG13	1:A:243:GLY:N	2.33	0.41
1:A:86:PRO:O	1:A:260:ARG:HD3	2.20	0.41
1:D:210:GLU:CD	1:D:210:GLU:N	2.73	0.41
1:D:207:LEU:HA	1:D:207:LEU:HD23	1.88	0.41
1:A:157:THR:HA	1:A:158:PRO:HD3	1.94	0.41
1:C:10:GLY:O	1:C:27:ARG:HG2	2.20	0.41
1:A:20:PRO:HG2	1:B:50:LYS:HB3	2.03	0.41
1:C:29:GLU:O	1:C:29:GLU:HG3	2.21	0.40
1:C:229:TYR:CZ	1:C:243:GLY:HA3	2.56	0.40
1:B:213:GLU:HB3	1:B:292:ILE:CD1	2.51	0.40
1:A:13:ARG:NE	1:A:15:GLU:OE2	2.42	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:90:ARG:HD3	4:B:413:HOH:O	2.21	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	269/304 (88%)	257 (96%)	11 (4%)	1 (0%)	39	31
1	B	270/304 (89%)	261 (97%)	9 (3%)	0	100	100
1	C	268/304 (88%)	255 (95%)	13 (5%)	0	100	100
1	D	271/304 (89%)	262 (97%)	9 (3%)	0	100	100
All	All	1078/1216 (89%)	1035 (96%)	42 (4%)	1 (0%)	56	51

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	253	VAL

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	238/262 (91%)	227 (95%)	11 (5%)	33	25

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	239/262 (91%)	235 (98%)	4 (2%)	68	69
1	C	238/262 (91%)	227 (95%)	11 (5%)	33	25
1	D	240/262 (92%)	229 (95%)	11 (5%)	33	25
All	All	955/1048 (91%)	918 (96%)	37 (4%)	39	32

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	ASN
1	A	18	GLN
1	A	27	ARG
1	A	37	THR
1	A	49	PRO
1	A	73	TYR
1	A	124	MET
1	A	170	THR
1	A	199	CYS
1	A	242	ILE
1	A	294	ASN
1	B	37	THR
1	B	124	MET
1	B	141	PRO
1	B	201	GLN
1	C	17	ASP
1	C	37	THR
1	C	129	GLN
1	C	133	GLN
1	C	151	LEU
1	C	170	THR
1	C	199	CYS
1	C	215	MET
1	C	220	ARG
1	C	242	ILE
1	C	269	LYS
1	D	6	LEU
1	D	7	ILE
1	D	24	MET
1	D	27	ARG
1	D	38	LYS
1	D	77	LEU
1	D	129	GLN

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Mol	Chain	Res	Type
1	D	133	GLN
1	D	151	LEU
1	D	199	CYS
1	D	201	GLN

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	18	GLN
1	A	201	GLN
1	A	294	ASN
1	B	129	GLN
1	B	233	HIS
1	C	16	ASN
1	C	133	GLN
1	C	233	HIS
1	D	113	HIS
1	D	233	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

6 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length

(or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#|Z| > 2$	Counts	RMSZ	$\#|Z| > 2$
2	S4M	A	301	-	23,26,26	1.21	4 (17%)	17,37,37	2.11	5 (29%)
2	S4M	B	301	-	23,26,26	0.93	2 (8%)	17,37,37	1.78	4 (23%)
3	4JV	B	302	-	23,23,23	1.16	2 (8%)	29,32,32	1.33	4 (13%)
2	S4M	C	301	-	23,26,26	1.10	2 (8%)	17,37,37	1.38	5 (29%)
2	S4M	D	301	-	23,26,26	0.83	1 (4%)	17,37,37	1.93	2 (11%)
3	4JV	D	302	-	23,23,23	1.11	1 (4%)	29,32,32	1.18	2 (6%)

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	S4M	A	301	-	-	0/7/28/28	0/3/3/3
2	S4M	B	301	-	-	0/7/28/28	0/3/3/3
3	4JV	B	302	-	-	0/5/5/5	0/3/3/3
2	S4M	C	301	-	-	0/7/28/28	0/3/3/3
2	S4M	D	301	-	-	0/7/28/28	0/3/3/3
3	4JV	D	302	-	-	0/5/5/5	0/3/3/3

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	302	4JV	C2-N6	-2.27	1.33	1.37
2	A	301	S4M	C4-N3	-2.06	1.32	1.35
2	D	301	S4M	C6-N6	2.06	1.42	1.34
2	C	301	S4M	C6-N6	2.11	1.42	1.34
2	B	301	S4M	C2-N3	2.13	1.35	1.32
2	A	301	S4M	C6-N6	2.14	1.42	1.34
2	A	301	S4M	CG-SD	2.17	1.85	1.80
2	B	301	S4M	CG-SD	2.21	1.85	1.80
2	A	301	S4M	O4'-C1'	2.66	1.45	1.41
3	D	302	4JV	C12-N14	2.97	1.40	1.34
2	C	301	S4M	O4'-C1'	3.28	1.45	1.41
3	B	302	4JV	C12-N14	3.48	1.41	1.34

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	301	S4M	C4'-O4'-C1'	-6.66	102.58	109.64
2	A	301	S4M	C4'-O4'-C1'	-5.09	104.24	109.64
2	B	301	S4M	C4'-O4'-C1'	-3.85	105.57	109.64
3	D	302	4JV	C13-O7-C3	-3.16	112.75	117.56
3	B	302	4JV	N6-C12-N9	-3.10	123.34	127.56
2	B	301	S4M	O3'-C3'-C4'	-3.08	101.80	111.01
2	B	301	S4M	C1'-N9-C4	-2.89	123.58	126.81
3	D	302	4JV	N6-C12-N9	-2.64	123.96	127.56
2	C	301	S4M	O3'-C3'-C4'	-2.13	104.64	111.01
2	A	301	S4M	O3'-C3'-C4'	-2.12	104.69	111.01
2	C	301	S4M	C2'-C3'-C4'	2.07	106.86	102.64
2	A	301	S4M	O4'-C4'-C5'	2.14	114.61	108.90
2	C	301	S4M	CG-CB-CA	2.23	117.21	112.53
2	C	301	S4M	O4'-C4'-C5'	2.27	114.94	108.90
3	B	302	4JV	C3-C1-C2	2.36	121.82	115.88
3	B	302	4JV	C13-O7-C3	2.46	121.30	117.56
2	C	301	S4M	O4'-C1'-N9	2.55	112.92	108.11
2	D	301	S4M	N6-C6-N1	2.58	122.84	118.52
3	B	302	4JV	N14-C12-N6	2.59	122.58	117.72
2	A	301	S4M	CG-CB-CA	2.92	118.65	112.53
2	B	301	S4M	O4'-C1'-N9	3.47	114.66	108.11
2	A	301	S4M	CB-CG-SD	4.61	122.61	112.17

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	301	S4M	1	0
3	B	302	4JV	1	0
3	D	302	4JV	4	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(Å²)	Q<0.9
1	A	273/304 (89%)	0.34	17 (6%)	24	27	15, 28, 50, 69	0
1	B	276/304 (90%)	0.28	17 (6%)	24	27	17, 26, 43, 65	0
1	C	274/304 (90%)	0.47	23 (8%)	14	16	17, 30, 52, 84	0
1	D	277/304 (91%)	0.35	20 (7%)	18	22	18, 30, 50, 90	0
All	All	1100/1216 (90%)	0.36	77 (7%)	19	23	15, 28, 49, 90	0

All (77) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	9	GLY	9.7
1	C	170	THR	5.1
1	D	16	ASN	5.0
1	C	10	GLY	4.6
1	C	7	ILE	4.5
1	D	17	ASP	4.5
1	B	170	THR	4.3
1	B	5	GLU	4.0
1	C	183	ALA	3.9
1	B	39	PHE	3.8
1	A	253	VAL	3.8
1	B	166	ILE	3.8
1	A	17	ASP	3.8
1	A	294	ASN	3.6
1	C	8	SER	3.6
1	D	38	LYS	3.3
1	C	237	TYR	3.3
1	B	38	LYS	3.2
1	D	37	THR	3.1
1	C	27	ARG	3.1
1	A	18	GLN	3.1

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Mol	Chain	Res	Type	RSRZ
1	C	11	TRP	3.1
1	B	93	ILE	3.1
1	C	16	ASN	3.0
1	C	77	LEU	3.0
1	B	77	LEU	3.0
1	B	199	CYS	3.0
1	C	17	ASP	3.0
1	D	77	LEU	2.9
1	D	294	ASN	2.9
1	A	166	ILE	2.8
1	A	16	ASN	2.8
1	A	252	GLY	2.8
1	D	93	ILE	2.8
1	D	166	ILE	2.8
1	A	136	ARG	2.7
1	C	136	ARG	2.7
1	D	15	GLU	2.7
1	A	77	LEU	2.7
1	D	151	LEU	2.7
1	C	166	ILE	2.7
1	D	39	PHE	2.7
1	B	35	ALA	2.6
1	B	136	ARG	2.6
1	A	170	THR	2.6
1	B	218	PHE	2.5
1	C	51	GLY	2.5
1	D	20	PRO	2.5
1	B	36	PRO	2.4
1	C	73	TYR	2.4
1	D	36	PRO	2.4
1	B	105	VAL	2.4
1	C	294	ASN	2.4
1	B	151	LEU	2.3
1	D	22	GLN	2.3
1	B	181	GLY	2.3
1	A	101	VAL	2.3
1	B	20	PRO	2.3
1	A	201	GLN	2.3
1	A	10	GLY	2.3
1	C	101	VAL	2.3
1	B	101	VAL	2.2
1	A	199	CYS	2.2

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Mol	Chain	Res	Type	RSRZ
1	D	101	VAL	2.2
1	A	49	PRO	2.1
1	C	169	THR	2.1
1	D	136	ARG	2.1
1	C	50	LYS	2.1
1	D	50	LYS	2.1
1	A	51	GLY	2.1
1	C	39	PHE	2.1
1	D	183	ALA	2.1
1	C	48	ASP	2.1
1	C	251	ALA	2.1
1	A	76	VAL	2.0
1	D	182	GLU	2.0
1	D	5	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no carbohydrates in this entry.

6.4 Ligands (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. 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(Å^2)	Q<0.9
3	4JV	B	302	21/21	0.94	0.12	0.06	28,30,38,40	0
2	S4M	A	301	24/24	0.93	0.12	-0.05	22,29,43,46	0
2	S4M	C	301	24/24	0.89	0.13	-0.27	25,34,50,61	0
3	4JV	D	302	21/21	0.90	0.13	-0.32	42,49,51,52	0
2	S4M	B	301	24/24	0.91	0.12	-0.37	22,30,42,54	0
2	S4M	D	301	24/24	0.91	0.11	-0.58	31,38,47,64	0

6.5 Other polymers (i)

There are no such residues in this entry.