



# Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 10:10 am BST

PDB ID : 3A5Y  
Title : Crystal structure of GenX from Escherichia coli in complex with lysyladenylate analog  
Authors : Sumida, T.; Yanagisawa, T.; Ishii, R.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)  
Deposited on : 2009-08-17  
Resolution : 1.90 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.11  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.11

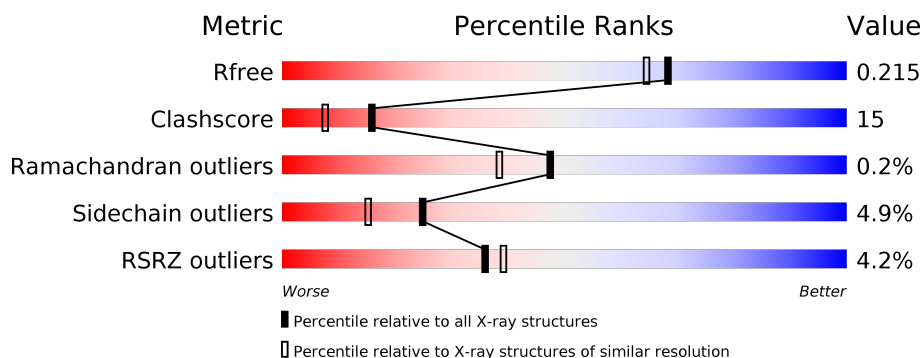
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.90 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))
$R_{free}$	130704	6207 (1.90-1.90)
Clashscore	141614	6847 (1.90-1.90)
Ramachandran outliers	138981	6760 (1.90-1.90)
Sidechain outliers	138945	6760 (1.90-1.90)
RSRZ outliers	127900	6082 (1.90-1.90)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	345	<div> <div>4%</div> <div>68% 16% • 14%</div> </div>
1	B	345	<div> <div>4%</div> <div>65% 22% • 10%</div> </div>
1	C	345	<div> <div>%</div> <div>66% 21% • • 10%</div> </div>
1	D	345	<div> <div>6%</div> <div>65% 23% • 10%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 11035 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 Putative lysyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	297	Total	C	N	O	S	0	0	0
			2379	1510	414	439	16			
1	B	310	Total	C	N	O	S	0	0	0
			2493	1575	435	467	16			
1	C	312	Total	C	N	O	S	0	0	0
			2502	1585	435	466	16			
1	D	311	Total	C	N	O	S	0	0	0
			2502	1585	435	466	16			

There are 80 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-19	MET	-	EXPRESSION TAG	UNP C3SGA2
A	-18	GLY	-	EXPRESSION TAG	UNP C3SGA2
A	-17	SER	-	EXPRESSION TAG	UNP C3SGA2
A	-16	SER	-	EXPRESSION TAG	UNP C3SGA2
A	-15	HIS	-	EXPRESSION TAG	UNP C3SGA2
A	-14	HIS	-	EXPRESSION TAG	UNP C3SGA2
A	-13	HIS	-	EXPRESSION TAG	UNP C3SGA2
A	-12	HIS	-	EXPRESSION TAG	UNP C3SGA2
A	-11	HIS	-	EXPRESSION TAG	UNP C3SGA2
A	-10	HIS	-	EXPRESSION TAG	UNP C3SGA2
A	-9	SER	-	EXPRESSION TAG	UNP C3SGA2
A	-8	SER	-	EXPRESSION TAG	UNP C3SGA2
A	-7	GLY	-	EXPRESSION TAG	UNP C3SGA2
A	-6	LEU	-	EXPRESSION TAG	UNP C3SGA2
A	-5	VAL	-	EXPRESSION TAG	UNP C3SGA2
A	-4	PRO	-	EXPRESSION TAG	UNP C3SGA2
A	-3	ARG	-	EXPRESSION TAG	UNP C3SGA2
A	-2	GLY	-	EXPRESSION TAG	UNP C3SGA2
A	-1	SER	-	EXPRESSION TAG	UNP C3SGA2
A	0	HIS	-	EXPRESSION TAG	UNP C3SGA2
B	-19	MET	-	EXPRESSION TAG	UNP C3SGA2

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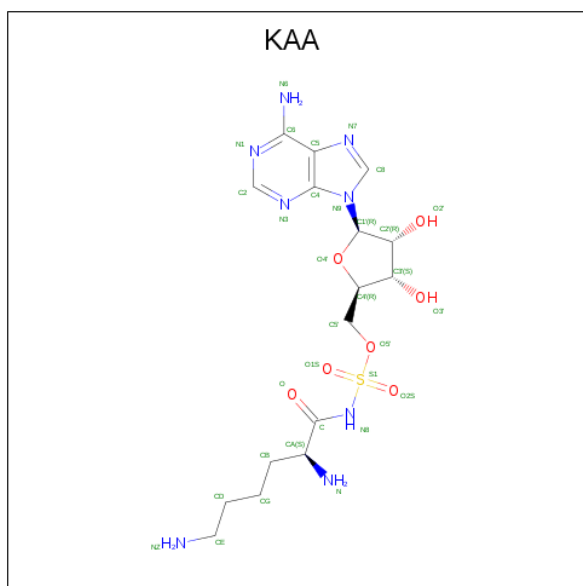
Chain	Residue	Modelled	Actual	Comment	Reference
B	-18	GLY	-	EXPRESSION TAG	UNP C3SGA2
B	-17	SER	-	EXPRESSION TAG	UNP C3SGA2
B	-16	SER	-	EXPRESSION TAG	UNP C3SGA2
B	-15	HIS	-	EXPRESSION TAG	UNP C3SGA2
B	-14	HIS	-	EXPRESSION TAG	UNP C3SGA2
B	-13	HIS	-	EXPRESSION TAG	UNP C3SGA2
B	-12	HIS	-	EXPRESSION TAG	UNP C3SGA2
B	-11	HIS	-	EXPRESSION TAG	UNP C3SGA2
B	-10	HIS	-	EXPRESSION TAG	UNP C3SGA2
B	-9	SER	-	EXPRESSION TAG	UNP C3SGA2
B	-8	SER	-	EXPRESSION TAG	UNP C3SGA2
B	-7	GLY	-	EXPRESSION TAG	UNP C3SGA2
B	-6	LEU	-	EXPRESSION TAG	UNP C3SGA2
B	-5	VAL	-	EXPRESSION TAG	UNP C3SGA2
B	-4	PRO	-	EXPRESSION TAG	UNP C3SGA2
B	-3	ARG	-	EXPRESSION TAG	UNP C3SGA2
B	-2	GLY	-	EXPRESSION TAG	UNP C3SGA2
B	-1	SER	-	EXPRESSION TAG	UNP C3SGA2
B	0	HIS	-	EXPRESSION TAG	UNP C3SGA2
C	-19	MET	-	EXPRESSION TAG	UNP C3SGA2
C	-18	GLY	-	EXPRESSION TAG	UNP C3SGA2
C	-17	SER	-	EXPRESSION TAG	UNP C3SGA2
C	-16	SER	-	EXPRESSION TAG	UNP C3SGA2
C	-15	HIS	-	EXPRESSION TAG	UNP C3SGA2
C	-14	HIS	-	EXPRESSION TAG	UNP C3SGA2
C	-13	HIS	-	EXPRESSION TAG	UNP C3SGA2
C	-12	HIS	-	EXPRESSION TAG	UNP C3SGA2
C	-11	HIS	-	EXPRESSION TAG	UNP C3SGA2
C	-10	HIS	-	EXPRESSION TAG	UNP C3SGA2
C	-9	SER	-	EXPRESSION TAG	UNP C3SGA2
C	-8	SER	-	EXPRESSION TAG	UNP C3SGA2
C	-7	GLY	-	EXPRESSION TAG	UNP C3SGA2
C	-6	LEU	-	EXPRESSION TAG	UNP C3SGA2
C	-5	VAL	-	EXPRESSION TAG	UNP C3SGA2
C	-4	PRO	-	EXPRESSION TAG	UNP C3SGA2
C	-3	ARG	-	EXPRESSION TAG	UNP C3SGA2
C	-2	GLY	-	EXPRESSION TAG	UNP C3SGA2
C	-1	SER	-	EXPRESSION TAG	UNP C3SGA2
C	0	HIS	-	EXPRESSION TAG	UNP C3SGA2
D	-19	MET	-	EXPRESSION TAG	UNP C3SGA2
D	-18	GLY	-	EXPRESSION TAG	UNP C3SGA2
D	-17	SER	-	EXPRESSION TAG	UNP C3SGA2

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Chain	Residue	Modelled	Actual	Comment	Reference
D	-16	SER	-	EXPRESSION TAG	UNP C3SGA2
D	-15	HIS	-	EXPRESSION TAG	UNP C3SGA2
D	-14	HIS	-	EXPRESSION TAG	UNP C3SGA2
D	-13	HIS	-	EXPRESSION TAG	UNP C3SGA2
D	-12	HIS	-	EXPRESSION TAG	UNP C3SGA2
D	-11	HIS	-	EXPRESSION TAG	UNP C3SGA2
D	-10	HIS	-	EXPRESSION TAG	UNP C3SGA2
D	-9	SER	-	EXPRESSION TAG	UNP C3SGA2
D	-8	SER	-	EXPRESSION TAG	UNP C3SGA2
D	-7	GLY	-	EXPRESSION TAG	UNP C3SGA2
D	-6	LEU	-	EXPRESSION TAG	UNP C3SGA2
D	-5	VAL	-	EXPRESSION TAG	UNP C3SGA2
D	-4	PRO	-	EXPRESSION TAG	UNP C3SGA2
D	-3	ARG	-	EXPRESSION TAG	UNP C3SGA2
D	-2	GLY	-	EXPRESSION TAG	UNP C3SGA2
D	-1	SER	-	EXPRESSION TAG	UNP C3SGA2
D	0	HIS	-	EXPRESSION TAG	UNP C3SGA2

- Molecule 2 is 5'-O-[(L-LYSYLAMINO)SULFONYL]ADENOSINE (three-letter code: KAA) (formula:  $C_{16}H_{26}N_8O_7S$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	S	0	0
			32	16	8	7	1		
2	B	1	Total	C	N	O	S	0	0
			32	16	8	7	1		

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	C	1	Total	C	N	O	S	0	0
			32	16	8	7	1		
2	D	1	Total	C	N	O	S	0	0
			32	16	8	7	1		

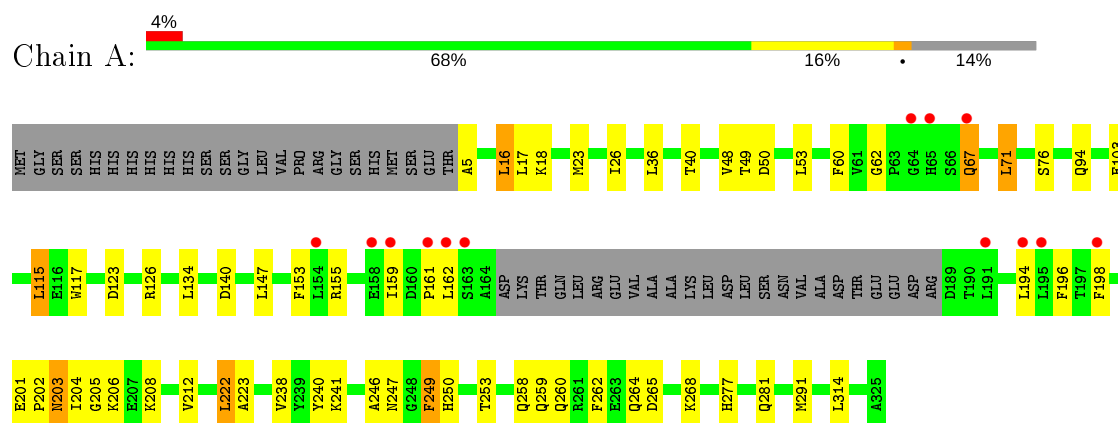
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	253	Total	O	0	0
			253	253		
3	B	256	Total	O	0	0
			256	256		
3	C	291	Total	O	0	0
			291	291		
3	D	231	Total	O	0	0
			231	231		

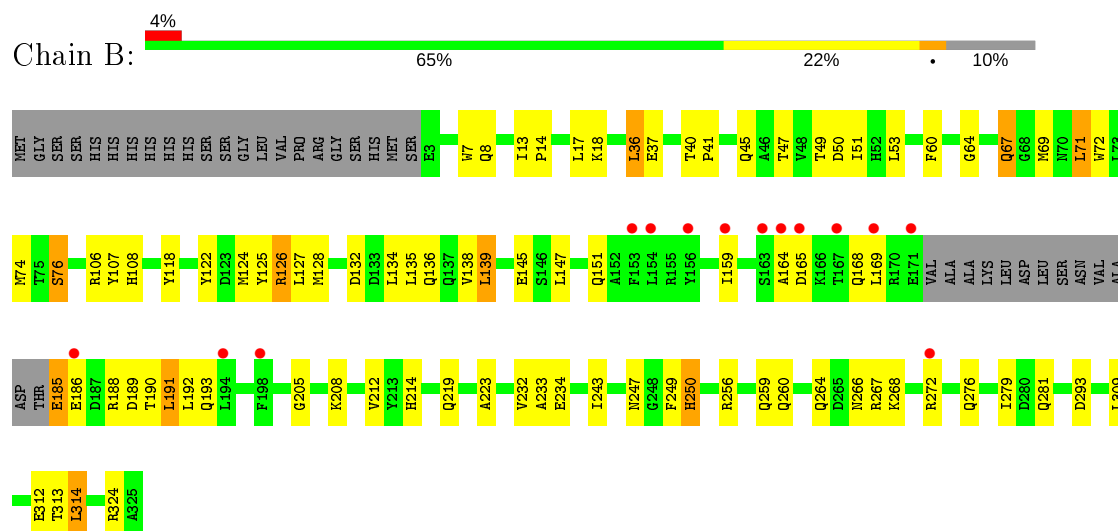
### 3 Residue-property plots [i](#)

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

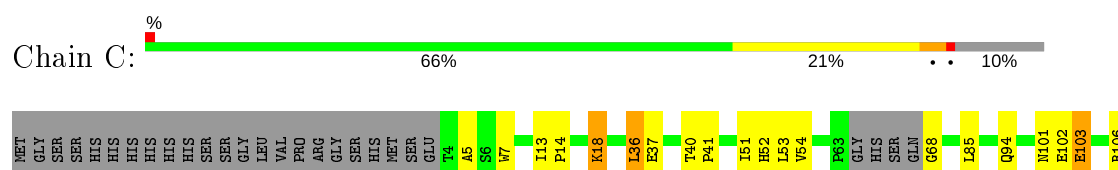
- Molecule 1: Putative lysyl-tRNA synthetase



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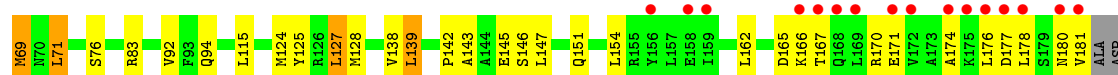
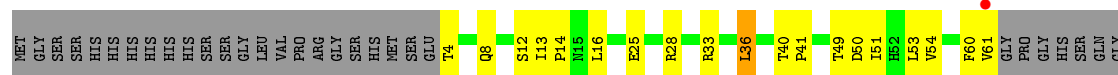


- Molecule 1: Putative lysyl-tRNA synthetase





• Molecule 1: Putative lysyl-tRNA synthetase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	54.80 Å 69.15 Å 94.08 Å 95.47° 106.51° 90.46°	Depositor
Resolution (Å)	44.87 – 1.90 44.87 – 1.90	Depositor EDS
% Data completeness (in resolution range)	95.2 (44.87-1.90) 95.4 (44.87-1.90)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.09	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.91 (at 1.89 Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, $R_{free}$	0.171 , 0.219 0.167 , 0.215	Depositor DCC
$R_{free}$ test set	9925 reflections (10.02%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	20.1	Xtriage
Anisotropy	0.510	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 60.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	11035	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.55% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

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

## 5 Model quality

### 5.1 Standard geometry

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

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	0.42	0/2435	0.68	1/3298 (0.0%)
1	B	0.47	2/2549 (0.1%)	0.69	1/3450 (0.0%)
1	C	0.45	1/2556 (0.0%)	0.68	2/3459 (0.1%)
1	D	0.43	1/2555 (0.0%)	0.67	2/3458 (0.1%)
All	All	0.44	4/10095 (0.0%)	0.68	6/13665 (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	B	0	1
1	C	0	1
All	All	0	2

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	185	GLU	CD-OE2	7.33	1.33	1.25
1	B	186	GLU	CD-OE2	7.18	1.33	1.25
1	D	186	GLU	CD-OE2	7.08	1.33	1.25
1	C	186	GLU	CD-OE2	6.83	1.33	1.25

All (6) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	250	HIS	N-CA-C	-8.65	87.65	111.00
1	A	250	HIS	N-CA-C	-7.66	90.32	111.00
1	D	250	HIS	N-CA-C	-7.51	90.73	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	250	HIS	N-CA-C	-5.42	96.36	111.00
1	D	249	PHE	CB-CA-C	-5.26	99.88	110.40
1	C	115	LEU	N-CA-C	-5.13	97.15	111.00

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	118	TYR	Sidechain
1	C	118	TYR	Sidechain

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2379	0	2323	56	0
1	B	2493	0	2427	66	0
1	C	2502	0	2454	76	0
1	D	2502	0	2456	99	0
2	A	32	0	26	2	0
2	B	32	0	26	2	0
2	C	32	0	26	2	0
2	D	32	0	26	1	0
3	A	253	0	0	7	0
3	B	256	0	0	6	0
3	C	291	0	0	11	0
3	D	231	0	0	7	0
All	All	11035	0	9764	289	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 15.

All (289) 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:124:MET:HG2	1:D:128:MET:HE2	1.33	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:243:ILE:HD11	1:C:303:ARG:HB3	1.44	1.00
1:D:139:LEU:HD11	1:D:304:LEU:HD11	1.42	0.99
1:D:272:ARG:HH21	1:D:273:GLY:H	1.10	0.98
1:D:214:HIS:HB3	1:D:232:VAL:HG21	1.48	0.94
1:D:125:TYR:HA	1:D:128:MET:HE3	1.51	0.93
1:A:23:MET:HE2	1:A:23:MET:HA	1.49	0.92
1:C:248:GLY:HA3	1:C:297:VAL:HG12	1.53	0.89
1:B:260:GLN:HG3	1:B:264:GLN:HE21	1.43	0.82
1:C:243:ILE:CD1	1:C:303:ARG:HB3	2.09	0.82
1:D:25:GLU:HA	1:D:28:ARG:HH22	1.48	0.78
1:B:60:PHE:HB2	1:B:71:LEU:HD22	1.63	0.78
1:C:7:TRP:O	1:D:83:ARG:HD2	1.83	0.77
1:D:61:VAL:HG12	3:D:827:HOH:O	1.83	0.77
1:A:26:ILE:HD13	1:A:134:LEU:HD11	1.67	0.76
1:C:170:ARG:HH21	1:C:186:GLU:HB2	1.49	0.76
1:D:180:ASN:OD1	1:D:181:VAL:HG23	1.88	0.73
1:C:178:LEU:HD13	1:C:194:LEU:HG	1.70	0.72
1:D:142:PRO:HG2	1:D:208:LYS:HB3	1.71	0.72
1:B:45:GLN:HG2	1:B:69:MET:HE1	1.70	0.72
1:D:40:THR:H	1:D:94:GLN:HE22	1.36	0.71
1:A:247:ASN:HD22	2:A:1990:KAA:HN8	1.36	0.71
1:C:102:GLU:HA	3:C:552:HOH:O	1.92	0.69
1:C:113:THR:HB	1:C:301:VAL:HG22	1.74	0.69
1:D:69:MET:CE	1:D:71:LEU:HD11	2.22	0.69
1:C:281:GLN:HG2	3:C:670:HOH:O	1.92	0.68
1:C:138:VAL:HG21	1:C:304:LEU:HD21	1.76	0.68
1:B:214:HIS:HB3	1:B:232:VAL:HG11	1.76	0.68
1:A:40:THR:H	1:A:94:GLN:HE22	1.41	0.67
1:D:272:ARG:HH21	1:D:273:GLY:N	1.89	0.67
1:D:187:ASP:OD2	1:D:190:THR:HG23	1.93	0.67
1:C:52:HIS:HB2	3:C:576:HOH:O	1.94	0.67
1:B:188:ARG:HH22	1:B:192:LEU:HD11	1.60	0.66
1:B:247:ASN:HD22	2:B:1991:KAA:HN8	1.41	0.66
1:D:139:LEU:HD12	1:D:139:LEU:N	2.11	0.66
1:D:4:THR:HB	1:D:8:GLN:NE2	2.10	0.66
1:D:247:ASN:HD22	2:D:1993:KAA:HN8	1.44	0.66
1:A:60:PHE:HB2	1:A:71:LEU:HD22	1.77	0.66
1:C:40:THR:H	1:C:94:GLN:HE22	1.42	0.66
1:A:123:ASP:OD2	1:C:155:ARG:HD3	1.97	0.65
1:B:214:HIS:CB	1:B:232:VAL:HG11	2.26	0.65
1:D:272:ARG:HH21	1:D:272:ARG:HG3	1.61	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:138:VAL:CG2	1:C:304:LEU:HD21	2.26	0.65
1:D:139:LEU:HD11	1:D:304:LEU:CD1	2.21	0.65
1:D:166:LYS:HD2	1:D:170:ARG:NH1	2.11	0.65
1:B:124:MET:HG2	1:B:128:MET:CE	2.28	0.64
1:C:127:LEU:HD21	1:C:297:VAL:HG13	1.79	0.64
1:A:206:LYS:CD	1:A:206:LYS:H	2.11	0.63
1:A:23:MET:CA	1:A:23:MET:HE2	2.28	0.63
1:D:25:GLU:HA	1:D:28:ARG:NH2	2.14	0.62
1:D:69:MET:HE1	1:D:71:LEU:HD11	1.81	0.62
1:A:206:LYS:N	1:A:206:LYS:HD3	2.15	0.62
1:D:60:PHE:HB2	1:D:71:LEU:HD22	1.80	0.62
1:C:247:ASN:HD22	2:C:1992:KAA:HN8	1.46	0.61
1:C:113:THR:HB	1:C:301:VAL:CG2	2.30	0.61
1:D:166:LYS:HZ1	1:D:186:GLU:HA	1.63	0.61
1:D:214:HIS:HB3	1:D:232:VAL:CG2	2.28	0.61
1:B:74:MET:CE	3:B:355:HOH:O	2.49	0.61
1:A:204:ILE:C	1:A:206:LYS:HD3	2.22	0.60
1:B:188:ARG:NH2	1:B:192:LEU:HD11	2.16	0.60
1:D:272:ARG:NH2	1:D:273:GLY:H	1.92	0.60
1:C:214:HIS:CG	1:C:232:VAL:HG11	2.35	0.60
1:D:260:GLN:O	1:D:264:GLN:HG3	2.01	0.60
1:A:206:LYS:H	1:A:206:LYS:HD3	1.67	0.60
1:C:214:HIS:HB3	1:C:232:VAL:HG11	1.83	0.60
1:C:51:ILE:HG12	1:C:268:LYS:HD2	1.82	0.60
1:C:214:HIS:CB	1:C:232:VAL:HG11	2.32	0.60
1:A:103:GLU:HG2	3:A:438:HOH:O	2.03	0.59
1:D:145:GLU:HB3	1:D:208:LYS:HE2	1.83	0.59
1:D:12:SER:O	1:D:16:LEU:HD22	2.02	0.59
1:B:18:LYS:HE3	1:B:309:LEU:HD22	1.83	0.59
1:C:51:ILE:HD11	1:C:265:ASP:HA	1.85	0.58
1:D:174:ALA:C	1:D:176:LEU:H	2.05	0.58
1:B:36:LEU:HD22	1:B:37:GLU:O	2.03	0.58
1:B:214:HIS:CG	1:B:232:VAL:HG11	2.38	0.58
1:C:127:LEU:CD2	1:C:297:VAL:HG13	2.32	0.58
1:C:170:ARG:NH2	1:C:186:GLU:HB2	2.19	0.58
1:D:166:LYS:HD3	1:D:191:LEU:HD22	1.86	0.57
1:B:45:GLN:CG	1:B:69:MET:HE1	2.34	0.57
1:C:68:GLY:N	3:C:569:HOH:O	2.36	0.57
1:C:322:VAL:HG22	1:D:69:MET:HE2	1.87	0.57
1:A:223:ALA:HB2	1:A:249:PHE:HB3	1.86	0.57
1:A:268:LYS:HG3	3:A:452:HOH:O	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:151:GLN:HG2	3:C:621:HOH:O	2.05	0.56
1:D:139:LEU:N	1:D:139:LEU:CD1	2.68	0.56
1:A:67:GLN:O	1:A:67:GLN:HG3	2.05	0.56
1:C:121:HIS:HB2	3:C:574:HOH:O	2.06	0.56
1:B:147:LEU:HD12	1:B:151:GLN:HE21	1.70	0.56
1:C:236:PHE:HZ	1:C:297:VAL:HG11	1.69	0.56
1:D:40:THR:H	1:D:94:GLN:NE2	2.03	0.56
1:B:124:MET:HG2	1:B:128:MET:HE1	1.88	0.56
1:A:40:THR:H	1:A:94:GLN:NE2	2.02	0.56
1:A:194:LEU:O	1:A:194:LEU:HD23	2.05	0.56
1:C:189:ASP:O	1:C:193:GLN:HG3	2.05	0.55
1:D:147:LEU:CD1	1:D:151:GLN:HG3	2.37	0.55
1:D:167:THR:O	1:D:171:GLU:HG3	2.05	0.55
1:C:322:VAL:HG22	1:D:69:MET:CE	2.37	0.55
1:D:69:MET:HE3	1:D:71:LEU:HD11	1.88	0.55
1:B:165:ASP:H	1:B:168:GLN:NE2	2.04	0.55
1:B:250:HIS:HE1	1:B:293:ASP:OD2	1.90	0.55
1:B:106:ARG:HD2	1:B:107:TYR:CZ	2.42	0.54
1:C:139:LEU:HD21	1:C:304:LEU:HD23	1.89	0.54
1:C:51:ILE:HD13	3:C:733:HOH:O	2.06	0.54
1:A:206:LYS:CD	1:A:206:LYS:N	2.70	0.54
1:B:51:ILE:HD11	1:B:268:LYS:HB2	1.90	0.54
1:B:259:GLN:NE2	1:B:279:ILE:HD13	2.22	0.54
1:B:125:TYR:CD1	1:B:128:MET:HE3	2.43	0.54
1:D:272:ARG:NH2	1:D:272:ARG:HG3	2.21	0.54
1:A:26:ILE:CD1	1:A:134:LEU:HD11	2.36	0.53
1:B:125:TYR:HD1	1:B:128:MET:HE3	1.74	0.53
1:C:223:ALA:HB2	1:C:249:PHE:CB	2.38	0.53
1:A:206:LYS:CE	1:A:206:LYS:H	2.21	0.53
1:B:147:LEU:O	1:B:212:VAL:HA	2.08	0.53
1:C:240:TYR:CZ	1:C:241:LYS:HE3	2.43	0.53
1:C:235:ARG:HG3	1:C:249:PHE:HD2	1.74	0.53
1:D:166:LYS:NZ	1:D:191:LEU:HD22	2.24	0.53
1:D:138:VAL:HG12	1:D:139:LEU:HD12	1.91	0.53
1:B:124:MET:HG2	1:B:128:MET:HE2	1.91	0.53
1:B:243:ILE:HD12	1:B:243:ILE:N	2.24	0.53
1:C:250:HIS:HE1	1:C:293:ASP:OD1	1.92	0.53
1:B:312:GLU:HG3	1:B:313:THR:HG23	1.91	0.52
1:C:40:THR:H	1:C:94:GLN:NE2	2.05	0.52
1:A:223:ALA:CB	1:A:249:PHE:HB3	2.39	0.52
1:B:108:HIS:HD2	3:B:397:HOH:O	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:176:LEU:C	1:D:178:LEU:H	2.13	0.52
1:D:166:LYS:HZ2	1:D:191:LEU:HD22	1.74	0.52
1:D:267:ARG:HH11	1:D:267:ARG:HG3	1.75	0.52
1:D:12:SER:HB2	1:D:14:PRO:HD2	1.91	0.52
1:C:54:VAL:O	1:C:54:VAL:HG13	2.09	0.52
1:A:203:ASN:HD22	1:A:203:ASN:C	2.13	0.52
1:A:18:LYS:HE3	3:A:379:HOH:O	2.08	0.52
1:D:264:GLN:HG2	1:D:267:ARG:HH21	1.74	0.51
1:C:234:GLU:OE1	1:C:250:HIS:HD2	1.94	0.51
1:A:123:ASP:OD2	1:C:155:ARG:CD	2.58	0.51
1:A:203:ASN:C	1:A:206:LYS:HD2	2.31	0.51
1:C:115:LEU:HB2	1:C:301:VAL:CG1	2.41	0.51
1:A:23:MET:CE	1:A:23:MET:HA	2.33	0.51
1:A:162:LEU:CD1	1:A:162:LEU:N	2.74	0.50
1:B:13:ILE:HB	1:B:14:PRO:HD3	1.93	0.50
1:C:236:PHE:CZ	1:C:297:VAL:CG1	2.94	0.50
1:C:36:LEU:HD22	1:C:37:GLU:O	2.11	0.50
1:D:36:LEU:HB3	1:D:92:VAL:HG12	1.92	0.50
1:D:40:THR:HB	1:D:41:PRO:CD	2.42	0.50
1:A:203:ASN:O	1:A:206:LYS:HD2	2.12	0.50
1:B:314:LEU:HD11	2:B:1991:KAA:H2	1.93	0.50
1:C:18:LYS:HB3	1:C:309:LEU:HD21	1.94	0.50
1:A:162:LEU:HD12	1:A:162:LEU:N	2.26	0.50
1:A:5:ALA:N	3:A:370:HOH:O	2.44	0.50
1:B:188:ARG:HG2	1:B:188:ARG:HH21	1.77	0.50
1:C:236:PHE:HZ	1:C:297:VAL:CG1	2.23	0.50
1:D:313:THR:OG1	1:D:316:GLU:HG3	2.12	0.50
1:B:135:LEU:O	1:B:139:LEU:HB2	2.12	0.50
1:D:166:LYS:NZ	1:D:191:LEU:HD13	2.27	0.50
1:D:51:ILE:HD11	1:D:268:LYS:HD2	1.94	0.50
1:D:272:ARG:HG3	1:D:273:GLY:H	1.76	0.49
1:A:222:LEU:HD13	1:A:258:GLN:OE1	2.12	0.49
3:C:518:HOH:O	1:D:61:VAL:HG13	2.11	0.49
1:C:314:LEU:HD11	2:C:1992:KAA:H2	1.94	0.49
1:C:223:ALA:HB2	1:C:249:PHE:CG	2.47	0.49
1:D:174:ALA:C	1:D:176:LEU:N	2.65	0.49
1:D:54:VAL:HG13	1:D:54:VAL:O	2.11	0.49
1:C:166:LYS:HB3	1:C:170:ARG:HH12	1.77	0.49
1:C:5:ALA:O	1:C:324:ARG:NH1	2.45	0.49
1:D:214:HIS:O	1:D:232:VAL:CG2	2.61	0.49
1:C:119:ARG:HD2	1:C:130:GLU:OE1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:60:PHE:CD2	1:D:61:VAL:N	2.81	0.48
1:A:147:LEU:O	1:A:212:VAL:HA	2.13	0.48
1:D:241:LYS:O	1:D:243:ILE:HD12	2.14	0.48
1:D:54:VAL:HG12	3:D:919:HOH:O	2.12	0.48
1:B:67:GLN:O	1:B:67:GLN:HG3	2.14	0.48
1:C:106:ARG:NH2	1:C:312:GLU:O	2.47	0.48
1:C:238:VAL:HG12	1:C:246:ALA:HB3	1.96	0.48
1:A:196:PHE:CE1	1:A:201:GLU:HG3	2.49	0.48
1:C:51:ILE:HD11	1:C:265:ASP:CA	2.45	0.47
1:D:166:LYS:CE	1:D:191:LEU:HD22	2.44	0.47
1:B:259:GLN:HE21	1:B:279:ILE:HD13	1.80	0.47
1:D:166:LYS:HE3	1:D:186:GLU:O	2.14	0.47
1:D:225:ILE:HD13	3:D:577:HOH:O	2.13	0.47
1:A:264:GLN:HG3	3:A:577:HOH:O	2.14	0.47
1:B:272:ARG:HG2	1:B:272:ARG:HH21	1.79	0.47
1:B:76:SER:HB3	3:B:435:HOH:O	2.14	0.47
1:C:115:LEU:HB2	1:C:301:VAL:HG12	1.96	0.47
1:C:147:LEU:O	1:C:212:VAL:HA	2.14	0.47
1:C:40:THR:HB	1:C:41:PRO:CD	2.44	0.47
1:C:205:GLY:HA2	1:C:208:LYS:O	2.14	0.47
1:D:147:LEU:O	1:D:212:VAL:HA	2.15	0.47
1:A:205:GLY:HA2	1:A:208:LYS:O	2.15	0.47
1:C:119:ARG:CD	1:C:130:GLU:OE1	2.63	0.47
1:A:201:GLU:HB2	1:A:202:PRO:HD3	1.97	0.47
1:A:36:LEU:HD13	1:B:17:LEU:HD23	1.96	0.47
1:D:12:SER:O	1:D:16:LEU:CD2	2.63	0.47
1:D:142:PRO:HG2	1:D:208:LYS:CB	2.45	0.47
1:A:17:LEU:HD13	1:A:17:LEU:O	2.15	0.46
1:B:165:ASP:O	1:B:169:LEU:HG	2.16	0.46
1:D:238:VAL:CG1	1:D:246:ALA:HB3	2.44	0.46
1:B:134:LEU:O	1:B:138:VAL:HG13	2.15	0.46
1:A:159:ILE:O	1:A:161:PRO:HD3	2.16	0.46
1:C:153:PHE:CB	1:C:161:PRO:HD3	2.45	0.46
1:A:60:PHE:CE1	1:A:62:GLY:HA2	2.50	0.46
1:D:40:THR:HB	1:D:41:PRO:HD2	1.97	0.46
1:B:49:THR:O	1:B:50:ASP:C	2.53	0.46
1:B:122:TYR:CD1	1:B:126:ARG:HD2	2.50	0.46
1:C:54:VAL:HG13	1:C:101:ASN:HB3	1.98	0.46
1:B:223:ALA:HB2	1:B:249:PHE:HB3	1.98	0.45
1:D:28:ARG:NH2	3:D:828:HOH:O	2.48	0.45
1:C:68:GLY:N	3:C:558:HOH:O	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:TYR:CZ	1:A:241:LYS:HE3	2.51	0.45
1:B:106:ARG:HG3	1:B:313:THR:HG22	1.98	0.45
1:D:189:ASP:O	1:D:193:GLN:HG2	2.17	0.45
1:D:205:GLY:HA2	1:D:208:LYS:O	2.17	0.45
1:B:189:ASP:O	1:B:193:GLN:HG3	2.16	0.45
1:D:166:LYS:HE3	1:D:186:GLU:C	2.36	0.45
1:A:49:THR:O	1:A:50:ASP:C	2.55	0.45
1:B:50:ASP:OD2	1:B:53:LEU:HD13	2.17	0.45
1:C:235:ARG:HA	1:C:249:PHE:HB3	2.00	0.45
1:A:115:LEU:HD13	1:A:117:TRP:CZ3	2.52	0.44
1:D:4:THR:N	3:D:825:HOH:O	2.50	0.44
1:B:185:GLU:OE1	1:B:190:THR:HG21	2.17	0.44
1:B:205:GLY:HA2	1:B:208:LYS:O	2.17	0.44
1:C:120:PRO:HA	1:C:294:CYS:HB3	1.99	0.44
1:D:69:MET:HE3	1:D:71:LEU:CD1	2.47	0.44
1:A:238:VAL:HG12	1:A:246:ALA:HB3	2.00	0.44
1:D:243:ILE:N	1:D:243:ILE:HD12	2.33	0.44
1:C:236:PHE:CZ	1:C:297:VAL:HG11	2.52	0.44
1:A:153:PHE:CG	1:A:161:PRO:HG3	2.53	0.43
1:B:132:ASP:O	1:B:136:GLN:HG3	2.17	0.43
1:A:281:GLN:HG2	3:A:476:HOH:O	2.17	0.43
1:D:272:ARG:HG3	1:D:273:GLY:N	2.33	0.43
1:B:219:GLN:NE2	3:B:374:HOH:O	2.48	0.43
1:D:143:ALA:O	1:D:208:LYS:HD2	2.18	0.43
1:B:51:ILE:CD1	1:B:268:LYS:HB2	2.49	0.43
1:B:47:THR:HB	1:B:72:TRP:CG	2.54	0.43
1:C:103:GLU:OE2	1:D:61:VAL:HG22	2.18	0.43
1:D:270:ALA:HB2	1:D:276:GLN:NE2	2.34	0.43
1:B:18:LYS:HE2	3:B:362:HOH:O	2.17	0.43
1:D:147:LEU:HD12	1:D:151:GLN:HG3	2.00	0.43
1:D:166:LYS:CD	1:D:191:LEU:HD22	2.49	0.43
1:D:214:HIS:HA	1:D:233:ALA:O	2.19	0.43
1:D:28:ARG:NH2	3:D:952:HOH:O	2.52	0.43
1:B:185:GLU:HB3	1:B:191:LEU:HD13	2.01	0.43
1:B:260:GLN:HG3	1:B:264:GLN:NE2	2.23	0.43
1:D:127:LEU:HD12	1:D:295:SER:HB3	2.01	0.43
1:A:17:LEU:HD13	1:A:17:LEU:C	2.40	0.43
1:B:159:ILE:HD11	1:B:164:ALA:HB1	2.01	0.43
1:C:13:ILE:HB	1:C:14:PRO:HD3	2.00	0.43
1:D:51:ILE:CD1	1:D:268:LYS:HD2	2.49	0.43
1:B:7:TRP:CZ2	1:B:8:GLN:HG2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:194:LEU:O	1:A:198:PHE:HD1	2.01	0.42
1:C:259:GLN:HG3	3:C:524:HOH:O	2.18	0.42
1:A:206:LYS:HE2	1:A:206:LYS:H	1.82	0.42
1:B:151:GLN:HG2	3:B:351:HOH:O	2.19	0.42
1:D:49:THR:O	1:D:50:ASP:C	2.58	0.42
1:D:278:PRO:HD2	3:D:865:HOH:O	2.19	0.42
1:A:194:LEU:C	1:A:194:LEU:HD23	2.39	0.42
1:A:253:THR:HG22	1:A:291:MET:CE	2.50	0.42
1:A:262:PHE:O	1:A:265:ASP:HB2	2.19	0.42
1:C:138:VAL:HG23	1:C:139:LEU:HG	2.01	0.42
1:C:256:ARG:HG3	3:C:610:HOH:O	2.19	0.42
1:D:190:THR:HA	1:D:193:GLN:CG	2.49	0.42
1:C:322:VAL:CG2	1:D:69:MET:HE2	2.49	0.42
1:B:234:GLU:OE2	1:B:250:HIS:HD2	2.03	0.42
1:C:164:ALA:HA	1:C:168:GLN:OE1	2.20	0.42
1:C:201:GLU:N	1:C:202:PRO:HD2	2.34	0.42
1:A:16:LEU:HD12	1:A:16:LEU:HA	1.91	0.41
1:D:13:ILE:N	1:D:14:PRO:CD	2.83	0.41
1:B:40:THR:HB	1:B:41:PRO:CD	2.49	0.41
1:C:138:VAL:HG23	1:C:304:LEU:HD21	2.02	0.41
1:B:7:TRP:CE2	1:B:8:GLN:HG2	2.55	0.41
1:D:166:LYS:HZ3	1:D:191:LEU:HD13	1.85	0.41
1:B:264:GLN:HG2	1:B:267:ARG:NH1	2.35	0.41
1:B:272:ARG:HG2	1:B:272:ARG:NH2	2.35	0.41
1:B:266:ASN:HB3	1:B:276:GLN:HE21	1.85	0.41
1:D:190:THR:HA	1:D:193:GLN:HG2	2.01	0.41
1:D:190:THR:HA	1:D:193:GLN:OE1	2.21	0.41
1:D:28:ARG:HB3	1:D:28:ARG:NH2	2.35	0.41
1:C:232:VAL:CG1	1:C:233:ALA:N	2.84	0.41
1:A:48:VAL:O	1:A:277:HIS:HD2	2.04	0.41
1:B:223:ALA:CB	1:B:249:PHE:HB3	2.50	0.41
1:D:146:SER:HG	1:D:213:TYR:HE2	1.66	0.41
1:D:171:GLU:O	1:D:174:ALA:HB3	2.19	0.41
1:C:214:HIS:HA	1:C:233:ALA:O	2.21	0.41
1:D:60:PHE:HD1	1:D:69:MET:HG3	1.85	0.41
1:B:188:ARG:NH2	1:B:188:ARG:HG2	2.36	0.41
1:B:232:VAL:CG1	1:B:233:ALA:N	2.82	0.41
1:A:314:LEU:HD21	2:A:1990:KAA:H2	2.03	0.40
1:D:257:GLU:O	1:D:261:ARG:HG3	2.21	0.40
1:D:33:ARG:HG3	1:D:33:ARG:HH21	1.85	0.40
1:A:260:GLN:NE2	3:A:375:HOH:O	2.55	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:272:ARG:CG	1:D:273:GLY:H	2.35	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	293/345 (85%)	283 (97%)	10 (3%)	0	100	100
1	B	306/345 (89%)	296 (97%)	9 (3%)	1 (0%)	41	31
1	C	306/345 (89%)	297 (97%)	9 (3%)	0	100	100
1	D	305/345 (88%)	296 (97%)	8 (3%)	1 (0%)	41	31
All	All	1210/1380 (88%)	1172 (97%)	36 (3%)	2 (0%)	47	38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	64	GLY
1	D	177	ASP

### 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	254/296 (86%)	241 (95%)	13 (5%)	24	14

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	B	267/296 (90%)	254 (95%)	13 (5%)	25	15
1	C	268/296 (90%)	254 (95%)	14 (5%)	23	14
1	D	269/296 (91%)	257 (96%)	12 (4%)	27	18
All	All	1058/1184 (89%)	1006 (95%)	52 (5%)	25	15

All (52) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	16	LEU
1	A	53	LEU
1	A	67	GLN
1	A	71	LEU
1	A	76	SER
1	A	115	LEU
1	A	126	ARG
1	A	140	ASP
1	A	155	ARG
1	A	203	ASN
1	A	222	LEU
1	A	249	PHE
1	A	259	GLN
1	B	36	LEU
1	B	67	GLN
1	B	71	LEU
1	B	76	SER
1	B	126	ARG
1	B	127	LEU
1	B	139	LEU
1	B	145	GLU
1	B	191	LEU
1	B	256	ARG
1	B	281	GLN
1	B	314	LEU
1	B	324	ARG
1	C	18	LYS
1	C	36	LEU
1	C	53	LEU
1	C	85	LEU
1	C	103	GLU
1	C	115	LEU
1	C	186	GLU

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Mol	Chain	Res	Type
1	C	191	LEU
1	C	243	ILE
1	C	249	PHE
1	C	259	GLN
1	C	272	ARG
1	C	304	LEU
1	C	314	LEU
1	D	36	LEU
1	D	53	LEU
1	D	69	MET
1	D	71	LEU
1	D	76	SER
1	D	115	LEU
1	D	127	LEU
1	D	139	LEU
1	D	154	LEU
1	D	162	LEU
1	D	165	ASP
1	D	238	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (39) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	8	GLN
1	A	45	GLN
1	A	67	GLN
1	A	94	GLN
1	A	129	ASN
1	A	151	GLN
1	A	193	GLN
1	A	203	ASN
1	A	219	GLN
1	A	224	GLN
1	A	277	HIS
1	B	8	GLN
1	B	15	ASN
1	B	45	GLN
1	B	67	GLN
1	B	108	HIS
1	B	151	GLN
1	B	168	GLN
1	B	203	ASN

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Mol	Chain	Res	Type
1	B	219	GLN
1	B	247	ASN
1	B	250	HIS
1	B	259	GLN
1	B	260	GLN
1	B	264	GLN
1	B	276	GLN
1	C	45	GLN
1	C	94	GLN
1	C	129	ASN
1	C	151	GLN
1	C	250	HIS
1	C	260	GLN
1	C	281	GLN
1	C	282	ASN
1	D	8	GLN
1	D	94	GLN
1	D	150	GLN
1	D	193	GLN
1	D	282	ASN

### 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](#)

4 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	KAA	B	1991	-	31,34,34	2.86	5 (16%)	33,49,49	2.10	5 (15%)
2	KAA	C	1992	-	31,34,34	2.86	5 (16%)	33,49,49	2.22	5 (15%)
2	KAA	D	1993	-	31,34,34	2.85	6 (19%)	33,49,49	2.21	4 (12%)
2	KAA	A	1990	-	31,34,34	2.88	6 (19%)	33,49,49	2.19	4 (12%)

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	KAA	B	1991	-	-	0/19/40/40	0/3/3/3
2	KAA	C	1992	-	-	0/19/40/40	0/3/3/3
2	KAA	D	1993	-	-	4/19/40/40	0/3/3/3
2	KAA	A	1990	-	-	1/19/40/40	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1990	KAA	O2S-S1	9.46	1.50	1.42
2	C	1992	KAA	O2S-S1	9.38	1.50	1.42
2	B	1991	KAA	O1S-S1	9.35	1.50	1.42
2	B	1991	KAA	O2S-S1	9.31	1.50	1.42
2	A	1990	KAA	O1S-S1	9.30	1.50	1.42
2	C	1992	KAA	O1S-S1	9.29	1.50	1.42
2	D	1993	KAA	O2S-S1	9.29	1.50	1.42
2	D	1993	KAA	O1S-S1	9.27	1.50	1.42
2	A	1990	KAA	O5'-S1	-7.60	1.43	1.59
2	B	1991	KAA	O5'-S1	-7.58	1.43	1.59
2	C	1992	KAA	O5'-S1	-7.58	1.43	1.59
2	D	1993	KAA	O5'-S1	-7.57	1.43	1.59
2	A	1990	KAA	O4'-C1'	2.30	1.44	1.41
2	C	1992	KAA	O4'-C1'	2.30	1.44	1.41
2	D	1993	KAA	O4'-C1'	2.27	1.44	1.41
2	B	1991	KAA	O4'-C1'	2.26	1.44	1.41
2	C	1992	KAA	C-N8	-2.21	1.33	1.37
2	A	1990	KAA	C-N8	-2.16	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	1993	KAA	C-N8	-2.15	1.33	1.37
2	B	1991	KAA	C-N8	-2.14	1.33	1.37
2	D	1993	KAA	S1-N8	2.10	1.63	1.59
2	A	1990	KAA	S1-N8	2.02	1.63	1.59

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	1993	KAA	O2S-S1-O1S	-7.57	108.96	120.76
2	A	1990	KAA	O2S-S1-O1S	-7.56	108.98	120.76
2	C	1992	KAA	O2S-S1-O1S	-7.51	109.05	120.76
2	D	1993	KAA	C-N8-S1	-7.28	112.83	124.61
2	B	1991	KAA	O2S-S1-O1S	-7.25	109.46	120.76
2	A	1990	KAA	C-N8-S1	-7.19	112.97	124.61
2	C	1992	KAA	C-N8-S1	-7.02	113.25	124.61
2	B	1991	KAA	C-N8-S1	-6.12	114.71	124.61
2	B	1991	KAA	N3-C2-N1	-4.58	121.52	128.68
2	D	1993	KAA	N3-C2-N1	-4.53	121.59	128.68
2	C	1992	KAA	N3-C2-N1	-4.45	121.72	128.68
2	A	1990	KAA	N3-C2-N1	-4.43	121.75	128.68
2	C	1992	KAA	O5'-C5'-C4'	2.51	112.31	107.62
2	B	1991	KAA	O5'-C5'-C4'	2.49	112.27	107.62
2	D	1993	KAA	O5'-C5'-C4'	2.33	111.97	107.62
2	A	1990	KAA	O5'-C5'-C4'	2.10	111.54	107.62
2	C	1992	KAA	C5'-O5'-S1	2.05	121.60	117.37
2	B	1991	KAA	O5'-S1-N8	2.05	111.31	105.60

There are no chirality outliers.

All (5) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	D	1993	KAA	O-C-CA-N
2	D	1993	KAA	N8-C-CA-N
2	D	1993	KAA	O-C-CA-CB
2	D	1993	KAA	N8-C-CA-CB
2	A	1990	KAA	O-C-CA-N

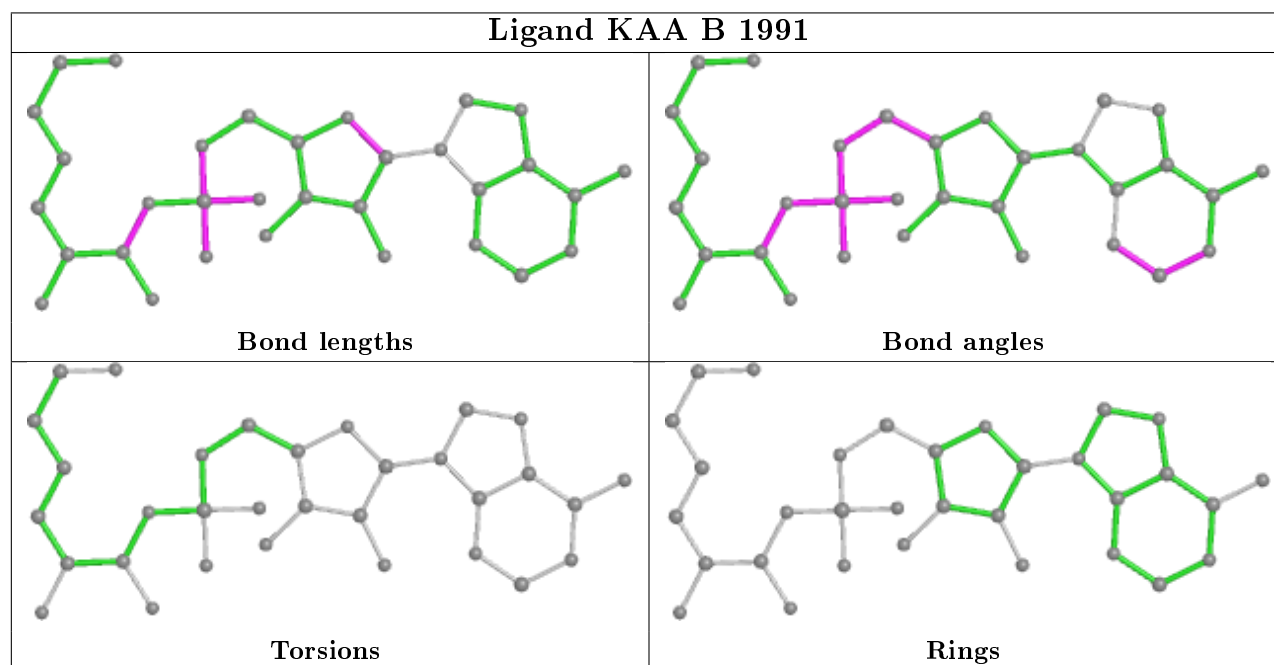
There are no ring outliers.

4 monomers are involved in 7 short contacts:

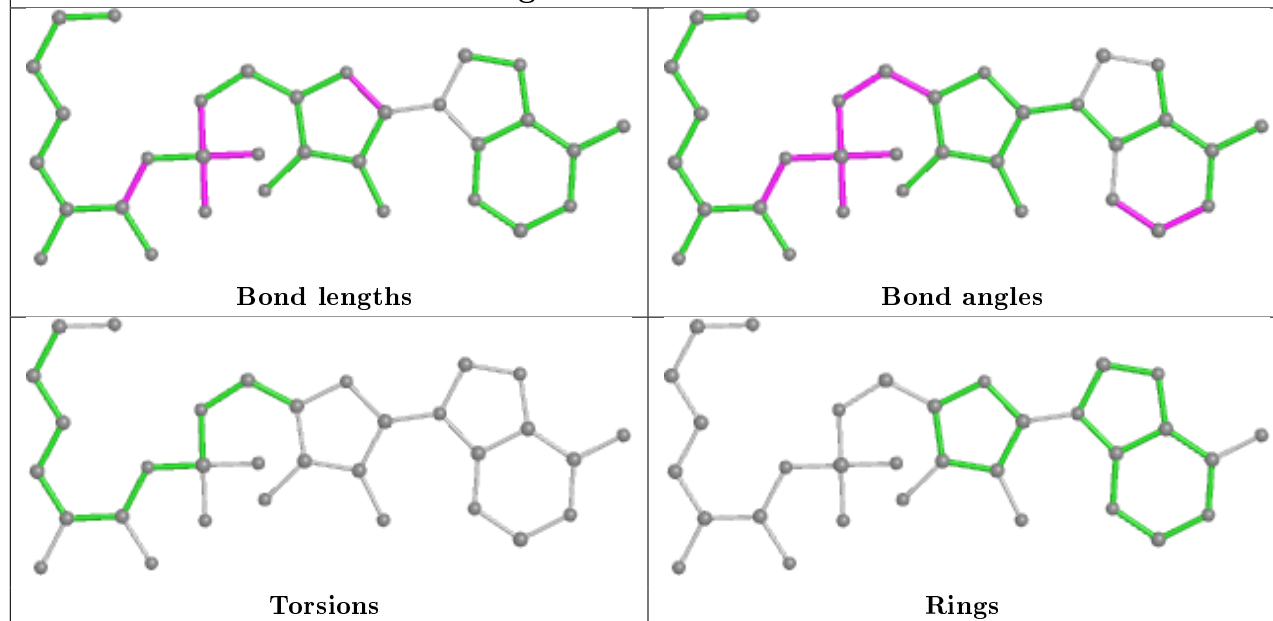


Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	1991	KAA	2	0
2	C	1992	KAA	2	0
2	D	1993	KAA	1	0
2	A	1990	KAA	2	0

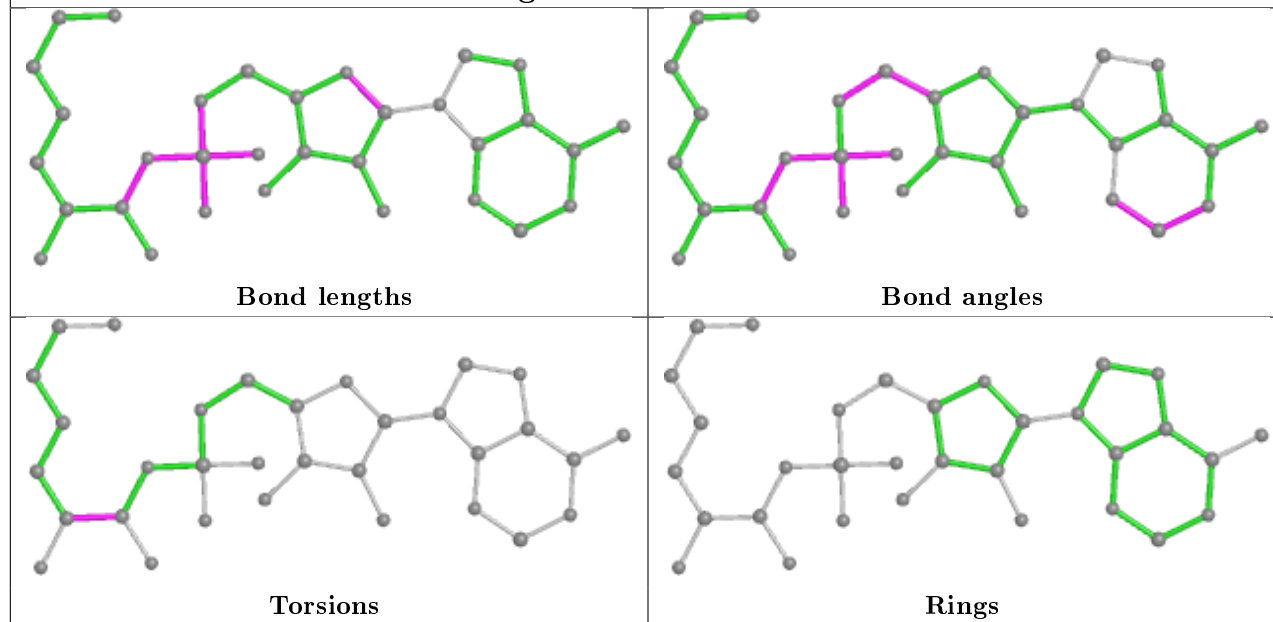
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

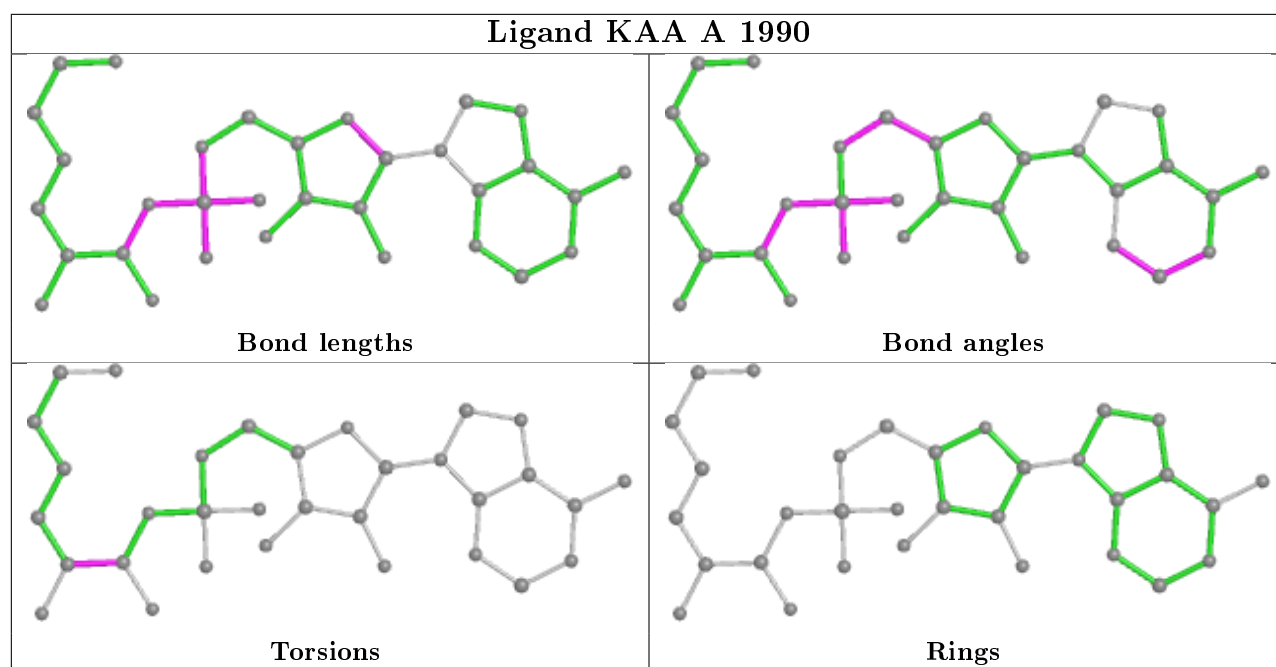


## Ligand KAA C 1992



## Ligand KAA D 1993





## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data ⓘ

### 6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å <sup>2</sup> )	Q<0.9
1	A	297/345 (86%)	-0.21	13 (4%) 34 37	12, 24, 57, 72	0
1	B	310/345 (89%)	-0.12	14 (4%) 33 36	12, 24, 50, 77	0
1	C	312/345 (90%)	-0.30	3 (0%) 82 84	12, 23, 47, 65	0
1	D	311/345 (90%)	0.04	22 (7%) 16 17	13, 26, 59, 90	0
All	All	1230/1380 (89%)	-0.15	52 (4%) 36 39	12, 24, 54, 90	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	178	LEU	6.1
1	D	176	LEU	5.1
1	C	178	LEU	4.9
1	A	191	LEU	4.6
1	D	181	VAL	3.8
1	D	177	ASP	3.7
1	A	159	ILE	3.7
1	D	169	LEU	3.6
1	D	180	ASN	3.6
1	D	172	VAL	3.6
1	D	159	ILE	3.5
1	A	194	LEU	3.5
1	C	174	ALA	3.5
1	D	174	ALA	3.4
1	B	165	ASP	3.4
1	D	191	LEU	3.4
1	D	175	LYS	3.3
1	A	65	HIS	3.3
1	D	171	GLU	3.3
1	B	272	ARG	3.3
1	D	198	PHE	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	154	LEU	3.3
1	B	169	LEU	3.1
1	B	167	THR	3.1
1	D	167	THR	3.1
1	D	166	LYS	3.0
1	B	156	TYR	3.0
1	A	198	PHE	2.9
1	A	195	LEU	2.8
1	A	64	GLY	2.8
1	B	164	ALA	2.7
1	C	179	SER	2.6
1	B	171	GLU	2.6
1	D	186	GLU	2.6
1	B	154	LEU	2.6
1	B	194	LEU	2.6
1	D	168	GLN	2.5
1	B	153	PHE	2.4
1	A	161	PRO	2.4
1	D	158	GLU	2.4
1	A	163	SER	2.3
1	B	163	SER	2.3
1	A	162	LEU	2.3
1	A	158	GLU	2.3
1	D	195	LEU	2.2
1	B	159	ILE	2.2
1	D	156	TYR	2.2
1	D	61	VAL	2.2
1	A	67	GLN	2.1
1	B	198	PHE	2.1
1	D	200	VAL	2.1
1	B	186	GLU	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 ⓘ

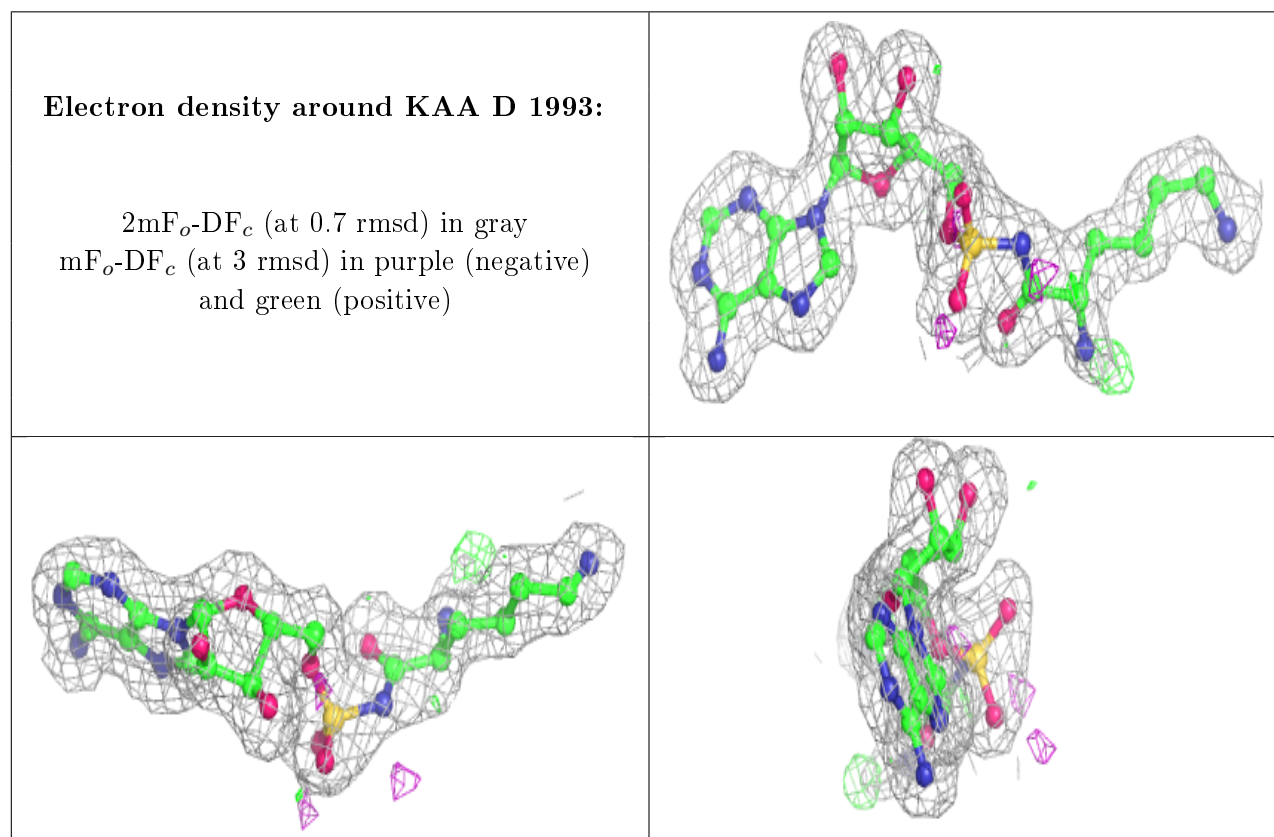
There are no carbohydrates in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

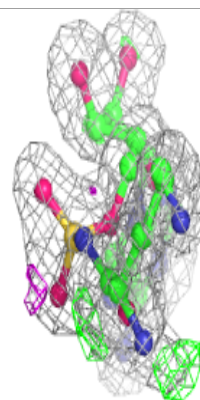
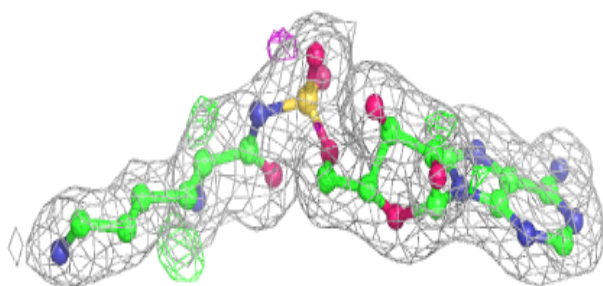
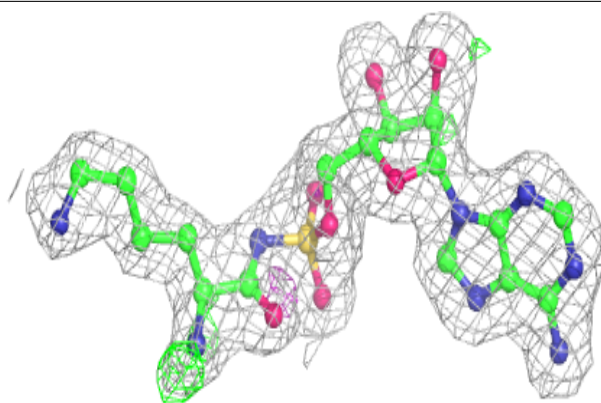
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	KAA	D	1993	32/32	0.97	0.07	12,18,35,40	0
2	KAA	A	1990	32/32	0.97	0.09	14,19,32,36	0
2	KAA	B	1991	32/32	0.98	0.07	11,17,27,28	0
2	KAA	C	1992	32/32	0.98	0.07	12,17,31,34	0

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

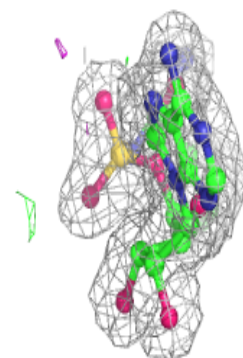
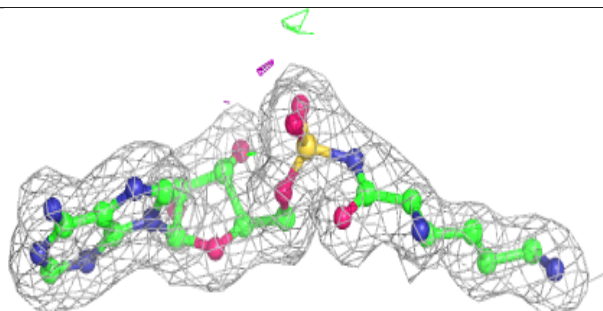
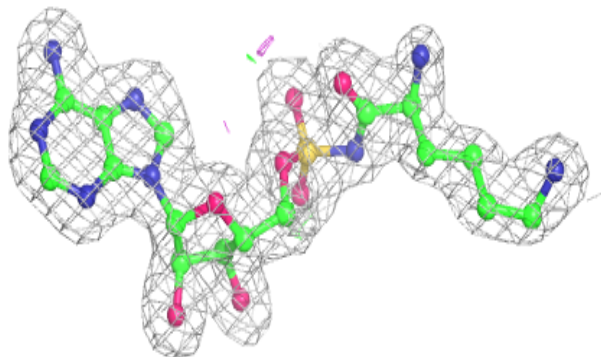


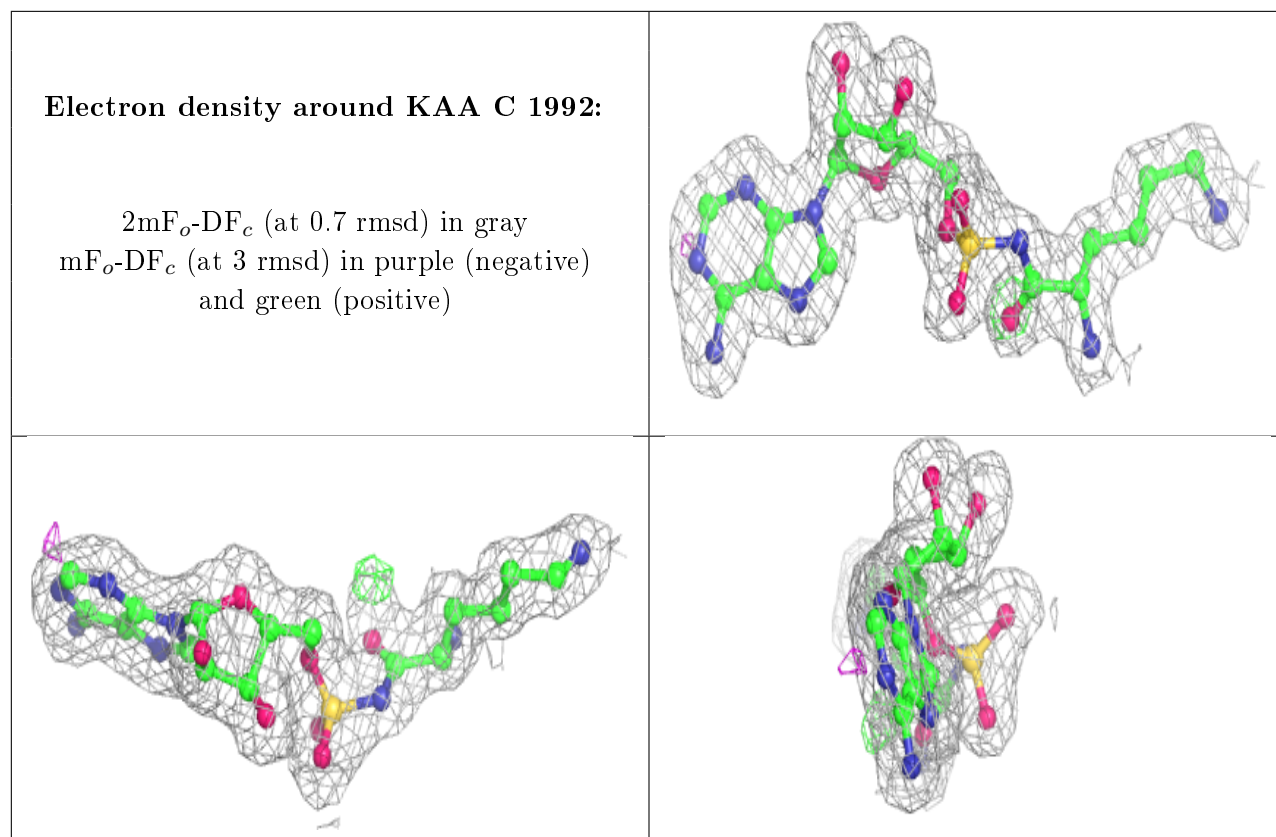
**Electron density around KAA A 1990:**

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

**Electron density around KAA B 1991:**

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





## 6.5 Other polymers [i](#)

There are no such residues in this entry.