



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 2, 2026 – 01:32 AM UTC

PDB ID : 5M9F / pdb_00005m9f
Title : Structure of the two C-terminal domains of bacteriophage K gp144
Authors : Liu, A.; Nguyen, T.H.; van Raaij, M.J.
Deposited on : 2016-11-01
Resolution : 1.80 Å(reported)

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

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A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

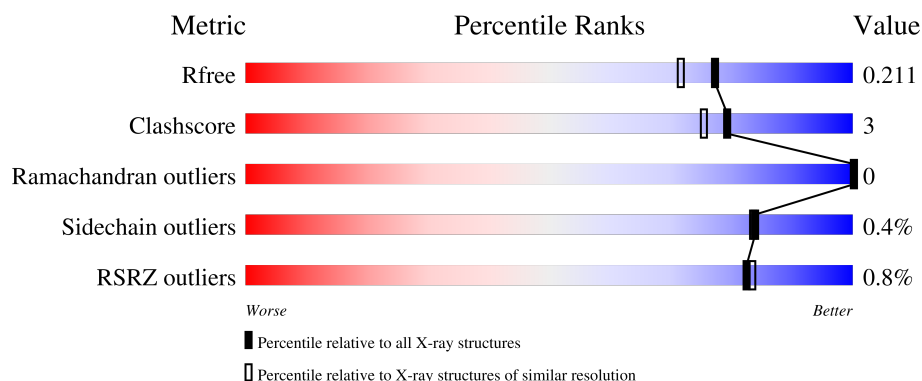
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.80 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}	180053	7662 (1.80-1.80)
Clashscore	190562	8479 (1.80-1.80)
Ramachandran outliers	187476	8391 (1.80-1.80)
Sidechain outliers	187428	8390 (1.80-1.80)
RSRZ outliers	180081	7663 (1.80-1.80)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 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	262	
1	B	262	
1	C	262	

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	ACT	A	501	-	-	X	-
2	ACT	C	502	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 5523 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 ORF68.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	212	Total	C	N	O	S	0	4	0
			1636	1023	272	334	7			
1	B	212	Total	C	N	O	S	0	3	0
			1632	1019	272	334	7			
1	C	210	Total	C	N	O	S	0	4	0
			1617	1008	270	332	7			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	197	GLY	-	expression tag	UNP Q6Y7P9
A	198	SER	-	expression tag	UNP Q6Y7P9
A	199	SER	-	expression tag	UNP Q6Y7P9
A	200	HIS	-	expression tag	UNP Q6Y7P9
A	201	HIS	-	expression tag	UNP Q6Y7P9
A	202	HIS	-	expression tag	UNP Q6Y7P9
A	203	HIS	-	expression tag	UNP Q6Y7P9
A	204	HIS	-	expression tag	UNP Q6Y7P9
A	205	HIS	-	expression tag	UNP Q6Y7P9
A	206	SER	-	expression tag	UNP Q6Y7P9
A	207	SER	-	expression tag	UNP Q6Y7P9
A	208	GLY	-	expression tag	UNP Q6Y7P9
A	209	LEU	-	expression tag	UNP Q6Y7P9
A	210	VAL	-	expression tag	UNP Q6Y7P9
A	211	PRO	-	expression tag	UNP Q6Y7P9
A	212	ARG	-	expression tag	UNP Q6Y7P9
A	213	GLY	-	expression tag	UNP Q6Y7P9
A	214	SER	-	expression tag	UNP Q6Y7P9
A	215	HIS	-	expression tag	UNP Q6Y7P9
A	216	MET	-	expression tag	UNP Q6Y7P9
A	217	ALA	-	expression tag	UNP Q6Y7P9
A	218	SER	-	expression tag	UNP Q6Y7P9
A	219	MET	-	expression tag	UNP Q6Y7P9

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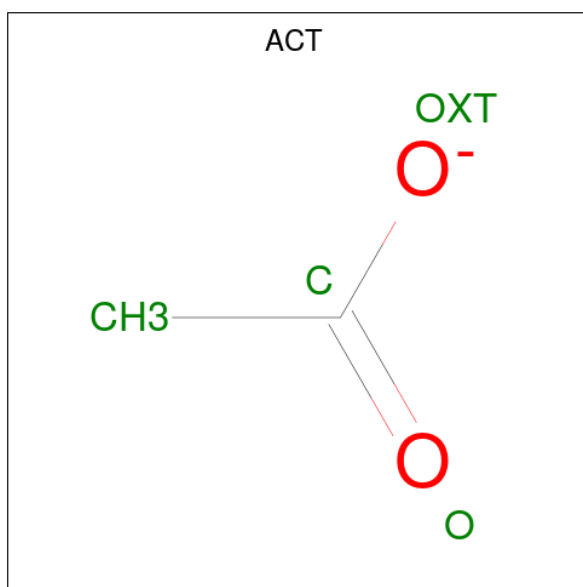
Chain	Residue	Modelled	Actual	Comment	Reference
A	220	THR	-	expression tag	UNP Q6Y7P9
A	221	GLY	-	expression tag	UNP Q6Y7P9
A	222	GLY	-	expression tag	UNP Q6Y7P9
A	223	GLN	-	expression tag	UNP Q6Y7P9
A	224	GLN	-	expression tag	UNP Q6Y7P9
A	225	MET	-	expression tag	UNP Q6Y7P9
A	226	GLY	-	expression tag	UNP Q6Y7P9
A	227	ARG	-	expression tag	UNP Q6Y7P9
A	228	GLY	-	expression tag	UNP Q6Y7P9
B	197	GLY	-	expression tag	UNP Q6Y7P9
B	198	SER	-	expression tag	UNP Q6Y7P9
B	199	SER	-	expression tag	UNP Q6Y7P9
B	200	HIS	-	expression tag	UNP Q6Y7P9
B	201	HIS	-	expression tag	UNP Q6Y7P9
B	202	HIS	-	expression tag	UNP Q6Y7P9
B	203	HIS	-	expression tag	UNP Q6Y7P9
B	204	HIS	-	expression tag	UNP Q6Y7P9
B	205	HIS	-	expression tag	UNP Q6Y7P9
B	206	SER	-	expression tag	UNP Q6Y7P9
B	207	SER	-	expression tag	UNP Q6Y7P9
B	208	GLY	-	expression tag	UNP Q6Y7P9
B	209	LEU	-	expression tag	UNP Q6Y7P9
B	210	VAL	-	expression tag	UNP Q6Y7P9
B	211	PRO	-	expression tag	UNP Q6Y7P9
B	212	ARG	-	expression tag	UNP Q6Y7P9
B	213	GLY	-	expression tag	UNP Q6Y7P9
B	214	SER	-	expression tag	UNP Q6Y7P9
B	215	HIS	-	expression tag	UNP Q6Y7P9
B	216	MET	-	expression tag	UNP Q6Y7P9
B	217	ALA	-	expression tag	UNP Q6Y7P9
B	218	SER	-	expression tag	UNP Q6Y7P9
B	219	MET	-	expression tag	UNP Q6Y7P9
B	220	THR	-	expression tag	UNP Q6Y7P9
B	221	GLY	-	expression tag	UNP Q6Y7P9
B	222	GLY	-	expression tag	UNP Q6Y7P9
B	223	GLN	-	expression tag	UNP Q6Y7P9
B	224	GLN	-	expression tag	UNP Q6Y7P9
B	225	MET	-	expression tag	UNP Q6Y7P9
B	226	GLY	-	expression tag	UNP Q6Y7P9
B	227	ARG	-	expression tag	UNP Q6Y7P9
B	228	GLY	-	expression tag	UNP Q6Y7P9
C	197	GLY	-	expression tag	UNP Q6Y7P9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	198	SER	-	expression tag	UNP Q6Y7P9
C	199	SER	-	expression tag	UNP Q6Y7P9
C	200	HIS	-	expression tag	UNP Q6Y7P9
C	201	HIS	-	expression tag	UNP Q6Y7P9
C	202	HIS	-	expression tag	UNP Q6Y7P9
C	203	HIS	-	expression tag	UNP Q6Y7P9
C	204	HIS	-	expression tag	UNP Q6Y7P9
C	205	HIS	-	expression tag	UNP Q6Y7P9
C	206	SER	-	expression tag	UNP Q6Y7P9
C	207	SER	-	expression tag	UNP Q6Y7P9
C	208	GLY	-	expression tag	UNP Q6Y7P9
C	209	LEU	-	expression tag	UNP Q6Y7P9
C	210	VAL	-	expression tag	UNP Q6Y7P9
C	211	PRO	-	expression tag	UNP Q6Y7P9
C	212	ARG	-	expression tag	UNP Q6Y7P9
C	213	GLY	-	expression tag	UNP Q6Y7P9
C	214	SER	-	expression tag	UNP Q6Y7P9
C	215	HIS	-	expression tag	UNP Q6Y7P9
C	216	MET	-	expression tag	UNP Q6Y7P9
C	217	ALA	-	expression tag	UNP Q6Y7P9
C	218	SER	-	expression tag	UNP Q6Y7P9
C	219	MET	-	expression tag	UNP Q6Y7P9
C	220	THR	-	expression tag	UNP Q6Y7P9
C	221	GLY	-	expression tag	UNP Q6Y7P9
C	222	GLY	-	expression tag	UNP Q6Y7P9
C	223	GLN	-	expression tag	UNP Q6Y7P9
C	224	GLN	-	expression tag	UNP Q6Y7P9
C	225	MET	-	expression tag	UNP Q6Y7P9
C	226	GLY	-	expression tag	UNP Q6Y7P9
C	227	ARG	-	expression tag	UNP Q6Y7P9
C	228	GLY	-	expression tag	UNP Q6Y7P9

- Molecule 2 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



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

- Molecule 3 is SODIUM ION (CCD ID: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Na 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	225	Total O 225 225	0	0
4	B	187	Total O 187 187	0	0
4	C	205	Total O 205 205	0	0

- Molecule 1: ORF68

- Molecule 1: ORF68

- Molecule 1: ORF68

Amino Acid	Protein (%)	Reference (%)
GLY	~1.5	~1.5
SER	~1.5	~1.5
HIS	~1.5	~1.5
HIS	~1.5	~1.5
HIS	~1.5	~1.5
HIS	~1.5	~1.5
SER	~1.5	~1.5
SER	~1.5	~1.5
GLY	~1.5	~1.5
LEU	~1.5	~1.5
VAL	~1.5	~1.5
PRO	~1.5	~1.5
ARG	~1.5	~1.5
GLY	~1.5	~1.5
SER	~1.5	~1.5
HIS	~1.5	~1.5
MET	~1.5	~1.5
ALA	~1.5	~1.5
SER	~1.5	~1.5
MET	~1.5	~1.5
THR	~1.5	~1.5
GLY	~1.5	~1.5
GLN	~1.5	~1.5
GLN	~1.5	~1.5
MET	~1.5	~1.5
GLY	~1.5	~1.5
ARG	~1.5	~1.5
GLY	~1.5	~1.5
PRO	~1.5	~1.5
LYS	~1.5	~1.5
ASP	~1.5	~1.5
MET	~1.5	~1.5
GLU	~1.5	~1.5
LYS	~1.5	~1.5
TYR	~1.5	~1.5
LEU	~1.5	~1.5
SER	~1.5	~1.5
SER	~1.5	~1.5
ILE	~1.5	~1.5
ASP	~1.5	~1.5
ASP	~1.5	~1.5
GLY	~1.5	~1.5
ALA	~1.5	~1.5
SER	~1.5	~1.5
SER	~1.5	~1.5
PHE	~1.5	~1.5
T377	~1.5	~1.5
G405	~1.5	~1.5
T415	~1.5	~1.5
I419	~1.5	~1.5
I455	~1.5	~1.5
M456	~1.5	~1.5
M457	~1.5	~1.5
P458	~1.5	~1.5
S257	~1.5	~1.5
P337	~1.5	~1.5
Y367	~1.5	~1.5

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	50.69Å 81.31Å 154.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	29.33 – 1.80 29.33 – 1.80	Depositor EDS
% Data completeness (in resolution range)	99.8 (29.33-1.80) 99.8 (29.33-1.80)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 1.80Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, R_{free}	0.161 , 0.206 0.171 , 0.211	Depositor DCC
R_{free} test set	3010 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	23.5	Xtriage
Anisotropy	0.280	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 31.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.97	EDS
Total number of atoms	5523	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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: NA, ACT

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	1.08	2/1690 (0.1%)	0.95	0/2299
1	B	1.02	0/1682	0.93	0/2289
1	C	1.02	1/1670 (0.1%)	0.93	0/2272
All	All	1.04	3/5042 (0.1%)	0.94	0/6860

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	405	GLY	C-O	6.21	1.30	1.23
1	A	342	LEU	N-CA	5.95	1.53	1.46
1	A	269	ASP	N-CA	5.39	1.52	1.46

There are no bond angle outliers.

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	1636	0	1567	7	0
1	B	1632	0	1560	9	0
1	C	1617	0	1548	8	0
2	A	12	0	9	6	0
2	C	8	0	6	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	1	0	0	0	0
4	A	225	0	0	2	0
4	B	187	0	0	2	0
4	C	205	0	0	2	0
All	All	5523	0	4690	26	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 3.

All (26) 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:B:457[B]:MET:HE3	2:C:502:ACT:H2	1.69	0.75
2:C:502:ACT:H1	4:C:601:HOH:O	1.85	0.74
1:B:457[B]:MET:HE3	2:C:502:ACT:CH3	2.29	0.62
2:A:501:ACT:CH3	1:C:457[B]:MET:HE3	2.29	0.62
2:A:501:ACT:H3	1:C:337:PRO:HB3	1.81	0.62
1:B:337:PRO:HB3	2:C:502:ACT:H3	1.83	0.58
2:C:501:ACT:H1	4:C:743:HOH:O	2.03	0.58
1:C:377:THR:HB	1:C:419:ILE:HD11	1.85	0.57
2:A:501:ACT:H2	1:C:457[B]:MET:HE3	1.90	0.52
1:A:377:THR:HB	1:A:419:ILE:HD11	1.92	0.50
1:B:378:GLU:HG2	4:B:676:HOH:O	2.11	0.50
1:B:457[A]:MET:SD	2:C:502:ACT:CH3	3.00	0.50
1:A:291:ASN:HB2	4:A:730:HOH:O	2.11	0.48
2:A:502:ACT:H1	4:B:621:HOH:O	2.14	0.47
1:A:371:TYR:CE2	1:A:390:CYS:HB2	2.50	0.47
2:A:501:ACT:CH3	1:C:457[A]:MET:SD	3.03	0.47
1:A:375:LYS:HD2	4:A:705:HOH:O	2.16	0.46
1:B:311:TYR:CZ	1:B:323:GLY:HA3	2.50	0.46
1:A:453:ILE:HG21	1:C:457[B]:MET:HE2	1.97	0.46
1:B:265:ILE:HG23	1:B:304:THR:HB	1.99	0.43
1:B:367:TYR:HB2	1:B:455:ILE:HB	2.01	0.43
1:A:367:TYR:HB2	1:A:455:ILE:HB	2.02	0.41
1:C:367:TYR:HB2	1:C:455:ILE:HB	2.03	0.41
2:A:501:ACT:H1	1:C:457[B]:MET:HE3	2.02	0.41
1:A:265[A]:ILE:HG23	1:A:304:THR:HB	2.03	0.40
1:B:295:GLY:HA3	1:B:312:ASN:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	214/262 (82%)	210 (98%)	4 (2%)	0	100	100
1	B	213/262 (81%)	208 (98%)	5 (2%)	0	100	100
1	C	212/262 (81%)	209 (99%)	3 (1%)	0	100	100
All	All	639/786 (81%)	627 (98%)	12 (2%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	191/227 (84%)	191 (100%)	0	100	100
1	B	190/227 (84%)	189 (100%)	1 (0%)	81	80
1	C	189/227 (83%)	188 (100%)	1 (0%)	81	80
All	All	570/681 (84%)	568 (100%)	2 (0%)	84	83

All (2) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	255	SER
1	C	257	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	308	HIS
1	A	320	ASN
1	C	262	GLN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 1 is monoatomic - leaving 5 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	ACT	C	502	-	3,3,3	0.89	0	3,3,3	0.84	0
2	ACT	A	502	-	3,3,3	0.73	0	3,3,3	1.40	0
2	ACT	A	503	-	3,3,3	0.79	0	3,3,3	0.84	0
2	ACT	C	501	-	3,3,3	0.63	0	3,3,3	1.73	1 (33%)
2	ACT	A	501	-	3,3,3	1.07	0	3,3,3	1.46	0

There are no bond length outliers.

All (1) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
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Mol	Chain	Res	Type	Atoms	Z	Observed($^{\circ}$)	Ideal($^{\circ}$)
2	C	501	ACT	O-C-CH3	-2.38	112.75	122.53

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	502	ACT	5	0
2	A	502	ACT	1	0
2	C	501	ACT	1	0
2	A	501	ACT	5	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	212/262 (80%)	-0.37	1 (0%) 87 88	13, 23, 42, 68	4 (1%)
1	B	212/262 (80%)	-0.05	2 (0%) 81 81	13, 27, 53, 65	3 (1%)
1	C	210/262 (80%)	-0.30	2 (0%) 79 80	13, 24, 42, 62	4 (1%)
All	All	634/786 (80%)	-0.24	5 (0%) 82 83	13, 24, 48, 68	11 (1%)

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	249	PRO	3.2
1	B	248	PHE	2.5
1	C	415	THR	2.5
1	B	271	THR	2.1
1	A	247	SER	2.1

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 oligosaccharides 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, 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	B-factors($\text{\AA}^2$)	Q<0.9
2	ACT	A	503	4/4	0.70	0.18	57,63,64,65	0
2	ACT	A	502	4/4	0.87	0.15	44,45,49,51	0
2	ACT	A	501	4/4	0.90	0.23	31,34,36,43	0
2	ACT	C	501	4/4	0.90	0.10	24,30,33,39	0
2	ACT	C	502	4/4	0.92	0.25	35,38,43,58	0
3	NA	A	504	1/1	0.98	0.09	20,20,20,20	0

6.5 Other polymers [i](#)

There are no such residues in this entry.