



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 03:36 PM UTC

PDB ID : 6D92 / pdb\_00006d92  
Title : Ternary RsAgo Complex with Guide RNA and Target DNA Containing A-A non-canonical pair at position 3  
Authors : Liu, Y.; Esyunina, D.; Olovnikov, I.; Teplova, M.; Patel, D.J.  
Deposited on : 2018-04-27  
Resolution : 1.81 Å (reported)

This is a wwPDB X-ray Structure Validation Summary 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.

The types of validation reports are described at

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

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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

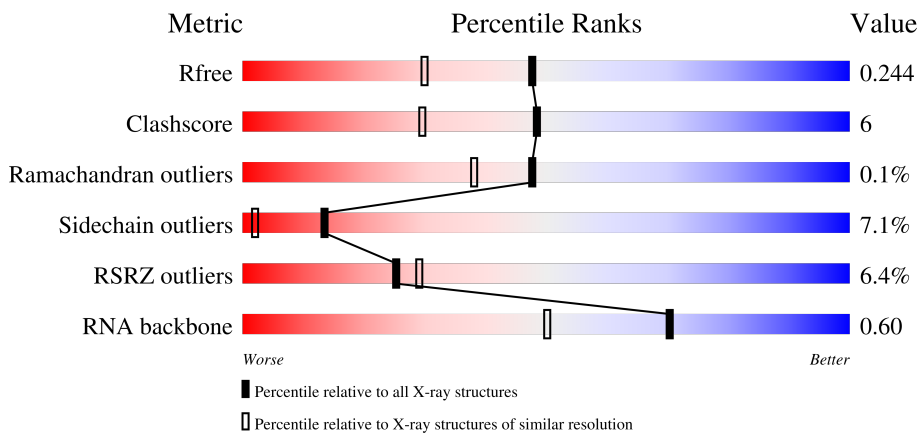
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

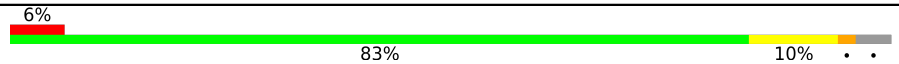
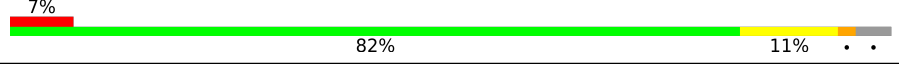
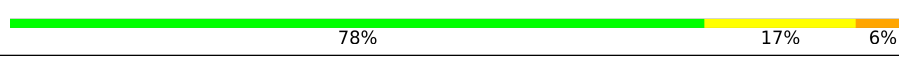

The reported resolution of this entry is 1.81 Å.

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	1112 (1.82-1.82)
Clashscore	190562	1148 (1.82-1.82)
Ramachandran outliers	187476	1140 (1.82-1.82)
Sidechain outliers	187428	1140 (1.82-1.82)
RSRZ outliers	180081	1112 (1.82-1.82)
RNA backbone	3983	1006 (2.22-1.42)

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 of 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	791	
1	F	791	
2	C	18	
2	H	18	

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Mol	Chain	Length	Quality of chain
3	G	19	 84% 16%
4	J	21	 5% 76% 24%

## 2 Entry composition [i](#)

There are 8 unique types of molecules in this entry. The entry contains 14158 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 Uncharacterized protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	758	5895	3742	1057	1080	16	0	1	0
1	F	758	5800	3693	1032	1059	16	0	0	0

There are 30 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-13	MET	-	initiating methionine	UNP A4WYU7
A	-12	HIS	-	expression tag	UNP A4WYU7
A	-11	HIS	-	expression tag	UNP A4WYU7
A	-10	HIS	-	expression tag	UNP A4WYU7
A	-9	HIS	-	expression tag	UNP A4WYU7
A	-8	HIS	-	expression tag	UNP A4WYU7
A	-7	HIS	-	expression tag	UNP A4WYU7
A	-6	ASP	-	expression tag	UNP A4WYU7
A	-5	TYR	-	expression tag	UNP A4WYU7
A	-4	LYS	-	expression tag	UNP A4WYU7
A	-3	ASP	-	expression tag	UNP A4WYU7
A	-2	ASP	-	expression tag	UNP A4WYU7
A	-1	ASP	-	expression tag	UNP A4WYU7
A	0	ASP	-	expression tag	UNP A4WYU7
A	1	LYS	-	expression tag	UNP A4WYU7
F	-13	MET	-	initiating methionine	UNP A4WYU7
F	-12	HIS	-	expression tag	UNP A4WYU7
F	-11	HIS	-	expression tag	UNP A4WYU7
F	-10	HIS	-	expression tag	UNP A4WYU7
F	-9	HIS	-	expression tag	UNP A4WYU7
F	-8	HIS	-	expression tag	UNP A4WYU7
F	-7	HIS	-	expression tag	UNP A4WYU7
F	-6	ASP	-	expression tag	UNP A4WYU7
F	-5	TYR	-	expression tag	UNP A4WYU7
F	-4	LYS	-	expression tag	UNP A4WYU7

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Chain	Residue	Modelled	Actual	Comment	Reference
F	-3	ASP	-	expression tag	UNP A4WYU7
F	-2	ASP	-	expression tag	UNP A4WYU7
F	-1	ASP	-	expression tag	UNP A4WYU7
F	0	ASP	-	expression tag	UNP A4WYU7
F	1	LYS	-	expression tag	UNP A4WYU7

- Molecule 2 is a RNA chain called RNA (5'-R(P\*UP\*UP\*AP\*CP\*UP\*GP\*CP\*AP\*CP\*AP\*GP\*GP\*UP\*GP\*AP\*CP\*GP\*A)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	18	Total	C	N	O	P	0	0	0
			386	172	70	126	18			
2	H	18	Total	C	N	O	P	0	0	0
			386	172	70	126	18			

- Molecule 3 is a DNA chain called DNA (5'-D(P\*TP\*CP\*GP\*TP\*CP\*AP\*CP\*CP\*TP\*GP\*TP\*GP\*CP\*AP\*GP\*AP\*AP\*AP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	19	Total	C	N	O	P	0	0	0
			387	184	71	113	19			

- Molecule 4 is a DNA chain called DNA (5'-D(P\*TP\*GP\*TP\*CP\*GP\*TP\*CP\*AP\*CP\*CP\*TP\*GP\*TP\*GP\*CP\*AP\*GP\*AP\*AP\*AP\*C)-3').

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	J	21	Total	C	N	O	P	0	0	0
			430	204	78	127	21			

- Molecule 5 is ACETATE ION (CCD ID: ACT) (formula: C<sub>2</sub>H<sub>3</sub>O<sub>2</sub>).

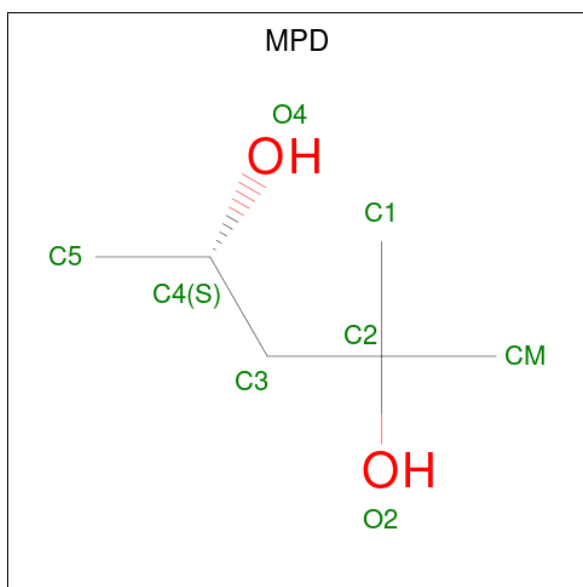


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O 4 2 2	0	0
5	A	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0
5	F	1	Total C O 4 2 2	0	0

- Molecule 6 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total Mg 1 1	0	0
6	H	1	Total Mg 1 1	0	0

- Molecule 7 is (4S)-2-METHYL-2,4-PENTANEDIOL (CCD ID: MPD) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>2</sub>).

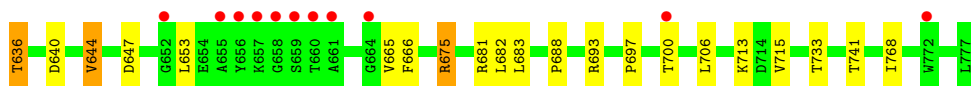


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	H	1	Total C O 8 6 2	0	0

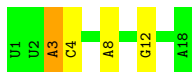
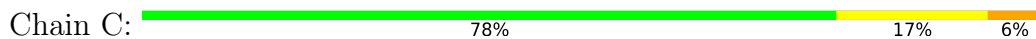
- Molecule 8 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
8	A	343	Total O 343 343	0	0
8	C	50	Total O 50 50	0	0
8	G	41	Total O 41 41	0	0
8	F	318	Total O 318 318	0	0
8	H	56	Total O 56 56	0	0
8	J	40	Total O 40 40	0	0

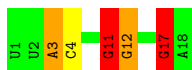




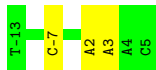
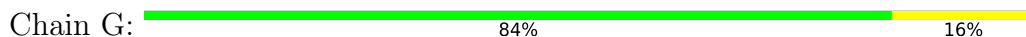
- Molecule 2: RNA (5'-R(P\*UP\*UP\*AP\*CP\*UP\*GP\*CP\*AP\*CP\*AP\*GP\*GP\*UP\*GP\*AP\*CP\*GP\*A)-3')



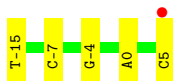
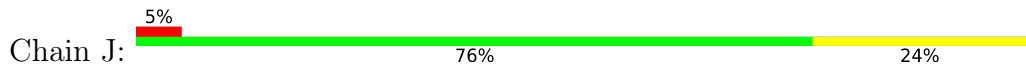
- Molecule 2: RNA (5'-R(P\*UP\*UP\*AP\*CP\*UP\*GP\*CP\*AP\*CP\*AP\*GP\*GP\*UP\*GP\*AP\*CP\*GP\*A)-3')



- Molecule 3: DNA (5'-D(P\*TP\*CP\*GP\*TP\*CP\*AP\*CP\*CP\*TP\*GP\*TP\*GP\*CP\*AP\*GP\*A\*P\*AP\*AP\*C)-3')



- Molecule 4: DNA (5'-D(P\*TP\*GP\*TP\*CP\*GP\*TP\*CP\*AP\*CP\*CP\*TP\*GP\*TP\*GP\*CP\*A\*P\*GP\*AP\*AP\*AP\*C)-3')



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	68.24Å 118.94Å 118.56Å 90.00° 95.72° 90.00°	Depositor
Resolution (Å)	42.81 – 1.81 42.81 – 1.81	Depositor EDS
% Data completeness (in resolution range)	93.4 (42.81-1.81) 93.6 (42.81-1.81)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.46 (at 1.81Å)	Xtrriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.198 , 0.240 0.202 , 0.244	Depositor DCC
$R_{free}$ test set	8084 reflections (4.72%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.5	Xtrriage
Anisotropy	0.285	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 32.6	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	14158	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	41.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.30% 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 i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: MG, ACT, MPD

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	0.72	0/6024	0.89	1/8179 (0.0%)
1	F	0.69	0/5929	0.89	6/8063 (0.1%)
2	C	0.52	0/431	0.95	1/668 (0.1%)
2	H	0.50	0/431	1.06	3/668 (0.4%)
3	G	0.43	0/433	0.78	0/665
4	J	0.39	0/481	0.79	0/738
All	All	0.68	0/13729	0.89	11/18981 (0.1%)

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	F	0	1

There are no bond length outliers.

The worst 5 of 11 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	11	G	C2'-C3'-O3'	-10.56	97.86	113.70
2	H	3	A	C4'-C3'-O3'	-5.85	104.23	113.00
1	A	630	ILE	CB-CA-C	-5.84	101.94	110.81
2	C	3	A	C4'-C3'-O3'	-5.60	104.60	113.00
1	F	568	TYR	N-CA-CB	5.58	118.05	109.91

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	F	566	CYS	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	5895	0	5810	56	0
1	F	5800	0	5663	70	0
2	C	386	0	195	3	0
2	H	386	0	195	7	0
3	G	387	0	214	2	0
4	J	430	0	237	7	0
5	A	8	0	6	0	0
5	F	8	0	6	0	0
6	C	1	0	0	0	0
6	H	1	0	0	0	0
7	H	8	0	14	1	0
8	A	343	0	0	7	1
8	C	50	0	0	1	0
8	F	318	0	0	10	1
8	G	41	0	0	0	0
8	H	56	0	0	3	0
8	J	40	0	0	2	0
All	All	14158	0	12340	141	1

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.

The worst 5 of 141 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)
4:J:-15:DT:O4	8:J:101:HOH:O	1.69	1.08
1:F:513:THR:HG23	1:F:557:TYR:O	1.65	0.97
1:A:61:VAL:HG13	1:A:68:LEU:HD21	1.59	0.85
1:A:585:GLU:OE2	1:A:589:ARG:NH2	2.13	0.81
1:F:193:ASP:OD1	1:F:195:ARG:HD3	1.80	0.80

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:A:1227:HOH:O	8:F:1174:HOH:O[2_455]	1.26	0.94

### 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	757/791 (96%)	744 (98%)	12 (2%)	1 (0%)	48 38
1	F	756/791 (96%)	740 (98%)	15 (2%)	1 (0%)	48 38
All	All	1513/1582 (96%)	1484 (98%)	27 (2%)	2 (0%)	48 38

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	508	ASN
1	F	768	ILE

#### 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	613/672 (91%)	566 (92%)	47 (8%)	12 1
1	F	591/672 (88%)	553 (94%)	38 (6%)	16 3
All	All	1204/1344 (90%)	1119 (93%)	85 (7%)	13 2

5 of 85 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	F	199	VAL
1	F	556	SER
1	F	223	VAL
1	F	406	LYS
1	F	567	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 10 such sidechains are listed below:

Mol	Chain	Res	Type
1	F	359	ASN
1	F	508	ASN
1	F	516	HIS
1	A	270	GLN
1	A	348	GLN

### 5.3.3 RNA [i](#)

Mol	Chain	Analysed	Backbone Outliers	Pucker Outliers
2	C	17/18 (94%)	1 (5%)	0
2	H	17/18 (94%)	3 (17%)	1 (5%)
All	All	34/36 (94%)	4 (11%)	1 (2%)

All (4) RNA backbone outliers are listed below:

Mol	Chain	Res	Type
2	C	12	G
2	H	11	G
2	H	12	G
2	H	17	G

All (1) RNA pucker outliers are listed below:

Mol	Chain	Res	Type
2	H	11	G

## 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 7 ligands modelled in this entry, 2 are 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
5	ACT	F	801	-	3,3,3	0.87	0	3,3,3	0.64	0
5	ACT	A	802	-	3,3,3	0.79	0	3,3,3	0.71	0
5	ACT	A	801	-	3,3,3	0.83	0	3,3,3	0.85	0
7	MPD	H	102	-	7,7,7	0.33	0	9,10,10	0.50	0
5	ACT	F	802	-	3,3,3	0.78	0	3,3,3	0.87	0

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
7	MPD	H	102	-	-	3/5/5/5	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	H	102	MPD	C1-C2-C3-C4
7	H	102	MPD	O2-C2-C3-C4
7	H	102	MPD	CM-C2-C3-C4

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
7	H	102	MPD	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, 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	758/791 (95%)	0.49	47 (6%) 26 30	22, 38, 72, 102	2 (0%)
1	F	758/791 (95%)	0.71	54 (7%) 22 25	22, 40, 64, 96	0
2	C	18/18 (100%)	-0.40	0 100 100	24, 30, 55, 83	0
2	H	18/18 (100%)	-0.35	0 100 100	27, 32, 45, 52	0
3	G	19/19 (100%)	-0.14	0 100 100	30, 38, 94, 115	0
4	J	21/21 (100%)	0.01	1 (4%) 35 41	29, 39, 87, 104	0
All	All	1592/1658 (96%)	0.56	102 (6%) 25 29	22, 39, 70, 115	2 (0%)

The worst 5 of 102 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	188	LEU	3.7
1	F	659	SER	3.5
1	F	658	GLY	3.5
1	F	323	LEU	3.4
1	A	187	LEU	3.3

### 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 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, 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(Å <sup>2</sup> )	Q<0.9
5	ACT	F	801	4/4	0.45	0.20	71,74,77,77	0
5	ACT	A	801	4/4	0.85	0.20	61,63,63,63	0
5	ACT	F	802	4/4	0.86	0.16	64,64,65,66	0
7	MPD	H	102	8/8	0.88	0.14	54,56,57,58	0
5	ACT	A	802	4/4	0.91	0.09	61,65,67,68	0
6	MG	C	101	1/1	0.98	0.04	21,21,21,21	0
6	MG	H	101	1/1	0.99	0.03	25,25,25,25	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.