



# Full wwPDB X-ray Structure Validation Report ⓘ

Jun 22, 2024 – 08:47 PM EDT

PDB ID : 4P37  
Title : Crystal structure of the Megavirus polyadenylate synthase  
Authors : Priet, S.; Lartigue, A.; Claverie, J.M.; Abergel, C.  
Deposited on : 2014-03-06  
Resolution : 2.24 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.

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 : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.37.1  
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) : 2.37.1

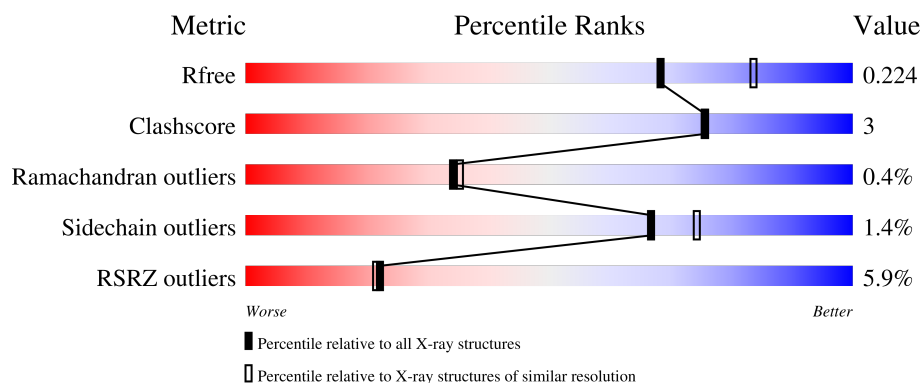
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

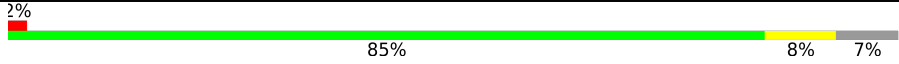

The reported resolution of this entry is 2.24 Å.

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	2391 (2.26-2.22)
Clashscore	141614	2539 (2.26-2.22)
Ramachandran outliers	138981	2489 (2.26-2.22)
Sidechain outliers	138945	2490 (2.26-2.22)
RSRZ outliers	127900	2353 (2.26-2.22)

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	534	
2	B	534	

## 2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 8963 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 poly(A) polymerase catalytic subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
1	A	498	4148	2678	675	773	5	17	0	1	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP G5CT11
A	-1	PRO	-	expression tag	UNP G5CT11
A	0	GLY	-	expression tag	UNP G5CT11
A	1	SER	-	expression tag	UNP G5CT11

- Molecule 2 is a protein called Putative poly(A) polymerase catalytic subunit.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	N	O	S	Se			
2	B	498	4147	2678	675	772	5	17	0	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP G5CT11
B	-1	PRO	-	expression tag	UNP G5CT11
B	0	GLY	-	expression tag	UNP G5CT11
B	1	SER	-	expression tag	UNP G5CT11

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula:  $C_4H_{12}NO_3$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 5 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



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

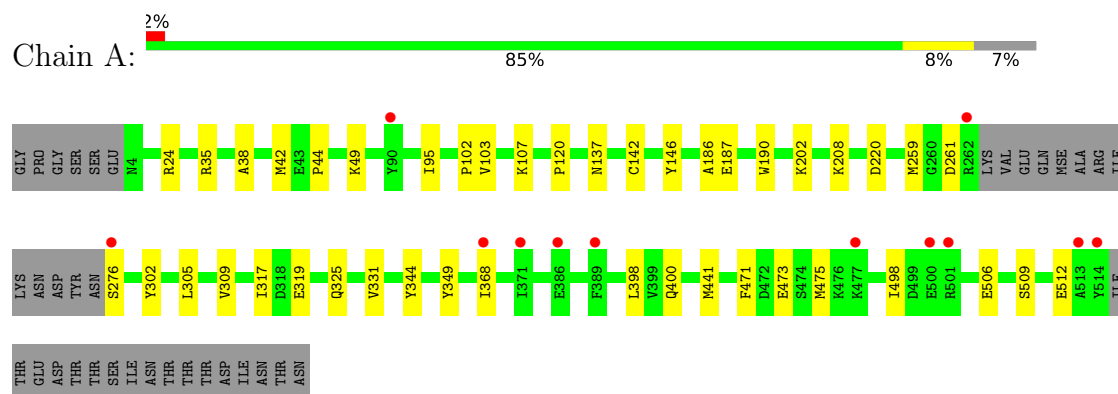
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	303	Total 303	O 303	0	0
6	B	275	Total 275	O 275	0	0

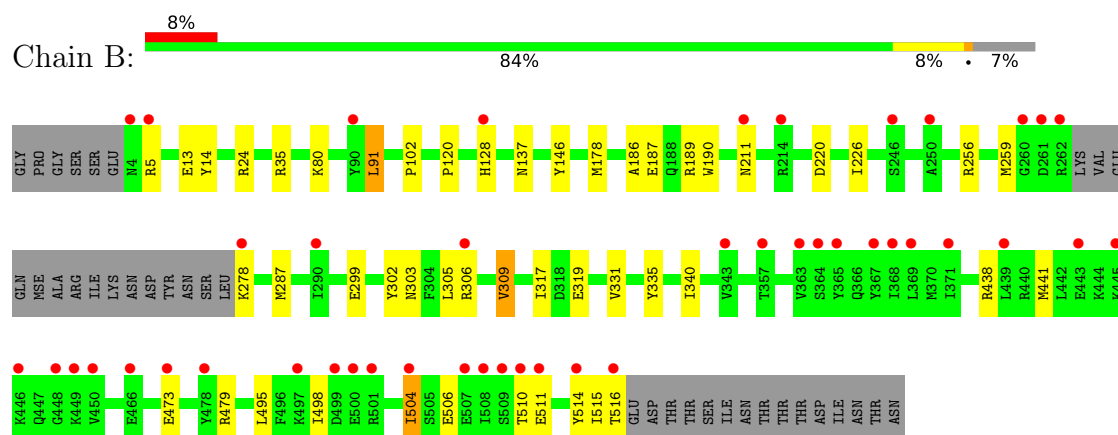
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide 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 poly(A) polymerase catalytic subunit



- Molecule 2: Putative poly(A) polymerase catalytic subunit



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	86.69Å 96.13Å 153.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.38 – 2.24 32.51 – 2.24	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.38-2.24) 98.7 (32.51-2.24)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.00 (at 2.24Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, $R_{free}$	0.187 , 0.214 0.201 , 0.224	Depositor DCC
$R_{free}$ test set	3135 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	42.7	Xtriage
Anisotropy	0.536	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 58.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	8963	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	55.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.24% 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: TRS, ALY, EDO, PEG

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	0.49	0/4229	0.64	0/5674
2	B	0.48	0/4212	0.63	0/5651
All	All	0.48	0/8441	0.63	0/11325

There are no bond length outliers.

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	4148	0	4131	24	0
2	B	4147	0	4130	30	0
3	A	42	0	60	2	0
3	B	28	0	40	0	0
4	A	8	0	12	1	0
5	A	8	0	12	0	0
5	B	4	0	6	3	0
6	A	303	0	0	1	0
6	B	275	0	0	1	0
All	All	8963	0	8391	52	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 (52) 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:A:325:GLN:HG2	4:A:607:TRS:H11	1.65	0.77
1:A:103:VAL:HG12	1:A:475:MSE:HE2	1.71	0.72
2:B:14:TYR:H	5:B:605:EDO:H22	1.63	0.62
2:B:299:GLU:HG3	2:B:504:ILE:HD13	1.84	0.59
1:A:441:MSE:HG2	6:A:950:HOH:O	2.03	0.58
2:B:178:MSE:SE	2:B:189:ARG:HD3	2.54	0.57
1:A:107:LYS:HB2	1:A:475:MSE:HE1	1.86	0.57
2:B:302:TYR:CD2	2:B:504:ILE:HG12	2.43	0.54
1:A:471:PHE:CE2	1:A:475:MSE:HE3	2.44	0.52
2:B:256:ARG:HA	2:B:259:MSE:HE2	1.91	0.52
2:B:515:ILE:HG13	2:B:516:THR:HA	1.91	0.52
2:B:128:HIS:HE1	6:B:812:HOH:O	1.93	0.52
1:A:349:TYR:HB3	3:A:606:PEG:H41	1.92	0.52
2:B:259:MSE:SE	2:B:278:LYS:HA	2.61	0.51
1:A:120:PRO:HD2	1:A:137:ASN:HA	1.93	0.50
1:A:202:LYS:HA	5:B:605:EDO:H12	1.93	0.50
1:A:302:TYR:CD1	1:A:317:ILE:HD11	2.47	0.50
2:B:319:GLU:HG2	2:B:331:VAL:HG12	1.94	0.50
1:A:102:PRO:HG3	1:A:146:TYR:HB2	1.93	0.49
1:A:319:GLU:HG2	1:A:331:VAL:HG12	1.93	0.49
2:B:120:PRO:HD2	2:B:137:ASN:HA	1.95	0.48
2:B:498:ILE:CD1	2:B:504:ILE:HG23	2.44	0.48
1:A:44:PRO:HG2	1:A:49:LYS:HE3	1.95	0.48
2:B:102:PRO:HG3	2:B:146:TYR:HB2	1.95	0.47
2:B:438:ARG:HA	2:B:441:MSE:HE2	1.95	0.47
2:B:479:ARG:HB3	2:B:514:TYR:HB3	1.96	0.47
2:B:305:LEU:O	2:B:309:VAL:HB	2.14	0.47
2:B:303:ASN:OD1	2:B:504:ILE:HD11	2.14	0.47
1:A:38:ALA:O	1:A:42:MSE:HB2	2.15	0.47
2:B:302:TYR:CD1	2:B:317:ILE:HD11	2.50	0.46
1:A:305:LEU:O	1:A:309:VAL:HB	2.16	0.46
2:B:226:ILE:HG23	2:B:287:MSE:HG2	1.99	0.45
2:B:317:ILE:HD12	2:B:498:ILE:HD11	1.99	0.45
2:B:302:TYR:CD2	2:B:504:ILE:CG1	3.00	0.45
2:B:335:TYR:HB2	2:B:340:ILE:HD11	1.99	0.44
1:A:259:MSE:HB3	1:A:276:SER:O	2.18	0.44
1:A:317:ILE:HD12	1:A:498:ILE:HD11	1.99	0.44
2:B:13:GLU:HG3	5:B:605:EDO:H11	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:368:ILE:HG23	1:A:398:LEU:HD21	2.01	0.43
2:B:186:ALA:HA	2:B:190:TRP:CG	2.54	0.43
1:A:186:ALA:HA	1:A:190:TRP:CG	2.54	0.43
2:B:479:ARG:NH2	2:B:514:TYR:HB2	2.34	0.43
1:A:344:TYR:CE2	3:A:605:PEG:H21	2.53	0.42
2:B:302:TYR:CE2	2:B:306:ARG:HD2	2.55	0.42
2:B:495:LEU:HD23	2:B:510:THR:HG21	2.01	0.42
1:A:187:GLU:HG3	2:B:35:ARG:HD2	2.01	0.42
2:B:91:LEU:HD12	2:B:91:LEU:HA	1.93	0.41
1:A:35:ARG:HD2	2:B:187:GLU:HG3	2.02	0.41
1:A:186:ALA:HA	1:A:190:TRP:CD1	2.56	0.41
2:B:186:ALA:HA	2:B:190:TRP:CD1	2.56	0.40
1:A:95:ILE:O	1:A:142:CYS:HA	2.21	0.40
1:A:208:LYS:HE2	1:A:400:GLN:OE1	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	495/534 (93%)	476 (96%)	16 (3%)	3 (1%)	25	23
2	B	493/534 (92%)	476 (97%)	16 (3%)	1 (0%)	47	53
All	All	988/1068 (92%)	952 (96%)	32 (3%)	4 (0%)	34	35

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	509	SER
1	A	512	GLU
1	A	261	ASP
2	B	5	ARG

### 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	462/476 (97%)	458 (99%)	4 (1%)	78	84
2	B	460/475 (97%)	451 (98%)	9 (2%)	55	62
All	All	922/951 (97%)	909 (99%)	13 (1%)	67	74

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

Mol	Chain	Res	Type
1	A	24	ARG
1	A	220	ASP
1	A	473	GLU
1	A	506	GLU
2	B	24	ARG
2	B	91	LEU
2	B	211	ASN
2	B	220	ASP
2	B	309	VAL
2	B	473	GLU
2	B	504	ILE
2	B	506	GLU
2	B	511	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	397	ASN

### 5.3.3 RNA

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is 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	ALY	B	80	2	10,11,12	0.74	1 (10%)	7,12,14	0.27	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
2	ALY	B	80	2	-	2/9/10/12	-

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	80	ALY	CB-CA	2.10	1.56	1.53

There are no bond angle outliers.

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	80	ALY	N-CA-CB-CG
2	B	80	ALY	C-CA-CB-CG

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

14 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	$\# Z  > 2$
3	PEG	A	605	-	6,6,6	0.26	0	5,5,5	0.24	0
3	PEG	A	604	-	6,6,6	0.14	0	5,5,5	0.12	0
3	PEG	B	602	-	6,6,6	0.28	0	5,5,5	0.28	0
3	PEG	A	603	-	6,6,6	0.12	0	5,5,5	0.12	0
3	PEG	A	602	-	6,6,6	0.16	0	5,5,5	0.08	0
3	PEG	B	603	-	6,6,6	0.19	0	5,5,5	0.13	0
4	TRS	A	607	-	7,7,7	0.28	0	9,9,9	0.38	0
5	EDO	A	608	-	3,3,3	0.62	0	2,2,2	0.10	0
5	EDO	A	609	-	3,3,3	0.59	0	2,2,2	0.31	0
3	PEG	A	606	-	6,6,6	0.28	0	5,5,5	0.17	0
3	PEG	A	601	-	6,6,6	0.11	0	5,5,5	0.05	0
3	PEG	B	601	-	6,6,6	0.25	0	5,5,5	0.13	0
3	PEG	B	604	-	6,6,6	0.17	0	5,5,5	0.11	0
5	EDO	B	605	-	3,3,3	0.47	0	2,2,2	0.49	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
3	PEG	A	605	-	-	3/4/4/4	-
3	PEG	A	604	-	-	2/4/4/4	-
3	PEG	B	602	-	-	4/4/4/4	-
3	PEG	A	603	-	-	0/4/4/4	-
3	PEG	A	602	-	-	3/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	PEG	B	603	-	-	0/4/4/4	-
4	TRS	A	607	-	-	4/9/9/9	-
5	EDO	A	608	-	-	0/1/1/1	-
5	EDO	A	609	-	-	0/1/1/1	-
3	PEG	A	606	-	-	1/4/4/4	-
3	PEG	A	601	-	-	3/4/4/4	-
3	PEG	B	601	-	-	2/4/4/4	-
3	PEG	B	604	-	-	2/4/4/4	-
5	EDO	B	605	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (24) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	607	TRS	N-C-C3-O3
3	A	602	PEG	O2-C3-C4-O4
3	B	601	PEG	O2-C3-C4-O4
4	A	607	TRS	C1-C-C3-O3
3	B	601	PEG	O1-C1-C2-O2
3	A	605	PEG	O2-C3-C4-O4
3	A	602	PEG	C4-C3-O2-C2
3	A	601	PEG	C4-C3-O2-C2
3	A	604	PEG	O1-C1-C2-O2
3	A	605	PEG	O1-C1-C2-O2
3	B	602	PEG	O1-C1-C2-O2
3	A	602	PEG	C1-C2-O2-C3
3	B	602	PEG	C4-C3-O2-C2
3	B	602	PEG	O2-C3-C4-O4
3	A	605	PEG	C4-C3-O2-C2
3	A	601	PEG	C1-C2-O2-C3
3	B	602	PEG	C1-C2-O2-C3
3	A	606	PEG	C4-C3-O2-C2
4	A	607	TRS	C2-C-C1-O1
3	A	601	PEG	O2-C3-C4-O4
3	B	604	PEG	C4-C3-O2-C2
3	A	604	PEG	C1-C2-O2-C3
4	A	607	TRS	N-C-C1-O1
3	B	604	PEG	O2-C3-C4-O4

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	605	PEG	1	0
4	A	607	TRS	1	0
3	A	606	PEG	1	0
5	B	605	EDO	3	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

### 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	481/534 (90%)	-0.08	12 (2%) 57 58	31, 47, 78, 146	12 (2%)
2	B	480/534 (89%)	0.21	45 (9%) 8 8	32, 52, 98, 138	15 (3%)
All	All	961/1068 (89%)	0.07	57 (5%) 22 21	31, 50, 89, 146	27 (2%)

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	262	ARG	10.8
1	A	514	TYR	7.9
2	B	450	VAL	7.1
2	B	501	ARG	5.9
2	B	262	ARG	5.4
2	B	261	ASP	5.3
2	B	508	ILE	5.1
2	B	510	THR	4.9
2	B	368	ILE	4.8
2	B	509	SER	4.6
2	B	478	TYR	3.8
1	A	513	ALA	3.8
2	B	507	GLU	3.6
1	A	90	TYR	3.6
2	B	473	GLU	3.5
2	B	448	GLY	3.5
1	A	276	SER	3.5
2	B	290	ILE	3.4
2	B	516	THR	3.4
2	B	500	GLU	3.3
2	B	211	ASN	3.2
2	B	449	LYS	3.1
2	B	260	GLY	3.0
2	B	90	TYR	3.0

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Mol	Chain	Res	Type	RSRZ
1	A	477	LYS	3.0
2	B	497	LYS	2.9
2	B	446	LYS	2.9
2	B	371	ILE	2.7
1	A	371	ILE	2.7
2	B	367	TYR	2.7
2	B	214	ARG	2.6
2	B	443	GLU	2.6
2	B	511	GLU	2.6
1	A	368	ILE	2.6
1	A	500	GLU	2.5
2	B	466	GLU	2.5
2	B	343	VAL	2.5
2	B	365	TYR	2.5
2	B	369	LEU	2.5
1	A	389	PHE	2.5
1	A	501	ARG	2.4
2	B	246	SER	2.4
2	B	364	SER	2.4
2	B	357	THR	2.4
2	B	504	ILE	2.3
2	B	306	ARG	2.3
2	B	250	ALA	2.2
2	B	278	LYS	2.2
1	A	386	GLU	2.2
2	B	5	ARG	2.2
2	B	514	TYR	2.2
2	B	4	ASN	2.2
2	B	363	VAL	2.2
2	B	499	ASP	2.1
2	B	439	LEU	2.1
2	B	128	HIS	2.0
2	B	445	LYS	2.0

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

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	ALY	B	80	12/13	0.86	0.14	58,63,70,70	0

### 6.3 Carbohydrates [i](#)

There are no monosaccharides 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
4	TRS	A	607	8/8	0.65	0.26	42,45,48,50	8
3	PEG	B	604	7/7	0.70	0.32	60,61,63,63	0
3	PEG	B	602	7/7	0.75	0.16	54,61,64,65	0
3	PEG	A	606	7/7	0.77	0.26	39,47,60,61	7
3	PEG	B	603	7/7	0.81	0.17	65,65,74,75	0
3	PEG	B	601	7/7	0.81	0.20	65,69,71,71	0
3	PEG	A	602	7/7	0.81	0.19	70,73,74,74	7
3	PEG	A	603	7/7	0.82	0.20	68,69,71,73	0
5	EDO	A	609	4/4	0.86	0.15	75,75,76,76	0
3	PEG	A	605	7/7	0.88	0.41	54,56,58,59	0
5	EDO	A	608	4/4	0.92	0.12	50,52,56,59	0
3	PEG	A	604	7/7	0.92	0.15	57,57,62,63	7
5	EDO	B	605	4/4	0.92	0.20	50,50,51,51	4
3	PEG	A	601	7/7	0.94	0.12	66,67,70,71	0

### 6.5 Other polymers [i](#)

There are no such residues in this entry.