



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 01:22 PM UTC

PDB ID : 4P37 / pdb_00004p37
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

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

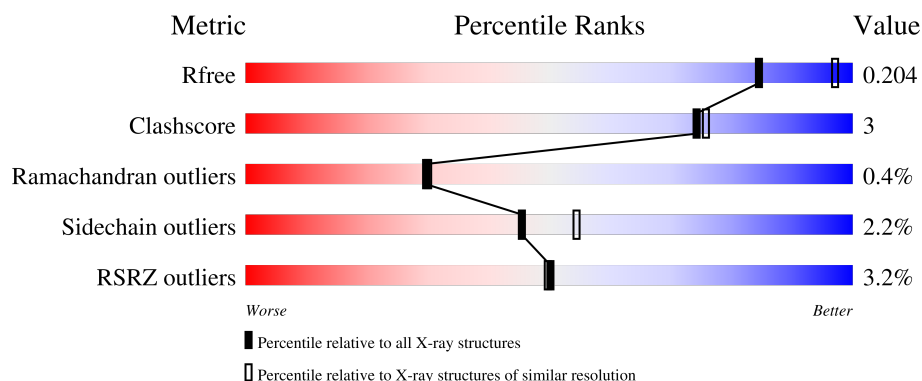
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 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}	180053	3416 (2.26-2.22)
Clashscore	190562	3556 (2.26-2.22)
Ramachandran outliers	187476	3500 (2.26-2.22)
Sidechain outliers	187428	3501 (2.26-2.22)
RSRZ outliers	180081	3415 (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 ≥ 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% 84% 9% 7%
2	B	534	3% 83% 9% 7%

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

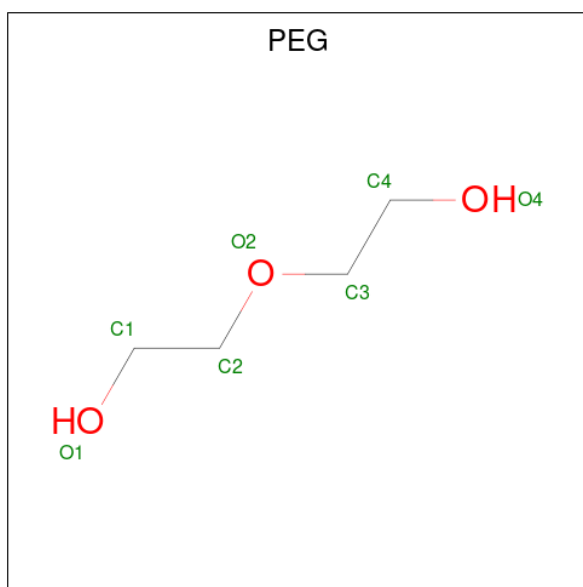
- Molecule 2 is a protein called Putative poly(A) polymerase catalytic subunit.

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:

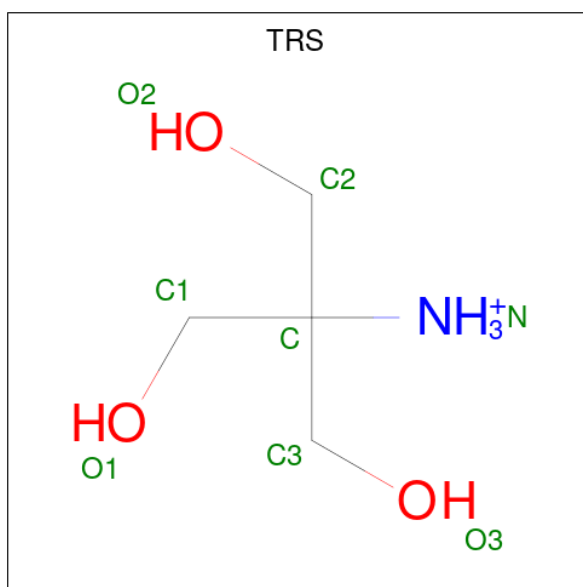
Chain	Residue	Modelled	Actual	Comment	Reference
B	-2	GLY	-	expression tag	UNP G5CT11
B	-1	PRO	-	expression tag	UNP G5CT11
B	0	GLY	-	expression tag	UNP G5CT11
B	1	SER	-	expression tag	UNP G5CT11

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: C₄H₁₀O₃).



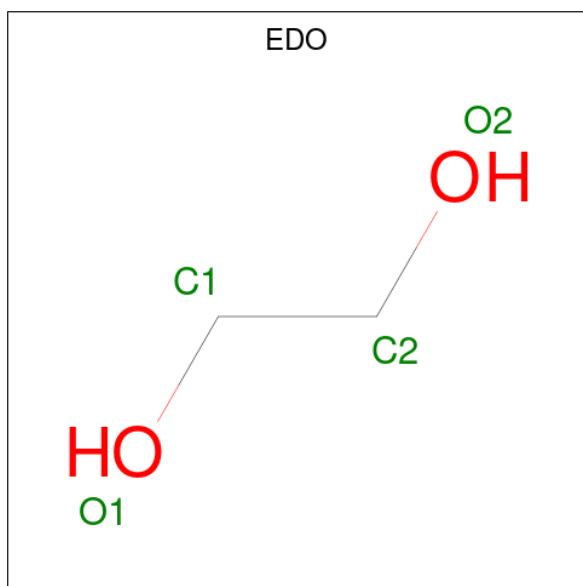
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	A	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		
3	B	1	Total	C	O	0	0
			7	4	3		

- Molecule 4 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (CCD ID: TRS) (formula: C₄H₁₂NO₃).



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 (CCD ID: EDO) (formula: C₂H₆O₂).



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

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.69Å 96.13Å 153.89Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.38 – 2.24 49.38 – 2.24	Depositor EDS
% Data completeness (in resolution range)	98.7 (49.38-2.24) 98.7 (49.38-2.24)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.00 (at 2.24Å)	Xtriage
Refinement program	BUSTER 2.10.2	Depositor
R, R_{free}	0.187 , 0.214 (Not available) , 0.204	Depositor DCC
R_{free} test set	3135 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	42.7	Xtriage
Anisotropy	0.536	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 55.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: TRS, EDO, PEG, ALY

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	0.84	0/4229	1.26	8/5674 (0.1%)
2	B	0.82	0/4212	1.25	5/5651 (0.1%)
All	All	0.83	0/8441	1.25	13/11325 (0.1%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	351	VAL	N-CA-C	6.41	114.23	107.76
1	A	511	GLU	CA-C-N	6.38	133.72	121.54
1	A	511	GLU	C-N-CA	6.38	133.72	121.54
2	B	407	ASN	CA-C-N	5.85	128.12	120.28
2	B	407	ASN	C-N-CA	5.85	128.12	120.28
2	B	351	VAL	N-CA-C	5.84	113.66	107.76
1	A	190	TRP	N-CA-C	5.81	117.28	111.07
2	B	170	PHE	N-CA-C	-5.78	104.41	112.45
1	A	433	TYR	CA-C-N	5.72	127.88	120.44
1	A	433	TYR	C-N-CA	5.72	127.88	120.44
2	B	190	TRP	N-CA-C	5.52	116.97	111.07
1	A	170	PHE	N-CA-C	-5.42	104.92	112.45
1	A	83	GLU	CB-CG-CD	5.07	121.22	112.60

There are no chirality outliers.

There are no planarity outliers.

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	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

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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 ⓘ

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	495/534 (93%)	476 (96%)	16 (3%)	3 (1%)	21	20
2	B	493/534 (92%)	476 (97%)	16 (3%)	1 (0%)	43	48
All	All	988/1068 (92%)	952 (96%)	32 (3%)	4 (0%)	30	30

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%)	455 (98%)	7 (2%)	57	66
2	B	460/475 (97%)	447 (97%)	13 (3%)	38	45
All	All	922/951 (97%)	902 (98%)	20 (2%)	45	54

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	24	ARG
1	A	220	ASP
1	A	309	VAL
1	A	443	GLU
1	A	473	GLU
1	A	490	ILE
1	A	506	GLU
2	B	24	ARG
2	B	91	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	211	ASN
2	B	220	ASP
2	B	309	VAL
2	B	443	GLU
2	B	451	ILE
2	B	473	GLU
2	B	475	MSE
2	B	490	ILE
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 (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	122	GLN
1	A	279	ASN
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	0.67	0	7,12,14	0.28	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	-

There are no bond length outliers.

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 oligosaccharides 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	602	-	6,6,6	0.17	0	5,5,5	0.08	0
3	PEG	B	601	-	6,6,6	0.26	0	5,5,5	0.12	0
3	PEG	B	603	-	6,6,6	0.19	0	5,5,5	0.14	0
4	TRS	A	607	-	7,7,7	0.34	0	9,9,9	0.46	0
3	PEG	A	601	-	6,6,6	0.12	0	5,5,5	0.05	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
5	EDO	A	608	-	3,3,3	0.56	0	2,2,2	0.16	0
3	PEG	A	606	-	6,6,6	0.28	0	5,5,5	0.16	0
5	EDO	B	605	-	3,3,3	0.43	0	2,2,2	0.53	0
3	PEG	A	604	-	6,6,6	0.15	0	5,5,5	0.12	0
3	PEG	B	602	-	6,6,6	0.28	0	5,5,5	0.27	0
3	PEG	B	604	-	6,6,6	0.18	0	5,5,5	0.11	0
3	PEG	A	605	-	6,6,6	0.27	0	5,5,5	0.24	0
5	EDO	A	609	-	3,3,3	0.53	0	2,2,2	0.35	0
3	PEG	A	603	-	6,6,6	0.12	0	5,5,5	0.13	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	602	-	-	3/4/4/4	-
3	PEG	B	601	-	-	3/4/4/4	-
3	PEG	B	603	-	-	0/4/4/4	-
4	TRS	A	607	-	-	5/9/9/9	-
3	PEG	A	601	-	-	3/4/4/4	-
5	EDO	A	608	-	-	0/1/1/1	-
3	PEG	A	606	-	-	1/4/4/4	-
5	EDO	B	605	-	-	0/1/1/1	-
3	PEG	A	604	-	-	2/4/4/4	-
3	PEG	B	602	-	-	4/4/4/4	-
3	PEG	B	604	-	-	2/4/4/4	-
3	PEG	A	605	-	-	3/4/4/4	-
5	EDO	A	609	-	-	0/1/1/1	-
3	PEG	A	603	-	-	0/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (26) 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

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
4	A	607	TRS	C1-C-C3-O3
3	B	601	PEG	O2-C3-C4-O4
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	604	PEG	O1-C1-C2-O2
3	A	605	PEG	O1-C1-C2-O2
3	B	602	PEG	O1-C1-C2-O2
3	B	602	PEG	O2-C3-C4-O4
3	A	601	PEG	C4-C3-O2-C2
3	A	602	PEG	C1-C2-O2-C3
3	B	602	PEG	C4-C3-O2-C2
4	A	607	TRS	C2-C-C1-O1
3	A	605	PEG	C4-C3-O2-C2
3	A	601	PEG	C1-C2-O2-C3
3	B	602	PEG	C1-C2-O2-C3
4	A	607	TRS	N-C-C1-O1
3	A	606	PEG	C4-C3-O2-C2
3	A	601	PEG	O2-C3-C4-O4
3	B	604	PEG	C4-C3-O2-C2
4	A	607	TRS	C2-C-C3-O3
3	A	604	PEG	C1-C2-O2-C3
3	B	601	PEG	C1-C2-O2-C3
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
4	A	607	TRS	1	0
3	A	606	PEG	1	0
5	B	605	EDO	3	0
3	A	605	PEG	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

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, 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	481/534 (90%)	0.05	13 (2%) 56 57	31, 47, 77, 143	13 (2%)
2	B	480/534 (89%)	0.19	18 (3%) 44 43	32, 52, 98, 138	15 (3%)
All	All	961/1068 (89%)	0.12	31 (3%) 50 50	31, 49, 87, 143	28 (2%)

All (31) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	516	THR	6.0
1	A	276	SER	5.5
2	B	450	VAL	4.9
2	B	515	ILE	4.8
1	A	277	LEU	3.8
2	B	451	ILE	3.8
1	A	514	TYR	3.4
1	A	513	ALA	3.4
1	A	128	HIS	3.2
2	B	504	ILE	3.2
2	B	128	HIS	3.1
2	B	90	TYR	3.0
2	B	209	TYR	3.0
2	B	471	PHE	2.9
2	B	478	TYR	2.9
1	A	389	PHE	2.8
2	B	508	ILE	2.7
2	B	210	ASP	2.5
2	B	449	LYS	2.5
1	A	90	TYR	2.4
1	A	262	ARG	2.4
1	A	511	GLU	2.4
2	B	262	ARG	2.3
2	B	87	TYR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
2	B	513	ALA	2.3
1	A	433	TYR	2.2
1	A	478	TYR	2.1
2	B	510	THR	2.1
1	A	360	TYR	2.1
2	B	11	TYR	2.0
1	A	315	ILE	2.0

6.2 Non-standard residues in protein, DNA, RNA chains [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(Å ²)	Q<0.9
2	ALY	B	80	12/13	0.75	0.16	58,63,70,70	0

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(Å ²)	Q<0.9
3	PEG	A	606	7/7	0.77	0.21	39,47,60,61	7
5	EDO	A	609	4/4	0.78	0.14	75,75,76,76	0
4	TRS	A	607	8/8	0.79	0.15	42,45,48,50	8
3	PEG	A	603	7/7	0.80	0.15	68,69,71,73	0
3	PEG	B	604	7/7	0.81	0.17	60,61,63,63	0
3	PEG	B	602	7/7	0.86	0.13	54,61,64,65	0
3	PEG	B	601	7/7	0.88	0.15	65,69,71,71	0
3	PEG	A	605	7/7	0.88	0.15	54,56,58,59	0
3	PEG	B	603	7/7	0.88	0.13	65,65,74,75	0
3	PEG	A	601	7/7	0.89	0.13	66,67,70,71	0

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	EDO	B	605	4/4	0.89	0.17	50,50,51,51	4
3	PEG	A	604	7/7	0.90	0.13	57,57,62,63	7
3	PEG	A	602	7/7	0.90	0.14	70,73,74,74	7
5	EDO	A	608	4/4	0.94	0.08	50,52,56,59	0

6.5 Other polymers [i](#)

There are no such residues in this entry.