



# wwPDB X-ray Structure Validation Summary Report ⓘ

Oct 10, 2021 – 09:14 PM EDT

PDB ID : 3FDS  
Title : Structural insight into recruitment of translesion DNA polymerase Dpo4 to sliding clamp PCNA  
Authors : Ling, H.  
Deposited on : 2008-11-26  
Resolution : 2.05 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.

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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 : 2.23.2  
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) : 2.23.2

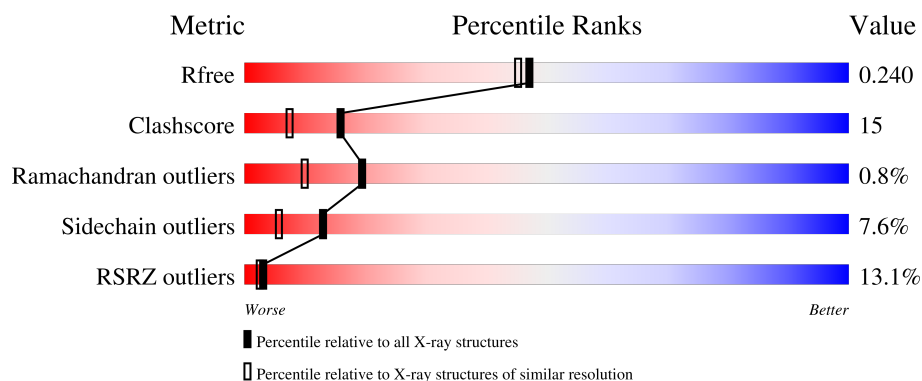
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.05 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	1692 (2.04-2.04)
Clashscore	141614	1773 (2.04-2.04)
Ramachandran outliers	138981	1752 (2.04-2.04)
Sidechain outliers	138945	1752 (2.04-2.04)
RSRZ outliers	127900	1672 (2.04-2.04)

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	352	<div> <div>14%</div> <div>75%</div> <div>20%</div> <div>• •</div> </div>
2	C	249	<div> <div>12%</div> <div>69%</div> <div>26%</div> <div>• •</div> </div>
3	D	245	<div> <div>13%</div> <div>77%</div> <div>17%</div> <div>• •</div> </div>

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
4	EDO	A	353	-	-	-	X
4	EDO	A	358	-	-	X	-
4	EDO	A	368	-	-	-	X
5	PEG	A	369	-	-	X	-
6	1PE	A	370	-	-	X	-
7	GOL	C	260	-	-	X	-
7	GOL	C	261	-	-	X	-
8	PGE	D	247	-	-	X	-

## 2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 7313 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 DNA polymerase IV.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	352	Total	C	N	O	S	6	12	0
			2913	1867	506	532	8			

- Molecule 2 is a protein called DNA polymerase sliding clamp B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	249	Total	C	N	O	S	0	10	0
			1991	1272	317	391	11			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	2	VAL	PHE	engineered mutation	UNP P57766

- Molecule 3 is a protein called DNA polymerase sliding clamp C.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	D	241	Total	C	N	O	S	0	4	0
			1930	1245	300	379	6			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	1	MET	-	initiating methionine	UNP Q97Z84

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



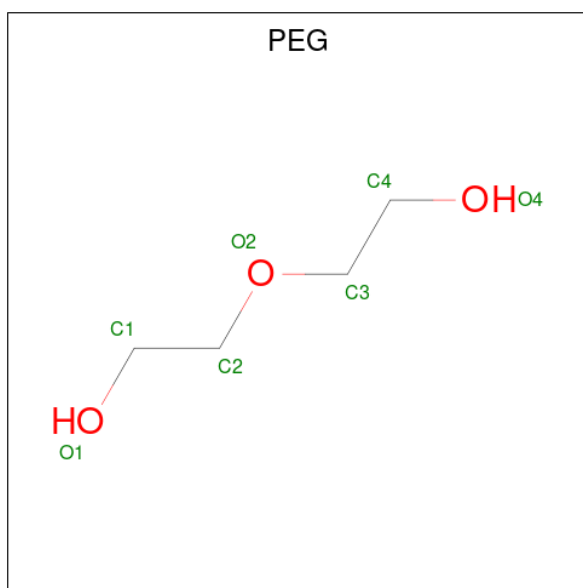
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total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

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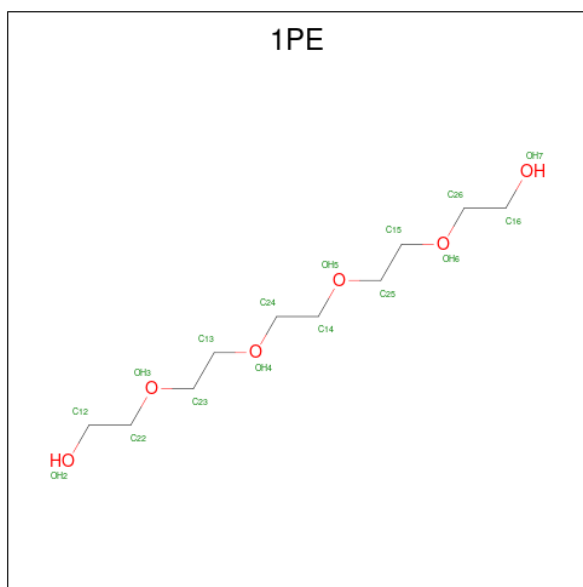
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			4	2	2		
4	A	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total	C	O	0	0
			4	2	2		
4	C	1	Total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

- Molecule 5 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C<sub>4</sub>H<sub>10</sub>O<sub>3</sub>).



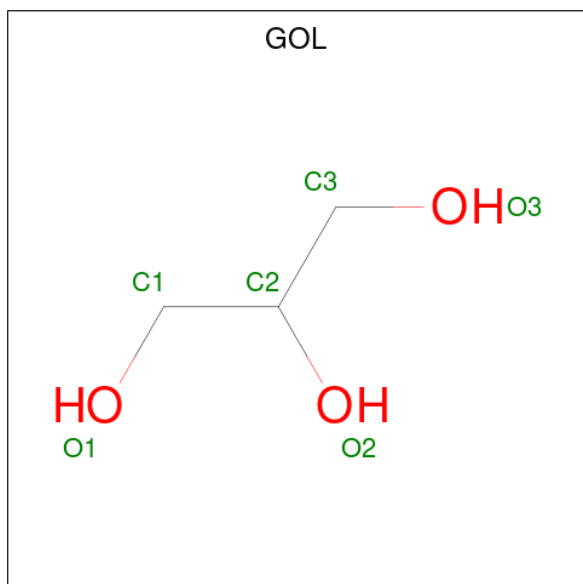
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	O	0	0
			7	4	3		
5	C	1	Total	C	O	0	0
			7	4	3		

- Molecule 6 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula:  $C_{10}H_{22}O_6$ ).



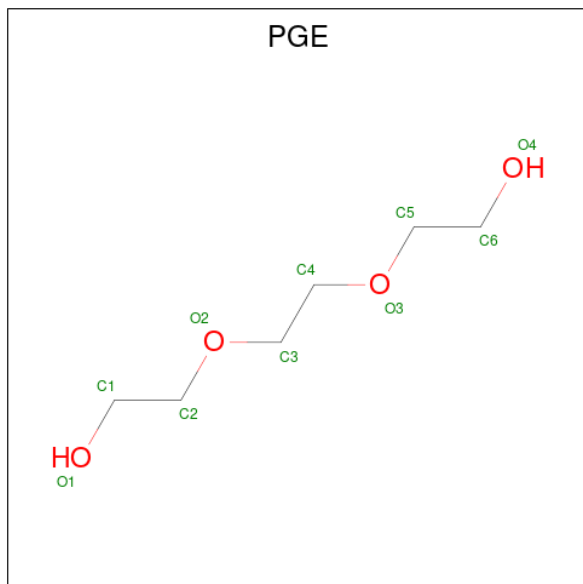
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			16	10	6		

- Molecule 7 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		
7	C	1	Total	C	O	0	0
			6	3	3		

- Molecule 8 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: C<sub>6</sub>H<sub>14</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
8	D	1	Total	C	O	0	0
			10	6	4		

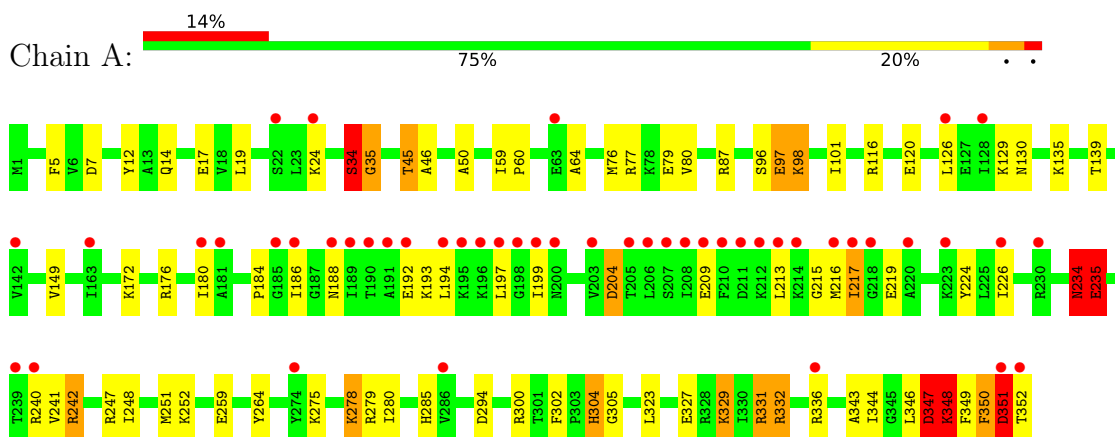
- Molecule 9 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
9	A	160	Total	O	0	0
			160	160		
9	C	99	Total	O	0	0
			99	99		
9	D	58	Total	O	0	0
			58	58		

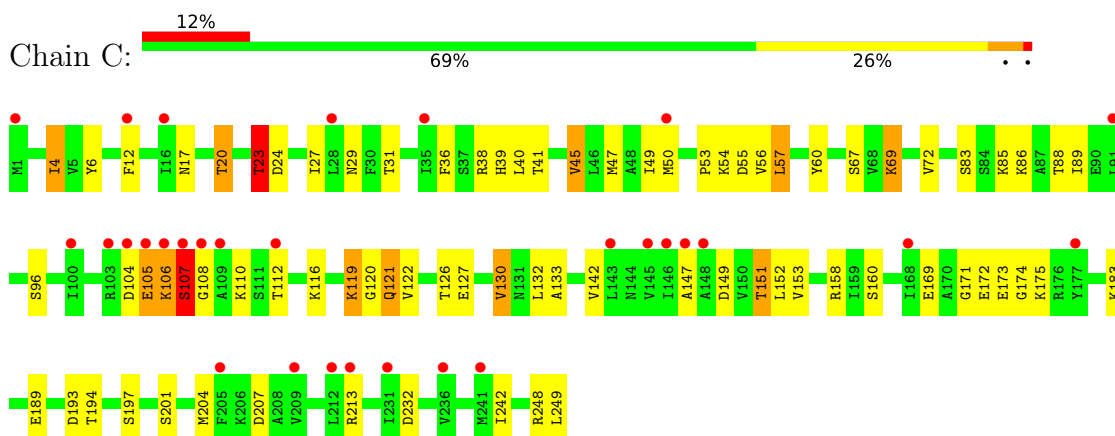
### 3 Residue-property plots [i](#)

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.

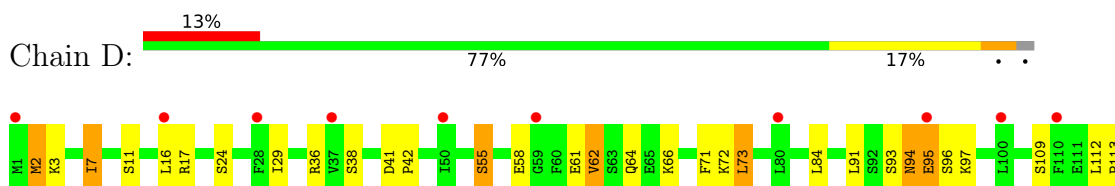
#### • Molecule 1: DNA polymerase IV

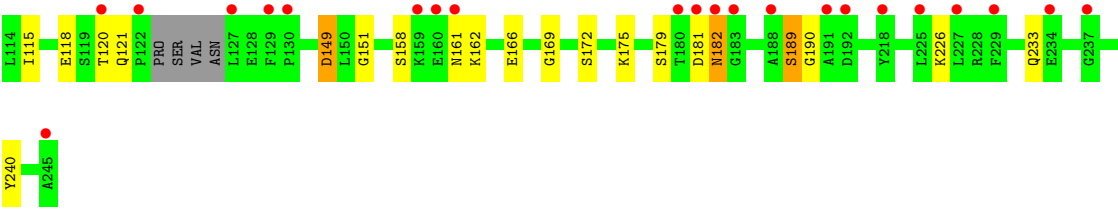


#### • Molecule 2: DNA polymerase sliding clamp B



#### • Molecule 3: DNA polymerase sliding clamp C





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	65.99Å 86.41Å 97.58Å 90.00° 107.30° 90.00°	Depositor
Resolution (Å)	29.88 – 2.05 29.90 – 2.00	Depositor EDS
% Data completeness (in resolution range)	100.0 (29.88-2.05) 97.1 (29.90-2.00)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.98 (at 2.00Å)	Xtriage
Refinement program	REFMAC	Depositor
R, $R_{free}$	0.190 , 0.240 0.192 , 0.240	Depositor DCC
$R_{free}$ test set	1371 reflections (2.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	38.0	Xtriage
Anisotropy	0.183	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 65.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-h-l	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	7313	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.45% 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: EDO, PGE, 1PE, GOL, 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	0.95	7/2975 (0.2%)	0.94	18/3989 (0.5%)
2	C	0.79	0/2036	0.88	5/2741 (0.2%)
3	D	0.89	1/1969 (0.1%)	0.89	1/2657 (0.0%)
All	All	0.89	8/6980 (0.1%)	0.91	24/9387 (0.3%)

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	A	0	5
2	C	0	1
3	D	0	1
All	All	0	7

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	176	ARG	CZ-NH2	8.79	1.44	1.33
1	A	259[A]	GLU	CD-OE1	-8.55	1.16	1.25
1	A	259[B]	GLU	CD-OE1	-8.55	1.16	1.25
1	A	209	GLU	CD-OE2	8.09	1.34	1.25
3	D	189	SER	C-N	6.77	1.45	1.33

The worst 5 of 24 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	35	GLY	N-CA-C	-9.82	88.55	113.10
1	A	176	ARG	NE-CZ-NH2	-8.98	115.81	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	348	LYS	N-CA-C	-8.49	88.07	111.00
3	D	73	LEU	CA-CB-CG	-8.37	96.05	115.30
1	A	235	GLU	N-CA-C	-7.90	89.67	111.00

There are no chirality outliers.

5 of 7 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	234	ASN	Peptide
1	A	347	ASP	Peptide
1	A	350	PHE	Peptide
1	A	351	ASP	Peptide
1	A	97	GLU	Peptide

## 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	2913	0	3062	89	1
2	C	1991	0	2071	76	0
3	D	1930	0	1943	44	1
4	A	64	0	96	11	0
4	C	36	0	54	6	0
4	D	4	0	6	3	0
5	A	7	0	10	4	0
5	C	7	0	10	2	0
6	A	16	0	22	7	0
7	A	6	0	8	1	0
7	C	12	0	16	19	0
8	D	10	0	14	17	0
9	A	160	0	0	10	1
9	C	99	0	0	4	1
9	D	58	0	0	0	0
All	All	7313	0	7312	209	2

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.

The worst 5 of 209 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)
2:C:171:GLY:O	7:C:260:GOL:H32	1.46	1.15
1:A:304:HIS:H	4:A:358:EDO:H12	1.10	1.13
3:D:72:LYS:H	8:D:247:PGE:H2	1.13	1.09
7:C:260:GOL:H2	9:C:618:HOH:O	1.54	1.07
2:C:147:ALA:O	2:C:151[B]:THR:HG22	1.53	1.07

All (2) 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)
9:A:404:HOH:O	9:C:544:HOH:O[1_655]	2.01	0.19
1:A:242:ARG:NH2	3:D:149:ASP:OD1[1_655]	2.08	0.12

## 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	363/352 (103%)	345 (95%)	12 (3%)	6 (2%)	9	2
2	C	257/249 (103%)	247 (96%)	8 (3%)	2 (1%)	19	10
3	D	240/245 (98%)	234 (98%)	6 (2%)	0	100	100
All	All	860/846 (102%)	826 (96%)	26 (3%)	8 (1%)	19	8

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	217	ILE
1	A	235	GLU
1	A	347	ASP
1	A	351	ASP

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Mol	Chain	Res	Type
2	C	107	SER

### 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	318/309 (103%)	300 (94%)	18 (6%)	20	12
2	C	230/220 (104%)	210 (91%)	20 (9%)	10	4
3	D	219/219 (100%)	198 (90%)	21 (10%)	8	3
All	All	767/748 (102%)	708 (92%)	59 (8%)	13	5

5 of 59 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	C	106	LYS
3	D	149	ASP
2	C	151[B]	THR
3	D	121	GLN
3	D	91	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 12 such sidechains are listed below:

Mol	Chain	Res	Type
3	D	64	GLN
3	D	94	ASN
3	D	233	GLN
3	D	161	ASN
1	A	234	ASN

### 5.3.3 RNA ⓘ

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 monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

33 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	$\# Z  > 2$
4	EDO	C	251	-	3,3,3	0.60	0	2,2,2	0.11	0
6	1PE	A	370	-	15,15,15	0.59	0	14,14,14	0.82	0
4	EDO	A	368	-	3,3,3	0.81	0	2,2,2	0.77	0
4	EDO	C	254	-	3,3,3	0.81	0	2,2,2	0.14	0
4	EDO	A	357	-	3,3,3	0.51	0	2,2,2	0.08	0
4	EDO	A	367	-	3,3,3	0.60	0	2,2,2	0.47	0
4	EDO	A	358	-	3,3,3	0.41	0	2,2,2	0.12	0
4	EDO	A	363	-	3,3,3	0.53	0	2,2,2	0.32	0
4	EDO	C	256	-	3,3,3	0.48	0	2,2,2	0.50	0
4	EDO	A	353	-	3,3,3	0.45	0	2,2,2	0.46	0
4	EDO	A	356	-	3,3,3	0.46	0	2,2,2	0.62	0
4	EDO	A	360	-	3,3,3	0.44	0	2,2,2	0.32	0
4	EDO	A	359	-	3,3,3	0.61	0	2,2,2	0.23	0
4	EDO	A	366	-	3,3,3	0.79	0	2,2,2	0.42	0
5	PEG	C	259	-	6,6,6	0.90	0	5,5,5	0.93	0
4	EDO	C	255	-	3,3,3	0.55	0	2,2,2	0.21	0
4	EDO	C	253	-	3,3,3	0.52	0	2,2,2	0.54	0
8	PGE	D	247	-	9,9,9	0.92	0	8,8,8	1.47	2 (25%)
5	PEG	A	369	-	6,6,6	0.59	0	5,5,5	0.48	0
4	EDO	A	361	-	3,3,3	0.42	0	2,2,2	0.56	0
4	EDO	A	355	-	3,3,3	0.57	0	2,2,2	0.32	0
7	GOL	C	261	-	5,5,5	1.03	0	5,5,5	1.53	1 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	C	250	-	3,3,3	0.64	0	2,2,2	0.46	0
4	EDO	C	258	-	3,3,3	0.54	0	2,2,2	0.44	0
4	EDO	C	257	-	3,3,3	0.56	0	2,2,2	0.16	0
4	EDO	A	364	-	3,3,3	0.58	0	2,2,2	0.10	0
4	EDO	A	365	-	3,3,3	0.57	0	2,2,2	0.28	0
4	EDO	D	246	-	3,3,3	0.66	0	2,2,2	0.24	0
7	GOL	C	260	-	5,5,5	0.63	0	5,5,5	1.15	0
7	GOL	A	371	-	5,5,5	0.52	0	5,5,5	0.84	0
4	EDO	C	252	-	3,3,3	0.50	0	2,2,2	0.39	0
4	EDO	A	354	-	3,3,3	0.62	0	2,2,2	0.21	0
4	EDO	A	362	-	3,3,3	0.54	0	2,2,2	0.48	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
4	EDO	C	251	-	-	1/1/1/1	-
6	1PE	A	370	-	-	8/13/13/13	-
4	EDO	A	368	-	-	1/1/1/1	-
4	EDO	C	254	-	-	1/1/1/1	-
4	EDO	A	357	-	-	1/1/1/1	-
4	EDO	A	367	-	-	0/1/1/1	-
4	EDO	A	358	-	-	0/1/1/1	-
4	EDO	A	363	-	-	1/1/1/1	-
4	EDO	C	256	-	-	1/1/1/1	-
4	EDO	A	353	-	-	1/1/1/1	-
4	EDO	A	356	-	-	1/1/1/1	-
4	EDO	A	360	-	-	1/1/1/1	-
4	EDO	A	359	-	-	0/1/1/1	-
4	EDO	A	366	-	-	1/1/1/1	-
5	PEG	C	259	-	-	2/4/4/4	-
4	EDO	C	255	-	-	1/1/1/1	-
4	EDO	C	253	-	-	1/1/1/1	-
8	PGE	D	247	-	-	5/7/7/7	-
5	PEG	A	369	-	-	4/4/4/4	-
4	EDO	A	361	-	-	1/1/1/1	-
4	EDO	A	355	-	-	1/1/1/1	-
7	GOL	C	261	-	-	2/4/4/4	-
4	EDO	C	250	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	C	258	-	-	0/1/1/1	-
4	EDO	C	257	-	-	1/1/1/1	-
4	EDO	A	364	-	-	0/1/1/1	-
4	EDO	A	365	-	-	0/1/1/1	-
4	EDO	D	246	-	-	0/1/1/1	-
7	GOL	C	260	-	-	2/4/4/4	-
7	GOL	A	371	-	-	1/4/4/4	-
4	EDO	C	252	-	-	1/1/1/1	-
4	EDO	A	354	-	-	0/1/1/1	-
4	EDO	A	362	-	-	1/1/1/1	-

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	D	247	PGE	C3-O2-C2	2.73	125.10	113.29
8	D	247	PGE	O3-C4-C3	2.25	120.55	110.39
7	C	261	GOL	O1-C1-C2	2.06	120.10	110.20

There are no chirality outliers.

5 of 42 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
7	C	261	GOL	C1-C2-C3-O3
5	C	259	PEG	C4-C3-O2-C2
8	D	247	PGE	C1-C2-O2-C3
5	A	369	PEG	O1-C1-C2-O2
6	A	370	1PE	OH4-C13-C23-OH3

There are no ring outliers.

17 monomers are involved in 70 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	251	EDO	1	0
6	A	370	1PE	7	0
4	A	358	EDO	7	0
4	C	256	EDO	1	0
4	A	360	EDO	2	0
4	A	366	EDO	1	0
5	C	259	PEG	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	255	EDO	1	0
4	C	253	EDO	2	0
8	D	247	PGE	17	0
5	A	369	PEG	4	0
7	C	261	GOL	15	0
4	C	250	EDO	1	0
4	D	246	EDO	3	0
7	C	260	GOL	4	0
7	A	371	GOL	1	0
4	A	354	EDO	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	352/352 (100%)	0.76	48 (13%) 3 2	31, 45, 53, 58	0
2	C	249/249 (100%)	0.77	30 (12%) 4 4	39, 46, 60, 66	0
3	D	241/245 (98%)	0.71	32 (13%) 3 2	37, 45, 55, 81	0
All	All	842/846 (99%)	0.75	110 (13%) 3 2	31, 45, 56, 81	0

The worst 5 of 110 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	196	LYS	8.7
1	A	213	LEU	7.8
1	A	352	THR	7.1
2	C	107	SER	6.8
1	A	210	PHE	6.8

### 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 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	EDO	C	255	4/4	0.63	0.28	50,51,51,52	4
4	EDO	C	252	4/4	0.65	0.20	53,54,54,54	4
4	EDO	D	246	4/4	0.67	0.32	51,53,55,55	0
4	EDO	A	355	4/4	0.68	0.24	48,48,49,50	4
4	EDO	A	368	4/4	0.73	0.45	52,54,54,55	0
4	EDO	C	257	4/4	0.74	0.20	44,46,48,48	4
4	EDO	A	353	4/4	0.77	0.46	52,52,53,53	4
4	EDO	C	254	4/4	0.78	0.19	55,57,58,59	0
4	EDO	C	258	4/4	0.79	0.29	48,49,49,50	4
4	EDO	A	367	4/4	0.80	0.19	51,61,62,63	0
4	EDO	A	360	4/4	0.81	0.19	61,63,63,66	0
7	GOL	C	260	6/6	0.82	0.26	41,44,50,50	0
4	EDO	A	354	4/4	0.83	0.20	47,49,50,51	4
4	EDO	A	361	4/4	0.84	0.17	50,51,51,51	4
4	EDO	A	357	4/4	0.85	0.41	46,47,48,49	4
4	EDO	C	253	4/4	0.85	0.44	46,55,56,61	0
4	EDO	A	366	4/4	0.85	0.20	53,60,61,61	0
4	EDO	C	251	4/4	0.85	0.15	56,63,65,69	0
5	PEG	A	369	7/7	0.86	0.22	59,61,64,64	0
8	PGE	D	247	10/10	0.86	0.33	15,39,49,53	2
4	EDO	A	363	4/4	0.87	0.16	64,65,65,67	0
4	EDO	C	256	4/4	0.87	0.33	53,56,58,62	0
4	EDO	A	356	4/4	0.88	0.10	54,56,56,59	0
5	PEG	C	259	7/7	0.88	0.21	31,47,54,55	0
6	1PE	A	370	16/16	0.88	0.17	50,58,70,73	0
4	EDO	A	364	4/4	0.88	0.23	44,45,45,48	4
4	EDO	A	365	4/4	0.88	0.18	51,51,51,51	4
4	EDO	A	359	4/4	0.90	0.25	46,57,58,64	0
4	EDO	A	362	4/4	0.90	0.15	56,56,56,57	4
4	EDO	C	250	4/4	0.93	0.45	40,49,49,57	0
7	GOL	C	261	6/6	0.94	0.34	39,47,48,49	0
4	EDO	A	358	4/4	0.95	0.27	43,45,46,46	0
7	GOL	A	371	6/6	0.96	0.12	34,46,49,51	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.