



# wwPDB X-ray Structure Validation Summary Report ⓘ

Jan 31, 2016 – 07:18 PM GMT

PDB ID : 1EX0  
Title : HUMAN FACTOR XIII, MUTANT W279F ZYMOGEN  
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Deposited on : 2000-04-28  
Resolution : 2.00 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  
<http://wwpdb.org/validation/2016/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 : 1.7 (RC4), CSD as536be (2015)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20026688  
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)  
Refmac : 5.8.0135  
CCP4 : 6.5.0  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : trunk26865

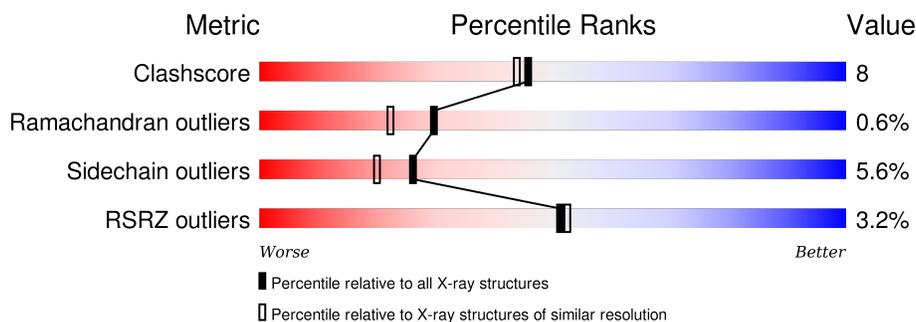
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.00 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))
Clashscore	102246	7340 (2.00-2.00)
Ramachandran outliers	100387	7248 (2.00-2.00)
Sidechain outliers	100360	7247 (2.00-2.00)
RSRZ outliers	91569	6262 (2.00-2.00)

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 on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria. 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	731	 3% 74% 20% ...
1	B	731	 3% 77% 16% ...

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	PGO	A	1340	-	-	-	X
4	PGO	A	1341	-	-	X	X

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<b>Mol</b>	<b>Type</b>	<b>Chain</b>	<b>Res</b>	<b>Chirality</b>	<b>Geometry</b>	<b>Clashes</b>	<b>Electron density</b>
4	PGO	B	1343	-	-	-	X
4	PGO	B	1344	-	-	-	X
4	PGO	B	1345	-	-	-	X

## 2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 12770 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 COAGULATION FACTOR XIII A CHAIN.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	705	5673	3595	980	1072	26	0	2	0
1	B	716	5744	3638	993	1086	27	0	2	0

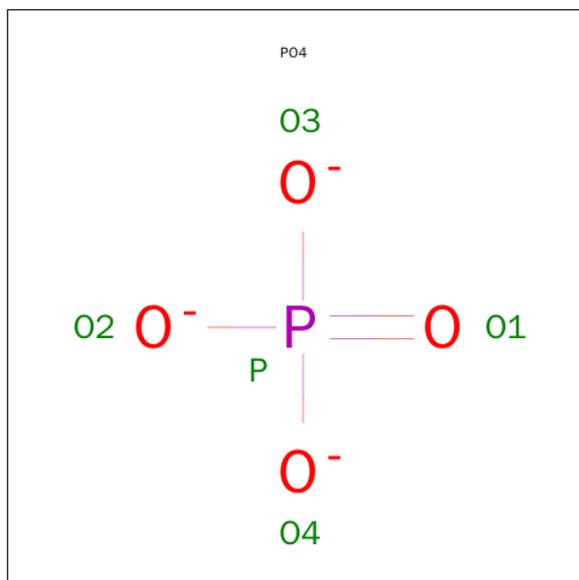
There are 13 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	SAC	SER	MODIFIED RESIDUE	UNP P00488
A	35	ASN	VAL	CONFLICT	UNP P00488
A	36	LEU	PRO	CONFLICT	UNP P00488
A	279	PHE	TRP	ENGINEERED	UNP P00488
A	509	SER	GLU	CONFLICT	UNP P00488
A	510	ARG	GLY	CONFLICT	UNP P00488
B	1	SAC	SER	MODIFIED RESIDUE	UNP P00488
B	35	ASN	VAL	CONFLICT	UNP P00488
B	36	LEU	PRO	CONFLICT	UNP P00488
B	279	PHE	TRP	ENGINEERED	UNP P00488
B	509	SER	GLU	CONFLICT	UNP P00488
B	510	ARG	GLY	CONFLICT	UNP P00488
B	511	SER	VAL	CONFLICT	UNP P00488

- Molecule 2 is CALCIUM ION (three-letter code: CA) (formula: Ca).

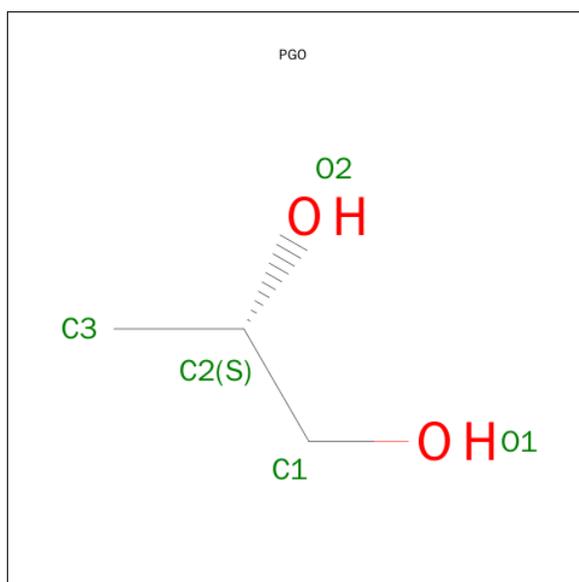
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	B	1	Total	Ca	0	0
			1	1		
2	A	1	Total	Ca	0	0
			1	1		

- Molecule 3 is PHOSPHATE ION (three-letter code: PO4) (formula: O<sub>4</sub>P).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0
3	B	1	Total O P 5 4 1	0	0

- Molecule 4 is S-1,2-PROPANEDIOL (three-letter code: PGO) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 5 3 2	0	0

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			5	3	2		
4	A	1	Total	C	O	0	0
			5	3	2		
4	B	1	Total	C	O	0	0
			5	3	2		
4	B	1	Total	C	O	0	0
			5	3	2		
4	B	1	Total	C	O	0	0
			5	3	2		

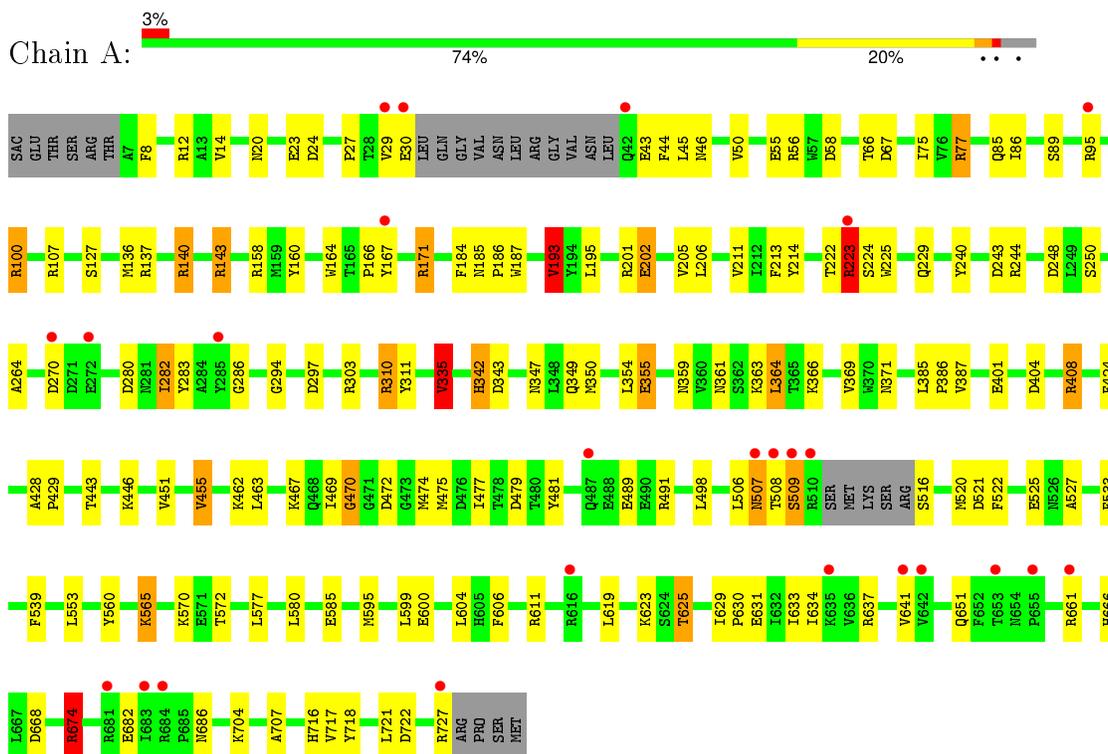
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	554	Total	O	0	0
			554	554		
5	B	752	Total	O	0	0
			752	752		

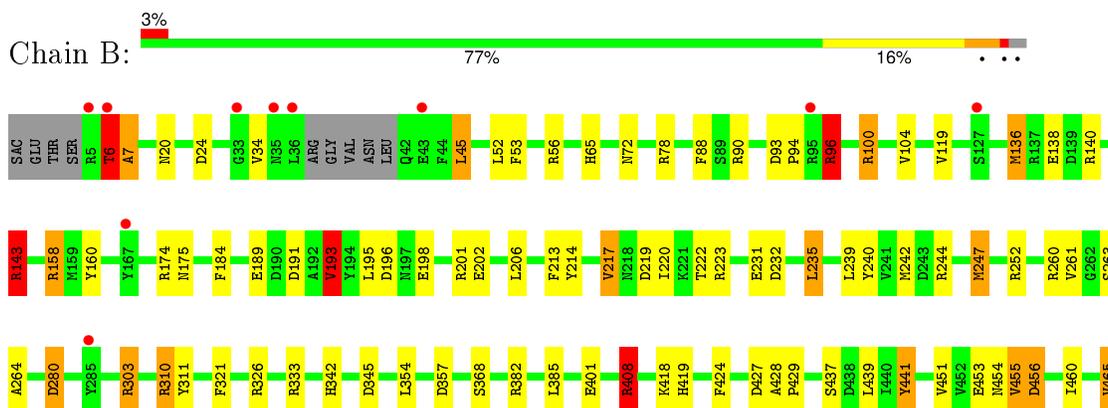
### 3 Residue-property plots

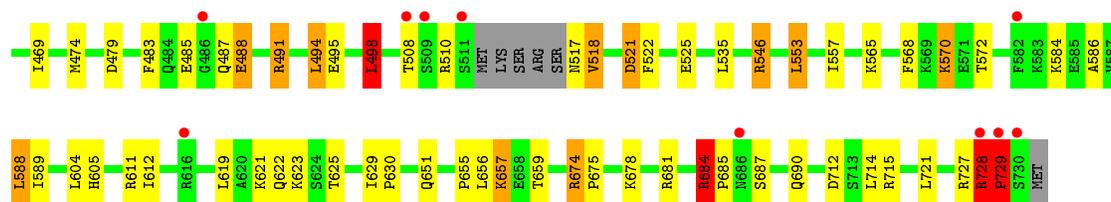
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according 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: COAGULATION FACTOR XIII A CHAIN



- Molecule 1: COAGULATION FACTOR XIII A CHAIN





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	100.54Å 70.64Å 133.38Å 90.00° 106.08° 90.00°	Depositor
Resolution (Å)	19.94 – 2.00 28.51 – 1.80	Depositor EDS
% Data completeness (in resolution range)	96.6 (19.94-2.00) 94.5 (28.51-1.80)	Depositor EDS
$R_{merge}$	0.05	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.18 (at 1.79Å)	Xtrriage
Refinement program	REFMAC 4.0.3.5	Depositor
R, $R_{free}$	0.187 , 0.234 0.186 , (Not available)	Depositor DCC
$R_{free}$ test set	No test flags present.	DCC
Wilson B-factor (Å <sup>2</sup> )	23.9	Xtrriage
Anisotropy	0.301	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 54.7	EDS
Estimated twinning fraction	No twinning to report.	Xtrriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Outliers	0 of 158697 reflections	Xtrriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	12770	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.87% 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, 0.375 respectively for untwinned datasets, and 0.333, 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: PGO, CA, PO4

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	0.60	0/5805	1.42	63/7874 (0.8%)
1	B	0.70	0/5877	1.49	77/7973 (1.0%)
All	All	0.65	0/11682	1.46	140/15847 (0.9%)

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	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

The worst 5 of 140 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed( $^{\circ}$ )	Ideal( $^{\circ}$ )
1	A	95	ARG	CD-NE-CZ	21.46	153.65	123.60
1	A	223[A]	ARG	NE-CZ-NH1	17.62	129.11	120.30
1	A	223[B]	ARG	NE-CZ-NH1	17.62	129.11	120.30
1	B	491	ARG	CD-NE-CZ	17.23	147.73	123.60
1	B	303	ARG	CD-NE-CZ	14.82	144.35	123.60

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	509	SER	Peptide

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Mol	Chain	Res	Type	Group
1	B	729	PRO	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	5673	0	5520	99	0
1	B	5744	0	5579	78	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	5	0	0	1	0
3	B	10	0	0	0	0
4	A	15	0	24	7	0
4	B	15	0	24	1	0
5	A	554	0	0	10	0
5	B	752	0	0	11	0
All	All	12770	0	11147	175	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 8.

The worst 5 of 175 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:651:GLN:HE21	1:B:690:GLN:HE21	1.15	0.94
1:B:630:PRO:HG3	1:B:655:PRO:HG3	1.51	0.91
1:A:143:ARG:HB2	4:A:1341:PGO:H12	1.54	0.87
1:B:136[A]:MET:HG2	1:B:143:ARG:HB2	1.59	0.84
1:B:659:THR:HG22	1:B:685:PRO:HD3	1.64	0.77

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	701/731 (96%)	677 (97%)	22 (3%)	2 (0%)	46	41
1	B	712/731 (97%)	682 (96%)	24 (3%)	6 (1%)	24	15
All	All	1413/1462 (97%)	1359 (96%)	46 (3%)	8 (1%)	30	22

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	509	SER
1	B	7	ALA
1	B	34	VAL
1	B	6	THR
1	B	510	ARG

### 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	621/644 (96%)	583 (94%)	38 (6%)	23	17
1	B	627/644 (97%)	592 (94%)	35 (6%)	26	20
All	All	1248/1288 (97%)	1175 (94%)	73 (6%)	26	19

5 of 73 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	585	GLU

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Mol	Chain	Res	Type
1	B	45	LEU
1	B	604	LEU
1	A	674	ARG
1	B	96	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 20 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	65	HIS
1	B	72	ASN
1	B	622	GLN
1	A	686	ASN
1	B	32	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 carbohydrates in this entry.

## 5.6 Ligand geometry [i](#)

Of 11 ligands modelled in this entry, 2 are monoatomic - leaving 9 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
3	PO4	A	1330	-	4,4,4	0.43	0	6,6,6	0.29	0
4	PGO	A	1340	-	4,4,4	1.18	1 (25%)	2,4,4	2.21	1 (50%)
4	PGO	A	1341	-	4,4,4	1.04	0	2,4,4	1.16	0
4	PGO	A	1342	-	4,4,4	0.85	0	2,4,4	2.00	1 (50%)
3	PO4	B	1331	-	4,4,4	0.35	0	6,6,6	0.28	0
3	PO4	B	1332	-	4,4,4	0.84	0	6,6,6	0.32	0
4	PGO	B	1343	-	4,4,4	1.23	1 (25%)	2,4,4	3.30	1 (50%)
4	PGO	B	1344	-	4,4,4	1.05	0	2,4,4	2.39	1 (50%)
4	PGO	B	1345	-	4,4,4	1.01	0	2,4,4	1.13	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	PO4	A	1330	-	-	0/0/0/0	0/0/0/0
4	PGO	A	1340	-	-	0/2/2/2	0/0/0/0
4	PGO	A	1341	-	-	0/2/2/2	0/0/0/0
4	PGO	A	1342	-	-	0/2/2/2	0/0/0/0
3	PO4	B	1331	-	-	0/0/0/0	0/0/0/0
3	PO4	B	1332	-	-	0/0/0/0	0/0/0/0
4	PGO	B	1343	-	-	0/2/2/2	0/0/0/0
4	PGO	B	1344	-	-	0/2/2/2	0/0/0/0
4	PGO	B	1345	-	-	0/2/2/2	0/0/0/0

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	1340	PGO	C1-C2	2.23	1.56	1.50
4	B	1343	PGO	C1-C2	2.31	1.56	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1343	PGO	O1-C1-C2	-4.66	99.82	110.87
4	B	1344	PGO	O1-C1-C2	-3.27	103.11	110.87
4	A	1340	PGO	O1-C1-C2	-2.99	103.77	110.87
4	A	1342	PGO	O1-C1-C2	-2.83	104.17	110.87

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

3 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	A	1330	PO4	1	0
4	A	1341	PGO	7	0
4	B	1345	PGO	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	705/731 (96%)	-0.25	25 (3%) 48 49	18, 30, 65, 88	2 (0%)
1	B	716/731 (97%)	-0.54	20 (2%) 56 57	14, 23, 52, 107	2 (0%)
All	All	1421/1462 (97%)	-0.40	45 (3%) 51 52	14, 27, 60, 107	4 (0%)

The worst 5 of 45 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	36	LEU	10.0
1	B	511	SER	9.4
1	B	6	THR	8.3
1	B	729	PRO	6.1
1	B	35	ASN	5.7

### 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 carbohydrates 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. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. 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	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PGO	B	1344	5/5	0.59	0.20	6.45	62,62,63,65	0
4	PGO	A	1340	5/5	0.93	0.17	6.38	45,46,47,48	0
4	PGO	B	1345	5/5	0.82	0.15	5.19	50,53,53,54	0
4	PGO	B	1343	5/5	0.84	0.15	2.86	46,49,50,51	0
4	PGO	A	1341	5/5	0.87	0.15	2.47	58,59,59,60	0
4	PGO	A	1342	5/5	0.97	0.08	1.51	48,48,49,49	0
3	PO4	B	1332	5/5	0.93	0.13	0.45	64,64,65,65	0
2	CA	A	1320	1/1	0.98	0.08	0.19	30,30,30,30	0
3	PO4	A	1330	5/5	0.96	0.09	0.10	36,36,40,40	0
3	PO4	B	1331	5/5	0.99	0.06	-1.13	25,26,29,29	0
2	CA	B	1321	1/1	0.98	0.03	-3.34	21,21,21,21	0

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

There are no such residues in this entry.