



# wwPDB X-ray Structure Validation Summary Report ⓘ

May 15, 2020 – 11:14 pm BST

PDB ID : 2HWG  
Title : Structure of phosphorylated Enzyme I of the phosphoenolpyruvate:sugar phosphotransferase system  
Authors : Lim, K.; Teplyakov, A.; Herzberg, O.  
Deposited on : 2006-08-01  
Resolution : 2.70 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	:	2.11
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)	:	2.11

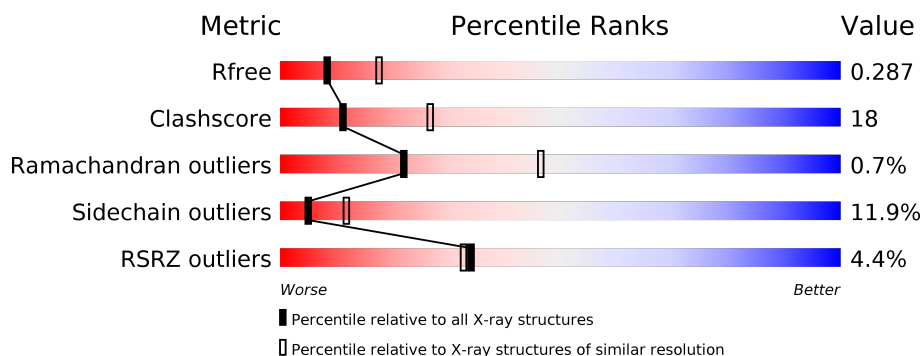
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 2.70 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	2808 (2.70-2.70)
Clashscore	141614	3122 (2.70-2.70)
Ramachandran outliers	138981	3069 (2.70-2.70)
Sidechain outliers	138945	3069 (2.70-2.70)
RSRZ outliers	127900	2737 (2.70-2.70)

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 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	575	<div> <div>2%</div> <div>64%</div> <div>29%</div> <div>6%</div> <div>..</div> </div>
1	B	575	<div> <div>6%</div> <div>65%</div> <div>30%</div> <div>..</div> </div>

## 2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 9102 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 Phosphoenolpyruvate-protein phosphotransferase.

Mol	Chain	Residues	Atoms							ZeroOcc	AltConf	Trace
1	A	572	Total	C	N	O	P	S	Se	0	0	0
			4437	2785	756	875	1	3	17			
1	B	572	Total	C	N	O	P	S	Se	0	0	0
			4437	2785	756	875	1	3	17			

There are 38 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MSE	MET	MODIFIED RESIDUE	UNP P08839
A	78	MSE	MET	MODIFIED RESIDUE	UNP P08839
A	98	MSE	MET	MODIFIED RESIDUE	UNP P08839
A	189	NEP	HIS	MODIFIED RESIDUE	UNP P08839
A	193	MSE	MET	MODIFIED RESIDUE	UNP P08839
A	239	MSE	MET	MODIFIED RESIDUE	UNP P08839
A	302	MSE	MET	MODIFIED RESIDUE	UNP P08839
A	334	MSE	MET	MODIFIED RESIDUE	UNP P08839
A	345	MSE	MET	MODIFIED RESIDUE	UNP P08839
A	364	MSE	MET	MODIFIED RESIDUE	UNP P08839
A	389	MSE	MET	MODIFIED RESIDUE	UNP P08839
A	392	MSE	MET	MODIFIED RESIDUE	UNP P08839
A	429	MSE	MET	MODIFIED RESIDUE	UNP P08839
A	469	MSE	MET	MODIFIED RESIDUE	UNP P08839
A	477	MSE	MET	MODIFIED RESIDUE	UNP P08839
A	501	MSE	MET	MODIFIED RESIDUE	UNP P08839
A	518	MSE	MET	MODIFIED RESIDUE	UNP P08839
A	525	MSE	MET	MODIFIED RESIDUE	UNP P08839
A	562	MSE	MET	MODIFIED RESIDUE	UNP P08839
B	1	MSE	MET	MODIFIED RESIDUE	UNP P08839
B	78	MSE	MET	MODIFIED RESIDUE	UNP P08839
B	98	MSE	MET	MODIFIED RESIDUE	UNP P08839
B	189	NEP	HIS	MODIFIED RESIDUE	UNP P08839
B	193	MSE	MET	MODIFIED RESIDUE	UNP P08839
B	239	MSE	MET	MODIFIED RESIDUE	UNP P08839

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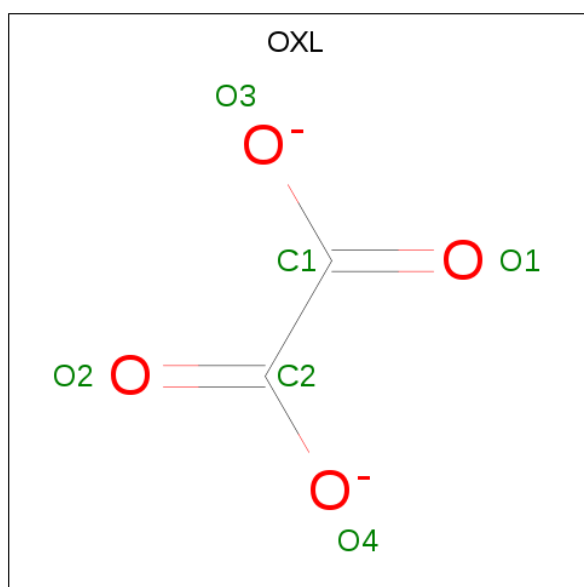
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Chain	Residue	Modelled	Actual	Comment	Reference
B	302	MSE	MET	MODIFIED RESIDUE	UNP P08839
B	334	MSE	MET	MODIFIED RESIDUE	UNP P08839
B	345	MSE	MET	MODIFIED RESIDUE	UNP P08839
B	364	MSE	MET	MODIFIED RESIDUE	UNP P08839
B	389	MSE	MET	MODIFIED RESIDUE	UNP P08839
B	392	MSE	MET	MODIFIED RESIDUE	UNP P08839
B	429	MSE	MET	MODIFIED RESIDUE	UNP P08839
B	469	MSE	MET	MODIFIED RESIDUE	UNP P08839
B	477	MSE	MET	MODIFIED RESIDUE	UNP P08839
B	501	MSE	MET	MODIFIED RESIDUE	UNP P08839
B	518	MSE	MET	MODIFIED RESIDUE	UNP P08839
B	525	MSE	MET	MODIFIED RESIDUE	UNP P08839
B	562	MSE	MET	MODIFIED RESIDUE	UNP P08839

- Molecule 2 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 3 is OXALATE ION (three-letter code: OXL) (formula: C<sub>2</sub>O<sub>4</sub>).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total 6	C 2	O 4	0	0
3	B	1	Total 6	C 2	O 4	0	0

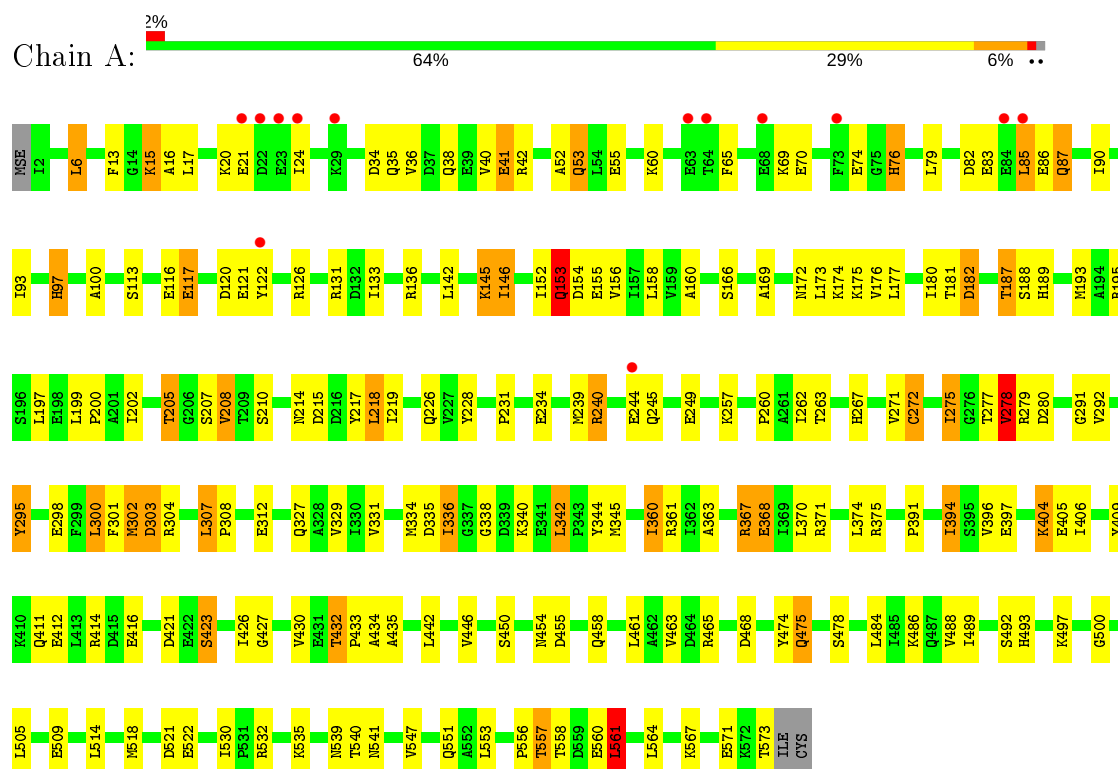
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	110	Total 110	O 110	0	0
4	B	104	Total 104	O 104	0	0

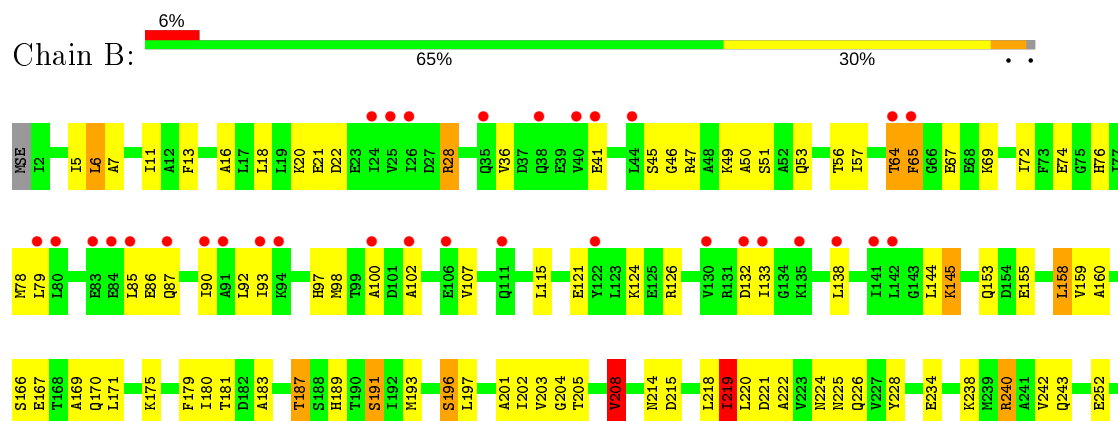
### 3 Residue-property plots

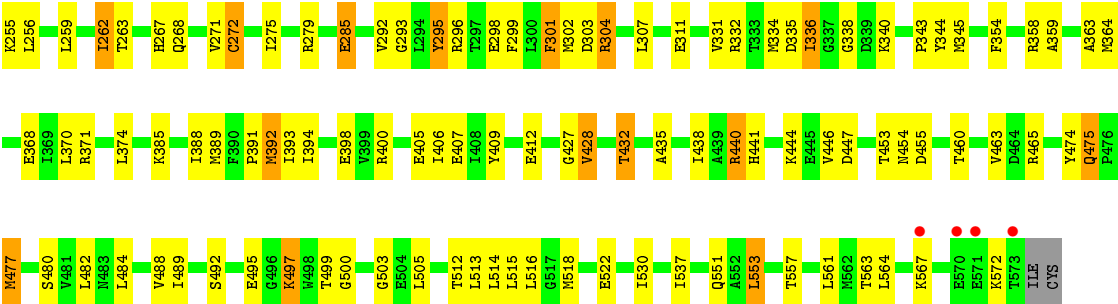
These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are 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: Phosphoenolpyruvate-protein phosphotransferase



- Molecule 1: Phosphoenolpyruvate-protein phosphotransferase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	85.49 Å 94.08 Å 161.01 Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.70 47.04 – 2.70	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.70) 99.5 (47.04-2.70)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.44 (at 2.69 Å)	Xtriage
Refinement program	REFMAC, CNS	Depositor
R, $R_{free}$	0.204 , 0.284 0.217 , 0.287	Depositor DCC
$R_{free}$ test set	1798 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	33.2	Xtriage
Anisotropy	0.498	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.32 , 34.0	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	0.91	EDS
Total number of atoms	9102	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	31.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 15.02% 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: OXL, MG, NEP

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	2/4457 (0.0%)	0.90	6/5982 (0.1%)
1	B	0.81	2/4457 (0.0%)	0.87	4/5982 (0.1%)
All	All	0.82	4/8914 (0.0%)	0.88	10/11964 (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	B	0	1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	285	GLU	CG-CD	7.15	1.62	1.51
1	A	60	LYS	CE-NZ	6.19	1.64	1.49
1	B	272	CYS	CB-SG	-5.56	1.72	1.81
1	A	272	CYS	CB-SG	-5.24	1.73	1.81

The worst 5 of 10 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	561	LEU	CA-CB-CG	10.50	139.44	115.30
1	B	262	ILE	CG1-CB-CG2	-7.79	94.27	111.40
1	B	219	ILE	CG1-CB-CG2	-6.35	97.42	111.40
1	B	208	VAL	CB-CA-C	-5.57	100.83	111.40
1	A	182	ASP	CB-CG-OD1	5.49	123.24	118.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	338	GLY	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	4437	0	4492	171	0
1	B	4437	0	4492	151	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	6	0	0	0	0
3	B	6	0	0	0	0
4	A	110	0	0	12	0
4	B	104	0	0	5	0
All	All	9102	0	8984	319	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 18.

The worst 5 of 319 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:345:MSE:CE	1:A:345:MSE:SE	2.14	1.46
1:A:169:ALA:HA	1:A:193:MSE:HE1	1.25	1.09
1:A:342:LEU:HD13	1:A:345:MSE:HG2	1.38	1.05
1:B:432:THR:HG22	1:B:435:ALA:H	1.22	1.04
1:B:440:ARG:CD	1:B:440:ARG:H	1.71	1.04

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	569/575 (99%)	533 (94%)	31 (5%)	5 (1%)	17	40
1	B	569/575 (99%)	531 (93%)	35 (6%)	3 (0%)	29	54
All	All	1138/1150 (99%)	1064 (94%)	66 (6%)	8 (1%)	22	46

5 of 8 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	344	TYR
1	A	35	GLN
1	A	172	ASN
1	A	278	VAL
1	B	303	ASP

### 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	472/457 (103%)	414 (88%)	58 (12%)	4	11
1	B	472/457 (103%)	418 (89%)	54 (11%)	5	13
All	All	944/914 (103%)	832 (88%)	112 (12%)	5	12

5 of 112 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	475	GLN

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Mol	Chain	Res	Type
1	B	47	ARG
1	B	463	VAL
1	A	505	LEU
1	A	561	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 17 such sidechains are listed below:

Mol	Chain	Res	Type
1	A	268	GLN
1	A	411	GLN
1	B	243	GLN
1	A	267	HIS
1	B	267	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues 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
1	NEP	B	189	1,2	10,14,15	2.19	3 (30%)	5,20,22	1.18	1 (20%)
1	NEP	A	189	1,2	10,14,15	1.79	4 (40%)	5,20,22	1.29	1 (20%)

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
1	NEP	B	189	1,2	-	0/5/12/14	0/1/1/1
1	NEP	A	189	1,2	-	3/5/12/14	0/1/1/1

The worst 5 of 7 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	189	NEP	P-O3P	5.20	1.51	1.47
1	A	189	NEP	CD2-NE2	-3.33	1.33	1.39
1	B	189	NEP	CD2-NE2	-2.77	1.34	1.39
1	A	189	NEP	P-O1P	-2.71	1.49	1.54
1	B	189	NEP	P-O1P	-2.49	1.49	1.54

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	189	NEP	O2P-P-O1P	2.43	116.12	106.57
1	B	189	NEP	O2P-P-O1P	2.16	115.04	106.57

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	189	NEP	CA-CB-CG-ND1
1	A	189	NEP	N-CA-CB-CG
1	A	189	NEP	C-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	B	189	NEP	2	0
1	A	189	NEP	3	0

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	OXL	A	903	2	0,5,5	0.00	-	0,6,6	0.00	-
3	OXL	B	904	2	0,5,5	0.00	-	0,6,6	0.00	-

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	OXL	A	903	2	-	0/0/4/4	-
3	OXL	B	904	2	-	0/0/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 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	554/575 (96%)	-0.03	13 (2%) 60 62	10, 27, 63, 84	0
1	B	554/575 (96%)	0.06	36 (6%) 18 17	10, 26, 67, 85	0
All	All	1108/1150 (96%)	0.02	49 (4%) 34 33	10, 26, 66, 85	0

The worst 5 of 49 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	65	PHE	4.2
1	A	24	ILE	4.1
1	B	85	LEU	4.1
1	B	573	THR	4.1
1	B	26	ILE	3.9

### 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, 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
1	NEP	B	189	14/15	0.99	0.15	9,15,18,18	0
1	NEP	A	189	14/15	0.99	0.15	20,21,22,23	0

### 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. 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
3	OXL	B	904	6/6	0.97	0.18	27,29,29,30	0
2	MG	A	901	1/1	0.98	0.13	21,21,21,21	0
3	OXL	A	903	6/6	0.98	0.14	18,19,21,23	0
2	MG	B	902	1/1	0.98	0.13	25,25,25,25	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.