



# wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 5, 2026 – 01:50 AM UTC

PDB ID : 5D7V / pdb\_00005d7v  
Title : Crystal structure of PTK6 kinase domain  
Authors : Thakur, M.K.; Birudukota, S.; Swaminathan, S.; Tyagi, R.; Gosu, R.  
Deposited on : 2015-08-14  
Resolution : 2.33 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.

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 : 4-5-2 with Phenix2.0  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtrriage (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

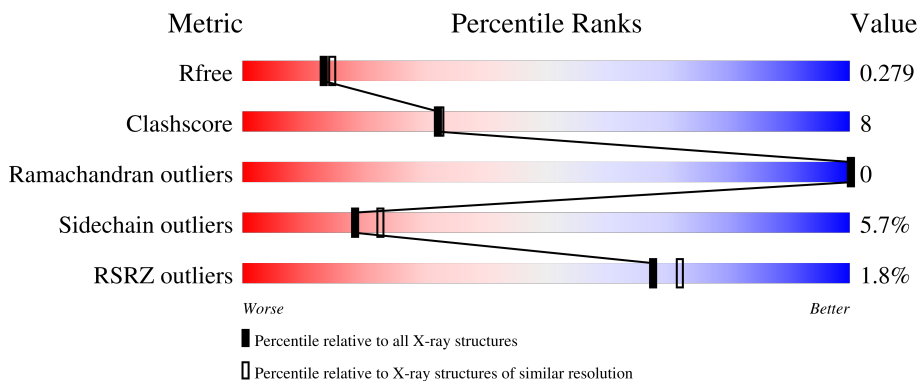
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

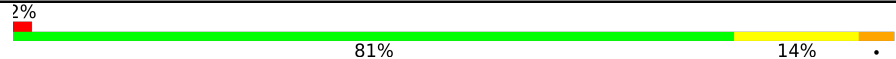



The reported resolution of this entry is 2.33 Å.

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	3031 (2.36-2.32)
Clashscore	190562	3127 (2.36-2.32)
Ramachandran outliers	187476	3095 (2.36-2.32)
Sidechain outliers	187428	3095 (2.36-2.32)
RSRZ outliers	180081	3033 (2.36-2.32)

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	269	 2% 81% 14% .
1	B	269	 2% 78% 19% ..
1	C	269	 % 82% 14% ..
1	D	269	 2% 82% 15% ..

## 2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 9141 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 Protein-tyrosine kinase 6.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	269	2214	1410	390	397	17	0	5	0
1	B	265	2161	1379	379	386	17	0	4	0
1	C	265	2165	1380	378	389	18	0	4	0
1	D	265	2143	1366	373	387	17	0	1	0

There are 32 discrepancies between the modelled and reference sequences:

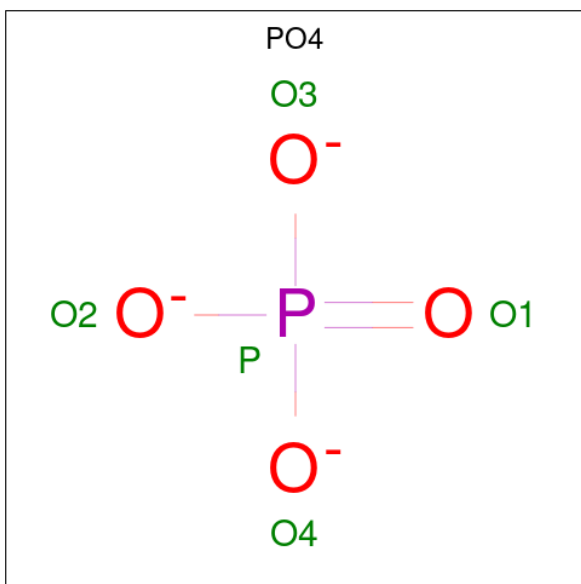
Chain	Residue	Modelled	Actual	Comment	Reference
A	184	CXM	-	expression tag	UNP Q13882
A	433	THR	CYS	engineered mutation	UNP Q13882
A	447	HIS	-	expression tag	UNP Q13882
A	448	HIS	-	expression tag	UNP Q13882
A	449	HIS	-	expression tag	UNP Q13882
A	450	HIS	-	expression tag	UNP Q13882
A	451	HIS	-	expression tag	UNP Q13882
A	452	HIS	-	expression tag	UNP Q13882
B	184	CXM	-	expression tag	UNP Q13882
B	433	THR	CYS	engineered mutation	UNP Q13882
B	447	HIS	-	expression tag	UNP Q13882
B	448	HIS	-	expression tag	UNP Q13882
B	449	HIS	-	expression tag	UNP Q13882
B	450	HIS	-	expression tag	UNP Q13882
B	451	HIS	-	expression tag	UNP Q13882
B	452	HIS	-	expression tag	UNP Q13882
C	184	CXM	-	expression tag	UNP Q13882
C	433	THR	CYS	engineered mutation	UNP Q13882
C	447	HIS	-	expression tag	UNP Q13882
C	448	HIS	-	expression tag	UNP Q13882
C	449	HIS	-	expression tag	UNP Q13882

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Chain	Residue	Modelled	Actual	Comment	Reference
C	450	HIS	-	expression tag	UNP Q13882
C	451	HIS	-	expression tag	UNP Q13882
C	452	HIS	-	expression tag	UNP Q13882
D	184	CXM	-	expression tag	UNP Q13882
D	433	THR	CYS	engineered mutation	UNP Q13882
D	447	HIS	-	expression tag	UNP Q13882
D	448	HIS	-	expression tag	UNP Q13882
D	449	HIS	-	expression tag	UNP Q13882
D	450	HIS	-	expression tag	UNP Q13882
D	451	HIS	-	expression tag	UNP Q13882
D	452	HIS	-	expression tag	UNP Q13882

- Molecule 2 is PHOSPHATE ION (CCD ID: PO4) (formula: O<sub>4</sub>P).



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

- Molecule 3 is GLYCEROL (CCD ID: GOL) (formula: C<sub>3</sub>H<sub>8</sub>O<sub>3</sub>).



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

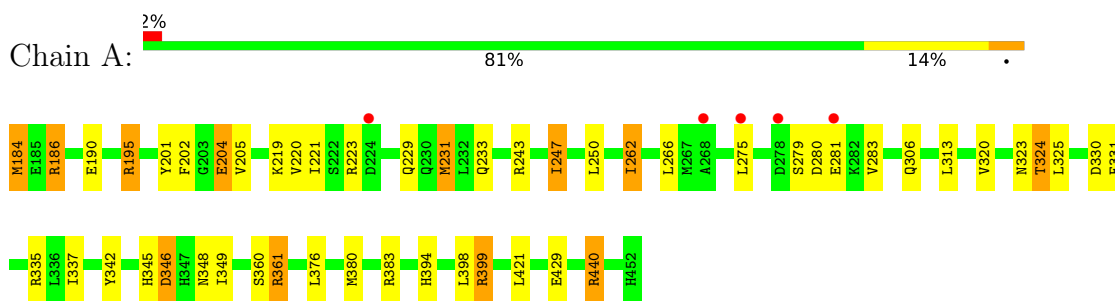
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	121	Total 121	O 121	0	0
4	B	78	Total 78	O 78	0	0
4	C	84	Total 84	O 84	0	0
4	D	83	Total 83	O 83	0	0

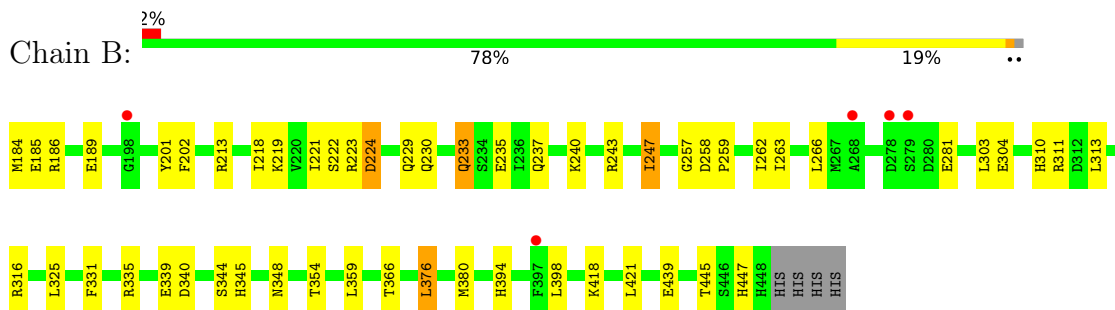
### 3 Residue-property plots [i](#)

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.

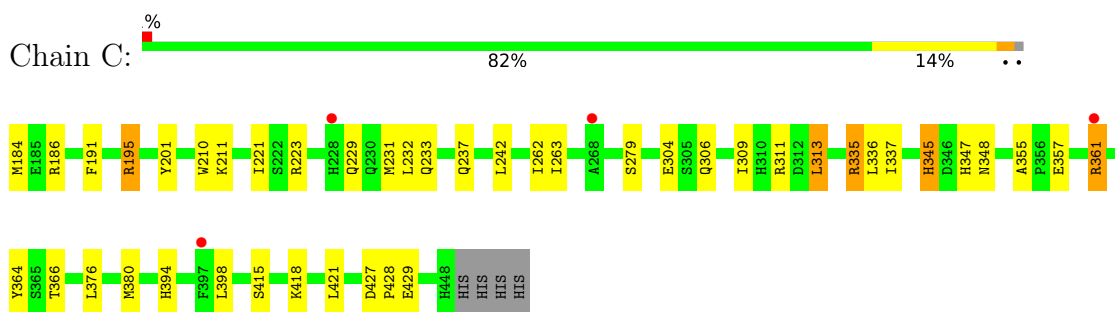
- Molecule 1: Protein-tyrosine kinase 6



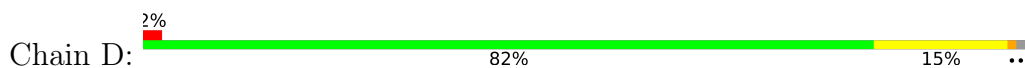
- Molecule 1: Protein-tyrosine kinase 6

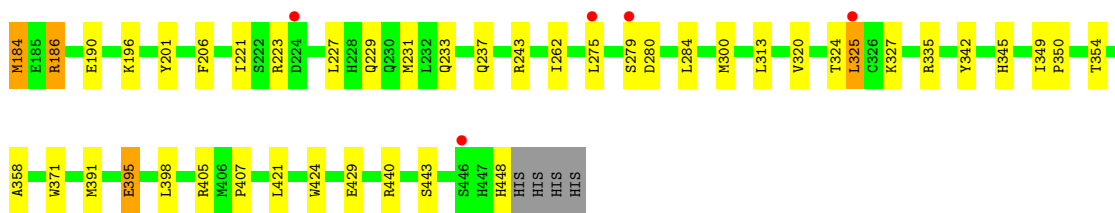


- Molecule 1: Protein-tyrosine kinase 6



- Molecule 1: Protein-tyrosine kinase 6





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	49.72Å 76.31Å 87.27Å 81.46° 75.92° 74.93°	Depositor
Resolution (Å)	50.00 – 2.33 50.00 – 2.33	Depositor EDS
% Data completeness (in resolution range)	96.0 (50.00-2.33) 96.0 (50.00-2.33)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.08 (at 2.34Å)	Xtrriage
Refinement program	REFMAC 5.2.0005	Depositor
R, $R_{free}$	0.219 , 0.282 0.218 , 0.279	Depositor DCC
$R_{free}$ test set	2476 reflections (4.87%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	27.2	Xtrriage
Anisotropy	0.337	Xtrriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.36 , 28.2	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.50$ , $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
$F_o, F_c$ correlation	0.93	EDS
Total number of atoms	9141	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	26.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.98% 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: GOL, CXM, 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	0.54	0/2265	0.86	0/3065
1	B	0.52	0/2205	0.83	1/2984 (0.0%)
1	C	0.51	0/2209	0.85	2/2989 (0.1%)
1	D	0.51	0/2177	0.84	0/2947
All	All	0.52	0/8856	0.85	3/11985 (0.0%)

There are no bond length outliers.

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	281	GLU	N-CA-C	6.07	120.23	112.34
1	C	355	ALA	CA-C-N	5.29	125.35	119.32
1	C	355	ALA	C-N-CA	5.29	125.35	119.32

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	2214	0	2187	43	0
1	B	2161	0	2149	37	0
1	C	2165	0	2152	35	0
1	D	2143	0	2123	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	5	0	0	0	0
2	B	5	0	0	0	0
2	C	5	0	0	0	0
2	D	5	0	0	0	0
3	A	18	0	24	0	0
3	B	18	0	24	2	0
3	C	18	0	24	6	0
3	D	18	0	24	3	0
4	A	121	0	0	2	0
4	B	78	0	0	3	0
4	C	84	0	0	0	0
4	D	83	0	0	2	0
All	All	9141	0	8707	140	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 140 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:399:ARG:HG2	1:A:399:ARG:HH11	1.20	1.06
1:A:440:ARG:HH11	1:A:440:ARG:HG3	1.22	1.05
1:C:376:LEU:HD23	1:C:380:MET:HE3	1.37	1.05
1:C:361:ARG:HG3	1:C:361:ARG:HH21	1.26	0.98
1:C:376:LEU:CD2	1:C:380:MET:HE3	1.97	0.93

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	271/269 (101%)	263 (97%)	8 (3%)	0	100	100
1	B	266/269 (99%)	257 (97%)	9 (3%)	0	100	100
1	C	266/269 (99%)	259 (97%)	7 (3%)	0	100	100
1	D	263/269 (98%)	254 (97%)	9 (3%)	0	100	100
All	All	1066/1076 (99%)	1033 (97%)	33 (3%)	0	100	100

There are no Ramachandran outliers to report.

### 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	241/238 (101%)	220 (91%)	21 (9%)	9	10
1	B	234/238 (98%)	221 (94%)	13 (6%)	19	23
1	C	236/238 (99%)	225 (95%)	11 (5%)	23	30
1	D	232/238 (98%)	223 (96%)	9 (4%)	28	37
All	All	943/952 (99%)	889 (94%)	54 (6%)	18	23

5 of 54 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	266	LEU
1	C	195	ARG
1	D	325	LEU
1	B	325	LEU
1	B	418	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 21 such sidechains are listed below:

Mol	Chain	Res	Type
1	C	447	HIS
1	D	345	HIS
1	D	448	HIS

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Mol	Chain	Res	Type
1	D	417	HIS
1	D	317	ASN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

8 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	CXM	B	184[A]	-	9,10,11	0.84	0	9,11,13	1.17	1 (11%)
1	CXM	C	184[B]	-	9,10,11	0.82	0	9,11,13	1.32	1 (11%)
1	CXM	A	184[A]	-	9,10,11	0.79	0	9,11,13	1.11	1 (11%)
1	CXM	B	184[B]	-	9,10,11	0.83	0	9,11,13	1.26	1 (11%)
1	CXM	C	184[A]	-	9,10,11	0.84	0	9,11,13	1.40	1 (11%)
1	CXM	D	184[A]	-	9,10,11	0.80	0	9,11,13	1.41	2 (22%)
1	CXM	A	184[B]	-	9,10,11	0.85	0	9,11,13	1.17	1 (11%)
1	CXM	D	184[B]	-	9,10,11	0.83	0	9,11,13	1.53	2 (22%)

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	CXM	B	184[A]	-	-	4/9/10/12	-
1	CXM	C	184[B]	-	-	6/9/10/12	-
1	CXM	A	184[A]	-	-	4/9/10/12	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	CXM	B	184[B]	-	-	6/9/10/12	-
1	CXM	C	184[A]	-	-	4/9/10/12	-
1	CXM	D	184[A]	-	-	5/9/10/12	-
1	CXM	A	184[B]	-	-	3/9/10/12	-
1	CXM	D	184[B]	-	-	6/9/10/12	-

There are no bond length outliers.

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

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	184[A]	CXM	ON1-CN-N	-3.53	119.06	124.86
1	D	184[B]	CXM	ON1-CN-N	-3.40	119.29	124.86
1	C	184[B]	CXM	ON1-CN-N	-3.39	119.30	124.86
1	D	184[A]	CXM	ON1-CN-N	-3.38	119.31	124.86
1	B	184[A]	CXM	ON1-CN-N	-2.75	120.35	124.86

There are no chirality outliers.

5 of 38 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	184[A]	CXM	N-CA-CB-CG
1	B	184[A]	CXM	N-CA-CB-CG
1	B	184[B]	CXM	C-CA-CB-CG
1	C	184[A]	CXM	ON2-CN-N-CA
1	C	184[A]	CXM	N-CA-CB-CG

There are no ring outliers.

2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	184[B]	CXM	1	0
1	D	184[B]	CXM	2	0

## 5.5 Carbohydrates

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry

16 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	GOL	A	503	-	5,5,5	0.36	0	5,5,5	0.27	0
3	GOL	A	504	-	5,5,5	0.34	0	5,5,5	0.50	0
2	PO4	D	501	-	4,4,4	0.90	0	6,6,6	0.54	0
3	GOL	B	504	-	5,5,5	0.38	0	5,5,5	0.29	0
3	GOL	A	502	-	5,5,5	0.46	0	5,5,5	0.33	0
3	GOL	C	503	-	5,5,5	0.37	0	5,5,5	0.38	0
3	GOL	B	503	-	5,5,5	0.39	0	5,5,5	0.24	0
3	GOL	D	503	-	5,5,5	0.39	0	5,5,5	0.79	0
3	GOL	B	502	-	5,5,5	0.30	0	5,5,5	0.70	0
3	GOL	C	502	-	5,5,5	0.37	0	5,5,5	0.43	0
3	GOL	D	502	-	5,5,5	0.32	0	5,5,5	0.58	0
2	PO4	C	501	-	4,4,4	0.86	0	6,6,6	0.48	0
3	GOL	D	504	-	5,5,5	0.36	0	5,5,5	0.59	0
3	GOL	C	504	-	5,5,5	0.39	0	5,5,5	0.41	0
2	PO4	A	501	-	4,4,4	0.85	0	6,6,6	0.49	0
2	PO4	B	501	-	4,4,4	0.85	0	6,6,6	0.42	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	GOL	A	503	-	-	2/4/4/4	-
3	GOL	A	504	-	-	2/4/4/4	-
3	GOL	B	504	-	-	0/4/4/4	-
3	GOL	A	502	-	-	4/4/4/4	-
3	GOL	D	503	-	-	4/4/4/4	-
3	GOL	B	503	-	-	2/4/4/4	-
3	GOL	B	502	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	GOL	C	502	-	-	1/4/4/4	-
3	GOL	D	502	-	-	2/4/4/4	-
3	GOL	D	504	-	-	2/4/4/4	-
3	GOL	C	504	-	-	3/4/4/4	-
3	GOL	C	503	-	-	4/4/4/4	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

5 of 26 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	502	GOL	O1-C1-C2-C3
3	A	502	GOL	C1-C2-C3-O3
3	A	504	GOL	C1-C2-C3-O3
3	C	503	GOL	O1-C1-C2-C3
3	C	503	GOL	C1-C2-C3-O3

There are no ring outliers.

5 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	504	GOL	1	0
3	C	503	GOL	3	0
3	B	502	GOL	1	0
3	D	502	GOL	3	0
3	C	504	GOL	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 [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	268/269 (99%)	0.17	5 (1%) 66 71	13, 23, 33, 40	4 (1%)
1	B	264/269 (98%)	0.20	5 (1%) 66 71	13, 25, 33, 40	3 (1%)
1	C	264/269 (98%)	0.25	4 (1%) 72 76	14, 26, 38, 43	3 (1%)
1	D	264/269 (98%)	0.32	5 (1%) 66 71	20, 28, 40, 44	0
All	All	1060/1076 (98%)	0.23	19 (1%) 67 72	13, 26, 37, 44	10 (0%)

The worst 5 of 19 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	198	GLY	3.5
1	C	397	PHE	3.1
1	B	279	SER	2.7
1	B	268	ALA	2.7
1	D	279	SER	2.5

### 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	CXM	B	184[A]	11/12	0.84	0.14	25,25,25,26	8
1	CXM	B	184[B]	11/12	0.84	0.14	23,25,25,26	8
1	CXM	D	184[A]	11/12	0.85	0.14	26,29,29,29	8
1	CXM	D	184[B]	11/12	0.85	0.14	28,29,29,29	8
1	CXM	C	184[A]	11/12	0.90	0.12	30,32,32,32	8
1	CXM	C	184[B]	11/12	0.90	0.12	32,32,32,33	8
1	CXM	A	184[A]	11/12	0.90	0.11	17,20,20,21	8

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
1	CXM	A	184[B]	11/12	0.90	0.11	18,20,20,21	8

### 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, 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	PO4	A	501	5/5	0.69	0.14	66,66,66,66	0
2	PO4	C	501	5/5	0.71	0.17	71,71,71,72	0
2	PO4	D	501	5/5	0.77	0.13	68,68,68,68	0
3	GOL	D	502	6/6	0.80	0.16	32,34,34,35	0
3	GOL	D	504	6/6	0.80	0.14	34,34,35,35	0
2	PO4	B	501	5/5	0.82	0.16	60,61,61,61	0
3	GOL	D	503	6/6	0.84	0.13	31,33,34,35	0
3	GOL	C	503	6/6	0.85	0.12	37,39,39,40	0
3	GOL	A	504	6/6	0.85	0.12	37,38,38,38	0
3	GOL	A	502	6/6	0.87	0.13	35,36,36,37	0
3	GOL	C	504	6/6	0.89	0.14	40,41,41,41	0
3	GOL	A	503	6/6	0.89	0.10	33,34,35,35	0
3	GOL	B	504	6/6	0.91	0.09	34,35,35,35	0
3	GOL	B	503	6/6	0.92	0.07	29,29,30,30	0
3	GOL	C	502	6/6	0.95	0.08	25,26,26,26	0
3	GOL	B	502	6/6	0.95	0.08	20,22,24,25	0

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

There are no such residues in this entry.