



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 3, 2017 – 12:07 AM EST

PDB ID : 5U23  
Title : X-ray structure of the WlaRG aminotransferase from *Campylobacter jejuni* in complex with TDP-Qui3N  
Authors : Holden, H.M.; Thoden, J.B.; Dow, G.T.; Gilbert, M.  
Deposited on : 2016-11-29  
Resolution : 1.45 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](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 : 1.7.1 (RC1), CSD as537be (2016)  
Xtriage (Phenix) : 1.9-1692  
EDS : rb-20028442  
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) : rb-20028442

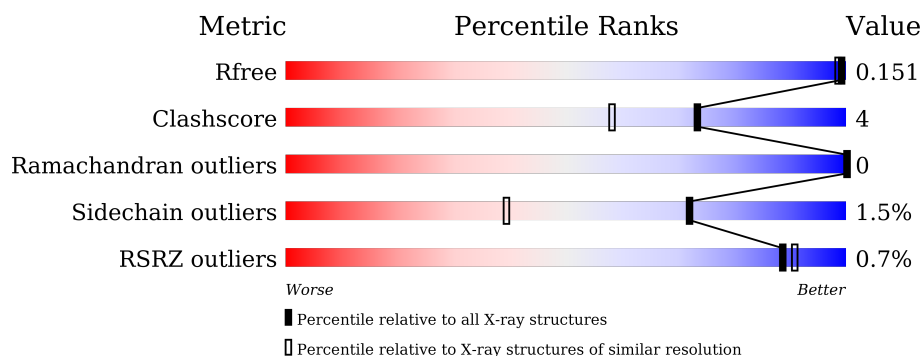
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.45 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))
$R_{free}$	91344	1278 (1.48-1.44)
Clashscore	102246	1336 (1.48-1.44)
Ramachandran outliers	100387	1320 (1.48-1.44)
Sidechain outliers	100360	1320 (1.48-1.44)
RSRZ outliers	91569	1279 (1.48-1.44)

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	382	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>87%</span> <span>7%</span> <span>5%</span> </div> </div>
1	B	382	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>87%</span> <span>7%</span> <span>5%</span> </div> </div>
1	C	382	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>85%</span> <span>9%</span> <span>5%</span> </div> </div>
1	D	382	<div> <div style="width: 100%; height: 10px; background: linear-gradient(to right, red, orange, yellow, green, grey);"></div> <div style="display: flex; justify-content: space-between; margin-top: 5px;"> <span>%</span> <span>88%</span> <span>8%</span> <span>•</span> </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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
6	MPO	C	407	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13733 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 aminotransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	C	361	Total	C	N	O	S	0	5	0
			2952	1901	496	540	15			
1	D	366	Total	C	N	O	S	0	3	0
			2984	1925	503	542	14			
1	A	361	Total	C	N	O	S	0	7	0
			2974	1914	503	542	15			
1	B	363	Total	C	N	O	S	0	5	0
			2986	1925	503	543	15			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-21	MET	-	initiating methionine	UNP Q9ALS9
C	-20	GLY	-	expression tag	UNP Q9ALS9
C	-19	SER	-	expression tag	UNP Q9ALS9
C	-18	SER	-	expression tag	UNP Q9ALS9
C	-17	HIS	-	expression tag	UNP Q9ALS9
C	-16	HIS	-	expression tag	UNP Q9ALS9
C	-15	HIS	-	expression tag	UNP Q9ALS9
C	-14	HIS	-	expression tag	UNP Q9ALS9
C	-13	HIS	-	expression tag	UNP Q9ALS9
C	-12	HIS	-	expression tag	UNP Q9ALS9
C	-11	SER	-	expression tag	UNP Q9ALS9
C	-10	SER	-	expression tag	UNP Q9ALS9
C	-9	ARG	-	expression tag	UNP Q9ALS9
C	-8	ASN	-	expression tag	UNP Q9ALS9
C	-7	LEU	-	expression tag	UNP Q9ALS9
C	-6	TYR	-	expression tag	UNP Q9ALS9
C	-5	PHE	-	expression tag	UNP Q9ALS9
C	-4	GLN	-	expression tag	UNP Q9ALS9
C	-3	GLY	-	expression tag	UNP Q9ALS9
C	-2	GLY	-	expression tag	UNP Q9ALS9
C	-1	GLY	-	expression tag	UNP Q9ALS9

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Chain	Residue	Modelled	Actual	Comment	Reference
C	0	HIS	-	expression tag	UNP Q9ALS9
D	-21	MET	-	initiating methionine	UNP Q9ALS9
D	-20	GLY	-	expression tag	UNP Q9ALS9
D	-19	SER	-	expression tag	UNP Q9ALS9
D	-18	SER	-	expression tag	UNP Q9ALS9
D	-17	HIS	-	expression tag	UNP Q9ALS9
D	-16	HIS	-	expression tag	UNP Q9ALS9
D	-15	HIS	-	expression tag	UNP Q9ALS9
D	-14	HIS	-	expression tag	UNP Q9ALS9
D	-13	HIS	-	expression tag	UNP Q9ALS9
D	-12	HIS	-	expression tag	UNP Q9ALS9
D	-11	SER	-	expression tag	UNP Q9ALS9
D	-10	SER	-	expression tag	UNP Q9ALS9
D	-9	ARG	-	expression tag	UNP Q9ALS9
D	-8	ASN	-	expression tag	UNP Q9ALS9
D	-7	LEU	-	expression tag	UNP Q9ALS9
D	-6	TYR	-	expression tag	UNP Q9ALS9
D	-5	PHE	-	expression tag	UNP Q9ALS9
D	-4	GLN	-	expression tag	UNP Q9ALS9
D	-3	GLY	-	expression tag	UNP Q9ALS9
D	-2	GLY	-	expression tag	UNP Q9ALS9
D	-1	GLY	-	expression tag	UNP Q9ALS9
D	0	HIS	-	expression tag	UNP Q9ALS9
A	-21	MET	-	initiating methionine	UNP Q9ALS9
A	-20	GLY	-	expression tag	UNP Q9ALS9
A	-19	SER	-	expression tag	UNP Q9ALS9
A	-18	SER	-	expression tag	UNP Q9ALS9
A	-17	HIS	-	expression tag	UNP Q9ALS9
A	-16	HIS	-	expression tag	UNP Q9ALS9
A	-15	HIS	-	expression tag	UNP Q9ALS9
A	-14	HIS	-	expression tag	UNP Q9ALS9
A	-13	HIS	-	expression tag	UNP Q9ALS9
A	-12	HIS	-	expression tag	UNP Q9ALS9
A	-11	SER	-	expression tag	UNP Q9ALS9
A	-10	SER	-	expression tag	UNP Q9ALS9
A	-9	ARG	-	expression tag	UNP Q9ALS9
A	-8	ASN	-	expression tag	UNP Q9ALS9
A	-7	LEU	-	expression tag	UNP Q9ALS9
A	-6	TYR	-	expression tag	UNP Q9ALS9
A	-5	PHE	-	expression tag	UNP Q9ALS9
A	-4	GLN	-	expression tag	UNP Q9ALS9
A	-3	GLY	-	expression tag	UNP Q9ALS9

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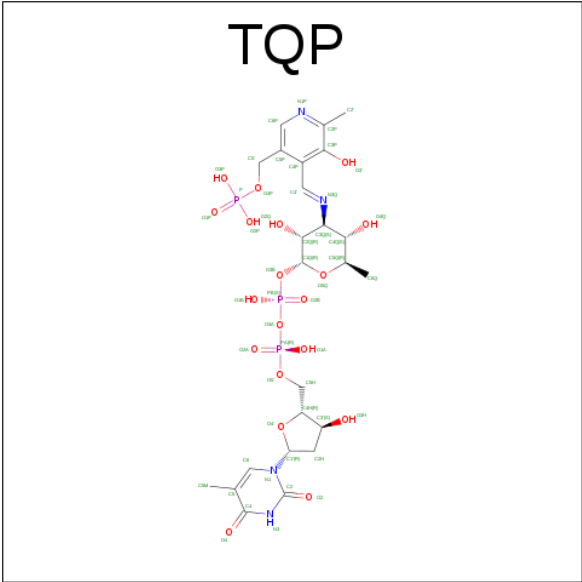
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Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	GLY	-	expression tag	UNP Q9ALS9
A	-1	GLY	-	expression tag	UNP Q9ALS9
A	0	HIS	-	expression tag	UNP Q9ALS9
B	-21	MET	-	initiating methionine	UNP Q9ALS9
B	-20	GLY	-	expression tag	UNP Q9ALS9
B	-19	SER	-	expression tag	UNP Q9ALS9
B	-18	SER	-	expression tag	UNP Q9ALS9
B	-17	HIS	-	expression tag	UNP Q9ALS9
B	-16	HIS	-	expression tag	UNP Q9ALS9
B	-15	HIS	-	expression tag	UNP Q9ALS9
B	-14	HIS	-	expression tag	UNP Q9ALS9
B	-13	HIS	-	expression tag	UNP Q9ALS9
B	-12	HIS	-	expression tag	UNP Q9ALS9
B	-11	SER	-	expression tag	UNP Q9ALS9
B	-10	SER	-	expression tag	UNP Q9ALS9
B	-9	ARG	-	expression tag	UNP Q9ALS9
B	-8	ASN	-	expression tag	UNP Q9ALS9
B	-7	LEU	-	expression tag	UNP Q9ALS9
B	-6	TYR	-	expression tag	UNP Q9ALS9
B	-5	PHE	-	expression tag	UNP Q9ALS9
B	-4	GLN	-	expression tag	UNP Q9ALS9
B	-3	GLY	-	expression tag	UNP Q9ALS9
B	-2	GLY	-	expression tag	UNP Q9ALS9
B	-1	GLY	-	expression tag	UNP Q9ALS9
B	0	HIS	-	expression tag	UNP Q9ALS9

- Molecule 2 is SODIUM ION (three-letter code: NA) (formula: Na).

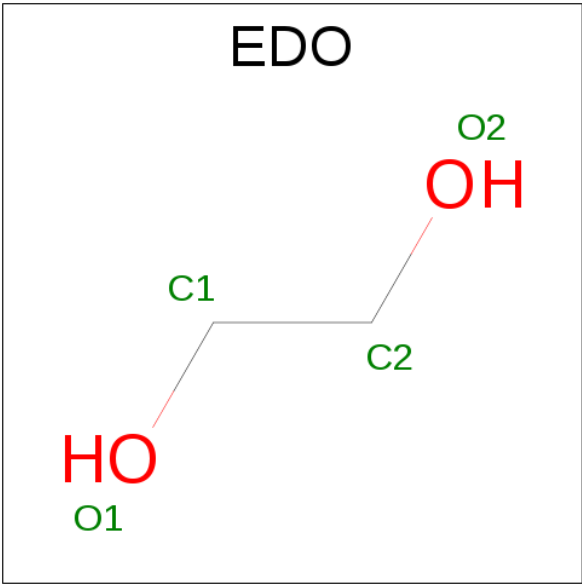
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	B	1	Total Na 1 1	0	0
2	C	1	Total Na 1 1	0	0

- Molecule 3 is (2R,3R,4S,5S,6R)-3,5-dihydroxy-4-[(1E)-{3-hydroxy-2-methyl-5-[(phosphono oxy)methyl]pyridin-4-yl)methylidene]amino}-6-methyltetrahydro-2H-pyran-2-yl [(2R,3S,5R)-3-hydroxy-5-(5-methyl-2,4-dioxo-3,4-dihydropyrimidin-1(2H)-yl)tetrahydrofuran-2-yl)methyl dihydrogen diphosphate (three-letter code: TQP) (formula: C<sub>24</sub>H<sub>35</sub>N<sub>4</sub>O<sub>19</sub>P<sub>3</sub>).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
3	C	1	Total	C	N	O	P	0	0
			50	24	4	19	3		
3	D	1	Total	C	N	O	P	0	0
			50	24	4	19	3		
3	A	1	Total	C	N	O	P	0	0
			50	24	4	19	3		
3	B	1	Total	C	N	O	P	0	0
			50	24	4	19	3		

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

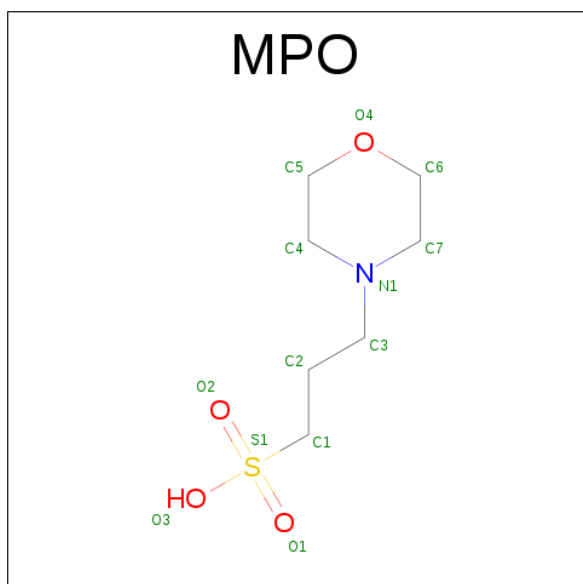


Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	D	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0

- Molecule 5 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total Cl 1 1	0	0

- Molecule 6 is 3[N-MORPHOLINO]PROPANE SULFONIC ACID (three-letter code: MPO) (formula: C<sub>7</sub>H<sub>15</sub>NO<sub>4</sub>S).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	C	1	Total C N O S 13 7 1 4 1	0	0



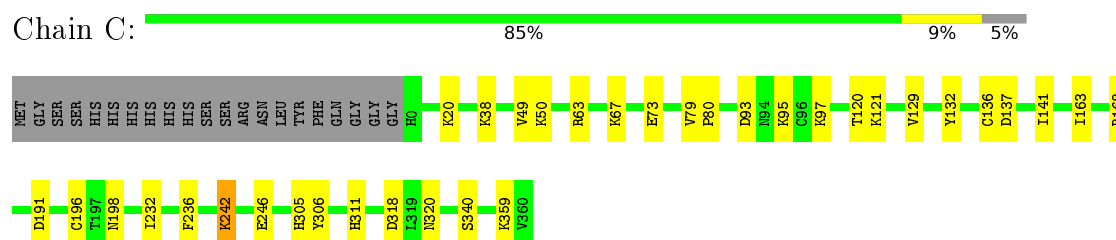
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	C	439	Total 439	O 439	0	0
7	D	399	Total 399	O 399	0	0
7	A	391	Total 391	O 391	0	0
7	B	364	Total 364	O 364	0	0

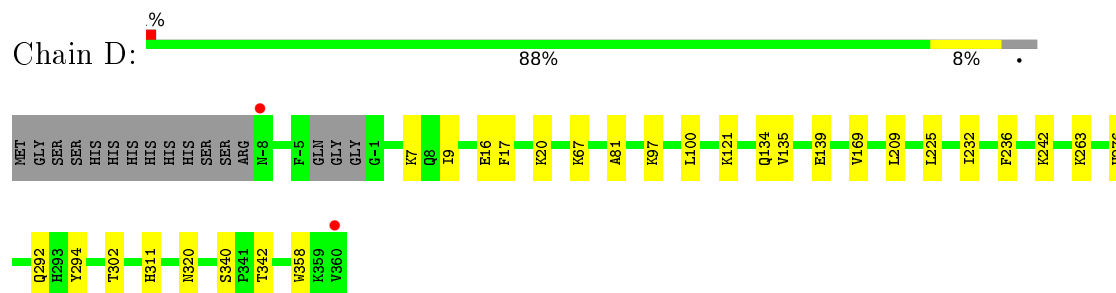
### 3 Residue-property plots [i](#)

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.

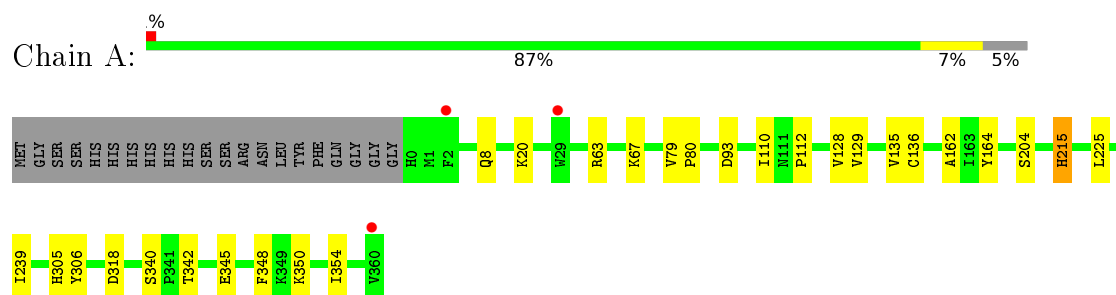
- Molecule 1: Putative aminotransferase



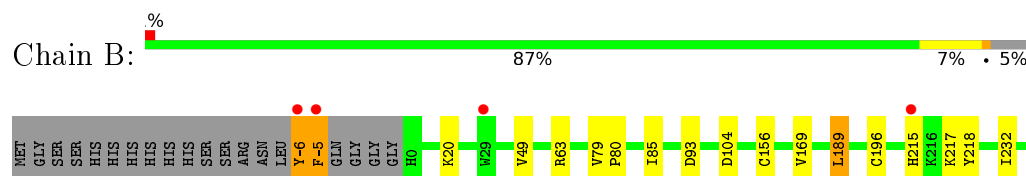
- Molecule 1: Putative aminotransferase



- Molecule 1: Putative aminotransferase



- Molecule 1: Putative aminotransferase





## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	107.82Å 56.64Å 124.55Å 90.00° 90.01° 90.00°	Depositor
Resolution (Å)	29.92 – 1.45 29.92 – 1.45	Depositor EDS
% Data completeness (in resolution range)	98.2 (29.92-1.45) 99.6 (29.92-1.45)	Depositor EDS
$R_{merge}$	0.08	Depositor
$R_{sym}$	0.08	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.36 (at 1.45Å)	Xtriage
Refinement program	REFMAC 5.8.0124	Depositor
R, $R_{free}$	0.127 , 0.153 0.133 , 0.151	Depositor DCC
$R_{free}$ test set	13149 reflections (5.22%)	DCC
Wilson B-factor (Å <sup>2</sup> )	9.8	Xtriage
Anisotropy	0.053	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 43.9	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.018 for h,-k,-l	Xtriage
Reported twinning fraction	0.383 for H, K, L 0.617 for -H, -K, L	Depositor
Outliers	4 of 265441 reflections (0.002%)	Xtriage
$F_o, F_c$ correlation	0.97	EDS
Total number of atoms	13733	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	13.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 9.13% 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: NA, MPO, TQP, EDO, CL

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	0.52	0/3049	0.83	0/4115
1	B	0.52	0/3052	0.82	1/4118 (0.0%)
1	C	0.57	0/3029	0.85	2/4089 (0.0%)
1	D	0.56	0/3057	0.86	1/4125 (0.0%)
All	All	0.54	0/12187	0.84	4/16447 (0.0%)

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	132	TYR	CB-CG-CD1	7.32	125.39	121.00
1	C	191	ASP	CB-CG-OD2	6.91	124.51	118.30
1	D	17	PHE	CB-CG-CD2	-5.30	117.09	120.80
1	B	104	ASP	CB-CG-OD1	5.15	122.94	118.30

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	2974	0	3010	20	0
1	B	2986	0	3016	28	0
1	C	2952	0	2988	29	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	2984	0	3014	23	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	50	0	30	0	0
3	B	50	0	30	0	0
3	C	50	0	30	0	0
3	D	50	0	30	0	0
4	A	4	0	6	0	0
4	B	8	0	12	0	0
4	C	12	0	18	0	0
4	D	4	0	6	0	0
5	C	1	0	0	0	0
6	C	13	0	14	2	0
7	A	391	0	0	2	0
7	B	364	0	0	6	1
7	C	439	0	0	9	1
7	D	399	0	0	8	0
All	All	13733	0	12204	100	1

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 4.

All (100) 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:C:63:ARG:HD2	1:C:93:ASP:OD2	1.41	1.16
1:A:63:ARG:HD2	1:A:93:ASP:OD2	1.45	1.15
1:B:63:ARG:HD2	1:B:93:ASP:OD2	1.53	1.09
1:C:141:ILE:HG13	7:C:501:HOH:O	1.52	1.08
1:B:-5:PHE:CE1	1:B:293:HIS:CE1	2.54	0.95
1:A:63:ARG:CD	1:A:93:ASP:OD2	2.19	0.90
1:B:-5:PHE:HE1	1:B:293:HIS:CE1	1.90	0.86
1:C:121:LYS:HD3	6:C:407:MPO:O2	1.81	0.79
1:C:163:ILE:HG23	7:C:763:HOH:O	1.84	0.77
1:A:128:VAL:CG2	1:A:136[B]:CYS:SG	2.73	0.77
1:A:128:VAL:HG22	1:A:136[B]:CYS:SG	2.25	0.76
1:B:272:ASN:ND2	7:B:501:HOH:O	2.20	0.71
1:B:63:ARG:CD	1:B:93:ASP:OD2	2.37	0.70
1:D:9:ILE:CD1	1:D:342:THR:OG1	2.39	0.70
1:B:289:ASP:HB3	7:B:627:HOH:O	1.93	0.69
1:B:85:ILE:HD11	1:B:316:TYR:HE2	1.56	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:137:ASP:O	7:C:501:HOH:O	2.13	0.66
1:D:16:GLU:HG3	7:D:516:HOH:O	1.94	0.66
1:B:156:CYS:SG	1:B:169:VAL:HG13	2.35	0.66
1:B:85:ILE:HD11	1:B:316:TYR:CE2	2.30	0.66
1:C:246:GLU:HG3	7:C:554:HOH:O	1.96	0.66
1:B:215:HIS:HD2	7:B:685:HOH:O	1.79	0.65
1:B:272:ASN:OD1	7:B:501:HOH:O	2.16	0.62
1:B:20:LYS:HG3	1:B:239:ILE:HD11	1.80	0.61
1:B:85:ILE:HD12	1:B:310:PRO:HB3	1.82	0.61
1:C:318:ASP:HB2	7:C:800:HOH:O	2.01	0.60
1:B:-5:PHE:CZ	1:B:293:HIS:CE1	2.90	0.59
1:C:63:ARG:CD	1:C:93:ASP:OD2	2.35	0.59
1:C:163:ILE:CG2	7:C:763:HOH:O	2.46	0.59
1:D:232[A]:ILE:HG22	1:D:236:PHE:CE2	2.38	0.59
1:C:232:ILE:HG22	1:C:236:PHE:CE2	2.38	0.59
1:C:232:ILE:CG2	1:C:236:PHE:CE2	2.86	0.58
1:C:67:LYS:HE2	7:C:876:HOH:O	2.03	0.57
1:C:63:ARG:HD2	1:C:93:ASP:CG	2.21	0.56
1:B:345:GLU:HA	1:B:348:PHE:CE2	2.41	0.55
1:B:49:VAL:HG21	1:B:196:CYS:HB3	1.89	0.55
1:D:232[A]:ILE:CG2	1:D:236:PHE:CE2	2.90	0.55
1:B:232:ILE:CG2	1:B:236:PHE:CE2	2.91	0.54
1:B:-5:PHE:CD1	1:B:-5:PHE:N	2.75	0.54
1:D:67:LYS:HE2	1:D:209:LEU:HD22	1.90	0.54
1:B:232:ILE:HG22	1:B:236:PHE:CE2	2.43	0.53
1:D:135:VAL:HG23	1:D:169:VAL:HG12	1.92	0.52
1:B:345:GLU:HA	1:B:348:PHE:CZ	2.45	0.52
1:C:93:ASP:OD1	7:C:503:HOH:O	2.19	0.52
1:D:9:ILE:HD13	1:D:342:THR:OG1	2.09	0.51
1:A:129:VAL:O	1:A:136[B]:CYS:SG	2.69	0.50
1:B:-5:PHE:HZ	1:B:293:HIS:CG	2.29	0.50
1:A:20:LYS:HG3	1:A:239:ILE:HD11	1.93	0.50
1:B:272:ASN:CG	7:B:501:HOH:O	2.46	0.50
1:A:110:ILE:O	1:A:112:PRO:HD3	2.11	0.50
1:D:9:ILE:HD12	1:D:342:THR:OG1	2.12	0.50
1:A:135[A]:VAL:HG13	1:A:162:ALA:HB1	1.94	0.50
1:A:8:GLN:HG2	1:A:342:THR:OG1	2.13	0.49
1:B:232:ILE:HG23	1:B:236:PHE:CZ	2.47	0.49
1:C:163:ILE:CD1	1:C:168:ARG:HD3	2.42	0.49
1:D:7:LYS:HE2	7:D:547:HOH:O	2.13	0.49
1:B:-6:TYR:HA	7:B:555:HOH:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:135[B]:VAL:HG11	1:A:164:TYR:HB2	1.93	0.48
1:D:242:LYS:HD2	7:D:828:HOH:O	2.12	0.48
1:A:305:HIS:HA	1:A:306:TYR:CD1	2.49	0.48
1:D:232[A]:ILE:HG23	1:D:236:PHE:CZ	2.48	0.48
1:D:121:LYS:HG2	7:D:826:HOH:O	2.13	0.48
1:C:49:VAL:HG21	1:C:196:CYS:HB3	1.96	0.48
1:C:232:ILE:HG23	1:C:236:PHE:CZ	2.48	0.47
1:A:350:LYS:HG2	1:A:354:ILE:HD12	1.95	0.47
1:D:292:GLN:HG3	1:D:302:THR:OG1	2.14	0.47
1:C:232:ILE:CG2	1:C:236:PHE:CZ	2.98	0.47
1:D:232[A]:ILE:CG2	1:D:236:PHE:CZ	2.98	0.46
1:C:137:ASP:HB2	7:C:787:HOH:O	2.15	0.46
1:C:305:HIS:HA	1:C:306:TYR:CD1	2.50	0.45
1:B:189:LEU:HD22	1:B:236:PHE:CD2	2.52	0.45
1:C:163:ILE:HD11	1:C:168:ARG:CD	2.47	0.45
1:A:135[A]:VAL:CG1	1:A:162:ALA:HB1	2.47	0.45
1:C:50:LYS:HE2	1:C:198:ASN:O	2.17	0.45
1:C:311:HIS:O	1:C:320:ASN:HA	2.18	0.44
1:B:79:VAL:CG2	1:B:80:PRO:HD2	2.47	0.43
1:C:129:VAL:O	1:C:136[B]:CYS:SG	2.77	0.43
1:C:242:LYS:HE2	1:C:242:LYS:HB3	1.52	0.43
1:A:345:GLU:HA	1:A:348:PHE:CZ	2.54	0.42
1:D:134:GLN:HB2	1:D:276:HIS:CD2	2.55	0.42
1:A:128:VAL:HG23	1:A:136[B]:CYS:SG	2.58	0.42
1:A:67:LYS:HE3	7:A:829:HOH:O	2.19	0.42
1:A:79:VAL:CG2	1:A:80:PRO:HD2	2.50	0.42
1:C:163:ILE:HD11	1:C:168:ARG:HD3	2.02	0.42
1:C:79:VAL:CG2	1:C:80:PRO:HD2	2.49	0.42
1:B:217:LYS:O	1:B:218:TYR:HB2	2.19	0.42
1:D:294:TYR:CE2	1:D:358:TRP:HB2	2.54	0.41
1:C:120:THR:O	6:C:407:MPO:H12	2.19	0.41
1:D:9:ILE:HD13	1:D:9:ILE:N	2.35	0.41
1:A:79:VAL:HG23	1:A:80:PRO:HD2	2.03	0.41
1:D:97:LYS:HG2	7:D:535:HOH:O	2.20	0.41
1:D:20:LYS:HD2	7:D:521:HOH:O	2.20	0.41
1:D:311:HIS:O	1:D:320:ASN:HA	2.21	0.41
1:B:85:ILE:CD1	1:B:310:PRO:HB3	2.50	0.41
1:C:73:GLU:HG3	1:C:95:LYS:HB3	2.02	0.41
1:A:204[A]:SER:OG	1:A:215:HIS:CE1	2.74	0.40
1:A:67:LYS:CE	7:A:829:HOH:O	2.68	0.40
1:D:67:LYS:HD3	7:D:842:HOH:O	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:97:LYS:HE2	7:D:535:HOH:O	2.21	0.40
1:D:81:ALA:HB2	1:D:100:LEU:HB3	2.04	0.40

All (1) 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)
7:C:505:HOH:O	7:B:501:HOH:O[1_556]	2.12	0.08

## 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	366/382 (96%)	356 (97%)	10 (3%)	0	100	100
1	B	364/382 (95%)	351 (96%)	13 (4%)	0	100	100
1	C	364/382 (95%)	351 (96%)	13 (4%)	0	100	100
1	D	365/382 (96%)	355 (97%)	10 (3%)	0	100	100
All	All	1459/1528 (96%)	1413 (97%)	46 (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	329/339 (97%)	325 (99%)	4 (1%)	78	48
1	B	328/339 (97%)	323 (98%)	5 (2%)	72	39
1	C	326/339 (96%)	320 (98%)	6 (2%)	66	30
1	D	327/339 (96%)	323 (99%)	4 (1%)	78	48
All	All	1310/1356 (97%)	1291 (98%)	19 (2%)	72	39

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	20	LYS
1	C	38	LYS
1	C	97	LYS
1	C	242	LYS
1	C	340	SER
1	C	359	LYS
1	D	139	GLU
1	D	225	LEU
1	D	263	LYS
1	D	340	SER
1	A	215	HIS
1	A	225	LEU
1	A	318	ASP
1	A	340	SER
1	B	-6	TYR
1	B	-5	PHE
1	B	189	LEU
1	B	296	ASN
1	B	340	SER

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	8	GLN
1	D	74	ASN
1	D	201	ASN
1	D	253	ASN
1	D	298	HIS
1	A	8	GLN
1	A	201	ASN
1	A	215	HIS

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Mol	Chain	Res	Type
1	A	253	ASN
1	A	256	ASN
1	A	260	GLN
1	A	293	HIS
1	A	297	ASN
1	B	215	HIS
1	B	253	ASN
1	B	296	ASN
1	B	321	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

## 5.6 Ligand geometry ⓘ

Of 15 ligands modelled in this entry, 3 are monoatomic - leaving 12 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	TQP	A	401	-	46,53,53	1.69	3 (6%)	60,81,81	1.86	8 (13%)
4	EDO	A	402	-	3,3,3	0.63	0	2,2,2	0.57	0
3	TQP	B	402	-	46,53,53	1.89	4 (8%)	60,81,81	2.13	10 (16%)
4	EDO	B	403	-	3,3,3	0.51	0	2,2,2	0.29	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	EDO	B	404	-	3,3,3	0.47	0	2,2,2	0.29	0
3	TQP	C	402	-	46,53,53	2.05	4 (8%)	60,81,81	2.33	13 (21%)
4	EDO	C	403	-	3,3,3	0.48	0	2,2,2	0.25	0
4	EDO	C	404	-	3,3,3	0.54	0	2,2,2	0.20	0
4	EDO	C	405	-	3,3,3	0.42	0	2,2,2	0.63	0
6	MPO	C	407	-	13,13,13	2.38	2 (15%)	16,17,17	3.16	5 (31%)
3	TQP	D	401	-	46,53,53	1.40	4 (8%)	60,81,81	2.20	11 (18%)
4	EDO	D	402	-	3,3,3	0.51	0	2,2,2	0.26	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	TQP	A	401	-	-	1/28/64/64	0/4/4/4
4	EDO	A	402	-	-	0/1/1/1	0/0/0/0
3	TQP	B	402	-	-	1/28/64/64	0/4/4/4
4	EDO	B	403	-	-	0/1/1/1	0/0/0/0
4	EDO	B	404	-	-	0/1/1/1	0/0/0/0
3	TQP	C	402	-	-	0/28/64/64	0/4/4/4
4	EDO	C	403	-	-	0/1/1/1	0/0/0/0
4	EDO	C	404	-	-	0/1/1/1	0/0/0/0
4	EDO	C	405	-	-	0/1/1/1	0/0/0/0
6	MPO	C	407	-	-	0/7/15/15	0/1/1/1
3	TQP	D	401	-	-	1/28/64/64	0/4/4/4
4	EDO	D	402	-	-	0/1/1/1	0/0/0/0

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	C	407	MPO	C1-S1	-5.39	1.69	1.77
3	C	402	TQP	C2-N3	-2.36	1.33	1.38
3	D	401	TQP	C2-N3	-2.28	1.33	1.38
3	B	402	TQP	C2-N3	-2.23	1.33	1.38
3	D	401	TQP	C4P-C3P	3.37	1.45	1.40
3	D	401	TQP	C4P-C5P	4.02	1.47	1.42
3	B	402	TQP	C4P-C3P	4.15	1.46	1.40
3	B	402	TQP	C4P-C5P	4.20	1.47	1.42
3	A	401	TQP	C4P-C3P	4.25	1.46	1.40
3	C	402	TQP	C4P-C5P	4.40	1.47	1.42
3	A	401	TQP	C4P-C5P	4.99	1.48	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	402	TQP	C4P-C3P	5.67	1.48	1.40
6	C	407	MPO	O1-S1	6.36	1.63	1.45
3	D	401	TQP	C3P-C2P	6.70	1.45	1.40
3	A	401	TQP	C3P-C2P	8.55	1.46	1.40
3	B	402	TQP	C3P-C2P	10.54	1.48	1.40
3	C	402	TQP	C3P-C2P	10.67	1.48	1.40

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	TQP	C5-C4-N3	-9.08	117.72	125.35
3	D	401	TQP	C5-C4-N3	-8.28	118.40	125.35
3	B	402	TQP	C5-C4-N3	-8.04	118.60	125.35
3	A	401	TQP	C5-C4-N3	-7.44	119.11	125.35
3	C	402	TQP	O3A-PB-O3B	-6.84	89.82	102.05
3	B	402	TQP	C3P-C4P-C5P	-5.18	114.51	118.26
3	D	401	TQP	O3A-PB-O3B	-5.14	92.85	102.05
3	B	402	TQP	O3A-PB-O3B	-5.09	92.94	102.05
3	C	402	TQP	C3P-C4P-C5P	-5.02	114.63	118.26
3	A	401	TQP	O3A-PB-O3B	-4.50	94.00	102.05
3	D	401	TQP	C3P-C4P-C5P	-4.40	115.07	118.26
3	D	401	TQP	C2'-C2P-C3P	-3.27	117.59	120.90
6	C	407	MPO	O2-S1-O1	-3.12	105.14	113.96
6	C	407	MPO	C6-C7-N1	-2.92	105.65	110.11
3	C	402	TQP	C2'-C2P-C3P	-2.81	118.06	120.90
3	A	401	TQP	C3P-C4P-C5P	-2.56	116.41	118.26
3	D	401	TQP	C1Q-O5Q-C5Q	-2.52	109.14	113.76
3	A	401	TQP	C2'-C2P-C3P	-2.51	118.36	120.90
3	D	401	TQP	O5Q-C1Q-C2Q	-2.47	105.15	110.28
3	D	401	TQP	P-O4P-C5'	-2.37	115.31	120.79
3	D	401	TQP	C2H-C1'-N1	-2.34	108.36	114.14
3	C	402	TQP	O5Q-C1Q-O3B	-2.26	108.38	111.36
3	C	402	TQP	C6Q-C5Q-C4Q	-2.22	108.72	113.02
3	C	402	TQP	O5'-PA-O2A	-2.13	100.51	109.21
3	B	402	TQP	C6Q-C5Q-C4Q	-2.12	108.91	113.02
3	A	401	TQP	O3P-P-O1P	2.00	117.17	110.63
3	B	402	TQP	O1B-PB-O3A	2.01	113.90	105.27
3	B	402	TQP	O1B-PB-O2B	2.03	123.14	112.56
3	C	402	TQP	C2H-C3'-C4H	2.05	106.93	102.77
3	A	401	TQP	O1B-PB-O2B	2.07	123.35	112.56
3	C	402	TQP	C1Q-O5Q-C5Q	2.12	117.64	113.76
3	B	402	TQP	C5P-C4P-C4'	2.18	124.79	121.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	402	TQP	O3P-P-O1P	2.25	117.96	110.63
3	C	402	TQP	C2'-C2P-N1P	2.40	123.26	117.96
6	C	407	MPO	C3-N1-C7	2.77	117.29	111.25
3	D	401	TQP	O5Q-C1Q-O3B	3.31	115.72	111.36
3	B	402	TQP	O3'-C3P-C2P	3.47	122.62	117.53
3	A	401	TQP	C3Q-N3Q-C4'	4.90	125.42	118.70
6	C	407	MPO	O2-S1-C1	5.03	110.42	106.87
3	B	402	TQP	C3Q-N3Q-C4'	5.11	125.71	118.70
3	C	402	TQP	C3Q-N3Q-C4'	5.17	125.79	118.70
3	D	401	TQP	C3Q-N3Q-C4'	5.73	126.56	118.70
3	A	401	TQP	C4-N3-C2	7.14	121.12	115.16
3	B	402	TQP	C4-N3-C2	7.63	121.52	115.16
3	D	401	TQP	C4-N3-C2	7.87	121.72	115.16
3	C	402	TQP	C4-N3-C2	7.94	121.78	115.16
6	C	407	MPO	O1-S1-C1	9.90	113.87	106.87

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	402	TQP	C4Q-C3Q-N3Q-C4'
3	D	401	TQP	C4Q-C3Q-N3Q-C4'
3	A	401	TQP	C4Q-C3Q-N3Q-C4'

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	407	MPO	2	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	361/382 (94%)	-0.46	3 (0%) 87 89	5, 11, 24, 42	0
1	B	363/382 (95%)	-0.39	5 (1%) 78 79	5, 11, 27, 34	0
1	C	361/382 (94%)	-0.52	0 100 100	4, 9, 20, 33	0
1	D	366/382 (95%)	-0.49	2 (0%) 91 94	4, 10, 23, 59	0
All	All	1451/1528 (94%)	-0.46	10 (0%) 89 91	4, 10, 23, 59	0

All (10) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	-5	PHE	4.5
1	D	360	VAL	3.8
1	A	360	VAL	3.2
1	D	-8	ASN	3.0
1	B	-6	TYR	2.8
1	B	215	HIS	2.8
1	B	360	VAL	2.5
1	A	29	TRP	2.1
1	B	29	TRP	2.1
1	A	2	PHE	2.0

### 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(Å <sup>2</sup> )	Q<0.9
6	MPO	C	407	13/13	0.95	0.20	8.22	23,26,31,35	0
4	EDO	C	405	4/4	0.93	0.10	1.76	18,18,23,26	0
2	NA	C	401	1/1	0.99	0.07	1.27	5,5,5,5	0
2	NA	B	401	1/1	1.00	0.07	0.88	5,5,5,5	0
4	EDO	C	403	4/4	0.96	0.08	0.28	12,15,15,20	0
4	EDO	A	402	4/4	0.96	0.07	0.19	12,16,17,20	0
4	EDO	C	404	4/4	0.98	0.06	0.19	8,9,10,11	0
4	EDO	B	403	4/4	0.98	0.07	0.08	12,12,12,20	0
4	EDO	D	402	4/4	0.93	0.07	-0.02	23,24,25,27	0
3	TQP	D	401	50/50	0.97	0.07	-0.28	5,11,19,27	0
3	TQP	B	402	50/50	0.97	0.07	-0.33	6,11,19,24	0
3	TQP	A	401	50/50	0.98	0.07	-0.39	6,10,15,22	0
3	TQP	C	402	50/50	0.98	0.07	-0.51	6,9,13,18	0
4	EDO	B	404	4/4	0.99	0.05	-1.91	10,10,11,13	0
5	CL	C	406	1/1	1.00	0.04	-	11,11,11,11	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.