



## Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2018 – 04:52 pm GMT

PDB ID : 4D0T  
Title : GalNAc-T2 crystal soaked with UDP-GalNAc, EA2 peptide and manganese  
Authors : Lira-Navarrete, E.; Iglesias-Fernandez, J.; Zandberg, W.F.; Companon, I.; Kong, Y.; Corzana, F.; Pinto, B.M.; Clausen, H.; Peregrina, J.M.; Vocadlo, D.; Rovira, C.; Hurtado-Guerrero, R.  
Deposited on : 2014-04-30  
Resolution : 2.45 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

<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	:	1.7.3 (157068), CSD as539be (2018)
Xtriage (Phenix)	:	1.13
EDS	:	trunk30967
Percentile statistics	:	20171227.v01 (using entries in the PDB archive December 27th 2017)
Refmac	:	5.8.0158
CCP4	:	7.0 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk30967

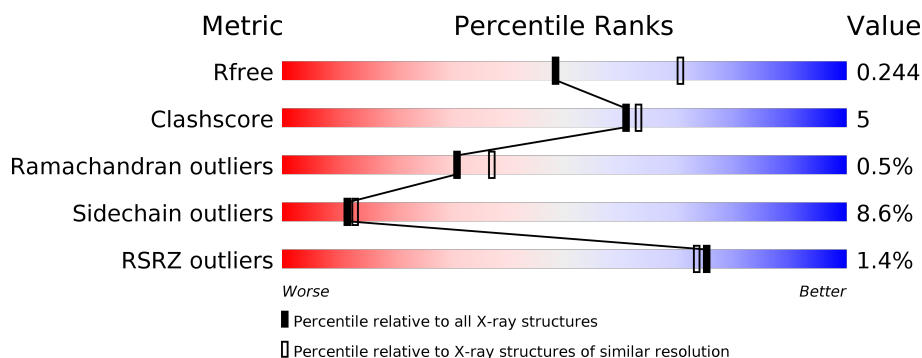
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.45 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))
$R_{free}$	111664	1259 (2.48-2.44)
Clashscore	122126	1323 (2.48-2.44)
Ramachandran outliers	120053	1314 (2.48-2.44)
Sidechain outliers	120020	1314 (2.48-2.44)
RSRZ outliers	108989	1238 (2.48-2.44)

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	571	<div> <div>73%</div> <div>11% • 13%</div> </div>
1	B	571	<div> <div>74%</div> <div>11% • 13%</div> </div>
1	C	571	<div> <div>%</div> <div>74%</div> <div>11% • 13%</div> </div>
1	D	571	<div> <div>%</div> <div>72%</div> <div>12% • 13%</div> </div>
1	E	571	<div> <div>74%</div> <div>10% • 13%</div> </div>
1	F	571	<div> <div>3%</div> <div>70%</div> <div>13% • 15%</div> </div>

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Mol	Chain	Length	Quality of chain
2	P	8	
2	Z	8	

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
7	NGA	P	1572	X	-	-	-

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 24500 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 POLYPEPTIDE N-ACETYL GALACTOSAMINYLTRANSFERASE 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	496	Total	C	N	O	S	0	0	0
			3956	2490	718	724	24			
1	B	495	Total	C	N	O	S	0	0	0
			3947	2485	716	722	24			
1	C	495	Total	C	N	O	S	0	1	0
			3955	2490	719	722	24			
1	D	495	Total	C	N	O	S	0	3	0
			3967	2498	720	725	24			
1	E	495	Total	C	N	O	S	0	0	0
			3947	2485	716	722	24			
1	F	487	Total	C	N	O	S	0	0	0
			3892	2449	707	712	24			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	516	ASP	ASN	engineered mutation	UNP Q10471
B	516	ASP	ASN	engineered mutation	UNP Q10471
C	516	ASP	ASN	engineered mutation	UNP Q10471
D	516	ASP	ASN	engineered mutation	UNP Q10471
E	516	ASP	ASN	engineered mutation	UNP Q10471
F	516	ASP	ASN	engineered mutation	UNP Q10471

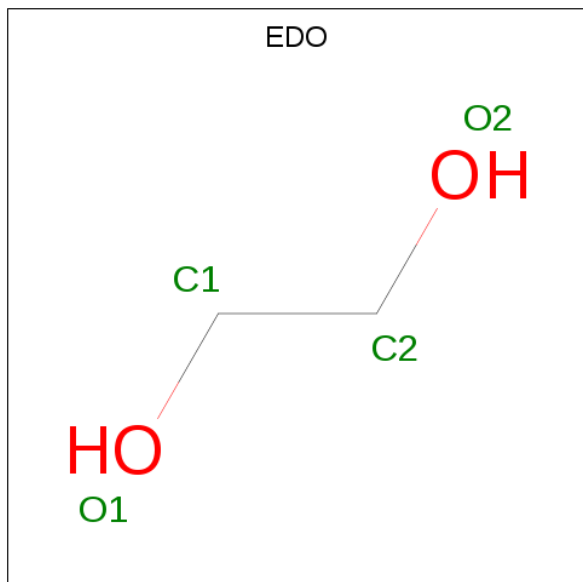
- Molecule 2 is a protein called PEPTIDE.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	P	7	Total	C	N	O	0	0	0
			47	28	7	12			
2	Z	6	Total	C	N	O	0	0	0
			40	25	6	9			

- Molecule 3 is MANGANESE (II) ION (three-letter code: MN) (formula: Mn).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	1	Total Mn 1 1	0	0
3	E	1	Total Mn 1 1	0	0
3	B	1	Total Mn 1 1	0	0
3	C	1	Total Mn 1 1	0	0
3	A	1	Total Mn 1 1	0	0
3	F	1	Total Mn 1 1	0	0

- Molecule 4 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



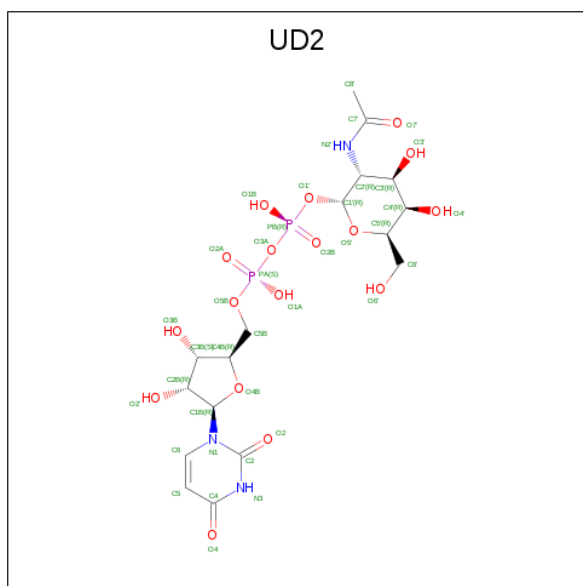
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 4 2 2	0	0
4	A	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	B	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0
4	C	1	Total C O 4 2 2	0	0

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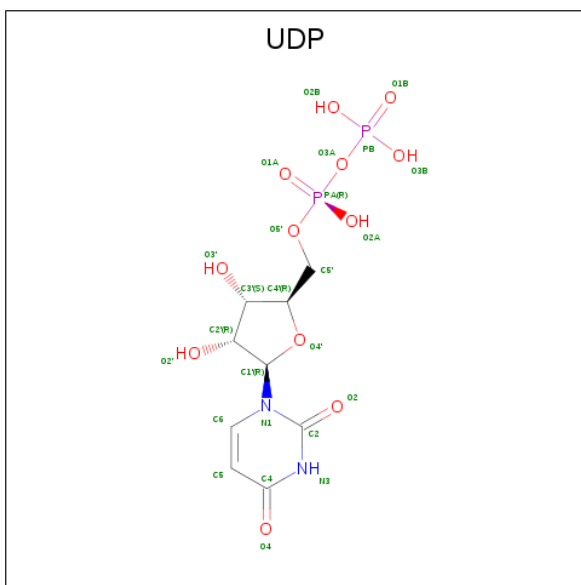
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	D	1	Total	C	O	0	0
			4	2	2		
4	D	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		
4	E	1	Total	C	O	0	0
			4	2	2		

- Molecule 5 is URIDINE-DIPHOSPHATE-N-ACETYLGLACTOSAMINE (three-letter code: UD2) (formula:  $C_{17}H_{27}N_3O_{17}P_2$ ).



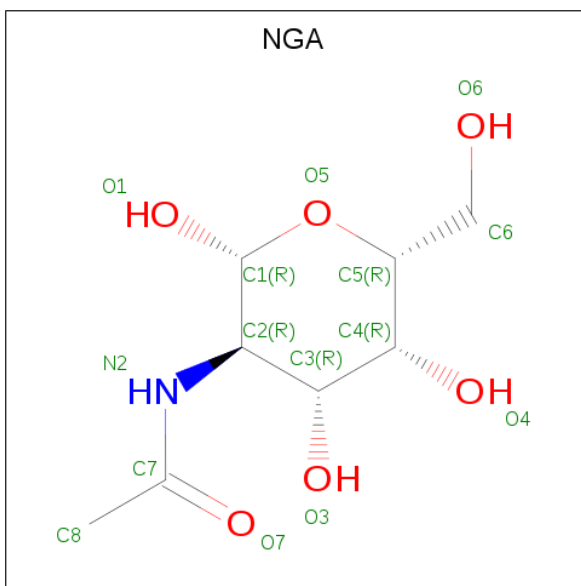
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
5	A	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
5	B	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
5	D	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
5	E	1	Total	C	N	O	P	0	0
			39	17	3	17	2		
5	F	1	Total	C	N	O	P	0	0
			39	17	3	17	2		

- Molecule 6 is URIDINE-5'-DIPHOSPHATE (three-letter code: UDP) (formula:  $C_9H_{14}N_2O_{12}P_2$ ).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	N	O	P	0	0
			25	9	2	12	2		

- Molecule 7 is N-ACETYL-D-GALACTOSAMINE (three-letter code: NGA) (formula:  $C_8H_{15}NO_6$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
7	P	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	108	Total 108	O 108	0	0
8	B	99	Total 99	O 99	0	0
8	C	67	Total 67	O 67	0	0
8	D	55	Total 55	O 55	0	0
8	E	105	Total 105	O 105	0	0
8	F	34	Total 34	O 34	0	0
8	P	1	Total 1	O 1	0	0

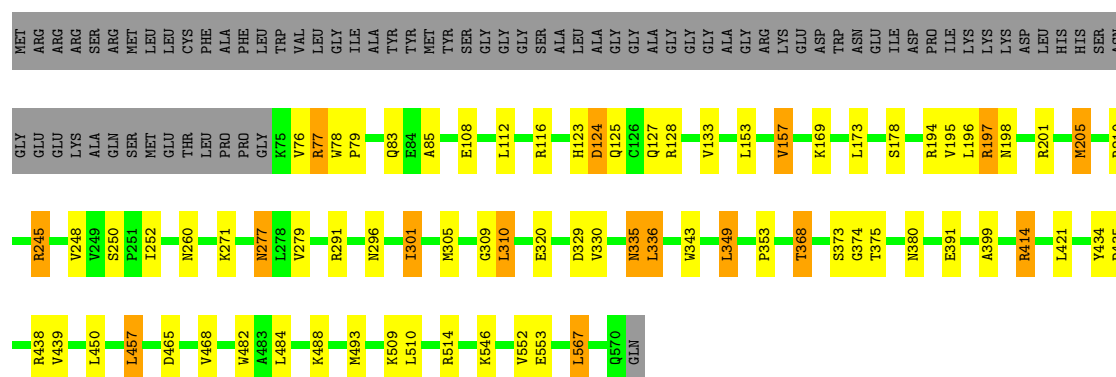


### 3 Residue-property plots

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.

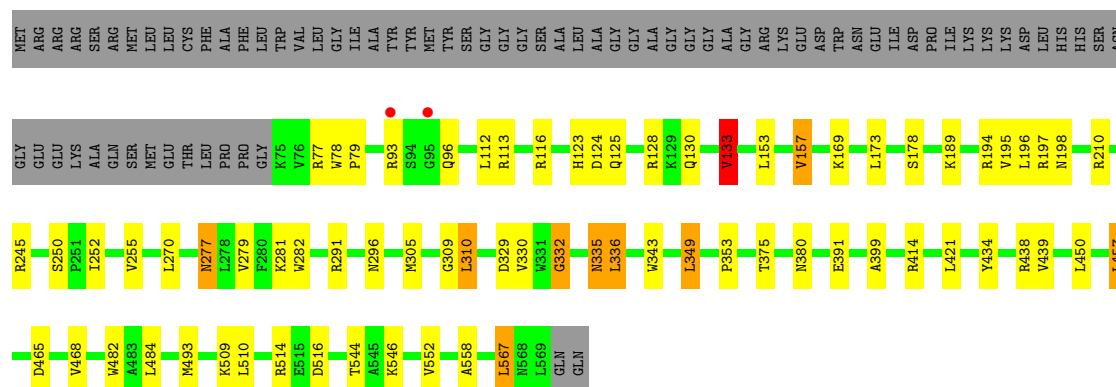
#### • Molecule 1: POLYPEPTIDE N-ACETYL GALACTOSAMINYLTRANSFERASE 2

Chain A: 



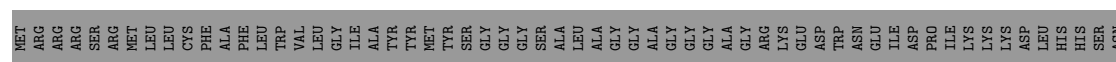
#### • Molecule 1: POLYPEPTIDE N-ACETYL GALACTOSAMINYLTRANSFERASE 2

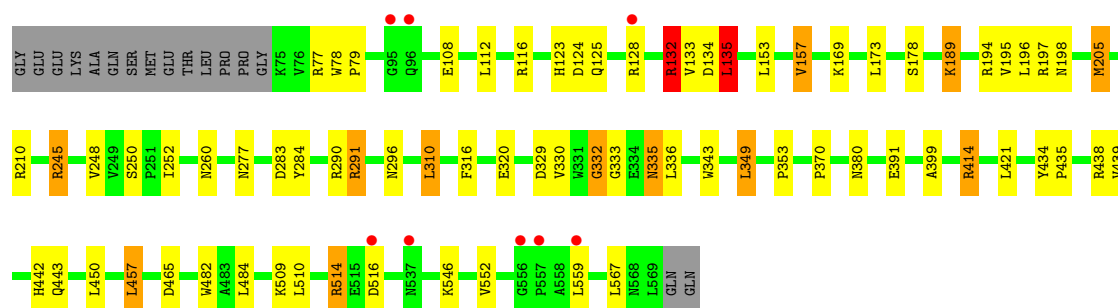
Chain B: 



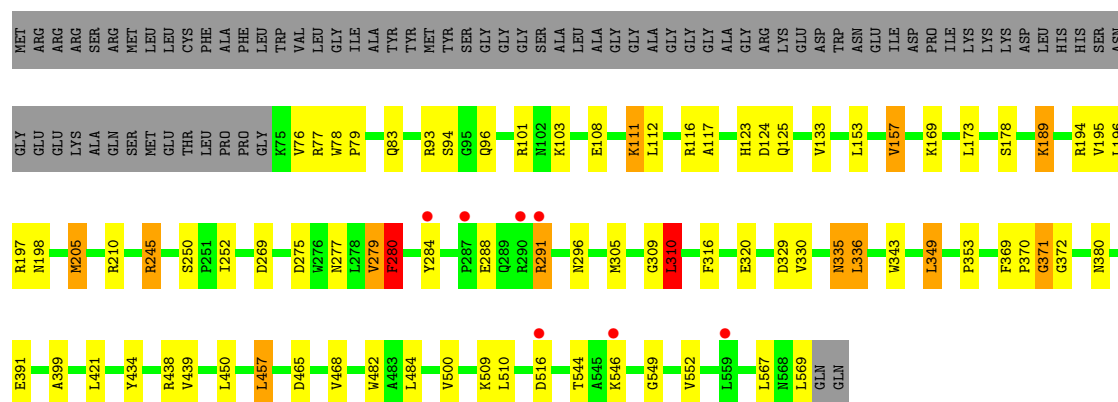
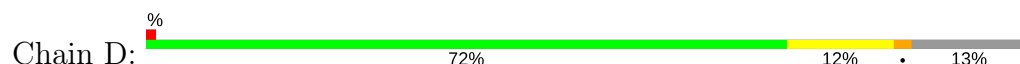
#### • Molecule 1: POLYPEPTIDE N-ACETYL GALACTOSAMINYLTRANSFERASE 2

Chain C: 

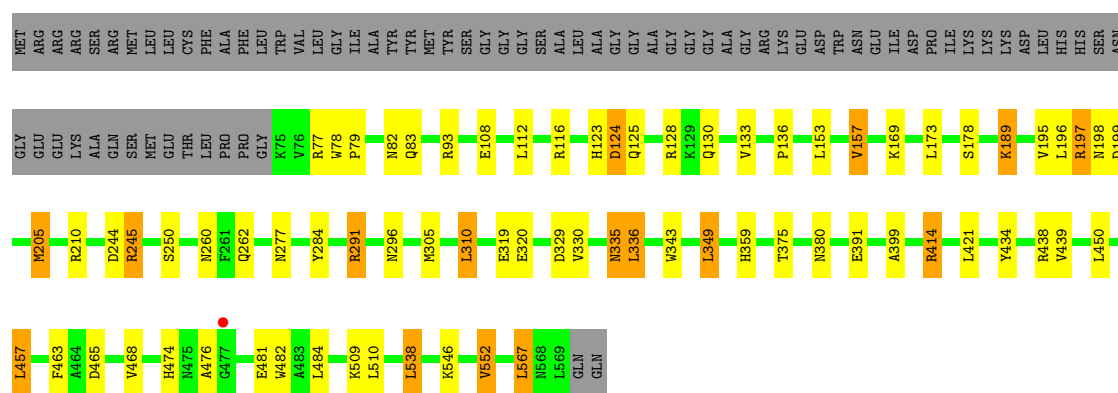




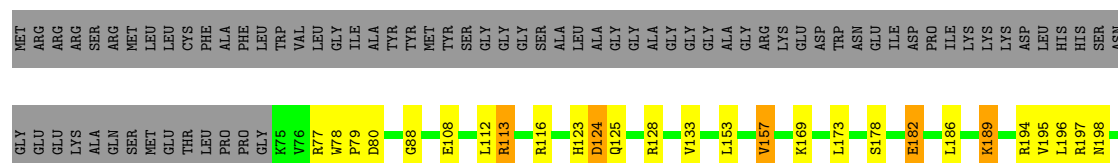
• Molecule 1: POLYPEPTIDE N-ACETYL GALACTOSAMINYLTRANSFERASE 2

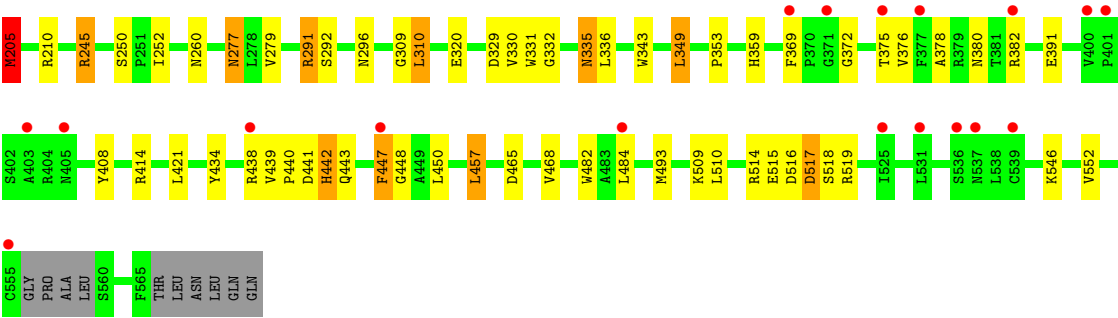


• Molecule 1: POLYPEPTIDE N-ACETYL GALACTOSAMINYLTRANSFERASE 2

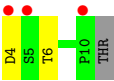


• Molecule 1: POLYPEPTIDE N-ACETYL GALACTOSAMINYLTRANSFERASE 2





● Molecule 2: PEPTIDE



● Molecule 2: PEPTIDE



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	117.22Å 122.37Å 249.72Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	249.72 – 2.45 70.07 – 2.45	Depositor EDS
% Data completeness (in resolution range)	99.7 (249.72-2.45) 99.7 (70.07-2.45)	Depositor EDS
$R_{merge}$	0.11	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.05 (at 2.45Å)	Xtriage
Refinement program	REFMAC 5.8.0049	Depositor
R, $R_{free}$	0.214 , 0.241 0.218 , 0.244	Depositor DCC
$R_{free}$ test set	3670 reflections (2.78%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.9	Xtriage
Anisotropy	0.233	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.29 , 32.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.015 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.94	EDS
Total number of atoms	24500	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	46.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.86% 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: UD2, UDP, MN, NGA, EDO

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	0.68	1/4048 (0.0%)	0.86	13/5478 (0.2%)
1	B	0.66	0/4039	0.86	10/5466 (0.2%)
1	C	0.65	1/4050 (0.0%)	0.89	12/5480 (0.2%)
1	D	0.62	1/4068 (0.0%)	0.85	6/5504 (0.1%)
1	E	0.67	2/4039 (0.0%)	0.85	12/5466 (0.2%)
1	F	0.61	2/3982 (0.1%)	0.89	11/5385 (0.2%)
2	P	0.91	0/48	1.22	0/67
2	Z	1.51	1/41 (2.4%)	1.57	1/58 (1.7%)
All	All	0.65	8/24315 (0.0%)	0.87	65/32904 (0.2%)

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	2
1	C	0	2
1	D	0	2
1	F	0	2
2	Z	0	1
All	All	0	9

All (8) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	292	SER	CB-OG	-6.18	1.34	1.42
1	A	553	GLU	CD-OE1	5.88	1.32	1.25
1	F	332	GLY	N-CA	5.86	1.54	1.46
1	E	319	GLU	CG-CD	5.55	1.60	1.51
2	Z	10	PRO	N-CD	5.18	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	319	GLU	CD-OE2	5.17	1.31	1.25
1	D	288	GLU	CG-CD	5.06	1.59	1.51
1	C	333	GLY	N-CA	-5.05	1.38	1.46

All (65) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	194	ARG	NE-CZ-NH2	-18.29	111.15	120.30
1	F	194	ARG	NE-CZ-NH1	11.41	126.01	120.30
1	C	135	LEU	CA-CB-CG	9.32	136.74	115.30
1	B	113	ARG	NE-CZ-NH1	8.91	124.75	120.30
1	C	135	LEU	CB-CG-CD1	7.34	123.48	111.00
1	C	132	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	F	292	SER	CB-CA-C	-7.09	96.62	110.10
1	A	368	THR	N-CA-CB	-6.88	97.24	110.30
1	F	88	GLY	N-CA-C	6.87	130.27	113.10
1	F	332	GLY	N-CA-C	-6.80	96.11	113.10
1	D	280	PHE	N-CA-CB	6.79	122.82	110.60
1	C	332	GLY	CA-C-N	6.68	129.57	116.20
1	A	374	GLY	N-CA-C	-6.65	96.47	113.10
2	Z	10	PRO	CA-N-CD	-6.55	102.33	111.50
1	B	194	ARG	NE-CZ-NH2	-6.41	117.10	120.30
1	B	77	ARG	CB-CA-C	6.35	123.11	110.40
1	B	133	VAL	CB-CA-C	6.33	123.42	111.40
1	A	77	ARG	NE-CZ-NH1	6.31	123.45	120.30
1	C	77	ARG	CB-CA-C	6.17	122.74	110.40
1	B	332	GLY	CA-C-N	6.15	128.50	116.20
1	E	414	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	C	332	GLY	O-C-N	-5.92	113.14	123.20
1	D	77	ARG	NE-CZ-NH1	5.88	123.24	120.30
1	C	194	ARG	NE-CZ-NH2	-5.86	117.37	120.30
1	C	310	LEU	CA-CB-CG	5.83	128.70	115.30
1	D	310	LEU	CA-CB-CG	5.79	128.63	115.30
1	F	77	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	B	310	LEU	CA-CB-CG	5.72	128.45	115.30
1	C	291	ARG	NE-CZ-NH1	5.69	123.14	120.30
1	A	197	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	E	197	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	D	205	MET	CA-CB-CG	5.60	122.82	113.30
1	F	332	GLY	C-N-CA	5.60	134.05	122.30
1	E	414	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	E	310	LEU	CA-CB-CG	5.56	128.09	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	414	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	D	194	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	B	567	LEU	CA-CB-CG	5.51	127.98	115.30
1	F	310	LEU	CA-CB-CG	5.50	127.95	115.30
1	A	567	LEU	CA-CB-CG	5.48	127.91	115.30
1	A	553	GLU	CG-CD-OE2	-5.47	107.36	118.30
1	A	373	SER	CA-C-N	5.41	127.02	116.20
1	E	291	ARG	NE-CZ-NH1	5.41	123.00	120.30
1	F	205	MET	CA-CB-CG	5.38	122.44	113.30
1	D	101	ARG	CG-CD-NE	-5.34	100.58	111.80
1	E	205	MET	CA-CB-CG	5.34	122.39	113.30
1	A	310	LEU	CA-CB-CG	5.34	127.59	115.30
1	E	567	LEU	CA-CB-CG	5.34	127.57	115.30
1	E	77	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	C	291	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	C	205	MET	CA-CB-CG	5.26	122.24	113.30
1	A	373	SER	N-CA-C	-5.25	96.82	111.00
1	C	414	ARG	NE-CZ-NH1	5.20	122.90	120.30
1	E	291	ARG	NE-CZ-NH2	-5.20	117.70	120.30
1	E	481	GLU	CG-CD-OE2	-5.20	107.90	118.30
1	F	414	ARG	NE-CZ-NH2	-5.19	117.70	120.30
1	B	332	GLY	O-C-N	-5.15	114.44	123.20
1	B	194	ARG	NE-CZ-NH1	5.14	122.87	120.30
1	A	205	MET	CA-CB-CG	5.13	122.03	113.30
1	E	244	ASP	CB-CG-OD1	5.10	122.89	118.30
1	A	553	GLU	CG-CD-OE1	5.09	128.48	118.30
1	F	113	ARG	CA-CB-CG	-5.09	102.21	113.40
1	B	414	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	A	194	ARG	NE-CZ-NH2	-5.04	117.78	120.30
1	E	481	GLU	OE1-CD-OE2	5.03	129.34	123.30

There are no chirality outliers.

All (9) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	133	VAL	Peptide
1	B	332	GLY	Peptide
1	C	332	GLY	Peptide
1	C	370	PRO	Peptide
1	D	370	PRO	Peptide
1	D	371	GLY	Peptide
1	F	331	TRP	Peptide

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Mol	Chain	Res	Type	Group
1	F	441	ASP	Peptide
2	Z	9	ALA	Peptide

## 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	3956	0	3862	38	0
1	B	3947	0	3854	43	0
1	C	3955	0	3867	27	0
1	D	3967	0	3881	44	0
1	E	3947	0	3854	29	0
1	F	3892	0	3792	49	0
2	P	47	0	40	0	0
2	Z	40	0	39	28	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
4	A	8	0	12	2	0
4	B	8	0	12	1	0
4	C	8	0	12	0	0
4	D	8	0	12	1	0
4	E	8	0	12	3	0
5	A	39	0	25	5	0
5	B	39	0	25	3	0
5	D	39	0	25	5	0
5	E	39	0	25	2	0
5	F	39	0	25	3	0
6	C	25	0	11	0	0
7	P	14	0	13	0	0
8	A	108	0	0	2	0
8	B	99	0	0	4	0
8	C	67	0	0	2	0
8	D	55	0	0	1	0
8	E	105	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	F	34	0	0	1	0
8	P	1	0	0	0	0
All	All	24500	0	23398	232	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 5.

All (232) 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:D:277:ASN:OD1	1:D:279:VAL:HB	1.56	1.06
1:B:270:LEU:HB2	2:Z:11:THR:HG21	1.37	1.06
1:B:270:LEU:HD12	2:Z:11:THR:CG2	1.87	1.04
1:F:442:HIS:HB3	1:F:443:GLN:HA	1.49	0.94
1:A:271:LYS:HG2	1:A:301:ILE:HD11	1.48	0.93
1:B:270:LEU:CB	2:Z:11:THR:HG21	2.00	0.91
1:B:270:LEU:HD12	2:Z:11:THR:HG21	1.52	0.91
1:C:290:ARG:NH1	1:F:493:MET:SD	2.45	0.90
1:D:245:ARG:HH11	1:D:245:ARG:HG2	1.36	0.88
1:A:435:PRO:HB2	1:D:291:ARG:NH1	1.89	0.88
1:B:270:LEU:CD1	2:Z:11:THR:HG21	2.05	0.85
1:F:369:PHE:HD2	1:F:376:VAL:HG11	1.42	0.85
1:B:270:LEU:CD1	2:Z:11:THR:CG2	2.57	0.82
1:E:305:MET:HE1	1:E:336:LEU:HA	1.63	0.80
1:F:182:GLU:HG3	1:F:186:LEU:HG	1.63	0.80
1:B:305:MET:HE1	1:B:336:LEU:HA	1.63	0.80
1:D:309:GLY:CA	5:D:1571:UD2:O3'	2.29	0.80
1:A:305:MET:HE1	1:A:336:LEU:HA	1.64	0.79
1:B:255:VAL:CG2	2:Z:10:PRO:HB3	2.13	0.78
1:D:305:MET:HE1	1:D:336:LEU:HA	1.65	0.77
1:F:369:PHE:HD2	1:F:376:VAL:CG1	1.97	0.77
1:A:414:ARG:HD3	8:A:2078:HOH:O	1.85	0.76
1:F:123:HIS:HD2	1:F:125:GLN:H	1.33	0.76
1:E:123:HIS:HD2	1:E:125:GLN:H	1.35	0.75
1:A:457:LEU:HD13	1:A:482:TRP:CE2	2.22	0.74
1:B:514:ARG:NE	1:B:516:ASP:OD1	2.20	0.74
1:B:255:VAL:HG22	2:Z:10:PRO:HB3	1.69	0.74
1:C:514:ARG:HH11	1:C:514:ARG:HG3	1.52	0.73
1:B:282:TRP:CZ3	2:Z:11:THR:HG23	2.24	0.73
1:C:123:HIS:HD2	1:C:125:GLN:H	1.37	0.73
1:E:457:LEU:HD13	1:E:482:TRP:CE2	2.24	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:442:HIS:CB	1:F:443:GLN:HA	2.18	0.72
1:B:457:LEU:HD13	1:B:482:TRP:CE2	2.24	0.72
1:F:457:LEU:HD13	1:F:482:TRP:CE2	2.25	0.71
1:A:123:HIS:HD2	1:A:125:GLN:H	1.39	0.71
1:B:123:HIS:HD2	1:B:125:GLN:H	1.37	0.71
1:C:457:LEU:HD13	1:C:482:TRP:CE2	2.27	0.70
1:D:123:HIS:HD2	1:D:125:GLN:H	1.38	0.70
1:A:201:ARG:HB3	4:A:1573:EDO:H21	1.73	0.69
1:D:309:GLY:HA3	5:D:1571:UD2:O3'	1.92	0.69
1:B:270:LEU:HD12	2:Z:11:THR:CB	2.22	0.69
1:D:457:LEU:HD13	1:D:482:TRP:CE2	2.27	0.69
1:F:447:PHE:HD1	1:F:448:GLY:N	1.91	0.68
1:A:277:ASN:ND2	1:A:279:VAL:HG12	2.08	0.68
1:F:442:HIS:HB3	1:F:443:GLN:CA	2.21	0.66
1:B:277:ASN:ND2	1:B:279:VAL:HG12	2.11	0.66
5:A:1574:UD2:H6	5:A:1574:UD2:H5'2	1.77	0.65
1:E:414:ARG:HD3	8:E:2080:HOH:O	1.96	0.65
1:A:435:PRO:O	1:D:291:ARG:NE	2.29	0.65
1:D:309:GLY:HA2	5:D:1571:UD2:O3'	1.94	0.65
1:D:369:PHE:O	1:D:371:GLY:HA2	1.99	0.62
1:F:277:ASN:ND2	1:F:279:VAL:HG12	2.14	0.62
1:A:198:ASN:HD22	1:A:210:ARG:HH11	1.47	0.62
1:D:108:GLU:OE2	1:D:111:LYS:HD3	1.99	0.62
1:B:399:ALA:HB2	1:B:567:LEU:HD22	1.80	0.61
1:B:329:ASP:H	1:B:380:ASN:HD21	1.49	0.61
1:C:435:PRO:HB2	1:F:291:ARG:CZ	2.31	0.60
2:Z:10:PRO:O	2:Z:11:THR:HG22	2.01	0.60
2:Z:6:THR:O	2:Z:7:THR:HB	2.01	0.60
1:A:399:ALA:HB2	1:A:567:LEU:HD22	1.83	0.60
1:D:329:ASP:H	1:D:380:ASN:HD21	1.50	0.59
1:E:359:HIS:CE1	5:E:1571:UD2:H8'2	2.37	0.59
1:F:205:MET:H	1:F:205:MET:HE2	1.67	0.58
1:A:309:GLY:CA	5:A:1574:UD2:O3'	2.52	0.58
1:B:270:LEU:HB2	2:Z:11:THR:CG2	2.26	0.58
1:D:245:ARG:HH11	1:D:245:ARG:CG	2.10	0.58
1:E:329:ASP:H	1:E:380:ASN:HD21	1.52	0.57
1:F:369:PHE:CD2	1:F:376:VAL:CG1	2.84	0.57
1:B:270:LEU:HD12	2:Z:11:THR:HB	1.86	0.57
1:A:329:ASP:H	1:A:380:ASN:HD21	1.53	0.56
1:E:198:ASN:HD22	1:E:210:ARG:HH11	1.53	0.56
5:F:1567:UD2:H6	5:F:1567:UD2:H5'2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:270:LEU:CG	2:Z:11:THR:HG21	2.36	0.55
1:B:93:ARG:HB2	1:B:96:GLN:NE2	2.21	0.55
1:F:517:ASP:OD1	1:F:519:ARG:HB2	2.07	0.55
1:C:329:ASP:H	1:C:380:ASN:HD21	1.54	0.55
1:F:329:ASP:H	1:F:380:ASN:HD21	1.54	0.55
1:F:372:GLY:H	1:F:376:VAL:HG12	1.71	0.55
1:B:277:ASN:HD21	1:B:279:VAL:HG12	1.71	0.55
1:A:309:GLY:HA3	5:A:1574:UD2:O3'	2.07	0.55
1:E:399:ALA:HB2	1:E:567:LEU:HD22	1.88	0.55
1:A:201:ARG:CB	4:A:1573:EDO:H21	2.36	0.55
1:D:198:ASN:HD22	1:D:210:ARG:HH11	1.55	0.55
1:C:399:ALA:HB2	1:C:567:LEU:HD22	1.89	0.54
1:A:277:ASN:HD21	1:A:279:VAL:HG12	1.71	0.54
1:B:282:TRP:CE3	2:Z:11:THR:CG2	2.90	0.54
1:F:447:PHE:CD1	1:F:448:GLY:N	2.75	0.54
1:A:271:LYS:HG2	1:A:301:ILE:CD1	2.31	0.53
1:D:245:ARG:NH1	1:D:245:ARG:HG2	2.14	0.53
1:F:198:ASN:HD22	1:F:210:ARG:HH11	1.55	0.53
1:F:517:ASP:OD2	1:F:519:ARG:NH2	2.33	0.53
1:A:85:ALA:HA	1:C:316:PHE:CE2	2.43	0.53
1:E:136:PRO:HD3	4:E:1573:EDO:H12	1.91	0.53
8:B:2083:HOH:O	1:E:262:GLN:NE2	2.36	0.53
1:C:284:TYR:CE1	1:F:493:MET:HG3	2.44	0.52
1:B:93:ARG:HB2	1:B:96:GLN:HE21	1.74	0.52
1:B:198:ASN:HD22	1:B:210:ARG:HH11	1.57	0.52
1:D:369:PHE:O	1:D:372:GLY:HA2	2.10	0.52
1:F:440:PRO:C	1:F:442:HIS:N	2.63	0.52
5:E:1571:UD2:H6	5:E:1571:UD2:H5'2	1.92	0.52
1:F:372:GLY:HA2	1:F:375:THR:HB	1.91	0.51
1:D:117:ALA:HA	4:D:1572:EDO:C2	2.40	0.51
1:D:399:ALA:HB2	1:D:567:LEU:HD21	1.91	0.51
1:E:335:ASN:N	1:E:335:ASN:HD22	2.08	0.51
1:F:382:ARG:NH2	1:F:408:TYR:CD1	2.78	0.51
1:D:335:ASN:N	1:D:335:ASN:HD22	2.09	0.51
1:F:335:ASN:N	1:F:335:ASN:HD22	2.09	0.51
8:B:2045:HOH:O	2:Z:10:PRO:HD2	2.11	0.51
1:B:255:VAL:CG2	2:Z:10:PRO:CB	2.88	0.50
1:F:359:HIS:CE1	5:F:1567:UD2:H8'2	2.46	0.50
1:B:270:LEU:CD1	2:Z:11:THR:HG22	2.42	0.50
1:B:78:TRP:CG	1:B:79:PRO:HD3	2.47	0.50
1:F:372:GLY:HA3	1:F:376:VAL:H	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:1573:UD2:H5'2	5:B:1573:UD2:H6	1.93	0.50
1:A:335:ASN:N	1:A:335:ASN:HD22	2.10	0.50
1:D:279:VAL:HG13	1:D:280:PHE:H	1.76	0.50
1:A:198:ASN:ND2	1:A:210:ARG:HH11	2.10	0.49
1:F:78:TRP:CG	1:F:79:PRO:HD3	2.47	0.49
1:C:198:ASN:HD22	1:C:210:ARG:HH11	1.59	0.49
1:C:132:ARG:HD3	1:C:135:LEU:HD13	1.95	0.49
1:A:78:TRP:CG	1:A:79:PRO:HD3	2.48	0.49
1:C:78:TRP:CG	1:C:79:PRO:HD3	2.48	0.49
1:F:440:PRO:C	1:F:442:HIS:H	2.16	0.49
1:C:335:ASN:N	1:C:335:ASN:HD22	2.10	0.48
1:D:78:TRP:CG	1:D:79:PRO:HD3	2.48	0.48
1:F:277:ASN:HD21	1:F:279:VAL:HG12	1.77	0.48
1:D:544:THR:HG23	1:D:549:GLY:O	2.12	0.48
1:D:245:ARG:NH1	1:D:245:ARG:CG	2.73	0.48
2:Z:7:THR:O	2:Z:7:THR:HG23	2.13	0.48
5:B:1573:UD2:O1B	2:Z:6:THR:HG22	2.13	0.48
1:B:178:SER:O	1:B:197:ARG:NH2	2.47	0.47
1:F:205:MET:H	1:F:205:MET:CE	2.27	0.47
1:B:279:VAL:HG13	8:B:2049:HOH:O	2.13	0.47
1:E:82:ASN:HB3	4:E:1572:EDO:C1	2.43	0.47
1:B:282:TRP:CE3	2:Z:11:THR:HG23	2.49	0.47
1:A:76:VAL:HG12	1:A:77:ARG:O	2.15	0.47
1:B:335:ASN:HD22	1:B:335:ASN:N	2.11	0.47
1:C:465:ASP:O	1:C:509:LYS:HE2	2.15	0.47
1:C:514:ARG:HG3	1:C:514:ARG:NH1	2.25	0.47
1:F:80:ASP:OD2	8:F:2001:HOH:O	2.20	0.47
1:F:309:GLY:HA3	5:F:1567:UD2:O3'	2.15	0.47
1:C:178:SER:O	1:C:197:ARG:NH2	2.46	0.47
1:D:178:SER:O	1:D:197:ARG:NH2	2.46	0.47
1:A:343:TRP:CD1	1:A:349:LEU:HD22	2.50	0.47
1:B:465:ASP:O	1:B:509:LYS:HE2	2.15	0.47
2:Z:10:PRO:HD2	2:Z:10:PRO:O	2.14	0.47
1:A:127:GLN:HB2	8:A:2023:HOH:O	2.14	0.46
1:E:124:ASP:OD1	1:E:128:ARG:NH1	2.48	0.46
1:E:343:TRP:CD1	1:E:349:LEU:HD22	2.50	0.46
1:F:178:SER:O	1:F:197:ARG:NH2	2.47	0.46
1:F:378:ALA:O	1:F:382:ARG:HG2	2.14	0.46
1:D:465:ASP:O	1:D:509:LYS:HE2	2.15	0.46
1:C:343:TRP:CD1	1:C:349:LEU:HD22	2.51	0.46
1:E:245:ARG:NH2	1:E:320:GLU:OE1	2.48	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:343:TRP:CD1	1:F:349:LEU:HD22	2.51	0.46
1:F:124:ASP:OD1	1:F:128:ARG:NH1	2.48	0.46
8:B:2045:HOH:O	2:Z:10:PRO:CD	2.64	0.46
1:F:465:ASP:O	1:F:509:LYS:HE2	2.16	0.46
1:E:465:ASP:O	1:E:509:LYS:HE2	2.15	0.45
1:A:178:SER:O	1:A:197:ARG:NH2	2.49	0.45
1:A:465:ASP:O	1:A:509:LYS:HE2	2.15	0.45
1:E:153:LEU:O	1:E:157:VAL:HG13	2.17	0.45
1:E:178:SER:O	1:E:197:ARG:NH2	2.49	0.45
1:D:309:GLY:HA3	5:D:1571:UD2:HO3'	1.82	0.45
1:B:343:TRP:CD1	1:B:349:LEU:HD22	2.51	0.45
1:C:132:ARG:HG3	1:C:134:ASP:OD1	2.17	0.45
1:C:153:LEU:O	1:C:157:VAL:HG13	2.17	0.45
1:D:343:TRP:CD1	1:D:349:LEU:HD22	2.52	0.45
1:D:93:ARG:HB2	1:D:96[B]:GLN:CD	2.37	0.44
1:A:124:ASP:OD1	1:A:128:ARG:NH1	2.50	0.44
1:A:245:ARG:NH2	1:A:320:GLU:OE1	2.50	0.44
1:F:153:LEU:O	1:F:157:VAL:HG13	2.16	0.44
1:C:245:ARG:NH2	1:C:320:GLU:OE1	2.51	0.44
1:C:414:ARG:HD3	8:C:2044:HOH:O	2.18	0.44
1:F:382:ARG:NH2	1:F:408:TYR:HD1	2.16	0.44
1:D:103:LYS:NZ	8:D:2006:HOH:O	2.51	0.44
1:E:538:LEU:HB3	1:E:552:VAL:HG22	2.00	0.44
1:D:245:ARG:HG3	1:D:245:ARG:H	1.60	0.43
1:D:189:LYS:HB2	1:D:189:LYS:HE2	1.74	0.43
1:C:108:GLU:HG2	1:C:260:ASN:HA	2.01	0.43
1:D:153:LEU:O	1:D:157:VAL:HG13	2.19	0.43
1:F:245:ARG:NH2	1:F:320:GLU:OE1	2.51	0.43
1:F:205:MET:HE1	1:F:329:ASP:CA	2.48	0.43
1:B:270:LEU:HD12	2:Z:11:THR:HG22	1.90	0.43
1:A:435:PRO:O	1:D:291:ARG:CD	2.67	0.43
1:F:108:GLU:HG2	1:F:260:ASN:HA	2.01	0.43
5:A:1574:UD2:H6	5:A:1574:UD2:C5B	2.45	0.43
1:E:82:ASN:HB3	4:E:1572:EDO:H12	2.01	0.43
1:E:189:LYS:HB2	1:E:189:LYS:HE2	1.72	0.43
1:A:153:LEU:O	1:A:157:VAL:HG13	2.19	0.42
1:D:569:LEU:HD23	1:D:569:LEU:N	2.34	0.42
1:B:252:ILE:HD12	1:B:353:PRO:HA	2.01	0.42
1:D:316:PHE:O	1:D:320[A]:GLU:HG2	2.18	0.42
1:F:189:LYS:HE2	1:F:189:LYS:HB2	1.72	0.42
1:D:252:ILE:HD12	1:D:353:PRO:HA	1.99	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:TRP:CZ3	2:Z:11:THR:CG2	3.00	0.42
1:F:205:MET:HE1	1:F:329:ASP:HA	2.02	0.42
1:F:514:ARG:O	1:F:515:GLU:C	2.56	0.42
1:C:252:ILE:HD12	1:C:353:PRO:HA	2.01	0.42
1:A:108:GLU:HG2	1:A:260:ASN:HA	2.01	0.42
1:B:309:GLY:HA3	5:B:1573:UD2:O3'	2.20	0.42
1:D:310:LEU:CD2	5:D:1571:UD2:H8'3	2.50	0.42
1:C:189:LYS:HD2	1:C:189:LYS:N	2.35	0.42
1:D:83:GLN:HG3	1:D:153:LEU:HD23	2.02	0.42
1:E:463:PHE:HB2	2:Z:10:PRO:HD3	2.01	0.42
1:C:248:VAL:HB	1:C:349:LEU:HD12	2.02	0.42
1:E:108:GLU:HG2	1:E:260:ASN:HA	2.02	0.42
1:F:252:ILE:HD12	1:F:353:PRO:HA	2.02	0.42
1:A:457:LEU:HD13	1:A:482:TRP:CD2	2.55	0.41
1:B:153:LEU:O	1:B:157:VAL:HG13	2.19	0.41
1:D:275:ASP:H	1:D:279:VAL:HG12	1.85	0.41
1:A:248:VAL:HB	1:A:349:LEU:HD12	2.03	0.41
1:A:435:PRO:HB2	1:D:291:ARG:CZ	2.48	0.41
1:C:283:ASP:HA	8:C:2034:HOH:O	2.20	0.41
1:E:83:GLN:HG3	1:E:153:LEU:HD23	2.01	0.41
1:E:78:TRP:CG	1:E:79:PRO:HD3	2.55	0.41
1:B:282:TRP:CH2	2:Z:11:THR:C	2.94	0.41
1:A:85:ALA:HB2	1:C:316:PHE:CG	2.56	0.41
1:B:198:ASN:ND2	1:B:210:ARG:HH11	2.19	0.41
1:B:558:ALA:HB1	4:B:1572:EDO:H22	2.02	0.41
1:F:198:ASN:ND2	1:F:210:ARG:HH11	2.18	0.41
1:E:83:GLN:HG3	1:E:153:LEU:CD2	2.51	0.41
1:A:493:MET:HB3	1:D:269:ASP:OD2	2.21	0.41
1:E:474:HIS:CD2	1:E:476:ALA:H	2.40	0.40
5:A:1574:UD2:H2B	5:A:1574:UD2:H5'2	1.96	0.40
1:A:252:ILE:HD12	1:A:353:PRO:HA	2.02	0.40
1:E:335:ASN:H	1:E:335:ASN:HD22	1.68	0.40
1:A:83:GLN:HG3	1:A:153:LEU:HD23	2.02	0.40
1:B:493:MET:HG3	1:E:284:TYR:CE1	2.56	0.40
1:D:198:ASN:ND2	1:D:210:ARG:HH11	2.17	0.40
1:D:83:GLN:HG3	1:D:153:LEU:CD2	2.52	0.40
1:F:516:ASP:O	1:F:518:SER:N	2.55	0.40

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	494/571 (86%)	482 (98%)	11 (2%)	1 (0%)	49	59
1	B	493/571 (86%)	481 (98%)	10 (2%)	2 (0%)	36	45
1	C	494/571 (86%)	478 (97%)	15 (3%)	1 (0%)	49	59
1	D	496/571 (87%)	480 (97%)	12 (2%)	4 (1%)	21	25
1	E	493/571 (86%)	481 (98%)	11 (2%)	1 (0%)	49	59
1	F	483/571 (85%)	466 (96%)	14 (3%)	3 (1%)	27	32
2	P	5/8 (62%)	4 (80%)	0	1 (20%)	0	0
2	Z	4/8 (50%)	1 (25%)	1 (25%)	2 (50%)	0	0
All	All	2962/3442 (86%)	2873 (97%)	74 (2%)	15 (0%)	31	37

All (15) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	94	SER
1	D	280	PHE
2	P	6	THR
2	Z	10	PRO
1	F	442	HIS
1	F	517	ASP
1	E	330	VAL
1	A	330	VAL
1	F	330	VAL
2	Z	7	THR
1	B	133	VAL
1	B	330	VAL
1	C	330	VAL
1	D	330	VAL
1	D	279	VAL

### 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	424/485 (87%)	388 (92%)	36 (8%)	12	13
1	B	423/485 (87%)	388 (92%)	35 (8%)	12	14
1	C	424/485 (87%)	385 (91%)	39 (9%)	10	10
1	D	426/485 (88%)	390 (92%)	36 (8%)	12	13
1	E	423/485 (87%)	386 (91%)	37 (9%)	11	12
1	F	417/485 (86%)	382 (92%)	35 (8%)	12	13
2	P	6/7 (86%)	5 (83%)	1 (17%)	2	1
2	Z	5/7 (71%)	5 (100%)	0	100	100
All	All	2548/2924 (87%)	2329 (91%)	219 (9%)	11	13

All (219) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	112	LEU
1	A	116	ARG
1	A	124	ASP
1	A	133	VAL
1	A	157	VAL
1	A	169	LYS
1	A	173	LEU
1	A	195	VAL
1	A	196	LEU
1	A	205	MET
1	A	245	ARG
1	A	250	SER
1	A	277	ASN
1	A	291	ARG
1	A	296	ASN
1	A	301	ILE
1	A	310	LEU
1	A	335	ASN
1	A	336	LEU

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Mol	Chain	Res	Type
1	A	349	LEU
1	A	368	THR
1	A	375	THR
1	A	391	GLU
1	A	421	LEU
1	A	434	TYR
1	A	438	ARG
1	A	439	VAL
1	A	450	LEU
1	A	457	LEU
1	A	468	VAL
1	A	484	LEU
1	A	488	LYS
1	A	510	LEU
1	A	514	ARG
1	A	546	LYS
1	A	552	VAL
1	B	112	LEU
1	B	116	ARG
1	B	124	ASP
1	B	128	ARG
1	B	130	GLN
1	B	157	VAL
1	B	169	LYS
1	B	173	LEU
1	B	189	LYS
1	B	195	VAL
1	B	196	LEU
1	B	245	ARG
1	B	250	SER
1	B	277	ASN
1	B	281	LYS
1	B	291	ARG
1	B	296	ASN
1	B	310	LEU
1	B	335	ASN
1	B	336	LEU
1	B	349	LEU
1	B	375	THR
1	B	391	GLU
1	B	421	LEU
1	B	434	TYR

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Mol	Chain	Res	Type
1	B	438	ARG
1	B	439	VAL
1	B	450	LEU
1	B	457	LEU
1	B	468	VAL
1	B	484	LEU
1	B	510	LEU
1	B	544	THR
1	B	546	LYS
1	B	552	VAL
1	C	112	LEU
1	C	116	ARG
1	C	124	ASP
1	C	128	ARG
1	C	132	ARG
1	C	133	VAL
1	C	135	LEU
1	C	157	VAL
1	C	169	LYS
1	C	173	LEU
1	C	189	LYS
1	C	195	VAL
1	C	196	LEU
1	C	205	MET
1	C	245	ARG
1	C	250	SER
1	C	277	ASN
1	C	291	ARG
1	C	296	ASN
1	C	310	LEU
1	C	335	ASN
1	C	336	LEU
1	C	349	LEU
1	C	391	GLU
1	C	421	LEU
1	C	434	TYR
1	C	438	ARG
1	C	439	VAL
1	C	442	HIS
1	C	443	GLN
1	C	450	LEU
1	C	457	LEU

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Mol	Chain	Res	Type
1	C	484	LEU
1	C	510	LEU
1	C	514	ARG
1	C	516	ASP
1	C	546	LYS
1	C	552	VAL
1	C	559	LEU
1	D	76	VAL
1	D	111	LYS
1	D	112	LEU
1	D	116	ARG
1	D	124	ASP
1	D	133	VAL
1	D	157	VAL
1	D	169	LYS
1	D	173	LEU
1	D	189	LYS
1	D	195	VAL
1	D	196	LEU
1	D	205	MET
1	D	245	ARG
1	D	250	SER
1	D	284	TYR
1	D	291	ARG
1	D	296	ASN
1	D	310	LEU
1	D	335	ASN
1	D	336	LEU
1	D	349	LEU
1	D	391	GLU
1	D	421	LEU
1	D	434	TYR
1	D	438	ARG
1	D	439	VAL
1	D	450	LEU
1	D	457	LEU
1	D	468	VAL
1	D	484	LEU
1	D	500	VAL
1	D	510	LEU
1	D	516	ASP
1	D	546	LYS

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Mol	Chain	Res	Type
1	D	552	VAL
1	E	93	ARG
1	E	112	LEU
1	E	116	ARG
1	E	124	ASP
1	E	130	GLN
1	E	133	VAL
1	E	157	VAL
1	E	169	LYS
1	E	173	LEU
1	E	189	LYS
1	E	195	VAL
1	E	196	LEU
1	E	199	ASP
1	E	205	MET
1	E	245	ARG
1	E	250	SER
1	E	277	ASN
1	E	291	ARG
1	E	296	ASN
1	E	310	LEU
1	E	335	ASN
1	E	336	LEU
1	E	349	LEU
1	E	375	THR
1	E	391	GLU
1	E	421	LEU
1	E	434	TYR
1	E	438	ARG
1	E	439	VAL
1	E	450	LEU
1	E	457	LEU
1	E	468	VAL
1	E	484	LEU
1	E	510	LEU
1	E	538	LEU
1	E	546	LYS
1	E	552	VAL
1	F	112	LEU
1	F	113	ARG
1	F	116	ARG
1	F	124	ASP

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Mol	Chain	Res	Type
1	F	133	VAL
1	F	157	VAL
1	F	169	LYS
1	F	173	LEU
1	F	182	GLU
1	F	189	LYS
1	F	195	VAL
1	F	196	LEU
1	F	205	MET
1	F	245	ARG
1	F	250	SER
1	F	277	ASN
1	F	291	ARG
1	F	296	ASN
1	F	310	LEU
1	F	335	ASN
1	F	336	LEU
1	F	349	LEU
1	F	391	GLU
1	F	421	LEU
1	F	434	TYR
1	F	438	ARG
1	F	439	VAL
1	F	447	PHE
1	F	450	LEU
1	F	457	LEU
1	F	468	VAL
1	F	484	LEU
1	F	510	LEU
1	F	546	LYS
1	F	552	VAL
2	P	4	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (87) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	123	HIS
1	A	127	GLN
1	A	198	ASN
1	A	262	GLN
1	A	277	ASN
1	A	296	ASN

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Mol	Chain	Res	Type
1	A	335	ASN
1	A	344	GLN
1	A	364	GLN
1	A	365	HIS
1	A	380	ASN
1	A	452	GLN
1	A	474	HIS
1	A	537	ASN
1	B	96	GLN
1	B	102	ASN
1	B	106	GLN
1	B	123	HIS
1	B	127	GLN
1	B	198	ASN
1	B	277	ASN
1	B	296	ASN
1	B	335	ASN
1	B	344	GLN
1	B	364	GLN
1	B	365	HIS
1	B	380	ASN
1	B	452	GLN
1	B	462	HIS
1	B	474	HIS
1	C	106	GLN
1	C	123	HIS
1	C	127	GLN
1	C	198	ASN
1	C	277	ASN
1	C	296	ASN
1	C	335	ASN
1	C	344	GLN
1	C	364	GLN
1	C	365	HIS
1	C	380	ASN
1	C	452	GLN
1	C	462	HIS
1	C	474	HIS
1	C	537	ASN
1	D	123	HIS
1	D	127	GLN
1	D	198	ASN

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Mol	Chain	Res	Type
1	D	296	ASN
1	D	335	ASN
1	D	344	GLN
1	D	364	GLN
1	D	365	HIS
1	D	380	ASN
1	D	442	HIS
1	D	452	GLN
1	D	462	HIS
1	D	474	HIS
1	D	537	ASN
1	D	568	ASN
1	E	106	GLN
1	E	123	HIS
1	E	127	GLN
1	E	198	ASN
1	E	277	ASN
1	E	296	ASN
1	E	335	ASN
1	E	344	GLN
1	E	365	HIS
1	E	380	ASN
1	E	452	GLN
1	E	462	HIS
1	E	474	HIS
1	F	123	HIS
1	F	127	GLN
1	F	198	ASN
1	F	277	ASN
1	F	296	ASN
1	F	335	ASN
1	F	344	GLN
1	F	364	GLN
1	F	365	HIS
1	F	380	ASN
1	F	452	GLN
1	F	462	HIS
1	F	474	HIS
1	F	537	ASN

### 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 23 ligands modelled in this entry, 6 are monoatomic - leaving 17 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$
4	EDO	A	1572	-	3,3,3	0.63	0	2,2,2	0.28	0
4	EDO	A	1573	-	3,3,3	0.70	0	2,2,2	0.10	0
5	UD2	A	1574	3	33,41,41	0.98	2 (6%)	45,62,62	2.36	15 (33%)
4	EDO	B	1571	-	3,3,3	0.62	0	2,2,2	0.06	0
4	EDO	B	1572	-	3,3,3	0.72	0	2,2,2	0.07	0
5	UD2	B	1573	3	33,41,41	0.75	0	45,62,62	2.25	15 (33%)
6	UDP	C	1571	3	20,26,26	0.89	1 (5%)	23,40,40	2.23	3 (13%)
4	EDO	C	1573	-	3,3,3	0.54	0	2,2,2	0.25	0
4	EDO	C	1574	-	3,3,3	0.76	0	2,2,2	0.51	0
5	UD2	D	1571	3	33,41,41	0.88	1 (3%)	45,62,62	2.03	11 (24%)
4	EDO	D	1572	-	3,3,3	0.78	0	2,2,2	0.31	0
4	EDO	D	1573	-	3,3,3	0.68	0	2,2,2	0.21	0
5	UD2	E	1571	3	33,41,41	1.00	1 (3%)	45,62,62	2.36	13 (28%)
4	EDO	E	1572	-	3,3,3	0.77	0	2,2,2	0.21	0
4	EDO	E	1573	-	3,3,3	0.77	0	2,2,2	0.78	0
5	UD2	F	1567	3	33,41,41	0.81	1 (3%)	45,62,62	1.95	9 (20%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
7	NGA	P	1572	2	14,14,15	1.01	1 (7%)	17,19,21	1.55	2 (11%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	EDO	A	1572	-	-	0/1/1/1	0/0/0/0
4	EDO	A	1573	-	-	0/1/1/1	0/0/0/0
5	UD2	A	1574	3	-	0/22/63/63	0/3/3/3
4	EDO	B	1571	-	-	0/1/1/1	0/0/0/0
4	EDO	B	1572	-	-	0/1/1/1	0/0/0/0
5	UD2	B	1573	3	-	0/22/63/63	0/3/3/3
6	UDP	C	1571	3	-	0/12/32/32	0/2/2/2
4	EDO	C	1573	-	-	0/1/1/1	0/0/0/0
4	EDO	C	1574	-	-	0/1/1/1	0/0/0/0
5	UD2	D	1571	3	-	0/22/63/63	0/3/3/3
4	EDO	D	1572	-	-	0/1/1/1	0/0/0/0
4	EDO	D	1573	-	-	0/1/1/1	0/0/0/0
5	UD2	E	1571	3	-	0/22/63/63	0/3/3/3
4	EDO	E	1572	-	-	0/1/1/1	0/0/0/0
4	EDO	E	1573	-	-	0/1/1/1	0/0/0/0
5	UD2	F	1567	3	-	0/22/63/63	0/3/3/3
7	NGA	P	1572	2	1/1/5/7	0/6/23/26	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	1574	UD2	C2-N3	-2.65	1.32	1.38
6	C	1571	UDP	C2-N3	-2.07	1.34	1.38
5	A	1574	UD2	C4-N3	2.04	1.36	1.33
5	F	1567	UD2	O4B-C1B	2.25	1.44	1.41
5	E	1571	UD2	C4-N3	2.75	1.38	1.33
5	D	1571	UD2	O4B-C1B	2.87	1.45	1.41
7	P	1572	NGA	C1-C2	3.10	1.56	1.52

All (68) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	1571	UD2	O5'-C1'-C2'	-6.50	97.36	110.56
5	B	1573	UD2	O5'-C1'-C2'	-6.40	97.55	110.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	P	1572	NGA	O5-C1-C2	-5.11	104.46	111.52
5	F	1567	UD2	O5'-C1'-C2'	-4.82	100.77	110.56
5	A	1574	UD2	O5'-C1'-C2'	-4.27	101.88	110.56
5	A	1574	UD2	C1'-C2'-N2'	-4.14	103.61	111.00
5	A	1574	UD2	O4B-C4B-C5B	-4.13	95.63	109.39
5	A	1574	UD2	O1B-PB-O1'	-3.92	91.01	106.81
5	D	1571	UD2	O5'-C1'-C2'	-3.79	102.86	110.56
5	E	1571	UD2	O4B-C4B-C5B	-3.53	97.64	109.39
5	B	1573	UD2	O4B-C4B-C5B	-3.47	97.84	109.39
5	E	1571	UD2	O1B-PB-O1'	-3.40	93.13	106.81
5	E	1571	UD2	C1'-C2'-N2'	-3.15	105.38	111.00
5	D	1571	UD2	O4B-C4B-C5B	-2.95	99.55	109.39
5	F	1567	UD2	PB-O3A-PA	-2.90	122.88	132.63
5	D	1571	UD2	PB-O3A-PA	-2.83	123.12	132.63
5	B	1573	UD2	C4'-C3'-C2'	-2.76	106.24	110.33
5	D	1571	UD2	O1B-PB-O1'	-2.59	96.36	106.81
5	E	1571	UD2	C4'-C3'-C2'	-2.55	106.56	110.33
5	D	1571	UD2	C2'-N2'-C7'	-2.55	116.90	123.23
5	A	1574	UD2	C4'-C3'-C2'	-2.52	106.60	110.33
5	B	1573	UD2	O5B-PA-O2A	-2.43	99.59	109.07
5	B	1573	UD2	C1'-C2'-N2'	-2.40	106.72	111.00
5	E	1571	UD2	C1'-O5'-C5'	-2.39	108.99	113.71
7	P	1572	NGA	C4-C3-C2	-2.35	107.58	111.02
5	F	1567	UD2	C1'-O5'-C5'	-2.30	109.17	113.71
5	F	1567	UD2	C4'-C3'-C2'	-2.29	106.93	110.33
5	D	1571	UD2	O5B-PA-O2A	-2.23	100.36	109.07
5	A	1574	UD2	C6'-C5'-C4'	-2.18	107.83	112.99
5	D	1571	UD2	O3B-C3B-C2B	-2.12	105.05	111.83
5	A	1574	UD2	C2'-N2'-C7'	-2.09	118.04	123.23
6	C	1571	UDP	O5'-PA-O1A	-2.07	100.96	109.07
5	B	1573	UD2	C5-C4-N3	-2.07	118.36	123.17
5	A	1574	UD2	C4B-O4B-C1B	-2.04	107.70	109.83
5	A	1574	UD2	C8'-C7'-N2'	-2.04	112.53	116.10
5	A	1574	UD2	O5B-C5B-C4B	2.02	116.01	109.00
5	B	1573	UD2	C3'-C2'-N2'	2.02	114.46	110.58
5	A	1574	UD2	O1A-PA-O2A	2.03	122.46	112.14
5	B	1573	UD2	O1A-PA-O2A	2.04	122.50	112.14
5	E	1571	UD2	O1'-C1'-C2'	2.05	112.10	108.40
5	A	1574	UD2	PB-O1'-C1'	2.07	127.75	119.74
5	D	1571	UD2	O1A-PA-O2A	2.08	122.71	112.14
5	F	1567	UD2	O5B-C5B-C4B	2.09	116.25	109.00
5	B	1573	UD2	O3'-C3'-C4'	2.14	115.33	110.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	1571	UD2	O3B-C3B-C4B	2.29	117.69	111.06
5	E	1571	UD2	O7'-C7'-N2'	2.29	126.28	121.94
5	B	1573	UD2	O1A-PA-O5B	2.32	118.50	107.75
5	F	1567	UD2	PB-O1'-C1'	2.32	128.72	119.74
5	A	1574	UD2	O5'-C5'-C4'	2.36	114.02	109.69
5	F	1567	UD2	O5'-C5'-C4'	2.42	114.12	109.69
5	E	1571	UD2	O4B-C1B-N1	2.50	113.02	108.05
6	C	1571	UDP	O2A-PA-O1A	2.76	126.18	112.14
5	B	1573	UD2	O5B-C5B-C4B	2.77	118.62	109.00
5	A	1574	UD2	O1B-PB-O2B	2.78	126.24	112.14
5	B	1573	UD2	O5'-C1'-O1'	2.78	115.00	111.36
5	B	1573	UD2	PB-O1'-C1'	2.96	131.18	119.74
5	B	1573	UD2	O1'-C1'-C2'	2.99	113.82	108.40
5	F	1567	UD2	O4B-C1B-N1	3.18	114.37	108.05
5	D	1571	UD2	O4B-C1B-N1	3.28	114.56	108.05
5	E	1571	UD2	O5'-C1'-O1'	3.38	115.78	111.36
5	E	1571	UD2	O1B-PB-O2B	3.57	130.28	112.14
5	E	1571	UD2	PB-O1'-C1'	4.67	137.79	119.74
5	F	1567	UD2	C4-N3-C2	7.24	120.37	114.14
5	E	1571	UD2	C4-N3-C2	7.52	120.61	114.14
5	D	1571	UD2	C4-N3-C2	7.58	120.66	114.14
5	B	1573	UD2	C4-N3-C2	8.88	121.78	114.14
6	C	1571	UDP	C4-N3-C2	9.23	122.08	114.14
5	A	1574	UD2	C4-N3-C2	10.07	122.80	114.14

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
7	P	1572	NGA	C1

There are no torsion outliers.

There are no ring outliers.

10 monomers are involved in 25 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	1573	EDO	2	0
5	A	1574	UD2	5	0
4	B	1572	EDO	1	0
5	B	1573	UD2	3	0
5	D	1571	UD2	5	0
4	D	1572	EDO	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	E	1571	UD2	2	0
4	E	1572	EDO	2	0
4	E	1573	EDO	1	0
5	F	1567	UD2	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

### 6.1 Protein, DNA and RNA chains

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	496/571 (86%)	-0.37	0 <span>100</span> <span>100</span>	22, 36, 63, 96	0
1	B	495/571 (86%)	-0.34	2 (0%) <span>92</span> <span>93</span>	25, 39, 67, 119	0
1	C	495/571 (86%)	-0.30	8 (1%) <span>72</span> <span>69</span>	26, 43, 72, 119	0
1	D	495/571 (86%)	-0.13	7 (1%) <span>75</span> <span>73</span>	30, 50, 80, 111	0
1	E	495/571 (86%)	-0.37	1 (0%) <span>94</span> <span>95</span>	21, 37, 60, 93	0
1	F	487/571 (85%)	0.11	18 (3%) <span>41</span> <span>38</span>	23, 56, 97, 123	0
2	P	7/8 (87%)	1.90	3 (42%) <span>0</span> <span>0</span>	25, 73, 78, 78	0
2	Z	6/8 (75%)	3.83	4 (66%) <span>0</span> <span>0</span>	65, 76, 103, 103	0
All	All	2976/3442 (86%)	-0.22	43 (1%) <span>75</span> <span>73</span>	21, 42, 80, 123	0

All (43) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	Z	11	THR	8.1
2	Z	7	THR	5.5
2	Z	10	PRO	4.6
1	D	291	ARG	4.3
1	D	284	TYR	4.3
1	F	401	PRO	3.7
2	P	4	ASP	3.7
1	F	405	ASN	3.6
1	F	400	VAL	3.5
2	P	10	PRO	3.4
1	C	128	ARG	3.3
2	Z	8	PRO	3.3
1	D	559	LEU	3.2
1	F	382	ARG	3.2
1	F	537	ASN	3.1
1	D	290	ARG	3.0

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Mol	Chain	Res	Type	RSRZ
1	C	556	GLY	3.0
1	F	375	THR	3.0
1	F	447	PHE	2.9
1	C	537	ASN	2.8
1	B	93	ARG	2.8
1	C	516	ASP	2.8
1	C	557	PRO	2.7
1	C	96	GLN	2.7
1	F	539	CYS	2.6
1	D	287	PRO	2.6
1	F	484	LEU	2.6
1	F	525	ILE	2.5
1	F	369	PHE	2.5
1	D	546	LYS	2.5
1	F	531	LEU	2.5
1	F	371	GLY	2.4
1	C	95	GLY	2.4
1	F	536	SER	2.4
1	E	477	GLY	2.3
1	D	516	ASP	2.3
2	P	5	SER	2.3
1	B	95	GLY	2.3
1	F	403	ALA	2.2
1	F	377	PHE	2.1
1	F	438	ARG	2.1
1	C	559	LEU	2.1
1	F	555	CYS	2.1

## 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. The B-factors column lists the minimum,

median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	EDO	E	1572	4/4	0.76	0.25	54,58,60,62	0
4	EDO	D	1572	4/4	0.78	0.34	48,48,55,62	0
4	EDO	A	1572	4/4	0.82	0.21	51,54,55,56	0
4	EDO	B	1572	4/4	0.85	0.18	51,55,56,59	0
4	EDO	C	1574	4/4	0.86	0.23	51,53,54,54	0
4	EDO	A	1573	4/4	0.86	0.34	48,48,49,51	0
4	EDO	D	1573	4/4	0.86	0.30	47,48,49,53	0
4	EDO	C	1573	4/4	0.89	0.16	44,46,50,51	0
4	EDO	B	1571	4/4	0.90	0.18	55,55,57,58	0
4	EDO	E	1573	4/4	0.92	0.14	39,41,43,44	0
5	UD2	F	1567	39/39	0.95	0.12	32,50,65,68	0
7	NGA	P	1572	14/15	0.95	0.13	31,41,47,50	0
3	MN	B	1570	1/1	0.96	0.14	34,34,34,34	0
5	UD2	B	1573	39/39	0.96	0.13	34,38,49,51	0
5	UD2	D	1571	39/39	0.97	0.11	29,37,44,47	0
5	UD2	E	1571	39/39	0.97	0.13	23,30,38,42	0
6	UDP	C	1571	25/25	0.98	0.11	31,34,36,38	0
3	MN	F	1566	1/1	0.98	0.10	40,40,40,40	0
5	UD2	A	1574	39/39	0.98	0.10	20,27,40,41	0
3	MN	E	1570	1/1	0.99	0.12	29,29,29,29	0
3	MN	C	1570	1/1	0.99	0.11	29,29,29,29	0
3	MN	D	1570	1/1	0.99	0.14	32,32,32,32	0
3	MN	A	1571	1/1	1.00	0.13	25,25,25,25	0

## 6.5 Other polymers ⓘ

There are no such residues in this entry.