



# Full wwPDB X-ray Structure Validation Report ⓘ

Feb 19, 2016 – 11:10 PM GMT

PDB ID : 5FOO  
Title : 6-phospho-beta-glucosidase  
Authors : Jin, Y.; Kwan, D.H.; Withers, S.G.; Davies, G.J.  
Deposited on : 2015-11-24  
Resolution : 2.10 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-20026982  
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-20026982

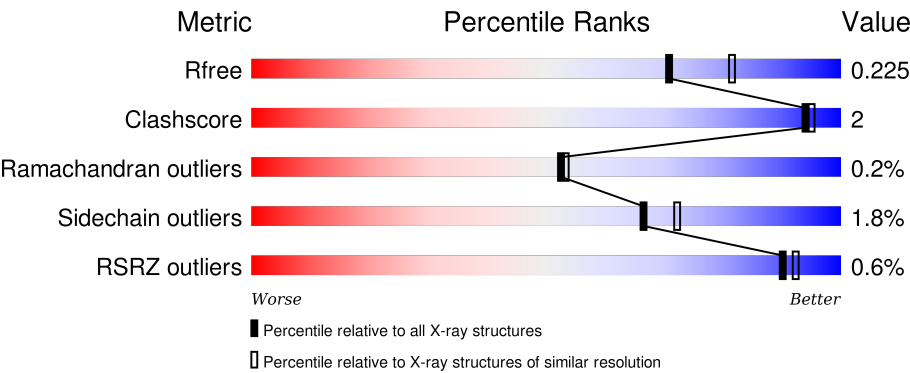
# 1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.10 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 <sub>free</sub>	91344	3939 (2.10-2.10)
Clashscore	102246	4460 (2.10-2.10)
Ramachandran outliers	100387	4413 (2.10-2.10)
Sidechain outliers	100360	4414 (2.10-2.10)
RSRZ outliers	91569	3948 (2.10-2.10)

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	480	<div><div></div><div>88%7% . .</div></div>
1	B	480	<div><div>%</div><div>90%6% .</div></div>
1	C	480	<div><div></div><div>90%6% . .</div></div>
1	D	480	<div><div>%</div><div>88%8% . .</div></div>
1	E	480	<div><div></div><div>90%6% .</div></div>

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Mol	Chain	Length	Quality of chain
1	F	480	<div> <div>%</div> <div> </div> <div>89% 6% . .</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 criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	EDO	A	1465	-	-	-	X
3	EDO	A	1467	-	-	-	X
3	EDO	A	1468	-	-	-	X
3	EDO	A	1469	-	-	-	X
3	EDO	B	1467	-	-	-	X
3	EDO	D	1465	-	-	-	X
3	EDO	D	1466	-	-	-	X
3	EDO	D	1467	-	-	-	X
3	EDO	D	1468	-	-	-	X
3	EDO	F	1465	-	-	-	X
4	PO4	A	1470	-	-	-	X
4	PO4	B	1470	-	-	-	X
4	PO4	C	1468	-	-	-	X

## 2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 23838 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.

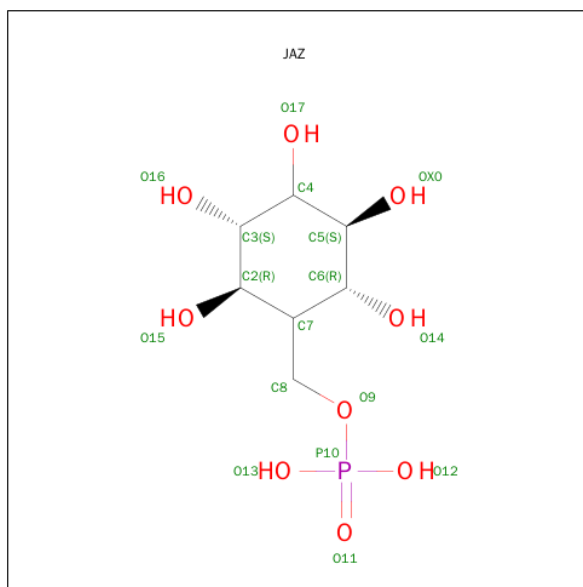
- Molecule 1 is a protein called 6-PHOSPHO-BETA-D GLYCOSIDASE.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	463	Total	C	N	O	S	0	0	0
			3772	2440	635	686	11			
1	B	463	Total	C	N	O	S	0	0	0
			3777	2443	635	688	11			
1	C	463	Total	C	N	O	S	0	0	0
			3773	2440	634	688	11			
1	D	463	Total	C	N	O	S	0	0	0
			3780	2445	636	688	11			
1	E	463	Total	C	N	O	S	0	0	0
			3775	2441	635	688	11			
1	F	462	Total	C	N	O	S	0	0	0
			3767	2435	634	687	11			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	331	HIS	ARG	ENGINEERED MUTATION	UNP Q99YP9
B	331	HIS	ARG	ENGINEERED MUTATION	UNP Q99YP9
C	331	HIS	ARG	ENGINEERED MUTATION	UNP Q99YP9
D	331	HIS	ARG	ENGINEERED MUTATION	UNP Q99YP9
E	331	HIS	ARG	ENGINEERED MUTATION	UNP Q99YP9
F	331	HIS	ARG	ENGINEERED MUTATION	UNP Q99YP9

- Molecule 2 is 6-PHOSPHOCYCLOPHELLITOL (three-letter code: JAZ) (formula:  $C_7H_{15}O_9P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	O	P	0	0
			16	7	8	1		
2	B	1	Total	C	O	P	0	0
			16	7	8	1		
2	C	1	Total	C	O	P	0	0
			16	7	8	1		
2	D	1	Total	C	O	P	0	0
			16	7	8	1		
2	E	1	Total	C	O	P	0	0
			16	7	8	1		
2	F	1	Total	C	O	P	0	0
			16	7	8	1		

- Molecule 3 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C<sub>2</sub>H<sub>6</sub>O<sub>2</sub>).



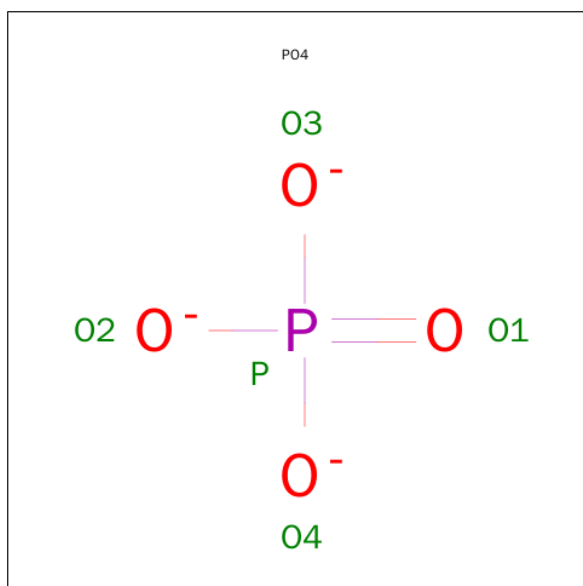
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total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

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

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

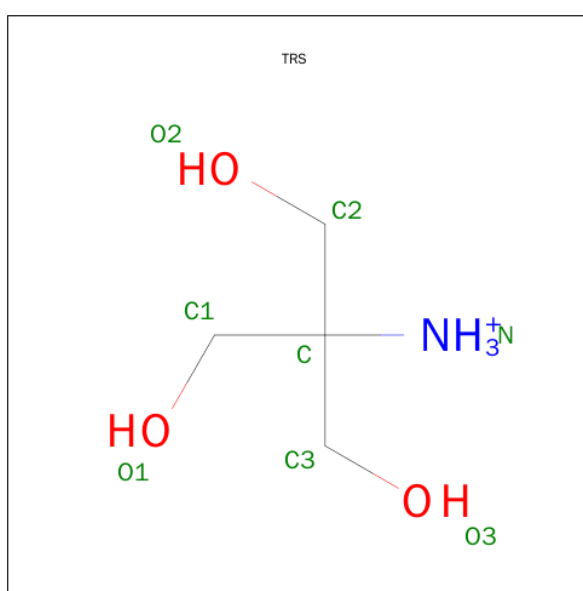


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	P	0	0
			5	4	1		
4	B	1	Total	O	P	0	0
			5	4	1		
4	C	1	Total	O	P	0	0
			5	4	1		
4	D	1	Total	O	P	0	0
			5	4	1		
4	E	1	Total	O	P	0	0
			5	4	1		
4	F	1	Total	O	P	0	0
			5	4	1		

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

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	B	1	Total	Cl	0	0
			1	1		
5	A	1	Total	Cl	0	0
			1	1		
5	D	1	Total	Cl	0	0
			1	1		

- Molecule 6 is 2-AMINO-2-HYDROXYMETHYL-PROPANE-1,3-DIOL (three-letter code: TRS) (formula: C<sub>4</sub>H<sub>12</sub>NO<sub>3</sub>).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	N	O	0	0
			8	4	1	3		

- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	214	Total	O	0	0
			214	214		
7	B	224	Total	O	0	0
			224	224		
7	C	173	Total	O	0	0
			173	173		
7	D	130	Total	O	0	0
			130	130		

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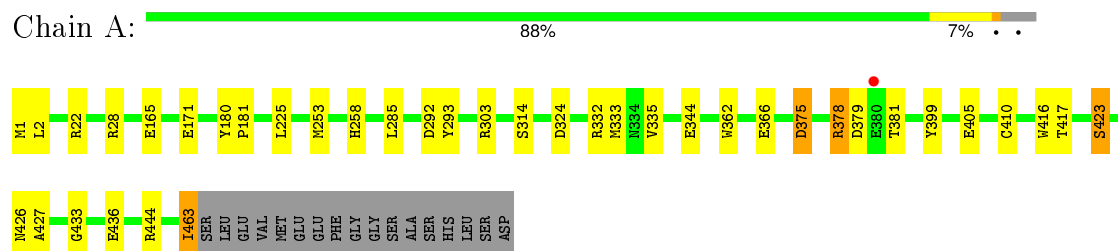
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	E	143	Total 143	O 143	0	0
7	F	97	Total 97	O 97	0	0

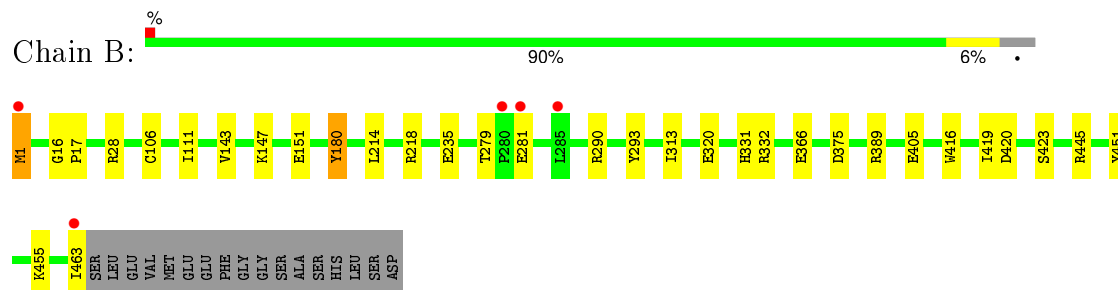
### 3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of 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 ( $\text{RSRZ} > 2$ ). 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.

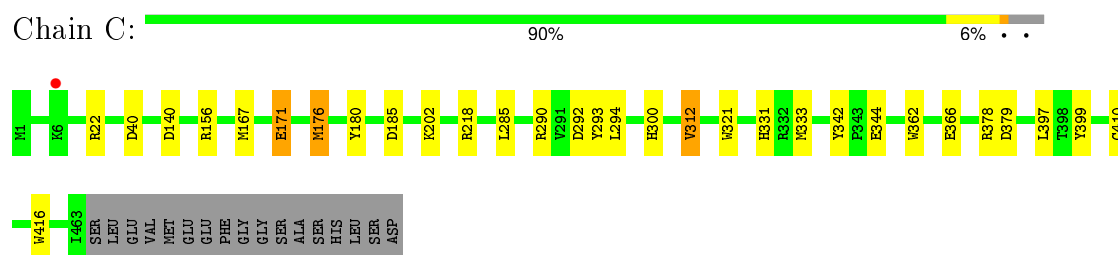
#### • Molecule 1: 6-PHOSPHO-BETA-D GLYCOSIDASE



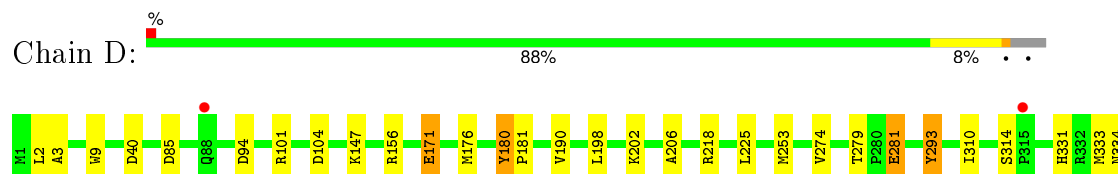
#### • Molecule 1: 6-PHOSPHO-BETA-D GLYCOSIDASE



#### • Molecule 1: 6-PHOSPHO-BETA-D GLYCOSIDASE



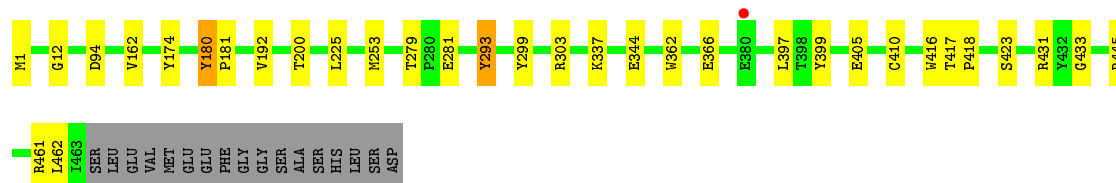
#### • Molecule 1: 6-PHOSPHO-BETA-D GLYCOSIDASE





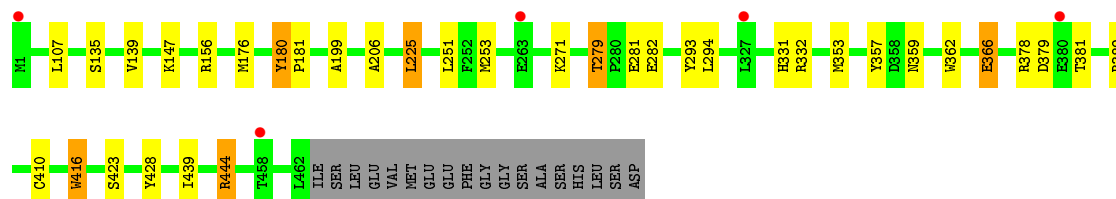
• Molecule 1: 6-PHOSPHO-BETA-D GLYCOSIDASE

Chain E: 90% 6% •



• Molecule 1: 6-PHOSPHO-BETA-D GLYCOSIDASE

Chain F: 89% 6% • •



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	103.02Å 109.90Å 158.50Å 90.00° 92.02° 90.00°	Depositor
Resolution (Å)	158.40 – 2.10 49.47 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.9 (158.40-2.10) 99.9 (49.47-2.10)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.01 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.174 , 0.220 0.183 , 0.225	Depositor DCC
$R_{free}$ test set	10459 reflections (5.36%)	DCC
Wilson B-factor (Å <sup>2</sup> )	33.2	Xtriage
Anisotropy	0.302	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.35 , 39.5	EDS
Estimated twinning fraction	0.018 for h,-k,-l	Xtriage
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Outliers	0 of 205508 reflections	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	23838	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.83% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

## 5 Model quality [i](#)

### 5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TRS, PO4, JAZ, 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	0.95	3/3897 (0.1%)	0.96	9/5315 (0.2%)
1	B	0.95	1/3902 (0.0%)	0.95	5/5321 (0.1%)
1	C	0.93	4/3898 (0.1%)	0.96	11/5317 (0.2%)
1	D	0.90	1/3905 (0.0%)	0.94	14/5324 (0.3%)
1	E	0.91	2/3900 (0.1%)	0.91	6/5319 (0.1%)
1	F	0.88	1/3892 (0.0%)	0.91	9/5308 (0.2%)
All	All	0.92	12/23394 (0.1%)	0.94	54/31904 (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	A	0	4
1	B	0	4
1	C	0	5
1	D	0	4
1	E	0	5
1	F	0	4
All	All	0	26

All (12) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	366	GLU	CD-OE2	9.71	1.36	1.25
1	F	366	GLU	CD-OE2	9.39	1.35	1.25
1	B	366	GLU	CD-OE2	8.73	1.35	1.25
1	A	366	GLU	CD-OE2	8.66	1.35	1.25
1	C	366	GLU	CD-OE2	7.00	1.33	1.25
1	A	171	GLU	CD-OE2	6.74	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	171	GLU	CD-OE2	6.54	1.32	1.25
1	C	366	GLU	CD-OE1	-6.40	1.18	1.25
1	A	165	GLU	CD-OE1	5.89	1.32	1.25
1	C	321	TRP	CB-CG	5.16	1.59	1.50
1	D	171	GLU	CD-OE2	5.08	1.31	1.25
1	E	94	ASP	CB-CG	5.07	1.62	1.51

All (54) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	176	MET	CG-SD-CE	11.92	119.28	100.20
1	F	378	ARG	NE-CZ-NH1	8.04	124.32	120.30
1	D	444	ARG	NE-CZ-NH1	7.97	124.29	120.30
1	C	292	ASP	CB-CG-OD2	7.75	125.28	118.30
1	C	379	ASP	CB-CG-OD1	7.51	125.06	118.30
1	F	378	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	A	292	ASP	CB-CG-OD2	7.08	124.67	118.30
1	E	431	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	F	176	MET	CG-SD-CE	7.01	111.41	100.20
1	A	22	ARG	NE-CZ-NH1	6.84	123.72	120.30
1	A	332	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	C	292	ASP	CB-CG-OD1	-6.74	112.23	118.30
1	A	292	ASP	CB-CG-OD1	-6.67	112.29	118.30
1	B	180	TYR	C-N-CD	-6.54	106.20	120.60
1	A	378	ARG	NE-CZ-NH2	-6.54	117.03	120.30
1	C	379	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	E	180	TYR	C-N-CD	-6.46	106.38	120.60
1	F	444	ARG	NE-CZ-NH2	-6.45	117.07	120.30
1	D	85	ASP	CB-CG-OD1	6.25	123.92	118.30
1	D	101	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	A	28	ARG	NE-CZ-NH2	-6.05	117.28	120.30
1	F	180	TYR	C-N-CD	-6.03	107.33	120.60
1	F	389	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	C	312	VAL	CB-CA-C	-5.92	100.16	111.40
1	C	22	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	D	104	ASP	CB-CG-OD1	5.89	123.60	118.30
1	D	444	ARG	NE-CZ-NH2	-5.87	117.36	120.30
1	D	180	TYR	C-N-CD	-5.85	107.73	120.60
1	F	444	ARG	NE-CZ-NH1	5.77	123.19	120.30
1	D	293	TYR	CB-CG-CD1	5.70	124.42	121.00
1	A	444	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	303	ARG	NE-CZ-NH1	5.59	123.10	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	445	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	E	94	ASP	CB-CG-OD1	5.56	123.30	118.30
1	E	293	TYR	CB-CG-CD1	5.54	124.33	121.00
1	C	185	ASP	CB-CG-OD1	5.54	123.29	118.30
1	D	218	ARG	NE-CZ-NH1	5.53	123.07	120.30
1	C	156	ARG	NE-CZ-NH1	5.51	123.06	120.30
1	B	389	ARG	NE-CZ-NH2	-5.51	117.55	120.30
1	D	445	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	B	290	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	A	378	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	D	378	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	F	332	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	B	28	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	B	332	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	E	293	TYR	CB-CG-CD2	-5.23	117.86	121.00
1	C	378	ARG	NE-CZ-NH1	5.15	122.87	120.30
1	D	40	ASP	CB-CG-OD1	5.12	122.91	118.30
1	C	40	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	F	225	LEU	CB-CG-CD1	5.08	119.64	111.00
1	D	94	ASP	CB-CG-OD1	5.04	122.83	118.30
1	D	156	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	D	156	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (26) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	180	TYR	Mainchain,Peptide
1	A	416	TRP	Mainchain,Peptide
1	B	180	TYR	Mainchain,Peptide
1	B	416	TRP	Mainchain,Peptide
1	C	180	TYR	Mainchain,Peptide
1	C	294	LEU	Peptide
1	C	416	TRP	Mainchain,Peptide
1	D	180	TYR	Mainchain,Peptide
1	D	416	TRP	Mainchain,Peptide
1	E	180	TYR	Mainchain,Peptide
1	E	299	TYR	Peptide
1	E	416	TRP	Mainchain,Peptide
1	F	180	TYR	Mainchain,Peptide
1	F	416	TRP	Mainchain,Peptide

## 5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3772	0	3569	15	0
1	B	3777	0	3575	13	0
1	C	3773	0	3564	9	0
1	D	3780	0	3584	16	0
1	E	3775	0	3571	13	0
1	F	3767	0	3560	20	0
2	A	16	0	11	2	0
2	B	16	0	11	0	0
2	C	16	0	11	0	0
2	D	16	0	11	0	0
2	E	16	0	11	0	0
2	F	16	0	11	0	0
3	A	20	0	30	2	0
3	B	20	0	30	2	0
3	C	8	0	12	0	0
3	D	16	0	24	0	0
3	E	4	0	6	1	0
3	F	8	0	12	0	0
4	A	5	0	0	0	0
4	B	5	0	0	0	0
4	C	5	0	0	0	0
4	D	5	0	0	0	0
4	E	5	0	0	0	0
4	F	5	0	0	0	0
5	A	1	0	0	0	0
5	B	1	0	0	1	0
5	D	1	0	0	0	0
6	C	8	0	12	0	0
7	A	214	0	0	0	0
7	B	224	0	0	2	0
7	C	173	0	0	0	0
7	D	130	0	0	0	0
7	E	143	0	0	2	0
7	F	97	0	0	0	0
All	All	23838	0	21615	82	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 2.

All (82) 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:F:279:THR:HG22	1:F:282:GLU:H	1.51	0.76
1:B:451:TYR:OH	7:B:2223:HOH:O	2.02	0.69
1:D:344:GLU:HG3	1:D:399:TYR:CZ	2.32	0.63
1:F:147:LYS:HD2	1:F:206:ALA:HB1	1.83	0.61
1:E:303:ARG:HH12	3:E:1465:EDO:H21	1.66	0.60
1:E:12:GLY:HA3	1:E:418:PRO:HG3	1.83	0.59
1:F:139:VAL:HG13	1:F:199:ALA:HB2	1.84	0.59
1:D:147:LYS:HD3	1:D:206:ALA:HB1	1.84	0.59
1:A:1:MET:CE	1:A:463:ILE:HD12	2.36	0.56
1:F:107:LEU:HD11	1:F:156:ARG:HB3	1.88	0.56
1:F:379:ASP:OD1	1:F:381:THR:HG22	2.05	0.56
1:A:423:SER:CB	2:A:1464:JAZ:O12	2.55	0.55
1:A:379:ASP:OD1	1:A:381:THR:HG22	2.06	0.54
1:F:362:TRP:O	1:F:410:CYS:HA	2.07	0.54
1:D:147:LYS:CD	1:D:206:ALA:HB1	2.37	0.54
1:B:320:GLU:O	7:B:2160:HOH:O	2.19	0.54
1:B:218:ARG:HE	3:B:1467:EDO:H12	1.74	0.53
1:F:225:LEU:CD2	1:F:353:MET:HE3	2.37	0.53
1:F:147:LYS:CD	1:F:206:ALA:HB1	2.39	0.53
1:B:463:ILE:HG22	5:B:1471:CL:CL	2.45	0.52
1:A:225:LEU:HD13	1:A:253:MET:HG3	1.90	0.52
1:C:362:TRP:O	1:C:410:CYS:HA	2.10	0.52
1:F:353:MET:HE1	1:F:357:TYR:CD2	2.46	0.51
1:B:1:MET:HE1	1:B:463:ILE:HD12	1.93	0.51
1:F:225:LEU:CD2	1:F:353:MET:CE	2.91	0.49
1:A:344:GLU:HG3	1:A:399:TYR:CZ	2.48	0.49
1:A:375:ASP:O	1:A:378:ARG:HG3	2.12	0.49
1:E:174:TYR:CE2	1:E:192:VAL:HG21	2.48	0.48
1:E:279:THR:HG22	1:E:281:GLU:N	2.28	0.48
1:C:312:VAL:HG22	1:D:341:ILE:HD12	1.96	0.48
1:F:251:LEU:C	1:F:251:LEU:HD23	2.34	0.48
1:A:324:ASP:HA	3:A:1469:EDO:H11	1.95	0.47
1:C:140:ASP:OD1	1:C:202:LYS:NZ	2.47	0.47
1:D:310:ILE:N	1:D:310:ILE:HD12	2.29	0.47
1:C:312:VAL:HG23	1:D:334:ASN:HA	1.97	0.47
1:E:279:THR:HG22	1:E:281:GLU:H	1.79	0.47
1:B:279:THR:HG23	1:B:281:GLU:OE1	2.14	0.47
1:A:362:TRP:O	1:A:410:CYS:HA	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:337:LYS:CE	7:E:2111:HOH:O	2.62	0.47
1:B:143:VAL:HG12	1:B:147:LYS:HD2	1.98	0.46
1:A:423:SER:HB3	2:A:1464:JAZ:O12	2.14	0.46
1:E:362:TRP:O	1:E:410:CYS:HA	2.16	0.46
1:D:225:LEU:HD13	1:D:253:MET:HG3	1.97	0.46
1:C:171:GLU:HB3	1:C:176:MET:HE2	1.98	0.46
1:D:3:ALA:O	1:D:401:HIS:NE2	2.47	0.46
1:F:253:MET:HE1	1:F:353:MET:CE	2.46	0.45
1:E:225:LEU:HD13	1:E:253:MET:HG3	1.97	0.45
1:D:333:MET:HE2	1:D:340:GLU:HA	1.99	0.45
1:A:333:MET:CE	1:A:335:VAL:HG22	2.46	0.45
1:C:312:VAL:HG22	1:D:341:ILE:CD1	2.47	0.45
1:D:171:GLU:HB3	1:D:176:MET:HE2	1.98	0.45
1:E:397:LEU:HB3	1:E:462:LEU:HD11	1.99	0.45
1:B:106:CYS:HB3	1:B:111:ILE:O	2.17	0.45
1:A:378:ARG:NH2	1:A:436:GLU:OE1	2.47	0.44
1:A:417:THR:O	1:A:433:GLY:HA2	2.17	0.44
1:F:279:THR:HG23	1:F:281:GLU:OE1	2.18	0.44
1:B:218:ARG:HE	3:B:1467:EDO:C1	2.30	0.44
1:F:366:GLU:HG3	1:F:416:TRP:HB2	2.00	0.44
1:B:16:GLY:N	1:B:17:PRO:CD	2.82	0.43
1:C:344:GLU:HG3	1:C:399:TYR:CZ	2.54	0.43
1:A:258:HIS:HD2	1:B:235:GLU:OE2	2.02	0.43
1:F:253:MET:HE1	1:F:353:MET:HE3	2.00	0.43
1:E:344:GLU:HG3	1:E:399:TYR:CZ	2.53	0.42
1:F:225:LEU:HD22	1:F:353:MET:HE3	2.02	0.42
1:F:225:LEU:HD13	1:F:253:MET:HG3	2.02	0.42
1:D:417:THR:O	1:D:433:GLY:HA2	2.19	0.42
1:E:337:LYS:HE2	7:E:2111:HOH:O	2.19	0.42
1:A:324:ASP:OD1	3:A:1469:EDO:O2	2.38	0.42
1:A:426:ASN:O	1:A:427:ALA:C	2.58	0.42
1:B:419:ILE:O	1:B:420:ASP:C	2.59	0.42
1:C:167:MET:O	1:C:171:GLU:HG3	2.20	0.41
1:D:9:TRP:HB2	1:D:412:GLY:HA3	2.01	0.41
1:D:190:VAL:HG11	1:D:274:VAL:O	2.20	0.41
1:C:342:TYR:CE2	1:C:344:GLU:HB2	2.55	0.41
1:F:294:LEU:O	1:F:362:TRP:HA	2.21	0.41
1:B:151:GLU:HA	1:B:214:LEU:HD13	2.02	0.41
1:E:417:THR:O	1:E:433:GLY:HA2	2.20	0.41
1:F:428:TYR:CG	1:F:439:ILE:HG21	2.55	0.41
1:D:198:LEU:O	1:D:202:LYS:HG3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:162:VAL:HG11	1:E:200:THR:HA	2.03	0.41
1:D:279:THR:HG22	1:D:281:GLU:N	2.35	0.40
1:F:362:TRP:CZ2	1:F:410:CYS:HB2	2.57	0.40

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	461/480 (96%)	448 (97%)	12 (3%)	1 (0%)	52	53
1	B	461/480 (96%)	447 (97%)	14 (3%)	0	100	100
1	C	461/480 (96%)	444 (96%)	17 (4%)	0	100	100
1	D	461/480 (96%)	446 (97%)	14 (3%)	1 (0%)	52	53
1	E	461/480 (96%)	445 (96%)	15 (3%)	1 (0%)	52	53
1	F	460/480 (96%)	446 (97%)	12 (3%)	2 (0%)	39	37
All	All	2765/2880 (96%)	2676 (97%)	84 (3%)	5 (0%)	52	53

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	F	359	ASN
1	D	181	PRO
1	F	181	PRO
1	E	181	PRO
1	A	181	PRO

### 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	388/405 (96%)	380 (98%)	8 (2%)	61	66
1	B	389/405 (96%)	380 (98%)	9 (2%)	58	62
1	C	388/405 (96%)	380 (98%)	8 (2%)	61	66
1	D	390/405 (96%)	384 (98%)	6 (2%)	72	78
1	E	389/405 (96%)	384 (99%)	5 (1%)	76	82
1	F	388/405 (96%)	381 (98%)	7 (2%)	66	72
All	All	2332/2430 (96%)	2289 (98%)	43 (2%)	66	72

All (43) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	2	LEU
1	A	285	LEU
1	A	293	TYR
1	A	314	SER
1	A	375	ASP
1	A	405	GLU
1	A	423	SER
1	A	463	ILE
1	B	1	MET
1	B	293	TYR
1	B	313	ILE
1	B	331	HIS
1	B	375	ASP
1	B	405	GLU
1	B	423	SER
1	B	445	ARG
1	B	455	LYS
1	C	218	ARG
1	C	285	LEU
1	C	290	ARG
1	C	293	TYR
1	C	300	HIS

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Mol	Chain	Res	Type
1	C	331	HIS
1	C	333	MET
1	C	397	LEU
1	D	2	LEU
1	D	281	GLU
1	D	293	TYR
1	D	314	SER
1	D	331	HIS
1	D	381	THR
1	E	1	MET
1	E	293	TYR
1	E	405	GLU
1	E	423	SER
1	E	461	ARG
1	F	135	SER
1	F	271	LYS
1	F	279	THR
1	F	293	TYR
1	F	331	HIS
1	F	423	SER
1	F	444	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	C	426	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 35 ligands modelled in this entry, 3 are monoatomic - leaving 32 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	$\# Z  > 2$
2	JAZ	A	1464	1	16,16,17	0.92	2 (12%)	18,24,26	1.08	1 (5%)
3	EDO	A	1465	-	3,3,3	0.21	0	2,2,2	0.73	0
3	EDO	A	1466	-	3,3,3	0.42	0	2,2,2	0.57	0
3	EDO	A	1467	-	3,3,3	0.39	0	2,2,2	0.79	0
3	EDO	A	1468	-	3,3,3	0.66	0	2,2,2	0.50	0
3	EDO	A	1469	-	3,3,3	0.89	0	2,2,2	0.70	0
4	PO4	A	1470	-	4,4,4	1.37	0	6,6,6	0.37	0
2	JAZ	B	1464	1	16,16,17	0.84	0	18,24,26	0.85	1 (5%)
3	EDO	B	1465	-	3,3,3	0.28	0	2,2,2	1.23	0
3	EDO	B	1466	-	3,3,3	0.22	0	2,2,2	0.94	0
3	EDO	B	1467	-	3,3,3	0.13	0	2,2,2	1.95	1 (50%)
3	EDO	B	1468	-	3,3,3	0.93	0	2,2,2	0.65	0
3	EDO	B	1469	-	3,3,3	0.56	0	2,2,2	0.32	0
4	PO4	B	1470	-	4,4,4	0.57	0	6,6,6	0.37	0
2	JAZ	C	1464	1	16,16,17	0.90	1 (6%)	18,24,26	1.11	1 (5%)
6	TRS	C	1465	-	7,7,7	0.76	0	9,9,9	1.44	2 (22%)
3	EDO	C	1466	-	3,3,3	0.38	0	2,2,2	1.16	0
3	EDO	C	1467	-	3,3,3	0.43	0	2,2,2	1.03	0
4	PO4	C	1468	-	4,4,4	0.86	0	6,6,6	0.35	0
2	JAZ	D	1464	1	16,16,17	1.21	0	18,24,26	1.14	1 (5%)
3	EDO	D	1465	-	3,3,3	0.42	0	2,2,2	1.42	0
3	EDO	D	1466	-	3,3,3	0.30	0	2,2,2	1.03	0
3	EDO	D	1467	-	3,3,3	0.21	0	2,2,2	1.48	0
3	EDO	D	1468	-	3,3,3	0.37	0	2,2,2	0.12	0
4	PO4	D	1469	-	4,4,4	0.74	0	6,6,6	0.36	0
2	JAZ	E	1464	1	16,16,17	0.64	0	18,24,26	1.05	1 (5%)
3	EDO	E	1465	-	3,3,3	0.29	0	2,2,2	0.99	0
4	PO4	E	1466	-	4,4,4	0.98	0	6,6,6	0.41	0
2	JAZ	F	1464	1	16,16,17	0.98	1 (6%)	18,24,26	1.73	5 (27%)
3	EDO	F	1465	-	3,3,3	0.31	0	2,2,2	0.44	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	EDO	F	1466	-	3,3,3	0.47	0	2,2,2	0.25	0
4	PO4	F	1467	-	4,4,4	0.99	0	6,6,6	0.31	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
2	JAZ	A	1464	1	-	0/6/26/30	0/1/1/1
3	EDO	A	1465	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1466	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1467	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1468	-	-	0/1/1/1	0/0/0/0
3	EDO	A	1469	-	-	0/1/1/1	0/0/0/0
4	PO4	A	1470	-	-	0/0/0/0	0/0/0/0
2	JAZ	B	1464	1	-	0/6/26/30	0/1/1/1
3	EDO	B	1465	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1466	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1467	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1468	-	-	0/1/1/1	0/0/0/0
3	EDO	B	1469	-	-	0/1/1/1	0/0/0/0
4	PO4	B	1470	-	-	0/0/0/0	0/0/0/0
2	JAZ	C	1464	1	-	0/6/26/30	0/1/1/1
6	TRS	C	1465	-	-	0/9/9/9	0/0/0/0
3	EDO	C	1466	-	-	0/1/1/1	0/0/0/0
3	EDO	C	1467	-	-	0/1/1/1	0/0/0/0
4	PO4	C	1468	-	-	0/0/0/0	0/0/0/0
2	JAZ	D	1464	1	-	0/6/26/30	0/1/1/1
3	EDO	D	1465	-	-	0/1/1/1	0/0/0/0
3	EDO	D	1466	-	-	0/1/1/1	0/0/0/0
3	EDO	D	1467	-	-	0/1/1/1	0/0/0/0
3	EDO	D	1468	-	-	0/1/1/1	0/0/0/0
4	PO4	D	1469	-	-	0/0/0/0	0/0/0/0
2	JAZ	E	1464	1	-	0/6/26/30	0/1/1/1
3	EDO	E	1465	-	-	0/1/1/1	0/0/0/0
4	PO4	E	1466	-	-	0/0/0/0	0/0/0/0
2	JAZ	F	1464	1	-	0/6/26/30	0/1/1/1
3	EDO	F	1465	-	-	0/1/1/1	0/0/0/0
3	EDO	F	1466	-	-	0/1/1/1	0/0/0/0
4	PO4	F	1467	-	-	0/0/0/0	0/0/0/0

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1464	JAZ	P10-O13	-2.23	1.47	1.54
2	A	1464	JAZ	P10-O12	-2.07	1.47	1.54
2	C	1464	JAZ	O17-C4	2.12	1.48	1.43
2	F	1464	JAZ	P10-O9	2.57	1.67	1.59

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	1464	JAZ	O16-C3-C4	-3.11	104.32	110.01
3	B	1467	EDO	O2-C2-C1	-2.72	93.61	112.23
2	B	1464	JAZ	O16-C3-C2	-2.30	105.17	110.36
2	D	1464	JAZ	C5-C4-C3	-2.26	107.52	110.54
2	F	1464	JAZ	C5-C6-C7	-2.24	107.88	112.64
6	C	1465	TRS	O3-C3-C	-2.18	105.75	110.92
2	C	1464	JAZ	O13-P10-O11	-2.03	104.00	110.63
2	E	1464	JAZ	O13-P10-O11	2.12	117.55	110.63
2	F	1464	JAZ	O13-P10-O11	2.27	118.04	110.63
2	F	1464	JAZ	O14-C6-C7	2.43	115.19	110.29
2	A	1464	JAZ	O12-P10-O11	2.82	119.83	110.63
2	F	1464	JAZ	C5-C4-C3	3.12	114.71	110.54
6	C	1465	TRS	C3-C-N	3.22	113.35	107.88

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1464	JAZ	2	0
3	A	1469	EDO	2	0
3	B	1467	EDO	2	0
3	E	1465	EDO	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



## 6 Fit of model and data ⓘ

### 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	463/480 (96%)	-0.34	1 (0%)	95 96	24, 31, 47, 66	1 (0%)
1	B	463/480 (96%)	-0.38	5 (1%)	82 86	20, 31, 48, 76	0
1	C	463/480 (96%)	-0.43	1 (0%)	95 96	24, 33, 46, 65	0
1	D	463/480 (96%)	-0.33	3 (0%)	90 92	25, 35, 53, 79	0
1	E	463/480 (96%)	-0.43	1 (0%)	95 96	24, 35, 52, 79	0
1	F	462/480 (96%)	-0.13	5 (1%)	82 86	28, 44, 63, 91	0
All	All	2777/2880 (96%)	-0.34	16 (0%)	90 92	20, 34, 54, 91	1 (0%)

All (16) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	1	MET	4.0
1	B	463	ILE	2.9
1	C	6	LYS	2.8
1	F	458	THR	2.7
1	B	281	GLU	2.5
1	B	285	LEU	2.5
1	E	380	GLU	2.4
1	D	88	GLN	2.4
1	F	263	GLU	2.3
1	D	463	ILE	2.3
1	F	380	GLU	2.2
1	B	280	PRO	2.2
1	A	380	GLU	2.1
1	B	1	MET	2.1
1	F	327	LEU	2.0
1	D	315	PRO	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( $\text{\AA}^2$ )	Q<0.9
4	PO4	B	1470	5/5	0.94	0.16	26.57	42,42,59,67	0
4	PO4	A	1470	5/5	0.97	0.15	16.01	35,42,55,58	0
3	EDO	A	1468	4/4	0.79	0.29	14.22	40,47,50,60	4
3	EDO	D	1468	4/4	0.91	0.23	7.34	38,39,41,42	4
3	EDO	A	1465	4/4	0.93	0.29	7.09	33,33,35,37	4
3	EDO	A	1469	4/4	0.89	0.17	6.88	36,46,49,54	0
3	EDO	D	1465	4/4	0.88	0.22	6.76	39,39,44,47	4
3	EDO	B	1467	4/4	0.94	0.22	6.60	33,38,39,41	4
3	EDO	D	1467	4/4	0.95	0.14	5.49	35,36,37,43	4
3	EDO	D	1466	4/4	0.90	0.15	3.87	38,40,41,42	4
3	EDO	A	1467	4/4	0.93	0.14	3.82	30,34,34,41	4
3	EDO	F	1465	4/4	0.95	0.15	2.76	39,40,40,42	4
4	PO4	C	1468	5/5	0.99	0.12	2.70	37,43,54,55	0
3	EDO	B	1469	4/4	0.91	0.15	1.77	37,42,43,44	4
3	EDO	B	1466	4/4	0.95	0.14	1.68	32,33,36,41	4
4	PO4	D	1469	5/5	0.97	0.11	1.38	43,45,54,57	0
3	EDO	A	1466	4/4	0.96	0.14	1.14	38,41,42,49	0
4	PO4	E	1466	5/5	0.97	0.10	1.03	42,44,59,66	0
3	EDO	B	1468	4/4	0.96	0.10	0.66	37,41,41,41	0
5	CL	A	1471	1/1	0.98	0.15	0.38	31,31,31,31	0
3	EDO	B	1465	4/4	0.93	0.13	0.23	39,40,44,52	0
2	JAZ	B	1464	16/17	0.98	0.10	0.05	21,23,25,25	0
2	JAZ	A	1464	16/17	0.98	0.11	-0.14	26,27,38,44	0
2	JAZ	D	1464	16/17	0.98	0.10	-0.23	22,27,29,31	0
2	JAZ	E	1464	16/17	0.99	0.08	-0.24	23,25,27,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors( $\text{\AA}^2$ )	Q<0.9
4	PO4	F	1467	5/5	0.97	0.10	-0.57	47,53,54,63	0
3	EDO	F	1466	4/4	0.97	0.08	-0.58	33,35,37,41	4
2	JAZ	C	1464	16/17	0.98	0.10	-0.58	20,25,27,28	0
2	JAZ	F	1464	16/17	0.97	0.09	-0.68	28,31,35,35	0
5	CL	B	1471	1/1	0.95	0.05	-	45,45,45,45	0
3	EDO	C	1467	4/4	0.85	0.20	-	39,41,51,59	0
3	EDO	E	1465	4/4	0.80	0.17	-	37,43,44,45	4
6	TRS	C	1465	8/8	0.89	0.12	-	43,48,50,50	0
3	EDO	C	1466	4/4	0.94	0.13	-	31,32,33,39	4
5	CL	D	1470	1/1	0.96	0.08	-	46,46,46,46	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.