



# Full wwPDB X-ray Structure Validation Report ⓘ

Dec 21, 2024 – 04:17 pm GMT

PDB ID : 8RG3  
Title : Crystal structure of PbFucA from Planctomycetes bacterium K23\_9 in P 1 21  
1  
Authors : Perez-Curz, C.; Moraleda-Montoya, A.; Liebana, R.; Lorizate, M.; Arrizabalaga, U.; Garcia-Alija, M.; Terrones, O.; Contreras, F.X.; Guerin, M.E.; Trastoy, B.; Alonso-Saez, L.  
Deposited on : 2023-12-13  
Resolution : 2.50 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.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

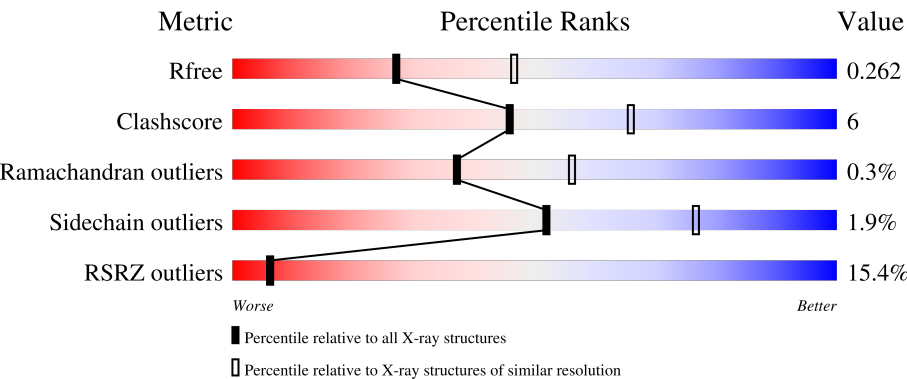
MolProbity	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.40

# 1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:  
*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.50 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))
$R_{free}$	164625	5504 (2.50-2.50)
Clashscore	180529	6282 (2.50-2.50)
Ramachandran outliers	177936	6191 (2.50-2.50)
Sidechain outliers	177891	6193 (2.50-2.50)
RSRZ outliers	164620	5504 (2.50-2.50)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	373	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>%86%9%5%</div>
1	B	373	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>%83%12%5%</div>
1	C	373	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>5%86%9%5%</div>
1	D	373	<div><div></div><div></div><div></div><div></div><div></div><div></div></div> <div>13%86%10%5%</div>

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Mol	Chain	Length	Quality of chain
1	E	373	<div><div></div><div>17%</div><div>79%</div><div>16%</div><div>5%</div></div>
1	F	373	<div><div></div><div>52%</div><div>74%</div><div>20%</div><div>• 5%</div></div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 16917 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 Glycoside-hydrolase family GH114 TIM-barrel domain-containing protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	356	Total	C	N	O	S	0	1	0
			2853	1831	501	506	15			
1	B	355	Total	C	N	O	S	0	1	0
			2813	1805	485	508	15			
1	C	356	Total	C	N	O	S	0	1	0
			2809	1806	484	504	15			
1	D	356	Total	C	N	O	S	0	0	0
			2733	1758	468	492	15			
1	E	355	Total	C	N	O	S	0	3	0
			2792	1793	479	504	16			
1	F	356	Total	C	N	O	S	0	1	0
			2739	1765	467	493	14			

There are 96 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	20	MET	-	initiating methionine	UNP A0A517NMB4
A	21	HIS	-	expression tag	UNP A0A517NMB4
A	22	HIS	-	expression tag	UNP A0A517NMB4
A	23	HIS	-	expression tag	UNP A0A517NMB4
A	24	HIS	-	expression tag	UNP A0A517NMB4
A	25	HIS	-	expression tag	UNP A0A517NMB4
A	26	HIS	-	expression tag	UNP A0A517NMB4
A	27	GLU	-	expression tag	UNP A0A517NMB4
A	28	ASN	-	expression tag	UNP A0A517NMB4
A	29	LEU	-	expression tag	UNP A0A517NMB4
A	30	TYR	-	expression tag	UNP A0A517NMB4
A	31	PHE	-	expression tag	UNP A0A517NMB4
A	32	GLN	-	expression tag	UNP A0A517NMB4
A	33	GLY	-	expression tag	UNP A0A517NMB4
A	34	SER	-	expression tag	UNP A0A517NMB4
A	35	GLY	-	expression tag	UNP A0A517NMB4

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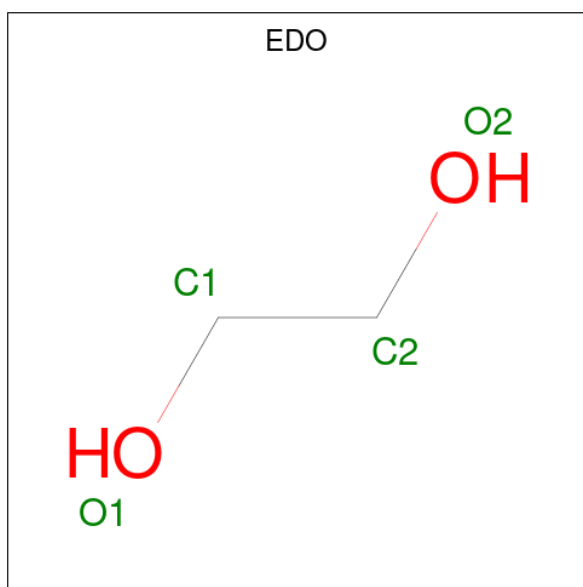
Chain	Residue	Modelled	Actual	Comment	Reference
B	20	MET	-	initiating methionine	UNP A0A517NMB4
B	21	HIS	-	expression tag	UNP A0A517NMB4
B	22	HIS	-	expression tag	UNP A0A517NMB4
B	23	HIS	-	expression tag	UNP A0A517NMB4
B	24	HIS	-	expression tag	UNP A0A517NMB4
B	25	HIS	-	expression tag	UNP A0A517NMB4
B	26	HIS	-	expression tag	UNP A0A517NMB4
B	27	GLU	-	expression tag	UNP A0A517NMB4
B	28	ASN	-	expression tag	UNP A0A517NMB4
B	29	LEU	-	expression tag	UNP A0A517NMB4
B	30	TYR	-	expression tag	UNP A0A517NMB4
B	31	PHE	-	expression tag	UNP A0A517NMB4
B	32	GLN	-	expression tag	UNP A0A517NMB4
B	33	GLY	-	expression tag	UNP A0A517NMB4
B	34	SER	-	expression tag	UNP A0A517NMB4
B	35	GLY	-	expression tag	UNP A0A517NMB4
C	20	MET	-	initiating methionine	UNP A0A517NMB4
C	21	HIS	-	expression tag	UNP A0A517NMB4
C	22	HIS	-	expression tag	UNP A0A517NMB4
C	23	HIS	-	expression tag	UNP A0A517NMB4
C	24	HIS	-	expression tag	UNP A0A517NMB4
C	25	HIS	-	expression tag	UNP A0A517NMB4
C	26	HIS	-	expression tag	UNP A0A517NMB4
C	27	GLU	-	expression tag	UNP A0A517NMB4
C	28	ASN	-	expression tag	UNP A0A517NMB4
C	29	LEU	-	expression tag	UNP A0A517NMB4
C	30	TYR	-	expression tag	UNP A0A517NMB4
C	31	PHE	-	expression tag	UNP A0A517NMB4
C	32	GLN	-	expression tag	UNP A0A517NMB4
C	33	GLY	-	expression tag	UNP A0A517NMB4
C	34	SER	-	expression tag	UNP A0A517NMB4
C	35	GLY	-	expression tag	UNP A0A517NMB4
D	20	MET	-	initiating methionine	UNP A0A517NMB4
D	21	HIS	-	expression tag	UNP A0A517NMB4
D	22	HIS	-	expression tag	UNP A0A517NMB4
D	23	HIS	-	expression tag	UNP A0A517NMB4
D	24	HIS	-	expression tag	UNP A0A517NMB4
D	25	HIS	-	expression tag	UNP A0A517NMB4
D	26	HIS	-	expression tag	UNP A0A517NMB4
D	27	GLU	-	expression tag	UNP A0A517NMB4
D	28	ASN	-	expression tag	UNP A0A517NMB4
D	29	LEU	-	expression tag	UNP A0A517NMB4

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Chain	Residue	Modelled	Actual	Comment	Reference
D	30	TYR	-	expression tag	UNP A0A517NMB4
D	31	PHE	-	expression tag	UNP A0A517NMB4
D	32	GLN	-	expression tag	UNP A0A517NMB4
D	33	GLY	-	expression tag	UNP A0A517NMB4
D	34	SER	-	expression tag	UNP A0A517NMB4
D	35	GLY	-	expression tag	UNP A0A517NMB4
E	20	MET	-	initiating methionine	UNP A0A517NMB4
E	21	HIS	-	expression tag	UNP A0A517NMB4
E	22	HIS	-	expression tag	UNP A0A517NMB4
E	23	HIS	-	expression tag	UNP A0A517NMB4
E	24	HIS	-	expression tag	UNP A0A517NMB4
E	25	HIS	-	expression tag	UNP A0A517NMB4
E	26	HIS	-	expression tag	UNP A0A517NMB4
E	27	GLU	-	expression tag	UNP A0A517NMB4
E	28	ASN	-	expression tag	UNP A0A517NMB4
E	29	LEU	-	expression tag	UNP A0A517NMB4
E	30	TYR	-	expression tag	UNP A0A517NMB4
E	31	PHE	-	expression tag	UNP A0A517NMB4
E	32	GLN	-	expression tag	UNP A0A517NMB4
E	33	GLY	-	expression tag	UNP A0A517NMB4
E	34	SER	-	expression tag	UNP A0A517NMB4
E	35	GLY	-	expression tag	UNP A0A517NMB4
F	20	MET	-	initiating methionine	UNP A0A517NMB4
F	21	HIS	-	expression tag	UNP A0A517NMB4
F	22	HIS	-	expression tag	UNP A0A517NMB4
F	23	HIS	-	expression tag	UNP A0A517NMB4
F	24	HIS	-	expression tag	UNP A0A517NMB4
F	25	HIS	-	expression tag	UNP A0A517NMB4
F	26	HIS	-	expression tag	UNP A0A517NMB4
F	27	GLU	-	expression tag	UNP A0A517NMB4
F	28	ASN	-	expression tag	UNP A0A517NMB4
F	29	LEU	-	expression tag	UNP A0A517NMB4
F	30	TYR	-	expression tag	UNP A0A517NMB4
F	31	PHE	-	expression tag	UNP A0A517NMB4
F	32	GLN	-	expression tag	UNP A0A517NMB4
F	33	GLY	-	expression tag	UNP A0A517NMB4
F	34	SER	-	expression tag	UNP A0A517NMB4
F	35	GLY	-	expression tag	UNP A0A517NMB4

- Molecule 2 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
2	A	1	Total	C	O	0	0
			4	2	2		
2	B	1	Total	C	O	0	0
			4	2	2		
2	C	1	Total	C	O	0	0
			4	2	2		

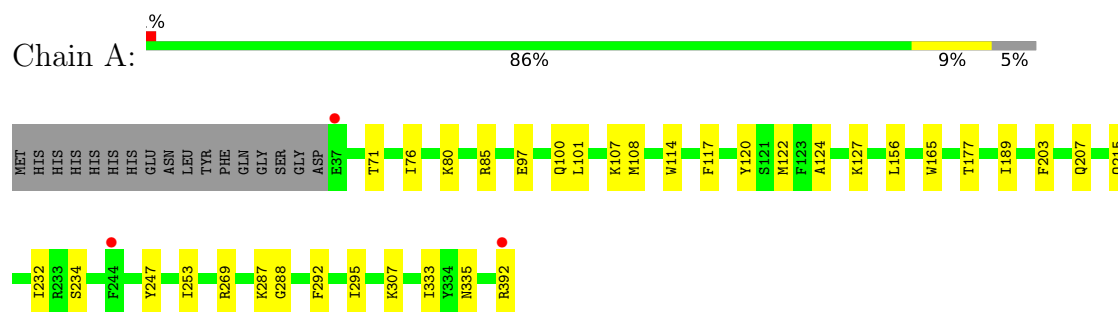
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	33	Total	O	0	0
			33	33		
3	B	47	Total	O	0	0
			47	47		
3	C	32	Total	O	0	0
			32	32		
3	D	27	Total	O	0	0
			27	27		
3	E	22	Total	O	0	0
			22	22		
3	F	5	Total	O	0	0
			5	5		

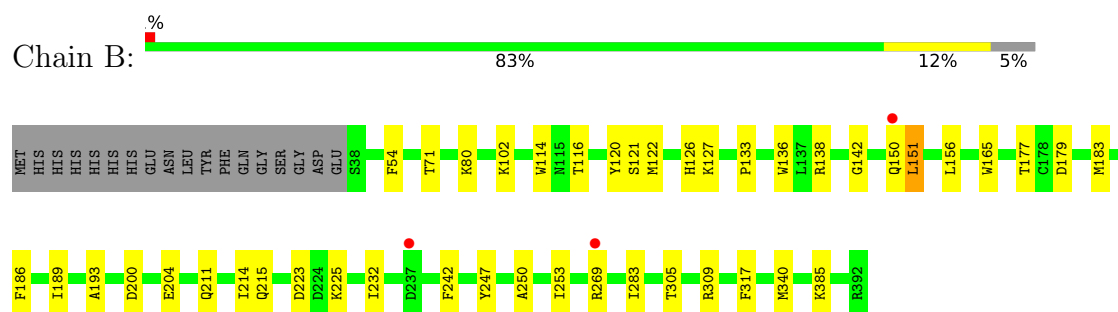
### 3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

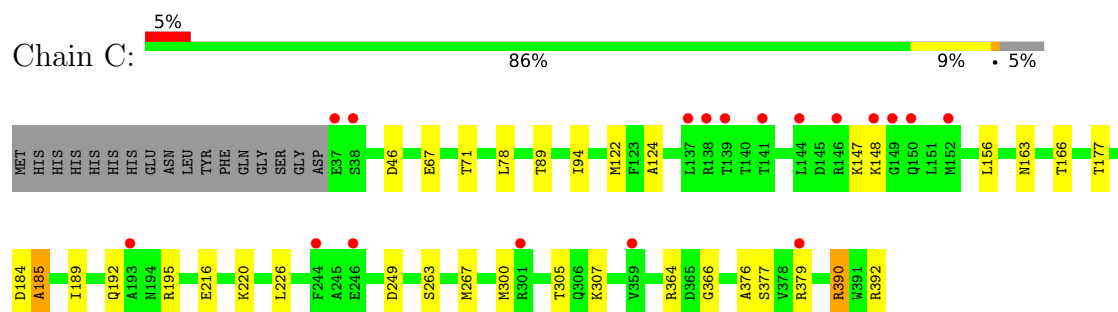
- Molecule 1: Glycoside-hydrolase family GH114 TIM-barrel domain-containing protein



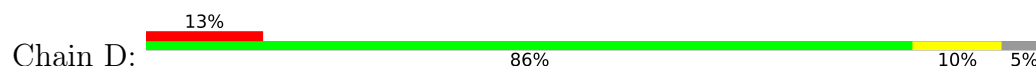
- Molecule 1: Glycoside-hydrolase family GH114 TIM-barrel domain-containing protein



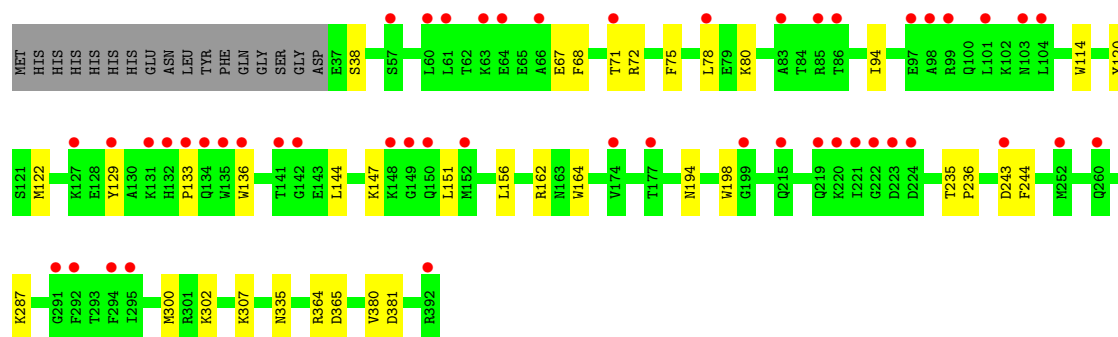
- Molecule 1: Glycoside-hydrolase family GH114 TIM-barrel domain-containing protein



- Molecule 1: Glycoside-hydrolase family GH114 TIM-barrel domain-containing protein

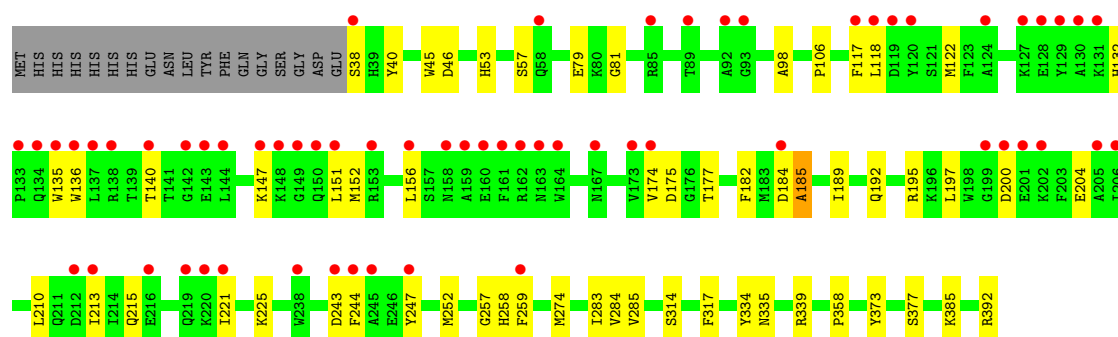






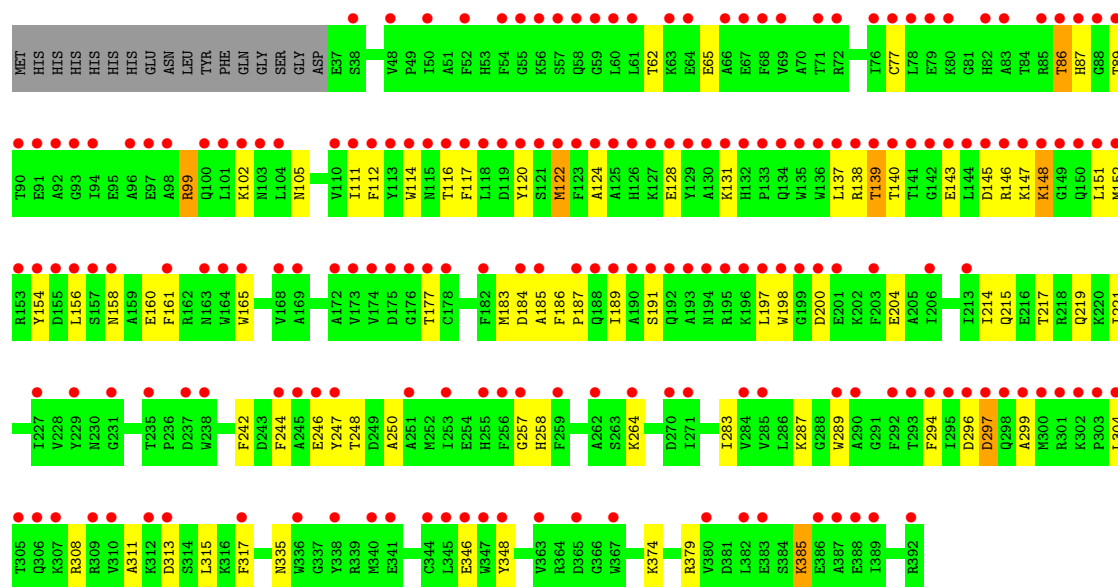
- Molecule 1: Glycoside-hydrolase family GH114 TIM-barrel domain-containing protein

Chain E: 17% 79% 16% 5%



- Molecule 1: Glycoside-hydrolase family GH114 TIM-barrel domain-containing protein

Chain F: 52% 74% 20% 5%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	91.84Å 81.90Å 160.31Å 90.00° 95.49° 90.00°	Depositor
Resolution (Å)	91.42 – 2.50 91.42 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.7 (91.42-2.50) 89.5 (91.42-2.50)	Depositor EDS
$R_{merge}$	0.14	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.47 (at 2.48Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, $R_{free}$	0.203 , 0.253 0.227 , 0.262	Depositor DCC
$R_{free}$ test set	80205 reflections (2.42%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	32.3	Xtriage
Anisotropy	0.465	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 32.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.91	EDS
Total number of atoms	16917	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	49.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 12.71% 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: 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	0.71	0/2932	0.77	0/3965
1	B	0.68	0/2892	0.77	0/3921
1	C	0.64	0/2888	0.74	0/3915
1	D	0.61	0/2810	0.72	0/3821
1	E	0.62	0/2881	0.70	0/3909
1	F	0.51	0/2818	0.68	0/3834
All	All	0.63	0/17221	0.73	0/23365

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	269	ARG	Sidechain

### 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	2853	0	2729	18	0
1	B	2813	0	2643	26	0
1	C	2809	0	2644	20	0
1	D	2733	0	2507	19	0
1	E	2792	0	2595	41	0
1	F	2739	0	2510	62	0
2	A	4	0	6	0	0
2	B	4	0	6	0	0
2	C	4	0	6	0	0
3	A	33	0	0	1	0
3	B	47	0	0	1	0
3	C	32	0	0	0	0
3	D	27	0	0	0	0
3	E	22	0	0	1	0
3	F	5	0	0	0	0
All	All	16917	0	15646	183	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 6.

All (183) 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:E:221:ILE:HD12	1:E:225:LYS:HB2	1.54	0.88
1:E:156:LEU:HD11	1:E:189:ILE:HD13	1.61	0.81
1:F:102:LYS:HE3	1:F:177:THR:HG22	1.71	0.72
1:F:183:MET:HE1	1:F:214:ILE:HG12	1.74	0.69
1:F:147:LYS:N	1:F:151:LEU:O	2.26	0.69
1:F:137:LEU:HD23	1:F:138:ARG:N	2.06	0.69
1:F:215:GLN:O	1:F:219:GLN:HG3	1.92	0.68
1:F:257:GLY:C	1:F:258:HIS:HD1	1.96	0.68
1:D:287:LYS:HE2	1:D:335:ASN:OD1	1.94	0.68
1:E:98:ALA:HB1	1:E:177:THR:HG22	1.76	0.67
1:E:215:GLN:HG3	1:E:247:TYR:CE2	2.29	0.67
1:F:215:GLN:HG2	1:F:219:GLN:NE2	2.10	0.66
1:F:120:TYR:HB3	1:F:122:MET:SD	2.38	0.63
1:F:137:LEU:HD22	1:F:145:ASP:CB	2.28	0.63
1:B:250:ALA:HB2	1:B:283:ILE:HB	1.82	0.62
1:B:225:LYS:NZ	3:B:503:HOH:O	2.33	0.61
1:E:132:HIS:CD2	1:E:135:TRP:CZ2	2.88	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:258[B]:HIS:NE2	1:E:259:PHE:CE1	2.69	0.61
1:D:67:GLU:O	1:D:71:THR:HG22	2.00	0.61
1:F:139:THR:HG22	1:F:143:GLU:O	2.01	0.60
1:E:274:MET:HG3	1:E:284:VAL:HG11	1.82	0.60
1:F:258:HIS:CD2	1:F:289:TRP:HB2	2.38	0.59
1:F:146:ARG:HA	1:F:152:MET:HA	1.83	0.59
1:F:287:LYS:HE3	1:F:335:ASN:OD1	2.02	0.59
1:F:244:PHE:O	1:F:248:THR:OG1	2.21	0.58
1:B:71:THR:O	1:B:71:THR:HG22	2.03	0.58
1:C:78:LEU:HD12	1:C:94:ILE:HG23	1.85	0.58
1:F:62:THR:HG23	1:F:65:GLU:OE1	2.03	0.58
1:F:304:LEU:HD21	1:F:308:ARG:NH2	2.20	0.57
1:E:377:SER:OG	1:E:392:ARG:NH1	2.37	0.57
1:C:166:THR:HG21	1:C:216:GLU:HB3	1.86	0.56
1:E:132:HIS:HB3	1:E:135:TRP:CE2	2.40	0.56
1:E:140:THR:HG23	1:E:197:LEU:O	2.05	0.56
1:D:68:PHE:O	1:D:72:ARG:HG3	2.05	0.56
1:F:308:ARG:NE	1:F:346:GLU:OE2	2.40	0.54
1:F:128:GLU:HA	1:F:131:LYS:HD3	1.90	0.54
1:C:263:SER:O	1:C:267:MET:HG3	2.08	0.54
1:A:177:THR:O	1:A:177:THR:HG22	2.08	0.53
1:E:252[B]:MET:SD	1:E:285:VAL:HB	2.47	0.53
1:E:132:HIS:HB3	1:E:135:TRP:NE1	2.23	0.53
1:E:257:GLY:O	1:E:258[A]:HIS:CD2	2.62	0.53
1:F:177:THR:HG22	1:F:177:THR:O	2.08	0.53
1:D:300:MET:O	1:D:307:LYS:HE3	2.08	0.52
1:F:296:ASP:O	1:F:297:ASP:C	2.48	0.52
1:F:385:LYS:HD2	1:F:385:LYS:O	2.09	0.52
1:B:121:SER:HA	1:B:126:HIS:CG	2.45	0.52
1:C:163:ASN:OD1	1:C:220:LYS:NZ	2.42	0.52
1:A:234:SER:OG	1:A:269[B]:ARG:NE	2.37	0.51
1:F:313:ASP:O	1:F:313:ASP:OD1	2.28	0.51
1:D:243:ASP:OD2	1:D:244:PHE:N	2.38	0.51
1:C:67:GLU:O	1:C:71:THR:HG23	2.09	0.51
1:D:147:LYS:N	1:D:151:LEU:O	2.43	0.51
1:B:150:GLN:O	1:B:151:LEU:HB2	2.10	0.51
1:F:200:ASP:O	1:F:204:GLU:HG2	2.11	0.51
1:F:317:PHE:CE1	1:F:385:LYS:HA	2.46	0.51
1:B:177:THR:HG22	1:B:177:THR:O	2.10	0.51
1:F:184:ASP:OD1	1:F:185:ALA:N	2.42	0.51
1:F:215:GLN:HG2	1:F:219:GLN:HE21	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:200:ASP:O	1:B:204:GLU:HG3	2.10	0.50
1:E:247:TYR:N	1:E:247:TYR:CD1	2.80	0.50
1:A:287:LYS:NZ	1:A:335:ASN:OD1	2.27	0.50
1:A:215:GLN:HG3	1:A:247:TYR:CZ	2.47	0.50
1:F:154:TYR:HB3	1:F:161:PHE:CE2	2.46	0.50
1:F:315:LEU:HD22	1:F:348:TYR:CD2	2.47	0.50
1:E:373:TYR:O	1:E:392:ARG:NH2	2.44	0.50
1:F:258:HIS:CD2	1:F:289:TRP:CB	2.95	0.49
1:B:156:LEU:HD11	1:B:189:ILE:HD13	1.95	0.49
1:E:152:MET:HE2	3:E:411:HOH:O	2.12	0.49
1:F:217:THR:O	1:F:221:ILE:HG13	2.12	0.49
1:A:203:PHE:O	1:A:207:GLN:HG2	2.13	0.49
1:A:287:LYS:HE2	3:A:512:HOH:O	2.13	0.48
1:F:77:CYS:HA	1:F:111:ILE:HB	1.94	0.48
1:F:158:ASN:OD1	1:F:161:PHE:N	2.37	0.48
1:C:184:ASP:O	1:C:185:ALA:HB3	2.12	0.48
1:E:215:GLN:HA	1:E:247:TYR:CD2	2.48	0.48
1:E:200:ASP:O	1:E:204:GLU:HG2	2.13	0.48
1:E:147:LYS:N	1:E:151:LEU:O	2.45	0.48
1:C:192:GLN:NE2	1:C:195:ARG:HE	2.11	0.48
1:F:147:LYS:O	1:F:148:LYS:C	2.52	0.48
1:E:152:MET:HE2	1:E:152:MET:HB3	1.70	0.47
1:F:296:ASP:O	1:F:299:ALA:N	2.45	0.47
1:E:243:ASP:OD2	1:E:244:PHE:CZ	2.67	0.47
1:F:86:THR:HG23	1:F:87:HIS:ND1	2.29	0.47
1:F:158:ASN:OD1	1:F:160:GLU:N	2.46	0.47
1:A:97:GLU:OE2	1:A:100:GLN:NE2	2.44	0.47
1:E:136:TRP:HB3	1:E:152:MET:HE3	1.94	0.47
1:A:232:ILE:HB	1:A:253:ILE:HG12	1.96	0.47
1:D:78:LEU:HD12	1:D:94:ILE:HG23	1.95	0.47
1:F:214:ILE:CD1	1:F:244:PHE:CD2	2.98	0.47
1:E:40:TYR:CG	1:E:283:ILE:HD11	2.50	0.47
1:E:184:ASP:O	1:E:185:ALA:HB3	2.14	0.47
1:B:102:LYS:HE3	1:B:179:ASP:OD2	2.15	0.46
1:F:311:ALA:HB1	1:F:348:TYR:OH	2.15	0.46
1:B:80:LYS:HE2	1:B:120:TYR:CZ	2.50	0.46
1:D:133:PRO:HA	1:D:136:TRP:CE2	2.51	0.46
1:F:89:THR:HG21	1:F:124:ALA:HB2	1.97	0.46
1:F:112:PHE:CE1	1:F:114:TRP:HB2	2.51	0.46
1:F:137:LEU:HD23	1:F:137:LEU:C	2.35	0.46
1:F:250:ALA:HB2	1:F:283:ILE:HB	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:133:PRO:HA	1:B:136:TRP:CE2	2.50	0.46
1:A:288:GLY:N	1:A:333:ILE:O	2.43	0.46
1:D:120:TYR:CE1	1:D:151:LEU:HD11	2.51	0.46
1:D:133:PRO:HA	1:D:136:TRP:CD2	2.51	0.46
1:C:177:THR:HG22	1:C:177:THR:O	2.16	0.45
1:B:309:ARG:O	1:B:309:ARG:HD3	2.17	0.45
1:E:258[B]:HIS:CE1	1:E:259:PHE:CZ	3.04	0.45
1:E:317:PHE:CE1	1:E:385:LYS:HA	2.51	0.45
1:F:186:PHE:N	1:F:187:PRO:CD	2.79	0.45
1:A:101:LEU:HD13	1:A:108:MET:HE3	1.98	0.45
1:F:246:GLU:HG2	1:F:247:TYR:CE2	2.51	0.45
1:A:76:ILE:O	1:A:76:ILE:HG23	2.17	0.45
1:C:46:ASP:OD1	1:F:374:LYS:HE2	2.17	0.45
1:E:57:SER:HA	1:E:81:GLY:O	2.16	0.45
1:E:182:PHE:CE1	1:E:252[B]:MET:HG3	2.52	0.45
1:F:161:PHE:CE1	1:F:165:TRP:HB2	2.52	0.45
1:E:45:TRP:CE2	1:E:358:PRO:HD3	2.52	0.45
1:D:80:LYS:HE2	1:D:120:TYR:CZ	2.51	0.45
1:E:210:LEU:O	1:E:213:ILE:HG22	2.17	0.45
1:E:314:SER:HB2	1:E:334:TYR:OH	2.16	0.44
1:C:300:MET:HA	1:C:307:LYS:NZ	2.32	0.44
1:E:132:HIS:HB3	1:E:135:TRP:CD1	2.52	0.44
1:A:156:LEU:HD11	1:A:189:ILE:HD13	2.00	0.44
1:C:300:MET:O	1:C:307:LYS:NZ	2.51	0.44
1:F:139:THR:OG1	1:F:140:THR:N	2.50	0.44
1:D:129:TYR:HB2	1:D:164:TRP:CH2	2.53	0.43
1:F:158:ASN:OD1	1:F:158:ASN:C	2.57	0.43
1:C:184:ASP:OD1	1:C:185:ALA:N	2.51	0.43
1:E:177:THR:O	1:E:177:THR:CG2	2.67	0.43
1:E:184:ASP:O	1:E:185:ALA:CB	2.66	0.43
1:B:138:ARG:HD3	1:B:142:GLY:O	2.18	0.43
1:E:174:VAL:HG12	1:E:175:ASP:N	2.34	0.43
1:F:137:LEU:HD23	1:F:138:ARG:O	2.18	0.43
1:A:292:PHE:CZ	1:A:307:LYS:HG2	2.53	0.43
1:C:364:ARG:HD2	1:C:366:GLY:O	2.19	0.43
1:D:364:ARG:HG3	1:D:365:ASP:N	2.34	0.43
1:E:117:PHE:O	1:E:118:LEU:HD23	2.19	0.43
1:B:232:ILE:HB	1:B:253:ILE:HG12	2.01	0.43
1:B:71:THR:O	1:B:71:THR:CG2	2.67	0.42
1:B:183:MET:HE1	1:B:214:ILE:HA	2.02	0.42
1:F:137:LEU:HD11	1:F:198:TRP:CE2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:377:SER:OG	1:C:392:ARG:NH1	2.53	0.42
1:D:380:VAL:HG22	1:D:381:ASP:N	2.34	0.42
1:F:116:THR:HA	1:F:165:TRP:CZ2	2.55	0.42
1:A:80:LYS:HE2	1:A:120:TYR:CZ	2.54	0.42
1:D:235:THR:HB	1:D:236:PRO:CD	2.49	0.42
1:A:124:ALA:O	1:A:127:LYS:HG3	2.19	0.42
1:D:194:ASN:HB3	1:D:198:TRP:CZ3	2.55	0.42
1:F:246:GLU:O	1:F:246:GLU:HG3	2.18	0.42
1:D:156:LEU:O	1:D:162:ARG:HD3	2.19	0.42
1:B:54:PHE:CE1	1:B:340:MET:HG3	2.55	0.42
1:F:62:THR:HG23	1:F:65:GLU:CD	2.40	0.42
1:B:114:TRP:CD1	1:B:165:TRP:CZ2	3.08	0.42
1:B:211:GLN:HE21	1:B:211:GLN:HB2	1.59	0.42
1:B:317:PHE:CE1	1:B:385:LYS:HA	2.55	0.42
1:D:114:TRP:HA	1:D:114:TRP:CE3	2.55	0.41
1:E:45:TRP:O	1:E:46:ASP:C	2.58	0.41
1:F:122:MET:SD	1:F:122:MET:N	2.93	0.41
1:F:156:LEU:HD11	1:F:189:ILE:HD13	2.02	0.41
1:B:215:GLN:HG3	1:B:247:TYR:CZ	2.56	0.41
1:A:114:TRP:CD1	1:A:165:TRP:CZ2	3.08	0.41
1:B:193:ALA:HB1	1:E:106:PRO:HD3	2.03	0.41
1:F:287:LYS:CE	1:F:335:ASN:OD1	2.67	0.41
1:E:135:TRP:CD1	1:E:135:TRP:N	2.88	0.41
1:A:71:THR:O	1:A:71:THR:CG2	2.68	0.41
1:B:186:PHE:N	1:B:186:PHE:CD1	2.89	0.41
1:C:300:MET:HA	1:C:307:LYS:HZ1	1.86	0.41
1:B:133:PRO:HA	1:B:136:TRP:CD2	2.55	0.41
1:B:186:PHE:N	1:B:186:PHE:HD1	2.19	0.41
1:E:53:HIS:CE1	1:E:79:GLU:HG2	2.56	0.41
1:E:192:GLN:OE1	1:E:195:ARG:HD2	2.20	0.41
1:F:99:ARG:HH11	1:F:99:ARG:HG3	1.86	0.41
1:F:183:MET:HE2	1:F:186:PHE:HZ	1.85	0.41
1:F:257:GLY:C	1:F:258:HIS:ND1	2.71	0.41
1:F:102:LYS:HA	1:F:105:ASN:O	2.21	0.41
1:F:140:THR:HG23	1:F:197:LEU:O	2.21	0.41
1:A:85:ARG:NE	1:B:223:ASP:OD2	2.54	0.40
1:C:89:THR:HG21	1:C:124:ALA:HB2	2.03	0.40
1:D:144:LEU:HD23	1:D:144:LEU:HA	1.94	0.40
1:C:147:LYS:O	1:C:148:LYS:C	2.60	0.40
1:C:156:LEU:HD11	1:C:189:ILE:HD13	2.02	0.40
1:C:226:LEU:HA	1:C:249:ASP:OD2	2.21	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:376:ALA:HA	1:C:390:ARG:O	2.21	0.40
1:F:117:PHE:CD2	1:F:189:ILE:HG13	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	355/373 (95%)	347 (98%)	8 (2%)	0	100	100
1	B	354/373 (95%)	341 (96%)	12 (3%)	1 (0%)	37	56
1	C	355/373 (95%)	345 (97%)	9 (2%)	1 (0%)	37	56
1	D	354/373 (95%)	344 (97%)	10 (3%)	0	100	100
1	E	356/373 (95%)	345 (97%)	9 (2%)	2 (1%)	22	39
1	F	355/373 (95%)	335 (94%)	18 (5%)	2 (1%)	22	39
All	All	2129/2238 (95%)	2057 (97%)	66 (3%)	6 (0%)	37	56

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	151	LEU
1	E	185	ALA
1	C	185	ALA
1	F	148	LYS
1	F	297	ASP
1	E	335	ASN

### 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	282/313 (90%)	277 (98%)	5 (2%)	54	78
1	B	276/313 (88%)	271 (98%)	5 (2%)	54	78
1	C	274/313 (88%)	270 (98%)	4 (2%)	60	82
1	D	255/313 (82%)	251 (98%)	4 (2%)	58	80
1	E	270/313 (86%)	267 (99%)	3 (1%)	70	87
1	F	257/313 (82%)	247 (96%)	10 (4%)	27	52
All	All	1614/1878 (86%)	1583 (98%)	31 (2%)	52	77

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	107	LYS
1	A	117	PHE
1	A	122	MET
1	A	295	ILE
1	A	392	ARG
1	B	116	THR
1	B	122	MET
1	B	127	LYS
1	B	242	PHE
1	B	305	THR
1	C	122	MET
1	C	305	THR
1	C	379	ARG
1	C	390	ARG
1	D	38	SER
1	D	75	PHE
1	D	122	MET
1	D	302	LYS
1	E	38	SER
1	E	122	MET
1	E	339	ARG
1	F	86	THR

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Mol	Chain	Res	Type
1	F	99	ARG
1	F	122	MET
1	F	139	THR
1	F	191	SER
1	F	242	PHE
1	F	264	LYS
1	F	294	PHE
1	F	379	ARG
1	F	385	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	215	GLN
1	B	39	HIS
1	C	211	GLN
1	C	342	ASN
1	E	53	HIS
1	F	219	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

3 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	EDO	A	401	-	3,3,3	0.63	0	2,2,2	0.97	0
2	EDO	C	401	-	3,3,3	0.69	0	2,2,2	0.68	0
2	EDO	B	401	-	3,3,3	0.57	0	2,2,2	0.92	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	EDO	A	401	-	-	0/1/1/1	-
2	EDO	C	401	-	-	0/1/1/1	-
2	EDO	B	401	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

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

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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	356/373 (95%)	0.13	3 (0%) 82 79	18, 34, 46, 54	1 (0%)
1	B	355/373 (95%)	0.27	3 (0%) 82 79	19, 38, 48, 56	1 (0%)
1	C	356/373 (95%)	0.76	18 (5%) 34 32	23, 45, 68, 86	1 (0%)
1	D	356/373 (95%)	0.99	49 (13%) 8 7	34, 51, 69, 81	0
1	E	355/373 (95%)	1.07	62 (17%) 5 5	25, 49, 83, 97	3 (0%)
1	F	356/373 (95%)	2.27	193 (54%) 0 0	48, 75, 103, 122	1 (0%)
All	All	2134/2238 (95%)	0.92	328 (15%) 6 6	18, 45, 86, 122	7 (0%)

All (328) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	F	152	MET	5.7
1	F	298	GLN	5.7
1	F	144	LEU	5.6
1	F	145	ASP	5.5
1	E	219	GLN	5.5
1	F	297	ASP	5.2
1	F	55	GLY	5.0
1	F	303	PRO	5.0
1	F	66	ALA	5.0
1	F	296	ASP	4.9
1	F	104	LEU	4.9
1	F	129	TYR	4.9
1	F	64	GLU	4.9
1	F	54	PHE	4.9
1	F	123	PHE	4.8
1	F	150	GLN	4.8
1	F	86	THR	4.6
1	F	57[A]	SER	4.6
1	F	153	ARG	4.5

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Mol	Chain	Res	Type	RSRZ
1	F	134	GLN	4.5
1	F	237	ASP	4.4
1	F	118	LEU	4.3
1	F	130	ALA	4.3
1	F	112	PHE	4.2
1	F	188	GLN	4.2
1	F	114	TRP	4.2
1	F	60	LEU	4.2
1	F	122	MET	4.2
1	F	78	LEU	4.2
1	F	125	ALA	4.1
1	F	121	SER	4.1
1	F	82	HIS	4.1
1	F	136	TRP	4.1
1	F	143	GLU	4.0
1	F	156	LEU	4.0
1	F	61	LEU	4.0
1	F	120	TYR	4.0
1	F	119	ASP	3.9
1	F	142	GLY	3.9
1	F	246	GLU	3.8
1	F	92	ALA	3.8
1	F	149	GLY	3.8
1	F	300	MET	3.8
1	E	150	GLN	3.8
1	F	347	TRP	3.8
1	D	222	GLY	3.7
1	F	151	LEU	3.7
1	F	198	TRP	3.7
1	C	148	LYS	3.7
1	D	64	GLU	3.6
1	C	149	GLY	3.6
1	D	295	ILE	3.6
1	F	135	TRP	3.6
1	E	134	GLN	3.6
1	F	294	PHE	3.6
1	F	141	THR	3.6
1	F	113	TYR	3.5
1	C	246	GLU	3.5
1	E	159	ALA	3.5
1	F	302	LYS	3.5
1	D	224	ASP	3.5

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Mol	Chain	Res	Type	RSRZ
1	F	154	TYR	3.4
1	E	133	PRO	3.4
1	F	90	THR	3.4
1	E	220	LYS	3.4
1	E	245	ALA	3.4
1	F	189	ILE	3.4
1	F	89	THR	3.3
1	F	124	ALA	3.3
1	F	190	ALA	3.3
1	F	203	PHE	3.3
1	F	292	PHE	3.3
1	D	60	LEU	3.3
1	F	197	LEU	3.3
1	F	301	ARG	3.3
1	F	345	LEU	3.3
1	F	264	LYS	3.3
1	F	164	TRP	3.3
1	F	137	LEU	3.3
1	D	223	ASP	3.3
1	F	100	GLN	3.3
1	E	142	GLY	3.3
1	F	238	TRP	3.3
1	F	127	LYS	3.3
1	F	201	GLU	3.2
1	C	150	GLN	3.2
1	F	340	MET	3.2
1	E	135	TRP	3.2
1	F	191	SER	3.2
1	F	244	PHE	3.2
1	F	94	ILE	3.2
1	F	139	THR	3.2
1	F	140	THR	3.2
1	F	76	ILE	3.2
1	E	131	LYS	3.1
1	E	137	LEU	3.1
1	F	193	ALA	3.1
1	D	71	THR	3.1
1	F	392	ARG	3.1
1	E	118	LEU	3.1
1	F	133	PRO	3.1
1	F	310	VAL	3.1
1	D	98	ALA	3.1

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Mol	Chain	Res	Type	RSRZ
1	E	124	ALA	3.1
1	F	96	ALA	3.1
1	F	63	LYS	3.1
1	D	132	HIS	3.1
1	D	134	GLN	3.1
1	F	168	VAL	3.0
1	F	103	ASN	3.0
1	F	87	HIS	3.0
1	D	129	TYR	3.0
1	D	142	GLY	3.0
1	C	139	THR	3.0
1	F	77	CYS	3.0
1	C	244	PHE	3.0
1	F	295	ILE	3.0
1	D	131	LYS	3.0
1	F	148	LYS	3.0
1	F	380	VAL	3.0
1	C	146	ARG	3.0
1	F	172	ALA	3.0
1	F	192	GLN	3.0
1	F	293	THR	3.0
1	F	206	ILE	3.0
1	E	148	LYS	3.0
1	E	138	ARG	3.0
1	F	85	ARG	3.0
1	D	220	LYS	2.9
1	F	367	TRP	2.9
1	C	37	GLU	2.9
1	E	158	ASN	2.9
1	D	86	THR	2.9
1	F	117	PHE	2.9
1	F	115	ASN	2.9
1	F	195	ARG	2.9
1	E	136	TRP	2.9
1	D	215	GLN	2.9
1	F	58	GLN	2.9
1	E	167	ASN	2.9
1	F	307	LYS	2.9
1	F	101	LEU	2.8
1	F	382	LEU	2.8
1	E	174	VAL	2.8
1	E	130	ALA	2.8

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Mol	Chain	Res	Type	RSRZ
1	F	131	LYS	2.8
1	F	185	ALA	2.8
1	F	50	ILE	2.8
1	F	93	GLY	2.8
1	E	160	GLU	2.8
1	F	306	GLN	2.8
1	E	127	LYS	2.8
1	E	164	TRP	2.8
1	F	165	TRP	2.8
1	F	138	ARG	2.8
1	F	251	ALA	2.8
1	F	299	ALA	2.8
1	D	61	LEU	2.8
1	D	104	LEU	2.7
1	E	144	LEU	2.7
1	F	387	ALA	2.7
1	B	237	ASP	2.7
1	F	98	ALA	2.7
1	F	111	ILE	2.7
1	F	102	LYS	2.7
1	F	388	GLU	2.7
1	C	38	SER	2.7
1	E	202	LYS	2.7
1	F	147	LYS	2.7
1	E	216	GLU	2.7
1	F	256	PHE	2.7
1	D	78	LEU	2.6
1	E	162	ARG	2.6
1	E	120	TYR	2.6
1	D	148	LYS	2.6
1	F	126	HIS	2.6
1	F	71	THR	2.6
1	E	163	ASN	2.6
1	F	79	GLU	2.6
1	D	85	ARG	2.6
1	E	140	THR	2.6
1	F	270	ASP	2.6
1	F	271	ILE	2.6
1	E	93	GLY	2.6
1	F	173	VAL	2.6
1	F	229	TYR	2.6
1	C	141	THR	2.6

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Mol	Chain	Res	Type	RSRZ
1	E	143	GLU	2.6
1	D	57	SER	2.6
1	F	38	SER	2.6
1	F	116	THR	2.6
1	F	177	THR	2.6
1	F	313	ASP	2.6
1	F	194	ASN	2.6
1	C	137	LEU	2.5
1	C	144	LEU	2.5
1	D	221	ILE	2.5
1	F	91	GLU	2.5
1	F	97	GLU	2.5
1	D	260	GLN	2.5
1	D	199	GLY	2.5
1	F	72	ARG	2.5
1	F	182	PHE	2.5
1	F	227	ILE	2.5
1	F	83	ALA	2.5
1	F	157	SER	2.5
1	F	67	GLU	2.5
1	F	305	THR	2.5
1	F	146	ARG	2.5
1	C	359	VAL	2.5
1	E	173	VAL	2.5
1	E	92	ALA	2.5
1	E	38	SER	2.5
1	E	201	GLU	2.5
1	E	213	ILE	2.5
1	F	259	PHE	2.5
1	F	132	HIS	2.4
1	F	178	CYS	2.4
1	C	193	ALA	2.4
1	D	136	TRP	2.4
1	E	128	GLU	2.4
1	F	383	GLU	2.4
1	B	150	GLN	2.4
1	F	163	ASN	2.4
1	F	348	TYR	2.4
1	F	169	ALA	2.4
1	F	196	LYS	2.4
1	F	59	GLY	2.4
1	D	103	ASN	2.4

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Mol	Chain	Res	Type	RSRZ
1	F	52	PHE	2.4
1	F	285	VAL	2.4
1	F	56	LYS	2.4
1	C	301	ARG	2.4
1	F	289	TRP	2.4
1	F	231	GLY	2.4
1	D	150	GLN	2.4
1	D	219	GLN	2.4
1	E	205	ALA	2.4
1	D	149	GLY	2.4
1	E	89	THR	2.4
1	E	149	GLY	2.4
1	F	88	GLY	2.4
1	F	257	GLY	2.4
1	F	304	LEU	2.3
1	E	244	PHE	2.3
1	F	161	PHE	2.3
1	F	184	ASP	2.3
1	E	247	TYR	2.3
1	D	127	LYS	2.3
1	F	80	LYS	2.3
1	D	83	ALA	2.3
1	F	262	ALA	2.3
1	D	141	THR	2.3
1	F	68	PHE	2.3
1	F	200	ASP	2.3
1	F	255	HIS	2.3
1	A	244	PHE	2.3
1	F	175	ASP	2.3
1	E	129	TYR	2.3
1	B	269	ARG	2.3
1	D	99	ARG	2.3
1	F	309	ARG	2.3
1	E	206	ILE	2.3
1	E	161	PHE	2.2
1	D	135	TRP	2.2
1	A	37	GLU	2.2
1	F	128	GLU	2.2
1	F	346	GLU	2.2
1	F	110	VAL	2.2
1	F	338	TYR	2.2
1	F	389	ILE	2.2

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Mol	Chain	Res	Type	RSRZ
1	F	245	ALA	2.2
1	E	119	ASP	2.2
1	F	253	ILE	2.2
1	F	176	GLY	2.2
1	F	235	THR	2.2
1	E	212	ASP	2.2
1	D	97	GLU	2.2
1	F	69	VAL	2.2
1	D	63	LYS	2.2
1	F	290	ALA	2.2
1	E	151	LEU	2.2
1	E	199	GLY	2.2
1	E	85	ARG	2.2
1	E	156	LEU	2.1
1	E	153	ARG	2.1
1	F	317	PHE	2.1
1	F	344	CYS	2.1
1	D	133	PRO	2.1
1	F	341	GLU	2.1
1	F	386	GLU	2.1
1	E	243	ASP	2.1
1	F	155	ASP	2.1
1	E	117	PHE	2.1
1	E	200	ASP	2.1
1	D	174	VAL	2.1
1	F	174	VAL	2.1
1	F	284	VAL	2.1
1	D	152	MET	2.1
1	C	379	ARG	2.1
1	D	291	GLY	2.1
1	F	247	TYR	2.1
1	D	177	THR	2.1
1	E	259	PHE	2.1
1	E	58	GLN	2.1
1	F	48	VAL	2.1
1	D	66	ALA	2.1
1	D	392	ARG	2.1
1	E	184	ASP	2.1
1	F	213	ILE	2.1
1	D	101	LEU	2.0
1	A	392	ARG	2.0
1	F	336	TRP	2.0

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Mol	Chain	Res	Type	RSRZ
1	F	187	PRO	2.0
1	D	292	PHE	2.0
1	E	147	LYS	2.0
1	F	312	LYS	2.0
1	C	152	MET	2.0
1	D	252	MET	2.0
1	E	221	ILE	2.0
1	D	243	ASP	2.0
1	F	158	ASN	2.0
1	F	365	ASP	2.0
1	C	138	ARG	2.0
1	F	363	VAL	2.0
1	F	199	GLY	2.0
1	E	238	TRP	2.0
1	D	294	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 monosaccharides 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(Å <sup>2</sup> )	Q<0.9
2	EDO	C	401	4/4	0.84	0.14	43,45,45,46	0
2	EDO	B	401	4/4	0.94	0.09	37,38,39,40	0
2	EDO	A	401	4/4	0.94	0.10	34,36,36,37	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.