



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 17, 2020 – 11:48 AM BST

PDB ID : 4ZFM  
Title : Structure of Gan1D-E170Q in complex with cellobiose-6-phosphate  
Authors : Lansky, S.; Zehavi, A.; Dvir, H.; Shoham, Y.; Shoham, G.  
Deposited on : 2015-04-21  
Resolution : 1.40 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 : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

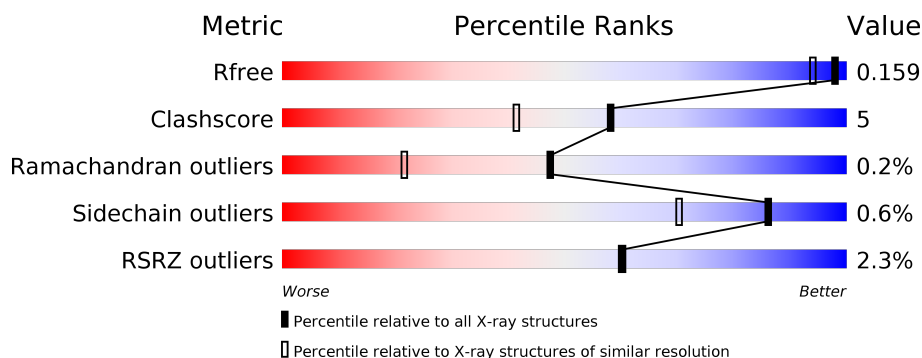
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 1.40 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))
$R_{free}$	130704	1714 (1.40-1.40)
Clashscore	141614	1812 (1.40-1.40)
Ramachandran outliers	138981	1763 (1.40-1.40)
Sidechain outliers	138945	1762 (1.40-1.40)
RSRZ outliers	127900	1674 (1.40-1.40)

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 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	485	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>19%</div> <div>• 5%</div> </div> </div>
1	B	485	<div> <div>2%</div> <div> <div></div> <div>79%</div> <div>15%</div> <div>• 5%</div> </div> </div>
1	C	485	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>18%</div> <div>• 5%</div> </div> </div>
1	D	485	<div> <div>2%</div> <div> <div></div> <div>77%</div> <div>18%</div> <div>• 5%</div> </div> </div>
2	E	2	<div> <div></div> <div> <div>50%</div> <div>50%</div> </div> </div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 18396 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Putative 6-phospho-beta-galactobiosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	461	Total	C	N	O	S	0	27	0
			3945	2545	680	706	14			
1	B	461	Total	C	N	O	S	0	20	0
			3911	2521	667	709	14			
1	C	461	Total	C	N	O	S	0	22	0
			3914	2525	664	710	15			
1	D	461	Total	C	N	O	S	0	17	0
			3875	2500	653	708	14			

There are 36 discrepancies between the modelled and reference sequences:

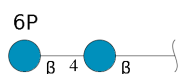
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP W8QF82
A	-5	ILE	-	expression tag	UNP W8QF82
A	-4	HIS	-	expression tag	UNP W8QF82
A	-3	HIS	-	expression tag	UNP W8QF82
A	-2	HIS	-	expression tag	UNP W8QF82
A	-1	HIS	-	expression tag	UNP W8QF82
A	0	HIS	-	expression tag	UNP W8QF82
A	1	HIS	-	expression tag	UNP W8QF82
A	170	GLN	GLU	engineered mutation	UNP W8QF82
B	-6	MET	-	initiating methionine	UNP W8QF82
B	-5	ILE	-	expression tag	UNP W8QF82
B	-4	HIS	-	expression tag	UNP W8QF82
B	-3	HIS	-	expression tag	UNP W8QF82
B	-2	HIS	-	expression tag	UNP W8QF82
B	-1	HIS	-	expression tag	UNP W8QF82
B	0	HIS	-	expression tag	UNP W8QF82
B	1	HIS	-	expression tag	UNP W8QF82
B	170	GLN	GLU	engineered mutation	UNP W8QF82
C	-6	MET	-	initiating methionine	UNP W8QF82
C	-5	ILE	-	expression tag	UNP W8QF82
C	-4	HIS	-	expression tag	UNP W8QF82

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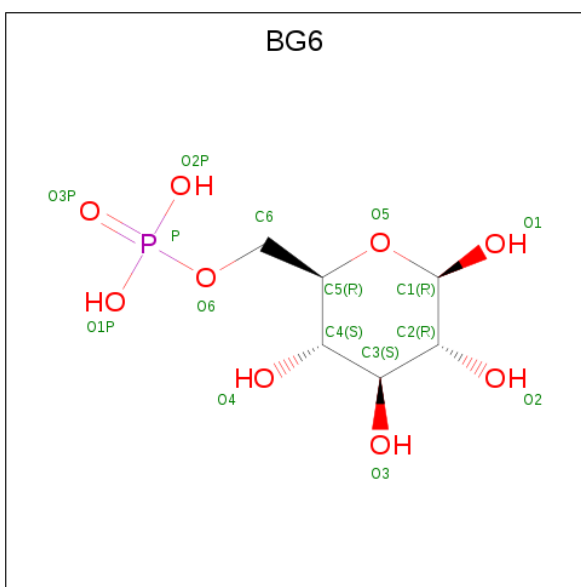
Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	HIS	-	expression tag	UNP W8QF82
C	-2	HIS	-	expression tag	UNP W8QF82
C	-1	HIS	-	expression tag	UNP W8QF82
C	0	HIS	-	expression tag	UNP W8QF82
C	1	HIS	-	expression tag	UNP W8QF82
C	170	GLN	GLU	engineered mutation	UNP W8QF82
D	-6	MET	-	initiating methionine	UNP W8QF82
D	-5	ILE	-	expression tag	UNP W8QF82
D	-4	HIS	-	expression tag	UNP W8QF82
D	-3	HIS	-	expression tag	UNP W8QF82
D	-2	HIS	-	expression tag	UNP W8QF82
D	-1	HIS	-	expression tag	UNP W8QF82
D	0	HIS	-	expression tag	UNP W8QF82
D	1	HIS	-	expression tag	UNP W8QF82
D	170	GLN	GLU	engineered mutation	UNP W8QF82

- Molecule 2 is an oligosaccharide called 1,5-anhydro-6-O-phosphono-D-glucitol-(1-4)-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
2	E	2	Total	C	O	P	0	0	0
			27	12	14	1			

- Molecule 3 is 6-O-phosphono-beta-D-glucopyranose (three-letter code: BG6) (formula: C<sub>6</sub>H<sub>13</sub>O<sub>9</sub>P).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	O	P	0	0
			16	6	9	1		
3	B	1	Total	C	O	P	0	0
			16	6	9	1		

- Molecule 4 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).



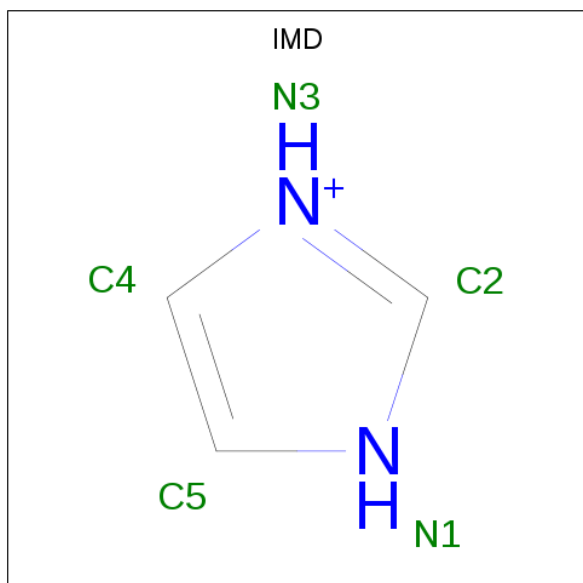
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

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

- Molecule 5 is IMIDAZOLE (three-letter code: IMD) (formula: C<sub>3</sub>H<sub>5</sub>N<sub>2</sub>).



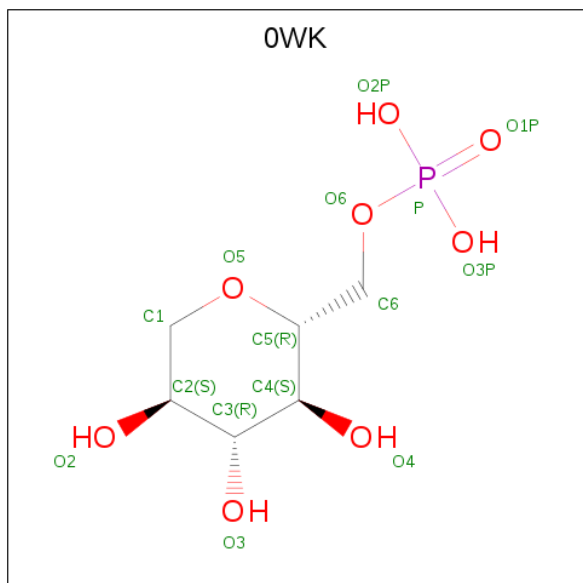
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			5	3	2		

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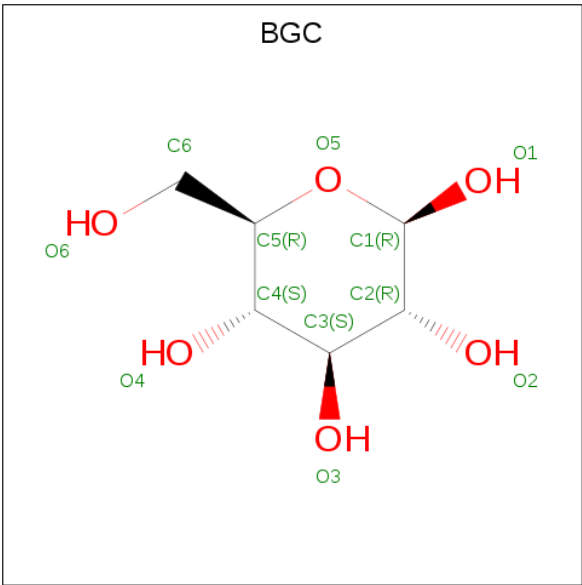
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	N	0	0
			5	3	2		
5	D	1	Total	C	N	0	0
			5	3	2		

- Molecule 6 is 1,5-anhydro-6-O-phosphono-D-glucitol (three-letter code: 0WK) (formula:  $C_6H_{13}O_8P$ ).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
6	C	1	Total	C	O	P	0	0
			15	6	8	1		

- Molecule 7 is beta-D-glucopyranose (three-letter code: BGC) (formula:  $C_6H_{12}O_6$ ).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	C	1	Total	C	O	0	0
			12	6	6		

- Molecule 8 is water.

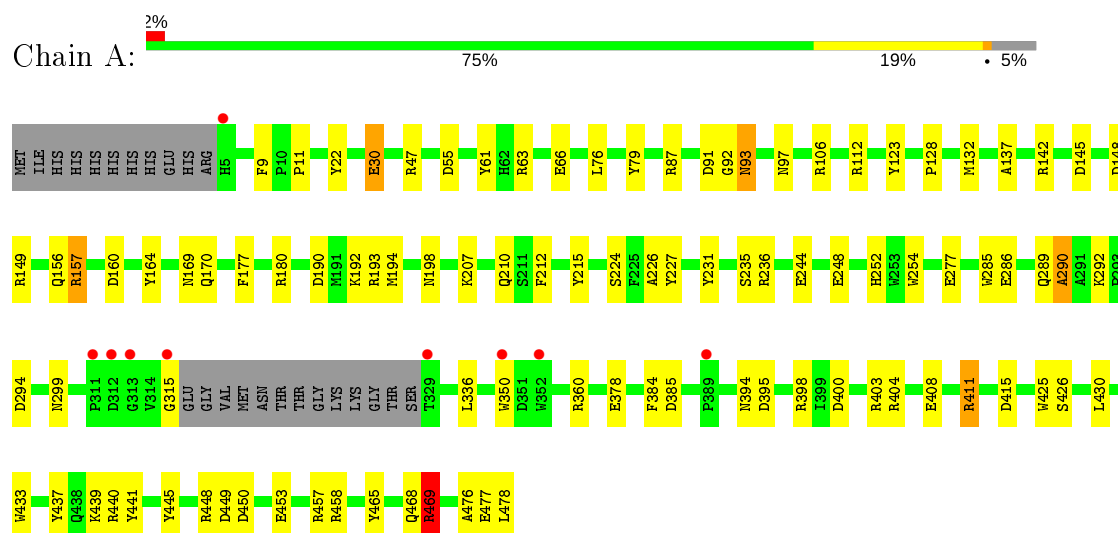
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	640	Total	O	0	0
			640	640		
8	B	638	Total	O	0	0
			638	638		
8	C	692	Total	O	0	0
			692	692		
8	D	608	Total	O	0	0
			608	608		



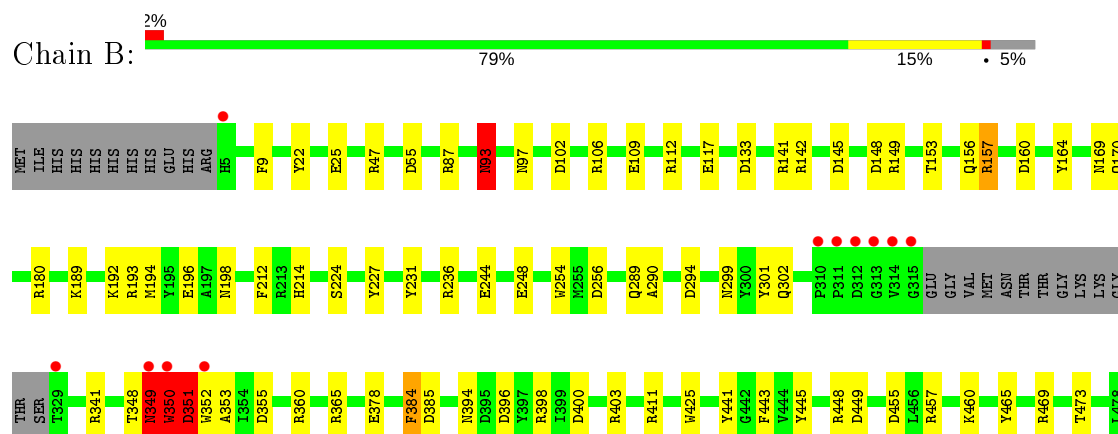
### 3 Residue-property plots [i](#)

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.

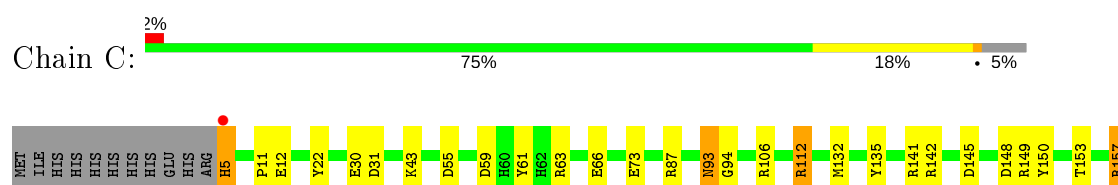
- Molecule 1: Putative 6-phospho-beta-galactobiosidase

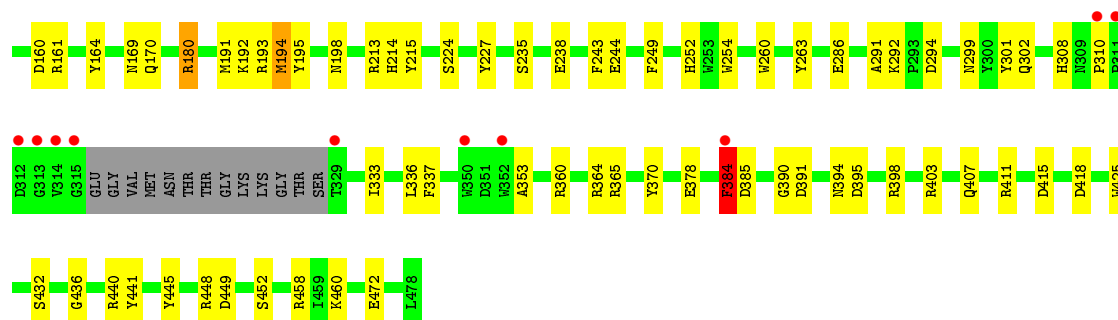


- Molecule 1: Putative 6-phospho-beta-galactobiosidase

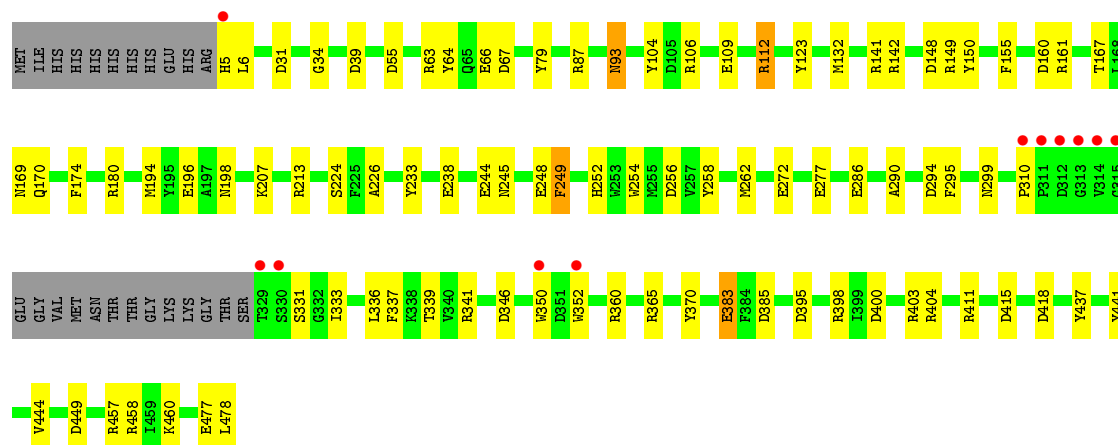
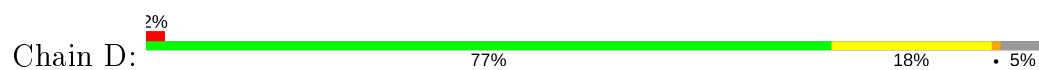


- Molecule 1: Putative 6-phospho-beta-galactobiosidase





• Molecule 1: Putative 6-phospho-beta-galactobiosidase



• Molecule 2: 1,5-anhydro-6-O-phosphono-D-glucitol-(1-4)-beta-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	101.59Å 97.47Å 105.27Å 90.00° 97.66° 90.00°	Depositor
Resolution (Å)	22.37 – 1.40 22.36 – 1.40	Depositor EDS
% Data completeness (in resolution range)	98.7 (22.37-1.40) 98.7 (22.36-1.40)	Depositor EDS
$R_{merge}$	0.07	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.22 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, $R_{free}$	0.130 , 0.158 0.131 , 0.159	Depositor DCC
$R_{free}$ test set	19771 reflections (5.03%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	10.1	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.38 , 47.7	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.000 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.98	EDS
Total number of atoms	18396	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	15.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 69.56 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.6228e-06. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<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: GOL, BGC, IMD, BG6, 0WK

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	1.49	31/4146 (0.7%)	1.50	65/5630 (1.2%)
1	B	1.47	25/4087 (0.6%)	1.59	80/5558 (1.4%)
1	C	1.44	25/4107 (0.6%)	1.56	84/5581 (1.5%)
1	D	1.44	18/4050 (0.4%)	1.61	78/5509 (1.4%)
All	All	1.46	99/16390 (0.6%)	1.57	307/22278 (1.4%)

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	2
1	B	0	4
1	C	0	1
1	D	0	1
All	All	0	8

All (99) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	286[A]	GLU	CD-OE1	9.52	1.36	1.25
1	A	286[B]	GLU	CD-OE1	9.52	1.36	1.25
1	B	350[A]	TRP	CB-CG	9.51	1.67	1.50
1	B	350[B]	TRP	CB-CG	9.51	1.67	1.50
1	A	441	TYR	CE2-CZ	-9.49	1.26	1.38
1	C	441	TYR	CE2-CZ	-9.41	1.26	1.38
1	B	117	GLU	CD-OE1	8.58	1.35	1.25
1	A	66	GLU	CD-OE1	8.34	1.34	1.25
1	C	63[A]	ARG	CZ-NH1	-8.32	1.22	1.33
1	C	63[B]	ARG	CZ-NH1	-8.32	1.22	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	64	TYR	CE1-CZ	-8.26	1.27	1.38
1	B	441	TYR	CE2-CZ	-8.15	1.27	1.38
1	D	286	GLU	CD-OE2	8.01	1.34	1.25
1	C	441	TYR	CD1-CE1	7.48	1.50	1.39
1	A	22	TYR	CD1-CE1	7.47	1.50	1.39
1	D	437	TYR	CE1-CZ	-7.33	1.29	1.38
1	B	227	TYR	CE2-CZ	-7.08	1.29	1.38
1	A	227	TYR	CE2-CZ	-7.00	1.29	1.38
1	A	106	ARG	CZ-NH2	-6.91	1.24	1.33
1	A	465	TYR	CE1-CZ	-6.88	1.29	1.38
1	B	244	GLU	CD-OE1	6.77	1.33	1.25
1	B	196	GLU	CD-OE2	6.70	1.33	1.25
1	B	160	ASP	CB-CG	6.54	1.65	1.51
1	A	22	TYR	CE1-CZ	-6.53	1.30	1.38
1	C	472	GLU	CD-OE2	6.53	1.32	1.25
1	D	441	TYR	CE2-CZ	-6.43	1.30	1.38
1	D	350	TRP	CB-CG	-6.41	1.38	1.50
1	C	244	GLU	CD-OE1	6.28	1.32	1.25
1	A	286[A]	GLU	CG-CD	6.27	1.61	1.51
1	A	286[B]	GLU	CG-CD	6.27	1.61	1.51
1	C	384	PHE	C-O	6.26	1.35	1.23
1	D	398	ARG	CD-NE	-6.21	1.35	1.46
1	C	164	TYR	CD1-CE1	6.10	1.48	1.39
1	C	441	TYR	CZ-OH	6.10	1.48	1.37
1	D	196	GLU	CD-OE2	6.08	1.32	1.25
1	C	215	TYR	CE1-CZ	-6.05	1.30	1.38
1	A	244	GLU	CD-OE1	6.02	1.32	1.25
1	A	437	TYR	CE1-CZ	-6.01	1.30	1.38
1	B	22	TYR	CE2-CZ	-5.99	1.30	1.38
1	A	160	ASP	CB-CG	5.94	1.64	1.51
1	B	457	ARG	CG-CD	5.93	1.66	1.51
1	A	441	TYR	CZ-OH	5.79	1.47	1.37
1	A	469[A]	ARG	CA-C	5.76	1.68	1.52
1	A	469[B]	ARG	CA-C	5.76	1.68	1.52
1	A	445	TYR	CE1-CZ	-5.69	1.31	1.38
1	C	180[A]	ARG	CZ-NH2	5.67	1.40	1.33
1	C	180[B]	ARG	CZ-NH2	5.67	1.40	1.33
1	B	441	TYR	CE1-CZ	-5.66	1.31	1.38
1	A	235	SER	CB-OG	5.65	1.49	1.42
1	B	301	TYR	CE1-CZ	-5.60	1.31	1.38
1	D	104	TYR	CE2-CZ	5.59	1.45	1.38
1	C	180[A]	ARG	CZ-NH1	5.59	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	180[B]	ARG	CZ-NH1	5.59	1.40	1.33
1	D	258	TYR	CE2-CZ	-5.58	1.31	1.38
1	A	457	ARG	CG-CD	5.55	1.65	1.51
1	C	87	ARG	CB-CG	-5.54	1.37	1.52
1	B	180[A]	ARG	CZ-NH1	5.54	1.40	1.33
1	B	180[B]	ARG	CZ-NH1	5.54	1.40	1.33
1	A	290	ALA	C-O	5.54	1.33	1.23
1	A	433	TRP	CD1-NE1	-5.53	1.28	1.38
1	B	349[A]	ASN	C-O	-5.53	1.12	1.23
1	B	349[B]	ASN	C-O	-5.53	1.12	1.23
1	C	235	SER	CB-OG	5.53	1.49	1.42
1	D	248	GLU	CD-OE1	-5.53	1.19	1.25
1	A	91	ASP	CB-CG	-5.48	1.40	1.51
1	B	156	GLN	CA-CB	-5.48	1.41	1.53
1	B	47	ARG	CD-NE	-5.47	1.37	1.46
1	C	452	SER	CB-OG	5.47	1.49	1.42
1	D	441	TYR	CD1-CE1	5.46	1.47	1.39
1	D	180[A]	ARG	CZ-NH1	5.42	1.40	1.33
1	D	180[B]	ARG	CZ-NH1	5.42	1.40	1.33
1	C	61	TYR	CE1-CZ	-5.42	1.31	1.38
1	A	22	TYR	CE2-CZ	-5.40	1.31	1.38
1	D	444	VAL	CB-CG2	-5.39	1.41	1.52
1	B	473	THR	CB-OG1	5.38	1.54	1.43
1	A	248	GLU	CG-CD	-5.37	1.44	1.51
1	B	109	GLU	CD-OE2	5.32	1.31	1.25
1	C	106	ARG	CZ-NH2	-5.31	1.26	1.33
1	D	249	PHE	CB-CG	-5.30	1.42	1.51
1	B	445	TYR	CE1-CZ	-5.30	1.31	1.38
1	A	61	TYR	CE1-CZ	-5.29	1.31	1.38
1	A	164	TYR	CZ-OH	5.28	1.46	1.37
1	B	248	GLU	CG-CD	-5.27	1.44	1.51
1	A	398	ARG	C-O	5.25	1.33	1.23
1	B	455	ASP	CB-CG	-5.25	1.40	1.51
1	C	61	TYR	CZ-OH	5.23	1.46	1.37
1	C	141	ARG	CZ-NH2	-5.22	1.26	1.33
1	C	390	GLY	N-CA	-5.22	1.38	1.46
1	D	350	TRP	CE3-CZ3	-5.17	1.29	1.38
1	D	34	GLY	N-CA	-5.17	1.38	1.46
1	B	441	TYR	CZ-OH	5.16	1.46	1.37
1	B	22	TYR	CD1-CE1	5.15	1.47	1.39
1	A	476	ALA	N-CA	5.14	1.56	1.46
1	A	445	TYR	CG-CD1	5.14	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	477	GLU	CD-OE2	5.04	1.31	1.25
1	A	277	GLU	CD-OE2	-5.04	1.20	1.25
1	C	260	TRP	CB-CG	-5.02	1.41	1.50
1	C	286[A]	GLU	CD-OE2	5.01	1.31	1.25
1	C	286[B]	GLU	CD-OE2	5.01	1.31	1.25

All (307) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	398	ARG	NE-CZ-NH2	20.91	130.75	120.30
1	B	141	ARG	NE-CZ-NH1	-18.47	111.07	120.30
1	D	411	ARG	NE-CZ-NH2	-15.06	112.77	120.30
1	C	180[A]	ARG	NE-CZ-NH2	-14.26	113.17	120.30
1	C	180[B]	ARG	NE-CZ-NH2	-14.26	113.17	120.30
1	B	180[A]	ARG	NE-CZ-NH2	-12.86	113.87	120.30
1	B	180[B]	ARG	NE-CZ-NH2	-12.86	113.87	120.30
1	B	403	ARG	NE-CZ-NH1	12.73	126.66	120.30
1	C	106	ARG	NE-CZ-NH1	12.40	126.50	120.30
1	C	398	ARG	NE-CZ-NH2	12.21	126.41	120.30
1	D	411	ARG	NE-CZ-NH1	12.18	126.39	120.30
1	B	360	ARG	NE-CZ-NH2	-12.17	114.22	120.30
1	D	161	ARG	NE-CZ-NH1	11.64	126.12	120.30
1	D	213	ARG	NE-CZ-NH1	11.47	126.04	120.30
1	C	365	ARG	NE-CZ-NH2	-11.45	114.58	120.30
1	D	404	ARG	NE-CZ-NH2	-11.11	114.75	120.30
1	A	215	TYR	CB-CG-CD2	11.06	127.64	121.00
1	B	398	ARG	NE-CZ-NH2	11.03	125.81	120.30
1	B	160	ASP	CB-CG-OD1	10.92	128.13	118.30
1	A	193	ARG	NE-CZ-NH1	-10.89	114.86	120.30
1	B	411	ARG	NE-CZ-NH2	-10.85	114.87	120.30
1	B	294	ASP	CB-CG-OD2	10.84	128.06	118.30
1	C	227	TYR	CB-CG-CD1	10.83	127.50	121.00
1	C	449	ASP	CB-CG-OD1	10.69	127.92	118.30
1	B	403	ARG	NE-CZ-NH2	-10.54	115.03	120.30
1	C	55	ASP	CB-CG-OD2	-10.49	108.86	118.30
1	B	47	ARG	NE-CZ-NH2	-10.46	115.07	120.30
1	C	112	ARG	NE-CZ-NH2	-10.32	115.14	120.30
1	D	106	ARG	NE-CZ-NH1	10.32	125.46	120.30
1	B	93	ASN	C-N-CA	-10.30	100.66	122.30
1	D	403	ARG	NE-CZ-NH1	10.29	125.45	120.30
1	B	449	ASP	CB-CG-OD1	10.19	127.47	118.30
1	A	55	ASP	CB-CG-OD2	-10.17	109.15	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	411	ARG	NE-CZ-NH1	10.09	125.34	120.30
1	B	194[A]	MET	CG-SD-CE	-10.04	84.13	100.20
1	B	194[B]	MET	CG-SD-CE	-10.04	84.13	100.20
1	D	360	ARG	NE-CZ-NH2	-9.97	115.31	120.30
1	B	87	ARG	NE-CZ-NH1	9.96	125.28	120.30
1	A	231	TYR	CB-CG-CD1	9.94	126.96	121.00
1	A	415	ASP	CB-CG-OD2	9.91	127.22	118.30
1	D	403	ARG	NE-CZ-NH2	-9.85	115.37	120.30
1	B	47	ARG	CG-CD-NE	-9.76	91.31	111.80
1	B	106	ARG	NE-CZ-NH1	9.71	125.16	120.30
1	D	112	ARG	NE-CZ-NH2	-9.66	115.47	120.30
1	D	458	ARG	NE-CZ-NH1	9.65	125.13	120.30
1	C	360	ARG	NE-CZ-NH2	-9.56	115.52	120.30
1	D	141	ARG	NE-CZ-NH1	-9.43	115.58	120.30
1	B	448	ARG	NE-CZ-NH1	9.42	125.01	120.30
1	D	194	MET	CG-SD-CE	-9.42	85.13	100.20
1	A	411	ARG	NE-CZ-NH1	9.31	124.96	120.30
1	C	411	ARG	NE-CZ-NH2	-9.27	115.67	120.30
1	D	31	ASP	CB-CG-OD2	9.22	126.60	118.30
1	C	384	PHE	O-C-N	-9.10	108.14	122.70
1	A	395	ASP	CB-CG-OD1	9.04	126.43	118.30
1	C	142	ARG	NE-CZ-NH2	-9.04	115.78	120.30
1	D	457	ARG	NE-CZ-NH1	9.01	124.81	120.30
1	C	403	ARG	NE-CZ-NH1	8.96	124.78	120.30
1	B	231	TYR	CB-CG-CD1	8.96	126.38	121.00
1	D	104	TYR	CB-CG-CD2	8.76	126.25	121.00
1	D	256	ASP	CB-CG-OD2	-8.68	110.49	118.30
1	D	63	ARG	NE-CZ-NH1	-8.63	115.99	120.30
1	A	227	TYR	CB-CG-CD1	8.59	126.16	121.00
1	A	194[B]	MET	CG-SD-CE	-8.57	86.49	100.20
1	A	194[C]	MET	CG-SD-CE	-8.57	86.49	100.20
1	C	403	ARG	NE-CZ-NH2	-8.51	116.05	120.30
1	D	160	ASP	CB-CG-OD1	8.42	125.88	118.30
1	B	133	ASP	CB-CG-OD2	-8.39	110.75	118.30
1	B	55	ASP	CB-CG-OD2	-8.39	110.75	118.30
1	D	449	ASP	CB-CG-OD2	-8.36	110.77	118.30
1	D	180[A]	ARG	NE-CZ-NH2	-8.35	116.12	120.30
1	D	180[B]	ARG	NE-CZ-NH2	-8.35	116.12	120.30
1	C	31	ASP	CB-CG-OD2	8.34	125.80	118.30
1	B	141	ARG	NH1-CZ-NH2	8.32	128.55	119.40
1	A	458	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	D	142	ARG	NE-CZ-NH2	-8.29	116.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	449	ASP	CB-CG-OD1	8.10	125.59	118.30
1	C	411	ARG	NE-CZ-NH1	8.10	124.35	120.30
1	C	244	GLU	OE1-CD-OE2	8.02	132.93	123.30
1	A	160	ASP	CB-CG-OD1	8.02	125.52	118.30
1	C	415	ASP	CB-CG-OD1	7.98	125.49	118.30
1	C	145	ASP	CB-CG-OD1	7.91	125.42	118.30
1	A	458	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	B	398	ARG	NE-CZ-NH1	-7.86	116.37	120.30
1	D	398	ARG	NE-CZ-NH1	-7.84	116.38	120.30
1	B	469	ARG	NE-CZ-NH2	-7.78	116.41	120.30
1	A	148	ASP	CB-CG-OD2	-7.75	111.32	118.30
1	A	142	ARG	NE-CZ-NH2	-7.66	116.47	120.30
1	D	87	ARG	NE-CZ-NH1	7.61	124.10	120.30
1	B	448	ARG	NE-CZ-NH2	-7.55	116.52	120.30
1	A	360	ARG	NE-CZ-NH2	-7.53	116.54	120.30
1	C	365	ARG	NE-CZ-NH1	7.49	124.05	120.30
1	C	364	ARG	NE-CZ-NH1	7.44	124.02	120.30
1	B	400	ASP	CB-CG-OD2	7.44	125.00	118.30
1	A	180[A]	ARG	NE-CZ-NH2	-7.41	116.60	120.30
1	A	180[B]	ARG	NE-CZ-NH2	-7.41	116.60	120.30
1	C	301	TYR	CD1-CE1-CZ	-7.40	113.14	119.80
1	A	404	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	A	190	ASP	CB-CG-OD1	7.36	124.92	118.30
1	D	294	ASP	CB-CG-OD2	7.36	124.92	118.30
1	C	448	ARG	NE-CZ-NH2	-7.33	116.63	120.30
1	B	193	ARG	NE-CZ-NH1	-7.33	116.64	120.30
1	B	55	ASP	CB-CG-OD1	7.31	124.88	118.30
1	C	30	GLU	OE1-CD-OE2	7.28	132.04	123.30
1	C	448	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	A	177	PHE	CB-CG-CD2	-7.24	115.73	120.80
1	D	142	ARG	NE-CZ-NH1	-7.24	116.68	120.30
1	A	231	TYR	CB-CG-CD2	-7.23	116.66	121.00
1	C	106	ARG	NE-CZ-NH2	-7.21	116.69	120.30
1	A	294	ASP	CB-CG-OD2	7.17	124.75	118.30
1	D	337	PHE	CB-CG-CD2	-7.16	115.79	120.80
1	C	418	ASP	CB-CG-OD2	-7.06	111.94	118.30
1	A	236	ARG	NE-CZ-NH2	-7.06	116.77	120.30
1	C	384	PHE	CB-CG-CD1	7.06	125.74	120.80
1	A	441	TYR	CD1-CE1-CZ	-7.04	113.47	119.80
1	A	286[A]	GLU	CG-CD-OE1	7.01	132.33	118.30
1	A	286[B]	GLU	CG-CD-OE1	7.01	132.33	118.30
1	C	112	ARG	NE-CZ-NH1	6.98	123.79	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	66	GLU	CG-CD-OE2	-6.97	104.36	118.30
1	B	400	ASP	CB-CG-OD1	-6.91	112.08	118.30
1	A	9	PHE	CB-CG-CD1	6.90	125.63	120.80
1	C	145	ASP	CB-CG-OD2	-6.89	112.10	118.30
1	D	449	ASP	CB-CG-OD1	6.88	124.50	118.30
1	C	441	TYR	CB-CG-CD2	-6.88	116.87	121.00
1	D	55	ASP	CB-CG-OD1	6.88	124.49	118.30
1	A	66	GLU	CG-CD-OE2	-6.86	104.59	118.30
1	C	391	ASP	CB-CG-OD2	-6.85	112.13	118.30
1	D	458	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	D	213	ARG	NE-CZ-NH2	-6.82	116.89	120.30
1	D	385	ASP	CB-CG-OD1	6.82	124.43	118.30
1	B	106	ARG	NE-CZ-NH2	-6.79	116.90	120.30
1	D	39	ASP	CB-CG-OD2	6.72	124.34	118.30
1	D	106	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	C	213	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	A	63[A]	ARG	NE-CZ-NH1	-6.65	116.97	120.30
1	A	63[B]	ARG	NE-CZ-NH1	-6.65	116.97	120.30
1	D	55	ASP	CB-CG-OD2	-6.63	112.33	118.30
1	C	215	TYR	CG-CD1-CE1	-6.63	116.00	121.30
1	C	160[A]	ASP	CB-CG-OD1	6.59	124.23	118.30
1	C	160[B]	ASP	CB-CG-OD1	6.59	124.23	118.30
1	D	64	TYR	CB-CG-CD1	-6.57	117.06	121.00
1	B	47	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	D	233	TYR	CB-CG-CD2	-6.55	117.07	121.00
1	C	66	GLU	OE1-CD-OE2	6.52	131.13	123.30
1	D	395	ASP	CB-CG-OD1	6.52	124.17	118.30
1	D	142	ARG	NH1-CZ-NH2	6.51	126.56	119.40
1	D	400	ASP	CB-CG-OD1	-6.51	112.44	118.30
1	B	256	ASP	CB-CG-OD2	-6.50	112.45	118.30
1	A	87	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	B	157[A]	ARG	CG-CD-NE	-6.46	98.23	111.80
1	B	157[B]	ARG	CG-CD-NE	-6.46	98.23	111.80
1	D	64	TYR	CZ-CE2-CD2	-6.41	114.03	119.80
1	C	59	ASP	CB-CG-OD1	6.37	124.03	118.30
1	B	350[A]	TRP	CA-CB-CG	6.36	125.78	113.70
1	B	350[B]	TRP	CA-CB-CG	6.36	125.78	113.70
1	A	30[A]	GLU	OE1-CD-OE2	6.34	130.90	123.30
1	A	30[B]	GLU	OE1-CD-OE2	6.34	130.90	123.30
1	D	415	ASP	CB-CG-OD1	6.33	123.99	118.30
1	B	9	PHE	CB-CG-CD1	6.32	125.23	120.80
1	B	22	TYR	CB-CG-CD2	-6.29	117.22	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	227	TYR	CB-CG-CD2	-6.28	117.23	121.00
1	B	164	TYR	CD1-CE1-CZ	-6.28	114.15	119.80
1	A	385	ASP	CB-CG-OD2	-6.28	112.65	118.30
1	B	142	ARG	NE-CZ-NH2	-6.27	117.16	120.30
1	B	157[A]	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	B	157[B]	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	B	384	PHE	O-C-N	-6.26	112.68	122.70
1	A	145	ASP	CB-CG-OD1	6.21	123.89	118.30
1	B	349[A]	ASN	N-CA-C	6.18	127.68	111.00
1	B	349[B]	ASN	N-CA-C	6.18	127.68	111.00
1	A	79	TYR	CB-CG-CD2	-6.17	117.30	121.00
1	D	437	TYR	CD1-CE1-CZ	6.16	125.34	119.80
1	B	385	ASP	CB-CG-OD1	6.15	123.83	118.30
1	A	142	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	D	109	GLU	OE1-CD-OE2	-6.14	115.93	123.30
1	A	76	LEU	CB-CG-CD2	6.13	121.42	111.00
1	A	66	GLU	CG-CD-OE1	6.13	130.55	118.30
1	B	148	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	C	364	ARG	NE-CZ-NH2	-6.10	117.25	120.30
1	B	341	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	B	398	ARG	CD-NE-CZ	6.04	132.05	123.60
1	C	194[A]	MET	CG-SD-CE	-6.02	90.57	100.20
1	C	194[B]	MET	CG-SD-CE	-6.02	90.57	100.20
1	D	238	GLU	CG-CD-OE1	-6.01	106.28	118.30
1	D	150	TYR	CB-CG-CD1	6.00	124.60	121.00
1	C	440	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	A	148	ASP	CB-CG-OD1	6.00	123.70	118.30
1	B	365	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	D	87	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	D	66	GLU	OE1-CD-OE2	5.95	130.44	123.30
1	D	398	ARG	NH1-CZ-NH2	-5.95	112.85	119.40
1	C	263	TYR	CB-CG-CD1	5.93	124.56	121.00
1	C	337	PHE	CB-CG-CD2	-5.91	116.66	120.80
1	C	63[A]	ARG	NE-CZ-NH1	-5.91	117.35	120.30
1	C	63[B]	ARG	NE-CZ-NH1	-5.91	117.35	120.30
1	B	93	ASN	CB-CA-C	5.89	122.18	110.40
1	D	398	ARG	CD-NE-CZ	5.89	131.84	123.60
1	D	370	TYR	CB-CG-CD2	-5.88	117.47	121.00
1	B	148	ASP	CB-CG-OD1	5.86	123.57	118.30
1	A	236	ARG	NE-CZ-NH1	5.85	123.23	120.30
1	C	213	ARG	NE-CZ-NH2	-5.85	117.37	120.30
1	C	286[A]	GLU	CG-CD-OE2	5.85	130.00	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	286[B]	GLU	CG-CD-OE2	5.85	130.00	118.30
1	C	150	TYR	CB-CG-CD1	5.82	124.49	121.00
1	C	395	ASP	CB-CG-OD1	5.80	123.52	118.30
1	A	137	ALA	CB-CA-C	5.80	118.79	110.10
1	D	104	TYR	CG-CD2-CE2	5.79	125.93	121.30
1	B	457	ARG	CA-CB-CG	5.78	126.12	113.40
1	A	215	TYR	CB-CG-CD1	-5.77	117.54	121.00
1	B	351[A]	ASP	N-CA-C	5.76	126.56	111.00
1	B	351[B]	ASP	N-CA-C	5.76	126.56	111.00
1	B	160	ASP	CB-CG-OD2	-5.75	113.12	118.30
1	A	476	ALA	O-C-N	-5.75	113.51	122.70
1	B	164	TYR	CB-CG-CD1	-5.73	117.56	121.00
1	B	441	TYR	OH-CZ-CE2	-5.71	104.68	120.10
1	B	465	TYR	CB-CG-CD2	-5.71	117.58	121.00
1	A	286[A]	GLU	CG-CD-OE2	-5.68	106.93	118.30
1	A	286[B]	GLU	CG-CD-OE2	-5.68	106.93	118.30
1	C	193	ARG	NE-CZ-NH1	-5.68	117.46	120.30
1	C	385	ASP	CB-CG-OD1	5.68	123.41	118.30
1	D	295	PHE	CB-CG-CD2	5.68	124.77	120.80
1	D	341	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	D	174	PHE	CB-CG-CD1	-5.67	116.83	120.80
1	B	289	GLN	CB-CG-CD	5.66	126.31	111.60
1	D	112	ARG	CA-CB-CG	-5.66	100.96	113.40
1	C	215	TYR	CD1-CE1-CZ	5.65	124.89	119.80
1	A	212	PHE	CB-CG-CD2	5.62	124.74	120.80
1	C	11	PRO	C-N-CA	-5.61	107.67	121.70
1	D	365	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	A	384	PHE	CB-CA-C	5.60	121.61	110.40
1	B	443	PHE	CB-CG-CD2	-5.60	116.88	120.80
1	C	370	TYR	CB-CG-CD1	5.59	124.35	121.00
1	A	440	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	D	277	GLU	CG-CD-OE2	5.56	129.42	118.30
1	A	177	PHE	CB-CG-CD1	5.55	124.69	120.80
1	D	148	ASP	CB-CG-OD2	-5.55	113.31	118.30
1	C	360	ARG	NH1-CZ-NH2	5.55	125.50	119.40
1	A	192	LYS	CD-CE-NZ	5.55	124.45	111.70
1	C	294	ASP	CB-CG-OD2	5.54	123.29	118.30
1	A	450	ASP	CB-CG-OD1	5.51	123.26	118.30
1	D	104	TYR	CB-CG-CD1	-5.51	117.69	121.00
1	B	22	TYR	CB-CG-CD1	5.51	124.31	121.00
1	C	157[A]	ARG	CG-CD-NE	-5.51	100.24	111.80
1	C	157[B]	ARG	CG-CD-NE	-5.51	100.24	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	22	TYR	CB-CG-CD2	-5.50	117.70	121.00
1	D	441	TYR	CD1-CE1-CZ	-5.50	114.85	119.80
1	C	243	PHE	CB-CG-CD1	5.49	124.64	120.80
1	B	441	TYR	CD1-CE1-CZ	-5.49	114.86	119.80
1	B	145	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	C	337	PHE	CB-CG-CD1	5.47	124.63	120.80
1	C	398	ARG	NH1-CZ-NH2	-5.46	113.40	119.40
1	C	458	ARG	NE-CZ-NH1	5.45	123.03	120.30
1	C	180[A]	ARG	NH1-CZ-NH2	5.45	125.39	119.40
1	C	180[B]	ARG	NH1-CZ-NH2	5.45	125.39	119.40
1	A	157[A]	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	157[B]	ARG	NE-CZ-NH2	-5.42	117.59	120.30
1	A	164	TYR	CZ-CE2-CD2	-5.41	114.93	119.80
1	C	445	TYR	CG-CD2-CE2	5.41	125.63	121.30
1	A	448	ARG	NE-CZ-NH2	-5.39	117.60	120.30
1	B	457	ARG	NE-CZ-NH1	5.37	122.98	120.30
1	C	135	TYR	CD1-CE1-CZ	5.37	124.63	119.80
1	C	141	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	D	336	LEU	CB-CG-CD1	-5.33	101.94	111.00
1	A	91	ASP	CB-CG-OD2	-5.32	113.52	118.30
1	D	67	ASP	CB-CG-OD2	5.31	123.08	118.30
1	C	148	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	411	ARG	NE-CZ-NH2	-5.30	117.65	120.30
1	B	441	TYR	CE1-CZ-CE2	5.25	128.19	119.80
1	D	478	LEU	CB-CG-CD1	5.24	119.91	111.00
1	A	468	GLN	O-C-N	5.23	131.07	122.70
1	C	227	TYR	CG-CD1-CE1	5.23	125.48	121.30
1	D	244	GLU	OE1-CD-OE2	5.23	129.57	123.30
1	A	448	ARG	NE-CZ-NH1	5.23	122.91	120.30
1	C	441	TYR	CG-CD1-CE1	-5.22	117.12	121.30
1	B	25	GLU	OE1-CD-OE2	-5.22	117.04	123.30
1	D	286	GLU	CG-CD-OE2	5.21	128.71	118.30
1	A	398	ARG	NE-CZ-NH1	-5.20	117.70	120.30
1	B	212	PHE	CB-CG-CD2	5.19	124.43	120.80
1	A	123	TYR	CB-CG-CD1	-5.18	117.89	121.00
1	D	123	TYR	CB-CG-CD2	5.17	124.10	121.00
1	D	79	TYR	CD1-CE1-CZ	5.16	124.44	119.80
1	D	294	ASP	CB-CG-OD1	-5.15	113.66	118.30
1	D	155	PHE	O-C-N	5.14	130.93	122.70
1	B	164	TYR	CE1-CZ-CE2	5.13	128.02	119.80
1	C	301	TYR	CG-CD1-CE1	5.13	125.41	121.30
1	D	233	TYR	CB-CG-CD1	5.12	124.08	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	117	GLU	CG-CD-OE2	-5.12	108.05	118.30
1	C	385	ASP	CB-CG-OD2	5.12	122.91	118.30
1	B	396	ASP	CB-CG-OD1	-5.12	113.69	118.30
1	C	452	SER	N-CA-CB	5.12	118.18	110.50
1	C	160[A]	ASP	OD1-CG-OD2	-5.12	113.58	123.30
1	C	160[B]	ASP	OD1-CG-OD2	-5.12	113.58	123.30
1	B	102	ASP	CB-CG-OD1	5.10	122.89	118.30
1	B	256	ASP	CB-CG-OD1	5.10	122.89	118.30
1	B	180[A]	ARG	NH1-CZ-NH2	5.10	125.01	119.40
1	B	180[B]	ARG	NH1-CZ-NH2	5.10	125.01	119.40
1	C	385	ASP	OD1-CG-OD2	-5.09	113.63	123.30
1	D	398	ARG	O-C-N	-5.08	114.57	122.70
1	D	383[A]	GLU	CG-CD-OE2	-5.07	108.16	118.30
1	D	383[B]	GLU	CG-CD-OE2	-5.07	108.16	118.30
1	B	355	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	C	291	ALA	O-C-N	-5.06	114.60	122.70
1	D	150	TYR	CB-CG-CD2	-5.04	117.98	121.00
1	C	445	TYR	CB-CG-CD2	5.03	124.02	121.00
1	B	231	TYR	CB-CG-CD2	-5.03	117.98	121.00
1	B	441	TYR	CB-CG-CD2	-5.03	117.98	121.00
1	C	22	TYR	CB-CG-CD1	5.02	124.01	121.00
1	D	418	ASP	CB-CG-OD2	-5.01	113.79	118.30

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	290	ALA	Mainchain
1	A	469[B]	ARG	Mainchain
1	B	290	ALA	Mainchain
1	B	349[B]	ASN	Peptide
1	B	351[A]	ASP	Mainchain
1	B	384	PHE	Mainchain
1	C	384	PHE	Mainchain
1	D	290	ALA	Mainchain

## 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	3945	0	3833	42	0
1	B	3911	0	3750	31	0
1	C	3914	0	3770	48	0
1	D	3875	0	3706	30	0
2	E	27	0	20	3	0
3	A	16	0	10	0	0
3	B	16	0	10	0	0
4	A	30	0	40	3	0
4	B	12	0	16	0	0
4	C	24	0	32	1	0
4	D	6	0	8	0	0
5	A	5	0	5	1	0
5	C	5	0	5	0	0
5	D	5	0	5	1	0
6	C	15	0	9	1	0
7	C	12	0	10	4	0
8	A	640	0	0	20	0
8	B	638	0	0	14	0
8	C	692	0	0	21	0
8	D	608	0	0	18	0
All	All	18396	0	15229	150	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 (150) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:ASP:HB2	8:A:838:HOH:O	1.37	1.19
1:C:170:GLN:HE22	7:C:507:BGC:H6C2	1.12	1.08
1:A:132[A]:MET:HE3	8:A:1072:HOH:O	1.56	1.05
1:C:132[A]:MET:HE3	8:C:1116:HOH:O	1.60	1.00
1:D:132[A]:MET:HE3	8:D:1075:HOH:O	1.65	0.96
1:B:348:THR:O	1:B:350[A]:TRP:HA	1.66	0.96
1:A:157[B]:ARG:HD2	8:A:752:HOH:O	1.66	0.95
1:A:132[A]:MET:CE	8:A:1072:HOH:O	2.11	0.93
1:C:170:GLN:NE2	7:C:507:BGC:H6C2	1.84	0.90
1:D:339[B]:THR:HG21	8:D:812:HOH:O	1.73	0.88
1:A:97[B]:ASN:ND2	8:A:601:HOH:O	2.09	0.86
1:D:249:PHE:CE2	1:D:333:ILE:HD11	2.13	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:112[B]:ARG:HG2	1:A:112[B]:ARG:NH1	1.92	0.82
1:B:112:ARG:HD2	8:B:612:HOH:O	1.83	0.79
1:A:112[B]:ARG:HG2	1:A:112[B]:ARG:HH11	1.48	0.78
1:A:169:ASN:HD21	1:A:299:ASN:HD21	1.29	0.78
1:C:169:ASN:HD21	1:C:299:ASN:HD21	1.34	0.76
1:D:149:ARG:HD3	8:D:737:HOH:O	1.84	0.76
1:A:198:ASN:HD21	1:A:254:TRP:HE1	1.33	0.75
1:D:169:ASN:HD21	1:D:299:ASN:HD21	1.33	0.74
1:B:348:THR:O	1:B:350[A]:TRP:CA	2.36	0.73
1:C:12:GLU:HG3	8:C:1140:HOH:O	1.89	0.72
1:C:170:GLN:HE22	7:C:507:BGC:C6	1.97	0.72
1:B:97:ASN:ND2	8:B:601:HOH:O	2.24	0.71
1:B:169:ASN:HD21	1:B:299:ASN:HD21	1.37	0.70
1:A:350:TRP:CD1	8:A:893:HOH:O	2.43	0.70
1:B:198:ASN:HD21	1:B:254:TRP:HE1	1.39	0.70
1:C:214:HIS:HE1	1:D:383[A]:GLU:HG2	1.57	0.69
1:D:198:ASN:HD21	1:D:254:TRP:HE1	1.40	0.69
1:A:112[B]:ARG:HH11	1:A:112[B]:ARG:CG	2.05	0.69
1:C:198:ASN:HD21	1:C:254:TRP:HE1	1.40	0.69
1:C:43:LYS:HE3	8:C:858:HOH:O	1.94	0.67
1:C:249:PHE:CD1	8:C:1225:HOH:O	2.48	0.66
1:A:403[B]:ARG:HG3	1:A:478:LEU:HB3	1.78	0.65
1:B:350[A]:TRP:O	1:B:351[A]:ASP:OD1	2.14	0.65
1:C:73:GLU:OE2	1:C:460[B]:LYS:HE2	1.97	0.64
1:A:11:PRO:HG2	8:A:1178:HOH:O	1.98	0.63
1:A:469[A]:ARG:NE	1:A:477:GLU:OE1	2.24	0.62
1:D:170:GLN:NE2	2:E:1:BGC:O6	2.32	0.62
1:D:331:SER:H	1:D:339[B]:THR:HG22	1.64	0.62
1:C:308[B]:HIS:ND1	8:C:606:HOH:O	2.31	0.61
5:D:502:IMD:H5	8:D:692:HOH:O	1.99	0.61
1:C:407[B]:GLN:NE2	8:C:602:HOH:O	2.25	0.61
1:D:112:ARG:HG2	8:D:907:HOH:O	1.99	0.61
1:B:149:ARG:HD3	8:B:820:HOH:O	2.02	0.59
1:C:308[B]:HIS:CE1	8:C:606:HOH:O	2.54	0.59
1:C:169:ASN:HD22	1:C:224:SER:HB3	1.68	0.59
1:A:315:GLY:HA3	8:A:1093:HOH:O	2.03	0.59
1:C:93:ASN:C	1:C:93:ASN:HD22	2.07	0.58
1:A:149:ARG:HD3	8:A:816:HOH:O	2.03	0.58
1:B:112:ARG:CG	8:B:612:HOH:O	2.51	0.58
8:D:611:HOH:O	2:E:1:BGC:H4	2.03	0.58
1:B:169:ASN:HD22	1:B:224:SER:HB3	1.69	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:169:ASN:HD22	1:A:224:SER:HB3	1.70	0.57
1:D:331:SER:H	1:D:339[B]:THR:CG2	2.17	0.57
1:A:252:HIS:HE1	8:A:846:HOH:O	1.88	0.57
1:D:352:TRP:HH2	8:D:611:HOH:O	1.87	0.57
1:C:191[B]:MET:HE1	8:C:1242:HOH:O	2.05	0.56
1:A:93:ASN:HD22	1:A:93:ASN:C	2.09	0.56
1:D:169:ASN:HD22	1:D:224:SER:HB3	1.71	0.56
1:A:336:LEU:CD2	4:A:506:GOL:H2	2.35	0.55
1:B:214:HIS:HD2	8:B:1096:HOH:O	1.88	0.55
1:B:302[B]:GLN:OE1	1:B:352:TRP:HA	2.07	0.55
1:C:170:GLN:NE2	7:C:507:BGC:C6	2.63	0.55
1:B:302[B]:GLN:HB2	1:B:353:ALA:HB3	1.89	0.55
1:A:47[A]:ARG:NH2	8:A:605:HOH:O	2.32	0.54
1:D:252:HIS:HE1	8:D:840:HOH:O	1.90	0.54
1:A:336:LEU:HD21	4:A:506:GOL:H2	1.89	0.54
1:A:157[B]:ARG:CD	8:A:752:HOH:O	2.40	0.53
1:B:302[B]:GLN:OE1	1:B:352:TRP:CA	2.56	0.53
1:B:236[A]:ARG:NH1	8:B:613:HOH:O	2.42	0.52
1:B:112:ARG:CD	8:B:612:HOH:O	2.47	0.52
1:D:460:LYS:HE2	8:D:1109:HOH:O	2.09	0.52
1:C:112:ARG:HD2	1:C:161:ARG:HB3	1.91	0.52
1:C:252:HIS:HE1	8:C:882:HOH:O	1.92	0.52
1:C:384:PHE:O	4:C:504:GOL:H11	2.09	0.52
1:B:112:ARG:HG2	8:B:612:HOH:O	2.09	0.51
1:C:192:LYS:HD2	8:C:865:HOH:O	2.10	0.50
1:C:191[B]:MET:CE	8:C:1242:HOH:O	2.60	0.50
1:C:73:GLU:CD	1:C:460[B]:LYS:HE2	2.32	0.50
1:D:331:SER:O	1:D:339[B]:THR:HG22	2.11	0.50
1:B:350[B]:TRP:CD1	1:B:350[B]:TRP:N	2.81	0.49
1:A:207:LYS:HD2	1:A:210[B]:GLN:HE21	1.77	0.49
1:D:207:LYS:NZ	8:D:614:HOH:O	2.46	0.48
1:B:93:ASN:C	1:B:93:ASN:HD22	2.16	0.48
1:B:394:ASN:ND2	8:B:615:HOH:O	2.47	0.48
1:A:400:ASP:CB	8:A:838:HOH:O	2.20	0.48
1:C:157[B]:ARG:HD3	1:D:346:ASP:OD1	2.13	0.47
1:A:408:GLU:OE2	1:A:411:ARG:NH1	2.45	0.47
1:B:302[B]:GLN:OE1	1:B:353:ALA:N	2.45	0.47
1:D:245:ASN:ND2	8:D:615:HOH:O	2.47	0.47
1:C:194[B]:MET:HE1	1:C:195:TYR:CE2	2.50	0.47
4:A:505:GOL:O2	8:A:602:HOH:O	2.21	0.47
1:B:460:LYS:HE2	8:B:1119:HOH:O	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:400:ASP:OD1	8:A:603:HOH:O	2.21	0.46
1:B:192:LYS:CE	8:B:608:HOH:O	2.63	0.46
1:D:262[A]:MET:CE	8:D:857:HOH:O	2.63	0.46
1:C:5:HIS:CG	1:C:5:HIS:O	2.68	0.46
1:D:272:GLU:CD	8:D:639:HOH:O	2.54	0.46
1:A:350:TRP:CD1	1:A:439:LYS:HD2	2.50	0.46
1:A:403[B]:ARG:HD3	1:A:478:LEU:C	2.36	0.45
1:B:350[A]:TRP:O	1:B:350[A]:TRP:CG	2.68	0.45
1:A:156:GLN:HE22	1:B:349[B]:ASN:HD22	1.65	0.45
1:C:194[B]:MET:CE	1:C:195:TYR:CE2	2.99	0.45
1:A:112[A]:ARG:HG2	8:A:889:HOH:O	2.14	0.45
1:A:285:TRP:O	1:A:289[A]:GLN:HG3	2.16	0.45
1:C:180[A]:ARG:NH1	8:C:621:HOH:O	2.49	0.45
1:D:93:ASN:HD22	1:D:93:ASN:C	2.20	0.45
1:A:210[B]:GLN:NE2	8:A:621:HOH:O	2.50	0.45
1:C:460[B]:LYS:NZ	8:C:610:HOH:O	2.37	0.45
1:A:453:GLU:OE1	5:A:507:IMD:N1	2.37	0.45
1:C:132[A]:MET:HE1	8:C:739:HOH:O	2.15	0.44
1:C:214:HIS:CE1	1:D:383[A]:GLU:HG2	2.44	0.44
1:C:308[B]:HIS:CE1	8:C:689:HOH:O	2.70	0.44
1:B:378:GLU:HG3	1:B:425:TRP:HB2	1.99	0.44
1:C:112:ARG:HG2	8:C:944:HOH:O	2.16	0.44
1:C:180[B]:ARG:HB2	1:C:194[B]:MET:SD	2.58	0.44
1:D:5:HIS:O	1:D:5:HIS:CG	2.69	0.44
1:A:170[A]:GLN:HE21	1:A:226:ALA:HB2	1.82	0.44
1:B:170:GLN:NE2	8:B:627:HOH:O	2.50	0.44
1:A:156:GLN:HE22	1:B:349[A]:ASN:HD22	1.65	0.44
1:D:132[A]:MET:CE	8:D:1075:HOH:O	2.42	0.44
1:C:292[B]:LYS:CG	8:C:1012:HOH:O	2.65	0.43
1:C:249:PHE:CE2	1:C:333:ILE:HD11	2.53	0.43
1:B:153:THR:O	1:B:157[B]:ARG:HG2	2.19	0.43
1:B:189:LYS:HE2	8:B:781:HOH:O	2.18	0.43
1:A:292[B]:LYS:HG2	8:A:974:HOH:O	2.18	0.43
1:C:336:LEU:HD13	8:C:1225:HOH:O	2.18	0.43
1:B:192:LYS:NZ	8:B:608:HOH:O	2.37	0.43
6:C:506:OWK:P	8:C:603:HOH:O	2.76	0.43
8:D:649:HOH:O	2:E:1:BGC:H3	2.18	0.43
1:D:352:TRP:CH2	8:D:611:HOH:O	2.57	0.42
1:A:30[A]:GLU:HG3	8:A:608:HOH:O	2.20	0.42
1:D:262[C]:MET:HE3	8:D:857:HOH:O	2.20	0.42
1:D:170:GLN:HE21	1:D:226:ALA:HB2	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:302:GLN:HB2	1:C:353:ALA:HB3	2.01	0.42
1:C:194[B]:MET:CE	1:C:195:TYR:CZ	3.02	0.42
1:C:432[B]:SER:HB3	1:C:436:GLY:O	2.20	0.41
1:C:214:HIS:HE1	1:D:383[A]:GLU:CG	2.28	0.41
1:C:94:GLY:O	1:C:149:ARG:NH2	2.39	0.41
1:A:425:TRP:HA	1:A:426:SER:HA	1.90	0.41
1:C:249:PHE:CE2	1:C:333:ILE:CD1	3.03	0.41
1:A:378:GLU:HG3	1:A:425:TRP:HB2	2.02	0.41
1:A:92:GLY:HA2	1:A:128:PRO:HG2	2.01	0.41
1:C:394:ASN:ND2	8:C:618:HOH:O	2.46	0.41
1:C:378:GLU:HG3	1:C:425:TRP:HB2	2.02	0.41
1:C:238[A]:GLU:HG3	8:C:1132:HOH:O	2.20	0.41
1:A:394:ASN:ND2	8:A:627:HOH:O	2.53	0.41
1:D:262[A]:MET:HE3	8:D:857:HOH:O	2.20	0.41
1:C:153:THR:O	1:C:157[B]:ARG:HG2	2.21	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	484/485 (100%)	468 (97%)	16 (3%)	0	100	100
1	B	478/485 (99%)	460 (96%)	18 (4%)	0	100	100
1	C	481/485 (99%)	464 (96%)	16 (3%)	1 (0%)	47	21
1	D	475/485 (98%)	457 (96%)	16 (3%)	2 (0%)	34	12
All	All	1918/1940 (99%)	1849 (96%)	66 (3%)	3 (0%)	47	21

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	167	THR
1	D	310	PRO
1	C	310	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	418/412 (102%)	416 (100%)	2 (0%)	88	74
1	B	412/412 (100%)	407 (99%)	5 (1%)	71	47
1	C	415/412 (101%)	413 (100%)	2 (0%)	88	74
1	D	409/412 (99%)	407 (100%)	2 (0%)	88	74
All	All	1654/1648 (100%)	1643 (99%)	11 (1%)	86	66

All (11) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	430	LEU
1	B	93	ASN
1	B	350[A]	TRP
1	B	350[B]	TRP
1	B	351[A]	ASP
1	B	351[B]	ASP
1	C	5	HIS
1	C	93	ASN
1	D	6	LEU
1	D	93	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	129	GLN
1	A	169	ASN

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Mol	Chain	Res	Type
1	A	171	GLN
1	A	198	ASN
1	A	202	ASN
1	A	205	ASN
1	A	251	ASN
1	A	252	HIS
1	A	265	GLN
1	A	269	ASN
1	A	349	ASN
1	A	379	ASN
1	A	394	ASN
1	B	93	ASN
1	B	129	GLN
1	B	169	ASN
1	B	170	GLN
1	B	171	GLN
1	B	198	ASN
1	B	202	ASN
1	B	205	ASN
1	B	251	ASN
1	B	265	GLN
1	B	269	ASN
1	B	379	ASN
1	B	435	ASN
1	C	93	ASN
1	C	129	GLN
1	C	169	ASN
1	C	170	GLN
1	C	171	GLN
1	C	198	ASN
1	C	202	ASN
1	C	205	ASN
1	C	251	ASN
1	C	252	HIS
1	C	265	GLN
1	C	269	ASN
1	C	379	ASN
1	C	394	ASN
1	C	435	ASN
1	D	93	ASN
1	D	129	GLN
1	D	169	ASN

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Mol	Chain	Res	Type
1	D	170	GLN
1	D	171	GLN
1	D	198	ASN
1	D	202	ASN
1	D	205	ASN
1	D	245	ASN
1	D	251	ASN
1	D	252	HIS
1	D	265	GLN
1	D	269	ASN
1	D	349	ASN
1	D	379	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 ⓘ

2 monosaccharides 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	BGC	E	1	2	12,12,12	0.73	0	17,17,17	2.10	7 (41%)
2	0WK	E	2	2	15,15,15	1.98	4 (26%)	22,22,22	2.92	7 (31%)

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	BGC	E	1	2	-	1/2/22/22	0/1/1/1
2	0WK	E	2	2	-	1/6/23/23	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	2	0WK	O2-C2	-4.61	1.33	1.43
2	E	2	0WK	P-O3P	-3.63	1.40	1.54
2	E	2	0WK	O3-C3	3.55	1.51	1.43
2	E	2	0WK	C4-C3	2.04	1.57	1.52

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	0WK	O3-C3-C4	7.38	127.41	110.35
2	E	2	0WK	C1-C2-C3	6.40	117.54	109.67
2	E	2	0WK	O3-C3-C2	-5.56	99.35	109.99
2	E	2	0WK	O2-C2-C1	-5.20	98.52	109.15
2	E	1	BGC	C1-C2-C3	-3.56	102.93	110.31
2	E	2	0WK	O2P-P-O1P	3.26	123.43	110.68
2	E	1	BGC	O2-C2-C3	3.19	117.72	110.35
2	E	1	BGC	O5-C1-C2	-3.02	104.90	110.28
2	E	1	BGC	O5-C5-C6	-2.96	99.08	106.44
2	E	2	0WK	O2-C2-C3	-2.91	104.30	110.14
2	E	1	BGC	O3-C3-C4	-2.90	103.64	110.35
2	E	1	BGC	O2-C2-C1	2.45	114.83	109.16
2	E	2	0WK	O4-C4-C5	-2.27	103.67	109.30
2	E	1	BGC	C6-C5-C4	2.05	117.80	113.00

There are no chirality outliers.

All (2) torsion outliers are listed below:

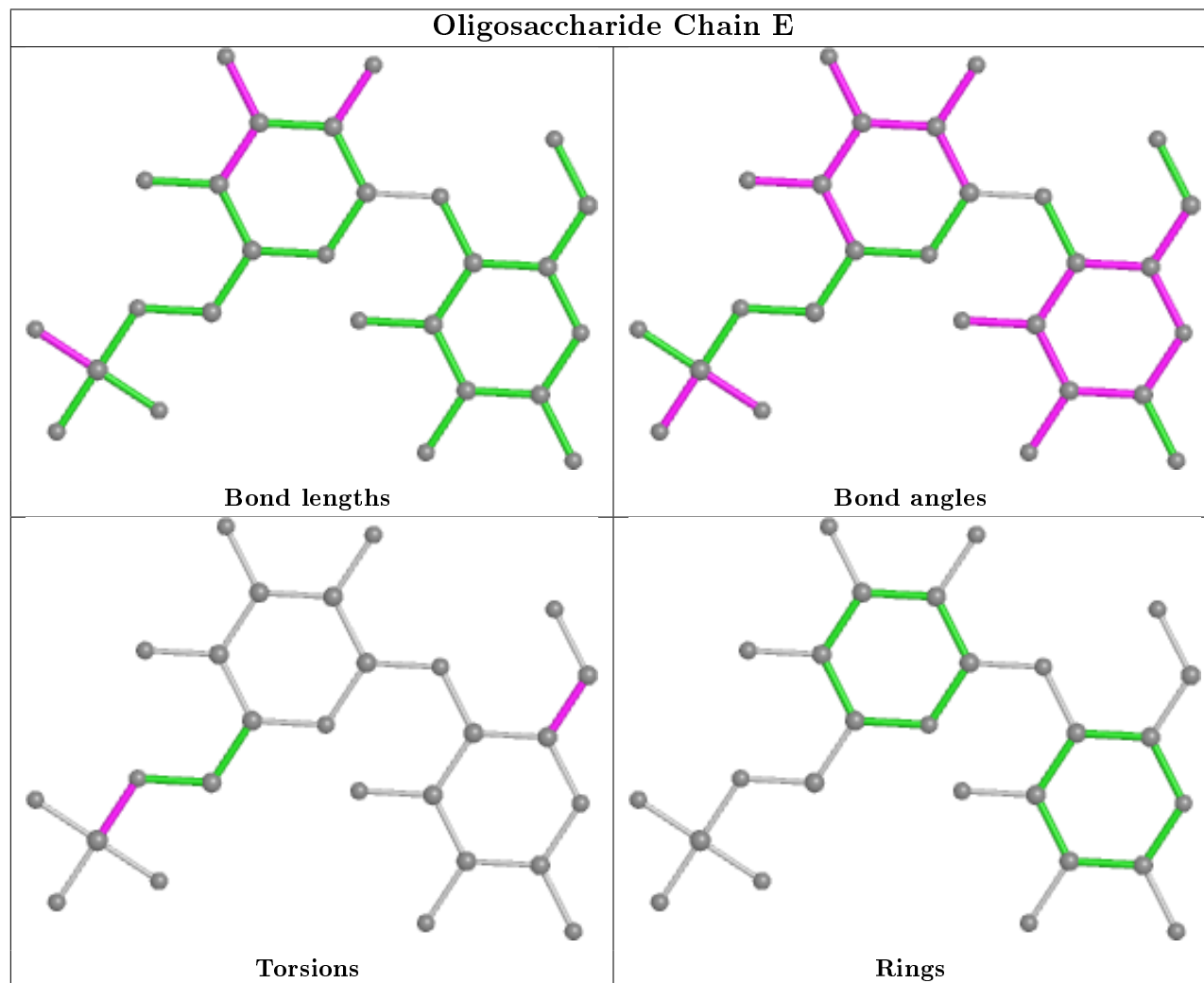
Mol	Chain	Res	Type	Atoms
2	E	1	BGC	O5-C5-C6-O6
2	E	2	0WK	C6-O6-P-O2P

There are no ring outliers.

1 monomer is involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	E	1	BGC	3	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for oligosaccharide.



## 5.6 Ligand geometry [i](#)

19 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
3	BG6	B	501	-	16,16,16	2.18	4 (25%)	24,24,24	3.38	12 (50%)
4	GOL	A	502	-	5,5,5	0.36	0	5,5,5	0.96	0
4	GOL	C	502	-	5,5,5	1.05	1 (20%)	5,5,5	1.22	0
6	0WK	C	506	-	15,15,15	2.15	5 (33%)	22,22,22	4.45	10 (45%)
4	GOL	B	503	-	5,5,5	0.41	0	5,5,5	1.02	0
4	GOL	A	503	-	5,5,5	0.29	0	5,5,5	1.54	1 (20%)
4	GOL	C	504	-	5,5,5	0.78	0	5,5,5	1.46	1 (20%)
4	GOL	C	503	-	5,5,5	0.72	0	5,5,5	0.95	0
4	GOL	A	504	-	5,5,5	1.00	0	5,5,5	1.51	1 (20%)
7	BGC	C	507	-	12,12,12	1.25	1 (8%)	17,17,17	3.37	12 (70%)
5	IMD	D	502	-	3,5,5	0.25	0	4,5,5	0.22	0
5	IMD	C	505	-	3,5,5	0.44	0	4,5,5	0.45	0
4	GOL	B	502	-	5,5,5	0.77	0	5,5,5	1.06	0
4	GOL	D	501	-	5,5,5	0.33	0	5,5,5	0.73	0
4	GOL	A	505	-	5,5,5	0.86	0	5,5,5	1.42	1 (20%)
3	BG6	A	501	-	16,16,16	2.25	4 (25%)	24,24,24	3.06	7 (29%)
4	GOL	C	501	-	5,5,5	0.97	0	5,5,5	1.73	2 (40%)
4	GOL	A	506	-	5,5,5	0.30	0	5,5,5	1.18	0
5	IMD	A	507	-	3,5,5	0.31	0	4,5,5	1.28	0

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	BG6	B	501	-	-	1/6/26/26	0/1/1/1
4	GOL	A	502	-	-	0/4/4/4	-
4	GOL	C	502	-	-	0/4/4/4	-
6	0WK	C	506	-	-	1/6/23/23	0/1/1/1
4	GOL	B	503	-	-	2/4/4/4	-
4	GOL	A	503	-	-	0/4/4/4	-
4	GOL	C	504	-	-	2/4/4/4	-
4	GOL	C	503	-	-	0/4/4/4	-
4	GOL	A	504	-	-	0/4/4/4	-
7	BGC	C	507	-	-	2/2/22/22	0/1/1/1
5	IMD	D	502	-	-	-	0/1/1/1
5	IMD	C	505	-	-	-	0/1/1/1
4	GOL	B	502	-	-	0/4/4/4	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	D	501	-	-	2/4/4/4	-
4	GOL	A	505	-	-	0/4/4/4	-
3	BG6	A	501	-	-	1/6/26/26	0/1/1/1
4	GOL	C	501	-	-	0/4/4/4	-
4	GOL	A	506	-	-	4/4/4/4	-
5	IMD	A	507	-	-	-	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	BG6	O2-C2	-5.41	1.30	1.43
3	B	501	BG6	O2-C2	-4.99	1.31	1.43
6	C	506	0WK	O2-C2	-4.84	1.33	1.43
3	A	501	BG6	O3-C3	4.81	1.54	1.43
3	B	501	BG6	O3-C3	4.50	1.53	1.43
6	C	506	0WK	O3-C3	4.19	1.52	1.43
3	B	501	BG6	C4-C3	3.46	1.61	1.52
6	C	506	0WK	C4-C3	3.11	1.60	1.52
3	A	501	BG6	P-O1P	-2.85	1.43	1.54
7	C	507	BGC	O5-C1	2.73	1.49	1.42
3	A	501	BG6	C4-C3	2.69	1.59	1.52
6	C	506	0WK	P-O3P	2.57	1.64	1.54
3	B	501	BG6	P-O2P	-2.20	1.46	1.54
4	C	502	GOL	O2-C2	2.11	1.49	1.43
6	C	506	0WK	O5-C1	-2.00	1.40	1.43

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	506	0WK	O3P-P-O6	-11.50	76.14	106.73
3	A	501	BG6	O3-C3-C4	9.90	133.24	110.35
6	C	506	0WK	C1-C2-C3	9.51	121.36	109.67
3	B	501	BG6	O3-C3-C4	9.19	131.59	110.35
6	C	506	0WK	O3-C3-C4	8.43	129.84	110.35
3	B	501	BG6	O2-C2-C1	-6.68	93.67	109.16
6	C	506	0WK	O3-C3-C2	-6.59	97.38	109.99
7	C	507	BGC	O2-C2-C1	6.14	123.40	109.16
6	C	506	0WK	P-O6-C6	5.88	134.48	118.30
3	A	501	BG6	O2-C2-C1	-5.69	95.96	109.16
3	B	501	BG6	O3-C3-C2	-5.62	97.35	110.35
7	C	507	BGC	C1-C2-C3	-5.45	99.00	110.31
7	C	507	BGC	O5-C5-C6	5.31	119.64	106.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	501	BG6	O3-C3-C2	-5.30	98.09	110.35
3	B	501	BG6	C1-C2-C3	5.14	120.97	110.31
6	C	506	0WK	O3P-P-O2P	5.01	126.79	107.64
3	A	501	BG6	C1-C2-C3	4.83	120.34	110.31
7	C	507	BGC	O3-C3-C4	4.37	120.46	110.35
3	B	501	BG6	O2-C2-C3	-3.77	101.63	110.35
7	C	507	BGC	C1-O5-C5	-3.43	107.19	113.66
7	C	507	BGC	C3-C4-C5	-3.42	104.15	110.24
3	B	501	BG6	O4-C4-C3	3.41	118.23	110.35
7	C	507	BGC	O1-C1-O5	3.39	120.56	110.38
3	B	501	BG6	O2P-P-O6	3.37	115.70	106.73
6	C	506	0WK	O2-C2-C1	-3.27	102.46	109.15
7	C	507	BGC	C4-C3-C2	-3.18	105.27	110.82
4	A	503	GOL	O3-C3-C2	3.14	125.25	110.20
7	C	507	BGC	O5-C1-C2	-3.13	104.70	110.28
3	B	501	BG6	C6-C5-C4	3.12	118.61	112.09
3	B	501	BG6	O4-C4-C5	-3.10	101.59	109.30
4	C	501	GOL	O3-C3-C2	2.96	124.38	110.20
3	B	501	BG6	O2P-P-O3P	-2.84	99.58	110.68
4	A	504	GOL	O3-C3-C2	2.81	123.65	110.20
3	A	501	BG6	O2P-P-O3P	2.72	121.35	110.68
6	C	506	0WK	O3P-P-O1P	2.70	121.25	110.68
3	A	501	BG6	O4-C4-C5	-2.68	102.63	109.30
7	C	507	BGC	O4-C4-C5	-2.60	102.84	109.30
3	A	501	BG6	O4-C4-C3	2.57	116.28	110.35
3	B	501	BG6	O1P-P-O3P	2.56	120.69	110.68
3	B	501	BG6	O1P-P-O6	-2.47	100.16	106.73
7	C	507	BGC	O6-C6-C5	2.44	119.66	111.29
4	A	505	GOL	O3-C3-C2	2.42	121.81	110.20
7	C	507	BGC	O4-C4-C3	2.40	115.89	110.35
6	C	506	0WK	O4-C4-C3	2.23	115.50	110.35
4	C	504	GOL	C3-C2-C1	2.22	120.34	111.70
6	C	506	0WK	O2-C2-C3	-2.22	105.70	110.14
4	C	501	GOL	C3-C2-C1	-2.15	103.36	111.70

There are no chirality outliers.

All (15) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	503	GOL	O1-C1-C2-C3
4	C	504	GOL	C1-C2-C3-O3
4	C	504	GOL	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
4	A	506	GOL	C1-C2-C3-O3
7	C	507	BGC	O5-C5-C6-O6
4	A	506	GOL	O1-C1-C2-O2
4	A	506	GOL	O1-C1-C2-C3
4	B	503	GOL	O1-C1-C2-O2
4	A	506	GOL	O2-C2-C3-O3
4	D	501	GOL	O1-C1-C2-O2
4	D	501	GOL	O1-C1-C2-C3
3	B	501	BG6	C6-O6-P-O1P
6	C	506	0WK	C6-O6-P-O3P
3	A	501	BG6	C6-O6-P-O2P
7	C	507	BGC	C4-C5-C6-O6

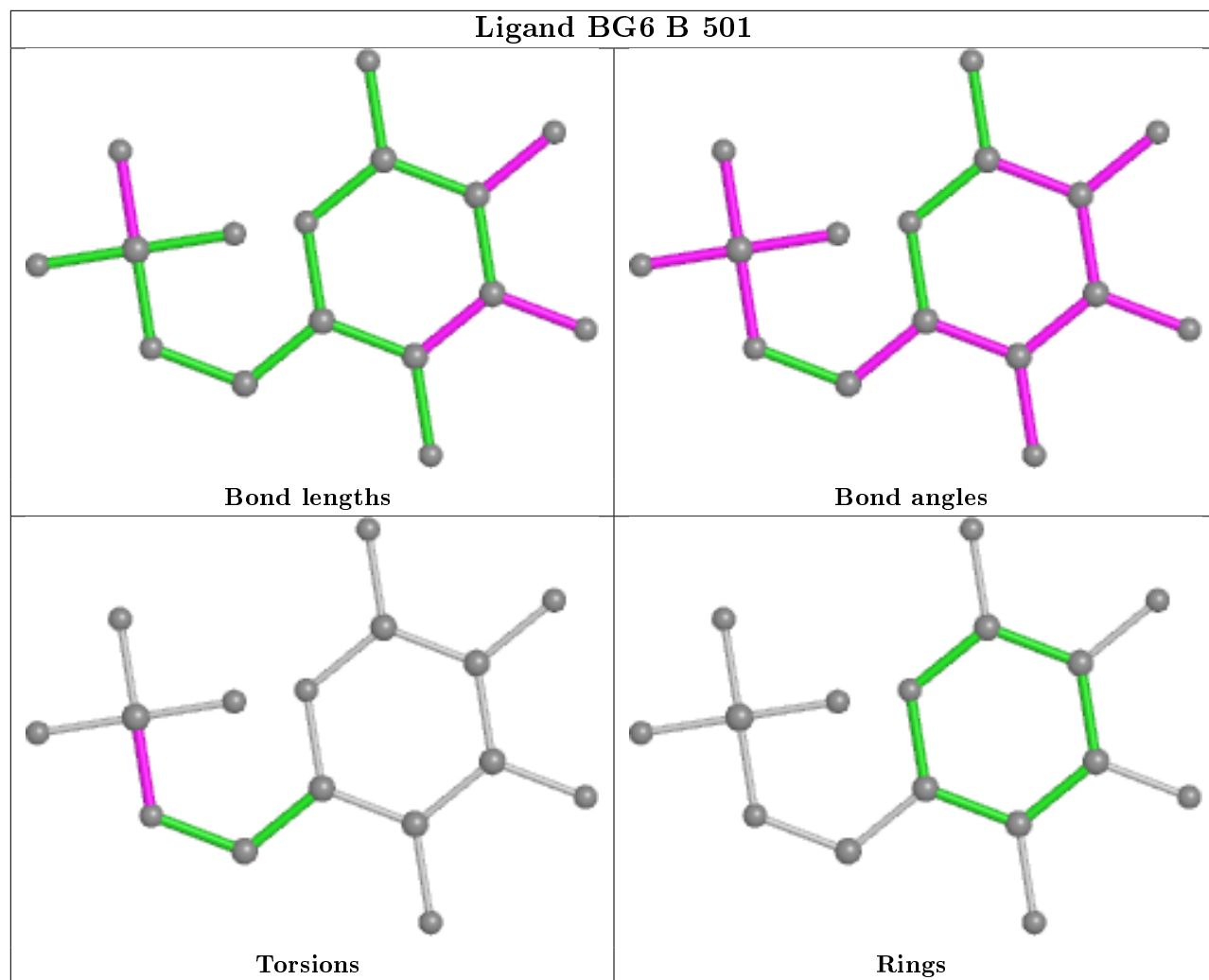
There are no ring outliers.

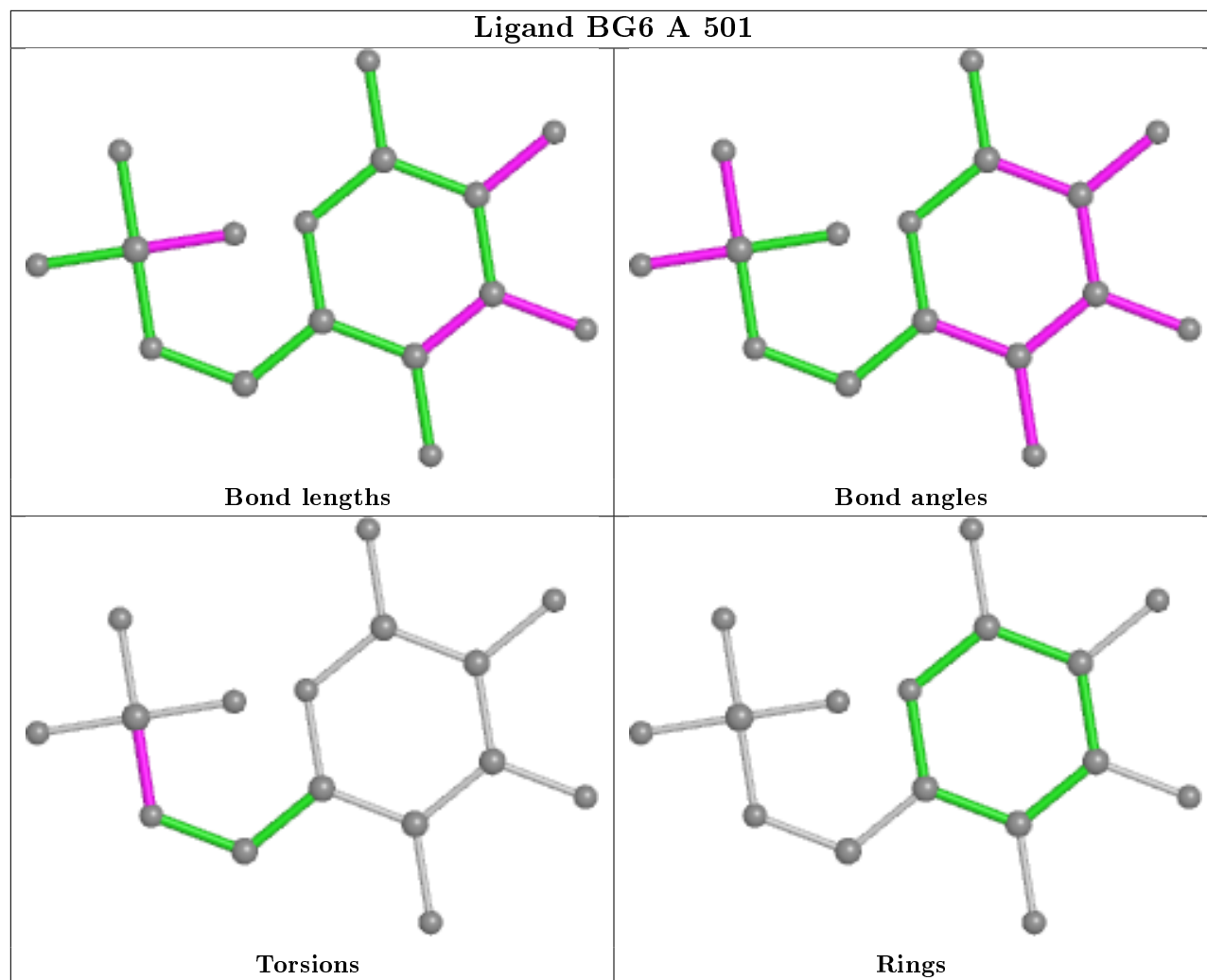
7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	C	506	0WK	1	0
4	C	504	GOL	1	0
7	C	507	BGC	4	0
5	D	502	IMD	1	0
4	A	505	GOL	1	0
4	A	506	GOL	2	0
5	A	507	IMD	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

## Ligand BG6 B 501





## 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	461/485 (95%)	-0.34	9 (1%) 65 65	6, 11, 27, 74	0
1	B	461/485 (95%)	-0.38	11 (2%) 59 58	6, 10, 24, 61	0
1	C	461/485 (95%)	-0.42	11 (2%) 59 58	5, 10, 22, 68	0
1	D	461/485 (95%)	-0.36	11 (2%) 59 58	6, 11, 25, 76	0
All	All	1844/1940 (95%)	-0.37	42 (2%) 60 60	5, 11, 25, 76	0

All (42) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	329	THR	7.5
1	A	329	THR	7.2
1	A	350	TRP	7.1
1	B	329	THR	6.2
1	C	329	THR	5.7
1	D	312	ASP	5.6
1	B	350[A]	TRP	5.5
1	A	313	GLY	5.3
1	B	315	GLY	5.0
1	A	352	TRP	4.7
1	B	312	ASP	4.7
1	D	314	VAL	4.7
1	C	313	GLY	4.6
1	C	312	ASP	4.6
1	B	352	TRP	4.5
1	D	352	TRP	4.5
1	C	5	HIS	4.4
1	D	311	PRO	4.4
1	D	313	GLY	4.4
1	D	315	GLY	4.2
1	C	314	VAL	4.2

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Mol	Chain	Res	Type	RSRZ
1	A	312	ASP	4.1
1	D	5	HIS	3.8
1	D	350	TRP	3.8
1	A	315	GLY	3.7
1	B	5	HIS	3.6
1	B	314	VAL	3.4
1	C	352	TRP	3.4
1	B	313	GLY	3.3
1	C	350	TRP	3.2
1	C	311	PRO	3.1
1	A	311	PRO	3.0
1	D	310	PRO	2.9
1	B	311	PRO	2.8
1	A	5	HIS	2.7
1	C	310	PRO	2.7
1	C	315	GLY	2.7
1	D	330	SER	2.5
1	A	389	PRO	2.4
1	C	384	PHE	2.2
1	B	349[A]	ASN	2.1
1	B	310	PRO	2.0

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

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

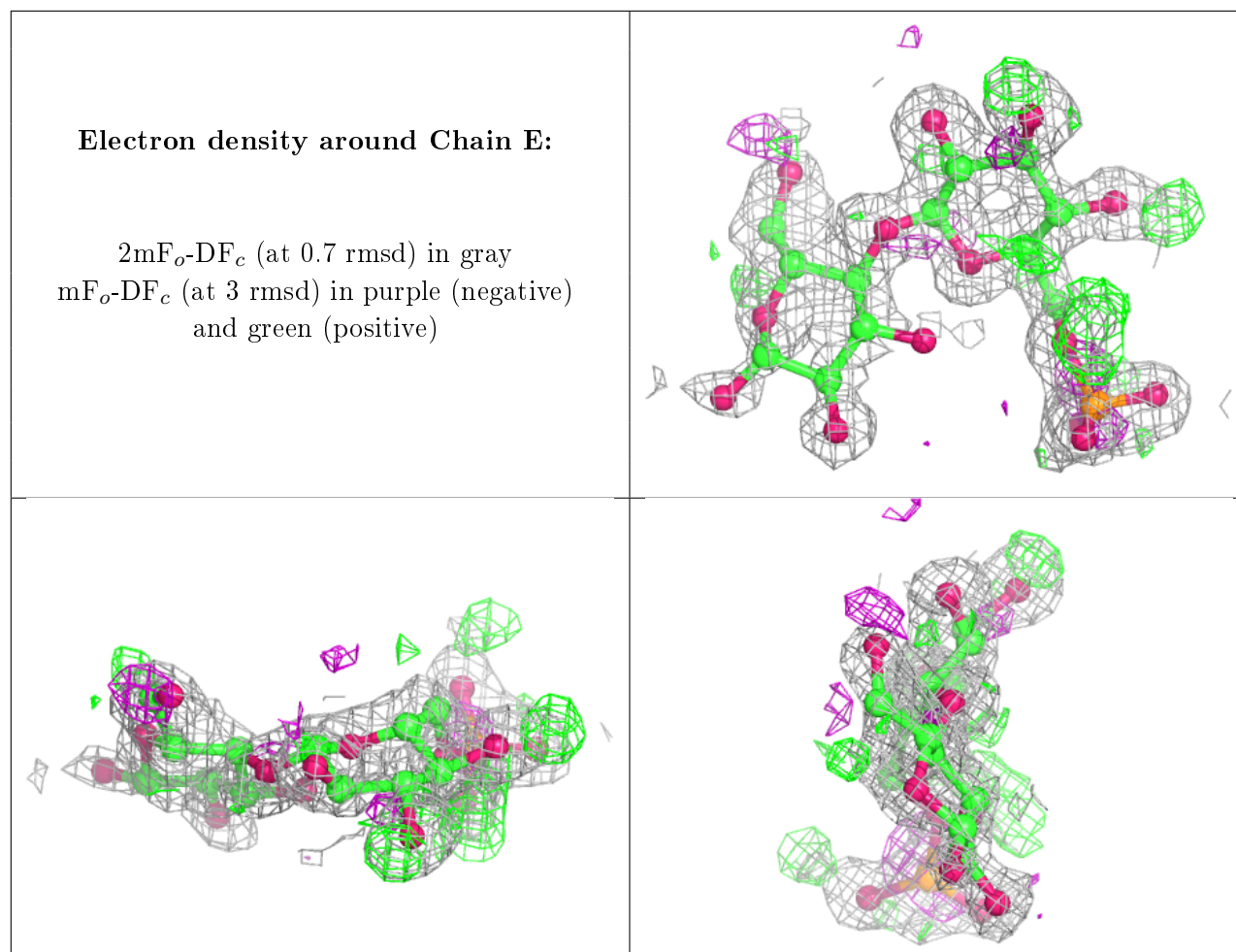
## 6.3 Carbohydrates ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
2	BGC	E	1	12/12	0.80	0.23	21,36,42,50	12
2	0WK	E	2	15/15	0.87	0.14	10,17,23,27	15

The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.





## 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
7	BGC	C	507	12/12	0.70	0.27	24,42,54,60	12
4	GOL	D	501	6/6	0.73	0.16	39,40,43,50	0
6	0WK	C	506	15/15	0.78	0.17	10,20,39,42	15
4	GOL	B	503	6/6	0.80	0.13	31,40,44,47	0
5	IMD	D	502	5/5	0.82	0.16	17,21,23,25	5
4	GOL	C	503	6/6	0.82	0.15	30,38,43,54	0
4	GOL	A	505	6/6	0.82	0.15	31,42,49,50	0
3	BG6	B	501	16/16	0.84	0.20	9,26,41,43	16
5	IMD	A	507	5/5	0.84	0.16	25,28,32,32	0
4	GOL	A	502	6/6	0.85	0.10	36,36,40,42	0
3	BG6	A	501	16/16	0.85	0.18	8,28,41,44	16

*Continued on next page...*

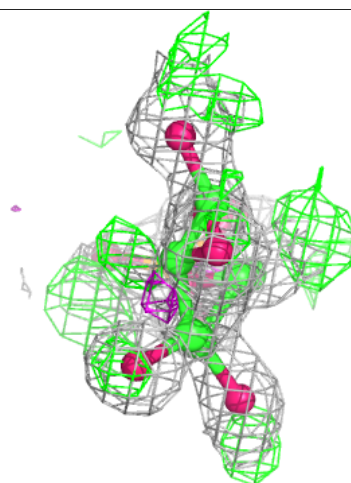
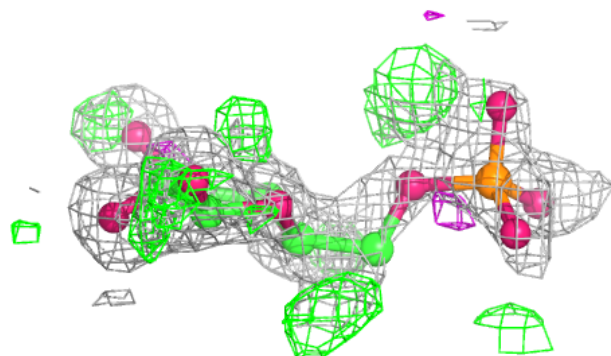
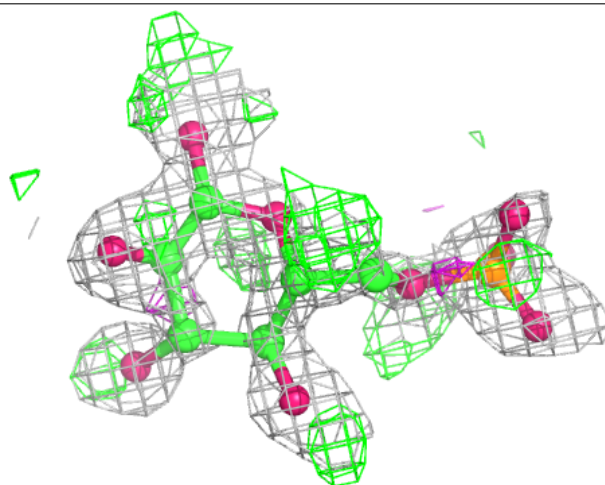
*Continued from previous page...*

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
4	GOL	C	504	6/6	0.85	0.25	37,44,46,59	0
5	IMD	C	505	5/5	0.89	0.18	23,29,30,32	0
4	GOL	B	502	6/6	0.90	0.12	25,41,43,46	0
4	GOL	A	506	6/6	0.93	0.15	36,40,44,45	0
4	GOL	A	504	6/6	0.94	0.12	13,19,24,26	0
4	GOL	C	502	6/6	0.94	0.10	15,18,21,26	0
4	GOL	C	501	6/6	0.95	0.12	13,17,24,27	0
4	GOL	A	503	6/6	0.96	0.09	14,19,23,27	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.

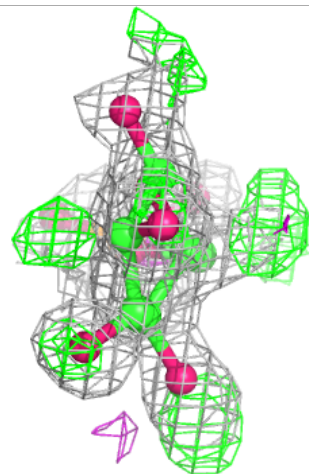
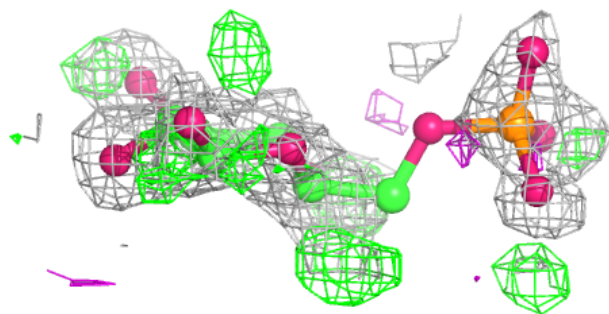
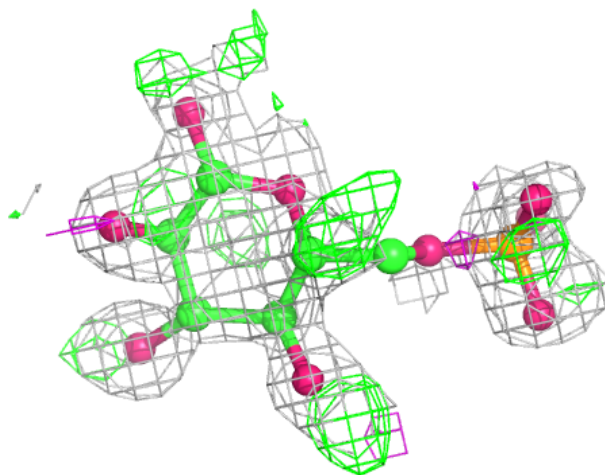
**Electron density around BG6 B 501:**

2mF<sub>o</sub>-DF<sub>c</sub> (at 0.7 rmsd) in gray  
mF<sub>o</sub>-DF<sub>c</sub> (at 3 rmsd) in purple (negative)  
and green (positive)



**Electron density around BG6 A 501:**

$2mF_o-DF_c$  (at 0.7 rmsd) in gray  
 $mF_o-DF_c$  (at 3 rmsd) in purple (negative)  
and green (positive)



## 6.5 Other polymers [i](#)

There are no such residues in this entry.