



# Full wwPDB X-ray Structure Validation Report ⓘ

Nov 9, 2024 – 12:19 PM EST

PDB ID : 6DFX  
Title : human diabetogenic TCR T1D3 in complex with DQ8-p8E9E peptide  
Authors : Wang, Y.; Dai, S.  
Deposited on : 2018-05-15  
Resolution : 2.03 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:

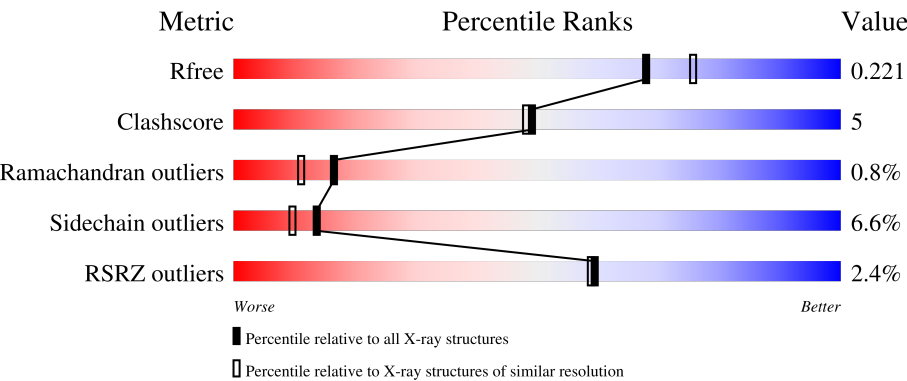
MolProbity : 4.02b-467  
Mogul : 2022.3.0, CSD as543be (2022)  
Xtriage (Phenix) : 1.20.1  
EDS : 3.0  
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)  
CCP4 : 9.0.003 (Gargrove)  
Density-Fitness : 1.0.11  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.39

# 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 2.03 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R <sub>free</sub>	164625	12358 (2.04-2.00)
Clashscore	180529	13897 (2.04-2.00)
Ramachandran outliers	177936	13770 (2.04-2.00)
Sidechain outliers	177891	13769 (2.04-2.00)
RSRZ outliers	164620	12358 (2.04-2.00)

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	188	<div><div>2%</div><div><div></div><div></div><div></div><div></div></div><div>81%13%..</div></div>
1	D	188	<div><div>%</div><div><div></div><div></div><div></div><div></div></div><div>85%10%..</div></div>
2	B	221	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>71%16%.10%</div></div>
2	E	221	<div><div>3%</div><div><div></div><div></div><div></div><div></div></div><div>67%19%..10%</div></div>
3	G	207	<div><div>4%</div><div><div></div><div></div><div></div><div></div></div><div>71%16%5%.6%</div></div>

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Mol	Chain	Length	Quality of chain
3	I	207	<div><div></div><div>3%</div><div>67%</div><div>19%</div><div>• •</div><div>9%</div></div>
4	H	238	<div><div></div><div>%</div><div>78%</div><div>17%</div><div>•</div></div>
4	J	238	<div><div></div><div>%</div><div>79%</div><div>15%</div><div>• •</div></div>
5	C	2	<div><div></div><div>100%</div></div>

## 2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 13693 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 MHC class II HLA-DQ-alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	180	Total	C	N	O	S	0	0	0
			1455	937	239	276	3			
1	D	180	Total	C	N	O	S	0	0	0
			1455	937	239	276	3			

There are 14 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	72	CYS	ILE	conflict	UNP Q30069
A	182	GLY	-	expression tag	UNP Q30069
A	183	GLY	-	expression tag	UNP Q30069
A	184	LEU	-	expression tag	UNP Q30069
A	185	VAL	-	expression tag	UNP Q30069
A	186	PRO	-	expression tag	UNP Q30069
A	187	ARG	-	expression tag	UNP Q30069
D	72	CYS	ILE	conflict	UNP Q30069
D	182	GLY	-	expression tag	UNP Q30069
D	183	GLY	-	expression tag	UNP Q30069
D	184	LEU	-	expression tag	UNP Q30069
D	185	VAL	-	expression tag	UNP Q30069
D	186	PRO	-	expression tag	UNP Q30069
D	187	ARG	-	expression tag	UNP Q30069

- Molecule 2 is a protein called MHC class II antigen.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	200	Total	C	N	O	S	0	0	0
			1623	1025	283	307	8			
2	E	199	Total	C	N	O	S	0	0	0
			1610	1018	277	307	8			

There are 64 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	-27	VAL	-	expression tag	UNP U3PYM0
B	-26	GLU	-	expression tag	UNP U3PYM0
B	-25	GLU	-	expression tag	UNP U3PYM0
B	-24	LEU	-	expression tag	UNP U3PYM0
B	-23	TYR	-	expression tag	UNP U3PYM0
B	-22	LEU	-	expression tag	UNP U3PYM0
B	-21	VAL	-	expression tag	UNP U3PYM0
B	-20	ALA	-	expression tag	UNP U3PYM0
B	-19	GLY	-	expression tag	UNP U3PYM0
B	-18	GLU	-	expression tag	UNP U3PYM0
B	-17	GLU	-	expression tag	UNP U3PYM0
B	-16	GLY	-	expression tag	UNP U3PYM0
B	-15	CYS	-	expression tag	UNP U3PYM0
B	-14	GLY	-	expression tag	UNP U3PYM0
B	-13	GLY	-	expression tag	UNP U3PYM0
B	-12	GLY	-	expression tag	UNP U3PYM0
B	-11	GLY	-	expression tag	UNP U3PYM0
B	-10	SER	-	expression tag	UNP U3PYM0
B	-9	LEU	-	expression tag	UNP U3PYM0
B	-4	VAL	-	expression tag	UNP U3PYM0
B	-3	GLY	-	expression tag	UNP U3PYM0
B	-2	GLY	-	expression tag	UNP U3PYM0
B	-1	SER	-	expression tag	UNP U3PYM0
B	0	GLY	-	expression tag	UNP U3PYM0
B	1	GLY	-	expression tag	UNP U3PYM0
B	2	GLY	-	expression tag	UNP U3PYM0
B	192	GLY	-	expression tag	UNP U3PYM0
B	193	GLY	-	expression tag	UNP U3PYM0
B	194	LEU	-	expression tag	UNP U3PYM0
B	195	VAL	-	expression tag	UNP U3PYM0
B	196	PRO	-	expression tag	UNP U3PYM0
B	197	ARG	-	expression tag	UNP U3PYM0
E	-27	VAL	-	expression tag	UNP U3PYM0
E	-26	GLU	-	expression tag	UNP U3PYM0
E	-25	GLU	-	expression tag	UNP U3PYM0
E	-24	LEU	-	expression tag	UNP U3PYM0
E	-23	TYR	-	expression tag	UNP U3PYM0
E	-22	LEU	-	expression tag	UNP U3PYM0
E	-21	VAL	-	expression tag	UNP U3PYM0
E	-20	ALA	-	expression tag	UNP U3PYM0
E	-19	GLY	-	expression tag	UNP U3PYM0
E	-18	GLU	-	expression tag	UNP U3PYM0
E	-17	GLU	-	expression tag	UNP U3PYM0

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Chain	Residue	Modelled	Actual	Comment	Reference
E	-16	GLY	-	expression tag	UNP U3PYM0
E	-15	CYS	-	expression tag	UNP U3PYM0
E	-14	GLY	-	expression tag	UNP U3PYM0
E	-13	GLY	-	expression tag	UNP U3PYM0
E	-12	GLY	-	expression tag	UNP U3PYM0
E	-11	GLY	-	expression tag	UNP U3PYM0
E	-10	SER	-	expression tag	UNP U3PYM0
E	-9	LEU	-	expression tag	UNP U3PYM0
E	-4	VAL	-	expression tag	UNP U3PYM0
E	-3	GLY	-	expression tag	UNP U3PYM0
E	-2	GLY	-	expression tag	UNP U3PYM0
E	-1	SER	-	expression tag	UNP U3PYM0
E	0	GLY	-	expression tag	UNP U3PYM0
E	1	GLY	-	expression tag	UNP U3PYM0
E	2	GLY	-	expression tag	UNP U3PYM0
E	192	GLY	-	expression tag	UNP U3PYM0
E	193	GLY	-	expression tag	UNP U3PYM0
E	194	LEU	-	expression tag	UNP U3PYM0
E	195	VAL	-	expression tag	UNP U3PYM0
E	196	PRO	-	expression tag	UNP U3PYM0
E	197	ARG	-	expression tag	UNP U3PYM0

- Molecule 3 is a protein called T1D3 alpha chain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	G	194	Total	C	N	O	S	0	0	0
			1506	928	264	306	8			
3	I	188	Total	C	N	O	S	0	0	0
			1453	899	253	293	8			

- Molecule 4 is a protein called T1D3 beta chain.

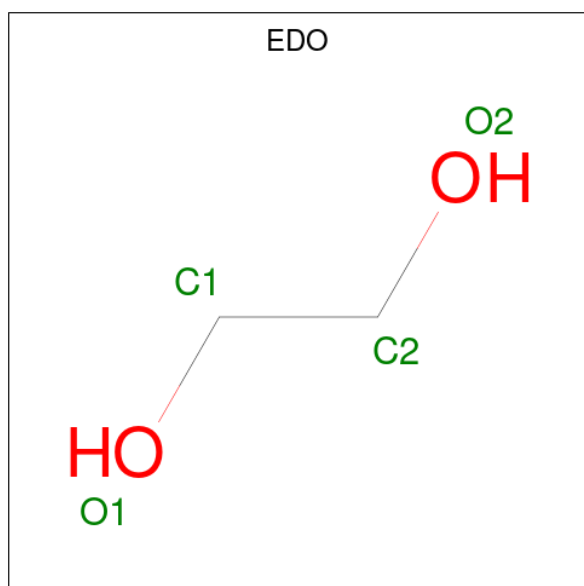
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	237	Total	C	N	O	S	0	0	0
			1885	1187	331	360	7			
4	J	237	Total	C	N	O	S	0	0	0
			1885	1187	331	360	7			

- Molecule 5 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula:  $C_2H_6O_2$ ).



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

- Molecule 7 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).



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

- Molecule 8 is water.

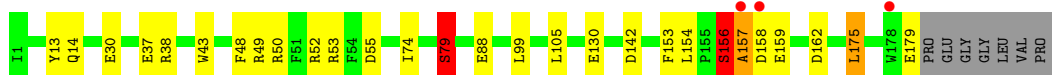
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	116	Total	O	0	0
			116	116		
8	B	146	Total	O	0	0
			146	146		
8	D	96	Total	O	0	0
			96	96		
8	E	84	Total	O	0	0
			84	84		
8	G	57	Total	O	0	0
			57	57		
8	H	131	Total	O	0	0
			131	131		
8	I	46	Total	O	0	0
			46	46		
8	J	99	Total	O	0	0
			99	99		



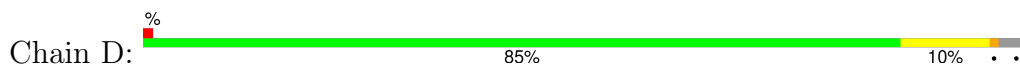
### 3 Residue-property plots [i](#)

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: MHC class II HLA-DQ-alpha chain

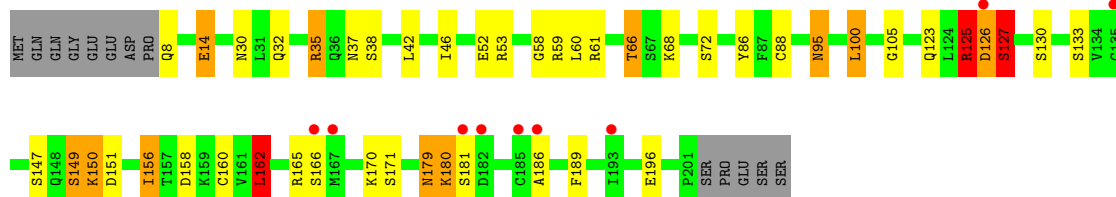


- Molecule 1: MHC class II HLA-DQ-alpha chain

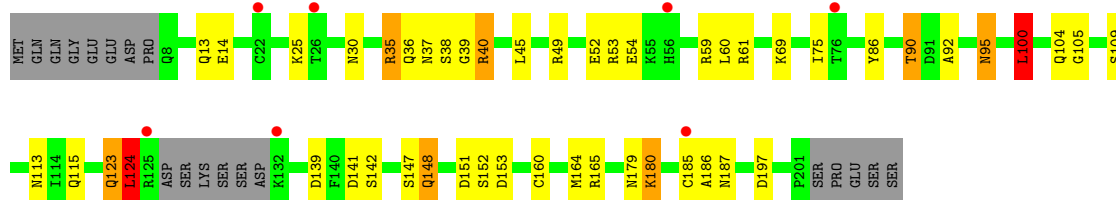


- Molecule 2: MHC class II antigen

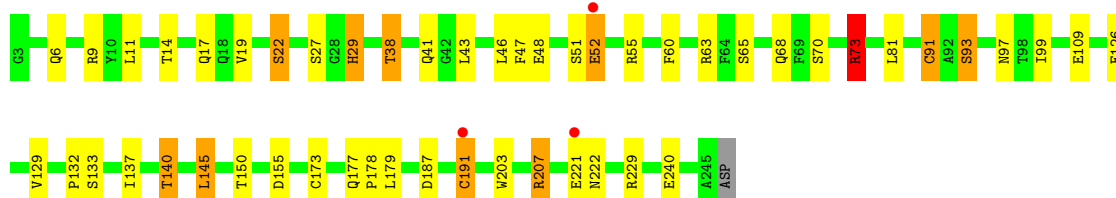
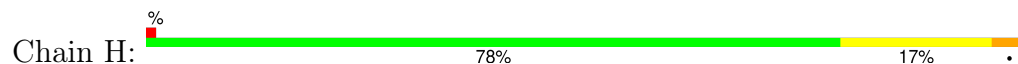




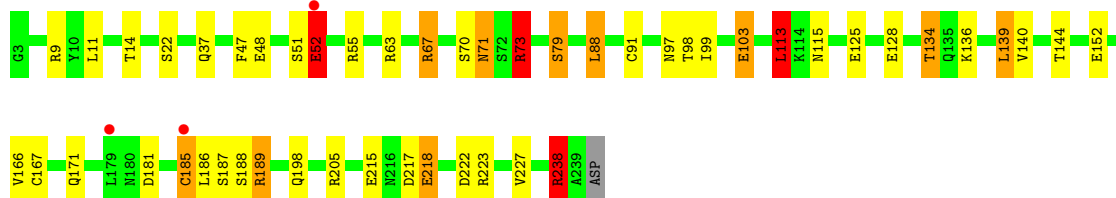
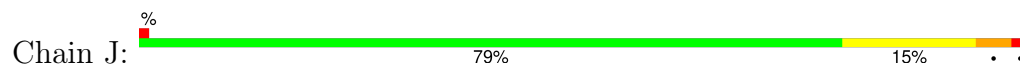
• Molecule 3: T1D3 alpha chain



• Molecule 4: T1D3 beta chain



• Molecule 4: T1D3 beta chain



• Molecule 5: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	111.70Å 88.90Å 116.78Å 90.00° 104.26° 90.00°	Depositor
Resolution (Å)	50.01 – 2.03 50.01 – 2.03	Depositor EDS
% Data completeness (in resolution range)	99.2 (50.01-2.03) 99.4 (50.01-2.03)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.58 (at 2.03Å)	Xtriage
Refinement program	REFMAC 5.8.0135	Depositor
R, $R_{free}$	0.181 , 0.217 0.189 , 0.221	Depositor DCC
$R_{free}$ test set	7235 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	40.5	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.33 , 39.1	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.49$ , $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.016 for l,-k,h	Xtriage
$F_o, F_c$ correlation	0.96	EDS
Total number of atoms	13693	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 11.62% of the height of the origin peak. No significant pseudotranslation is detected.*

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

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

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, NAG

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	1.46	13/1498 (0.9%)	1.23	11/2044 (0.5%)
1	D	1.30	3/1498 (0.2%)	1.16	3/2044 (0.1%)
2	B	1.53	16/1660 (1.0%)	1.35	18/2257 (0.8%)
2	E	1.45	11/1647 (0.7%)	1.46	25/2242 (1.1%)
3	G	1.41	11/1531 (0.7%)	1.32	14/2068 (0.7%)
3	I	1.25	6/1477 (0.4%)	1.31	17/1997 (0.9%)
4	H	1.49	13/1937 (0.7%)	1.29	18/2635 (0.7%)
4	J	1.43	14/1937 (0.7%)	1.27	23/2635 (0.9%)
All	All	1.42	87/13185 (0.7%)	1.30	129/17922 (0.7%)

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
2	E	0	6
3	G	0	3
3	I	0	2
All	All	0	11

All (87) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	103	GLU	CD-OE1	13.44	1.40	1.25
4	H	126	GLU	CD-OE2	13.20	1.40	1.25
2	B	74	GLU	CD-OE1	11.38	1.38	1.25
2	E	74	GLU	CD-OE2	9.76	1.36	1.25
4	H	191	CYS	CB-SG	-9.71	1.65	1.82
4	J	103	GLU	CG-CD	8.99	1.65	1.51
3	G	52	GLU	CD-OE2	8.99	1.35	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	52	GLU	CD-OE1	8.95	1.35	1.25
4	H	126	GLU	CG-CD	8.84	1.65	1.51
1	A	37	GLU	CD-OE2	8.71	1.35	1.25
4	J	103	GLU	CD-OE2	8.52	1.35	1.25
3	G	88	CYS	CB-SG	-8.18	1.68	1.82
1	A	88	GLU	CD-OE1	7.94	1.34	1.25
2	E	22	GLU	CG-CD	7.78	1.63	1.51
3	I	54	GLU	CG-CD	7.66	1.63	1.51
2	E	-26	GLU	CD-OE2	7.50	1.33	1.25
2	B	-23	TYR	CE2-CZ	-7.42	1.28	1.38
2	B	5	GLU	CG-CD	7.37	1.63	1.51
2	B	86	GLU	CD-OE2	7.36	1.33	1.25
2	E	69	GLU	CD-OE2	7.35	1.33	1.25
2	E	69	GLU	CG-CD	7.26	1.62	1.51
4	J	79	SER	CB-OG	-7.25	1.32	1.42
4	J	22	SER	CB-OG	7.21	1.51	1.42
4	H	52	GLU	CB-CG	7.05	1.65	1.52
4	J	48	GLU	CG-CD	6.98	1.62	1.51
1	A	37	GLU	CG-CD	6.97	1.62	1.51
2	B	-26	GLU	CD-OE1	6.94	1.33	1.25
3	I	52	GLU	CG-CD	6.83	1.62	1.51
2	B	69	GLU	CD-OE2	6.80	1.33	1.25
2	B	74	GLU	CG-CD	6.67	1.61	1.51
1	D	88	GLU	CD-OE2	6.60	1.32	1.25
4	H	65	SER	CB-OG	6.55	1.50	1.42
4	H	109	GLU	CG-CD	6.54	1.61	1.51
4	H	109	GLU	CD-OE1	6.53	1.32	1.25
3	G	126	ASP	N-CA	6.50	1.59	1.46
2	B	-26	GLU	CD-OE2	6.47	1.32	1.25
2	B	187	GLU	CD-OE2	6.46	1.32	1.25
4	J	185	CYS	CB-SG	-6.43	1.71	1.82
2	E	74	GLU	CG-CD	6.38	1.61	1.51
1	A	88	GLU	CD-OE2	6.37	1.32	1.25
2	E	-25	GLU	CD-OE1	6.34	1.32	1.25
1	A	156	SER	CB-OG	6.34	1.50	1.42
2	E	149	ARG	CD-NE	-6.33	1.35	1.46
2	E	94	ARG	CG-CD	-6.24	1.36	1.51
1	A	55	ASP	CB-CG	6.21	1.64	1.51
4	H	187	ASP	CB-CG	6.16	1.64	1.51
4	H	48	GLU	CG-CD	6.09	1.61	1.51
1	A	179	GLU	N-CA	6.08	1.58	1.46
3	I	109	SER	CB-OG	-6.07	1.34	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	52	GLU	CD-OE2	6.06	1.32	1.25
4	J	215	GLU	CG-CD	6.00	1.60	1.51
2	B	74	GLU	CD-OE2	5.91	1.32	1.25
3	G	160	CYS	CB-SG	-5.89	1.72	1.81
2	B	22	GLU	CG-CD	5.88	1.60	1.51
2	B	131	TRP	CB-CG	-5.88	1.39	1.50
3	G	14	GLU	CG-CD	5.84	1.60	1.51
2	B	-26	GLU	CG-CD	5.81	1.60	1.51
3	G	14	GLU	CD-OE1	5.78	1.32	1.25
1	A	30	GLU	CD-OE1	-5.75	1.19	1.25
1	A	88	GLU	CG-CD	5.75	1.60	1.51
2	E	92	GLN	CG-CD	-5.72	1.37	1.51
4	H	93	SER	CB-OG	-5.71	1.34	1.42
1	D	40	GLU	CD-OE2	5.70	1.31	1.25
1	A	30	GLU	CD-OE2	5.68	1.31	1.25
2	E	86	GLU	CD-OE2	5.66	1.31	1.25
1	A	179	GLU	CG-CD	5.58	1.60	1.51
2	B	-18	GLU	CG-CD	5.57	1.60	1.51
4	H	240	GLU	CG-CD	5.57	1.60	1.51
3	G	58	GLY	C-O	-5.53	1.14	1.23
3	G	133	SER	CB-OG	-5.48	1.35	1.42
4	J	128	GLU	CD-OE2	5.46	1.31	1.25
4	H	109	GLU	CD-OE2	5.46	1.31	1.25
4	J	70	SER	C-O	-5.45	1.12	1.23
3	G	72	SER	CB-OG	-5.40	1.35	1.42
1	D	179	GLU	N-CA	5.37	1.57	1.46
1	A	13	TYR	CZ-OH	-5.36	1.28	1.37
3	G	66	THR	CB-CG2	-5.29	1.34	1.52
1	A	79	SER	CB-OG	5.29	1.49	1.42
4	J	218	GLU	CG-CD	5.25	1.59	1.51
4	J	52	GLU	CD-OE1	5.25	1.31	1.25
4	J	152	GLU	CD-OE2	5.22	1.31	1.25
2	B	-10	SER	N-CA	5.20	1.56	1.46
4	H	48	GLU	CD-OE1	-5.15	1.20	1.25
3	I	14	GLU	CD-OE1	5.11	1.31	1.25
4	J	205	ARG	CZ-NH1	5.07	1.39	1.33
3	I	142	SER	CB-OG	5.03	1.48	1.42
2	B	69	GLU	CD-OE1	5.01	1.31	1.25

All (129) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	149	ARG	NE-CZ-NH1	-15.50	112.55	120.30
3	I	165	ARG	NE-CZ-NH2	14.08	127.34	120.30
2	E	149	ARG	NE-CZ-NH2	13.92	127.26	120.30
2	E	34	ARG	NE-CZ-NH2	-12.97	113.81	120.30
3	G	61	ARG	NE-CZ-NH1	11.07	125.84	120.30
3	I	165	ARG	NE-CZ-NH1	-10.49	115.05	120.30
2	B	149	ARG	NE-CZ-NH1	-10.18	115.21	120.30
2	B	149	ARG	NE-CZ-NH2	10.12	125.36	120.30
4	J	205	ARG	NE-CZ-NH1	9.95	125.28	120.30
2	B	34	ARG	NE-CZ-NH2	-9.93	115.33	120.30
1	A	142	ASP	CB-CG-OD1	9.84	127.15	118.30
2	B	130	ARG	NE-CZ-NH2	9.53	125.06	120.30
4	H	173	CYS	CA-CB-SG	-9.39	97.09	114.00
2	E	149	ARG	CG-CD-NE	-8.77	93.38	111.80
3	G	162	LEU	CA-CB-CG	8.71	135.33	115.30
4	H	229	ARG	NE-CZ-NH1	8.18	124.39	120.30
4	H	191	CYS	CA-CB-SG	-7.98	99.63	114.00
4	J	139	LEU	CA-CB-CG	7.96	133.60	115.30
4	H	145	LEU	CA-CB-CG	7.92	133.51	115.30
4	H	191	CYS	CB-CA-C	-7.89	94.61	110.40
2	E	149	ARG	CD-NE-CZ	7.77	134.48	123.60
2	B	34	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	A	50	ARG	NE-CZ-NH1	7.61	124.11	120.30
2	E	34	ARG	NE-CZ-NH1	7.61	124.10	120.30
4	J	217	ASP	CB-CG-OD2	7.59	125.13	118.30
1	D	142	ASP	CB-CG-OD1	7.57	125.11	118.30
3	I	59	ARG	NE-CZ-NH2	7.55	124.08	120.30
2	E	22	GLU	OE1-CD-OE2	-7.55	114.24	123.30
3	G	127	SER	N-CA-CB	7.50	121.76	110.50
4	H	73	ARG	NE-CZ-NH2	-7.48	116.56	120.30
3	I	35	ARG	N-CA-CB	-7.47	97.15	110.60
2	E	189	ARG	NE-CZ-NH2	7.36	123.98	120.30
1	A	38	ARG	NE-CZ-NH1	7.31	123.95	120.30
4	H	55	ARG	NE-CZ-NH1	7.10	123.85	120.30
4	H	187	ASP	CB-CG-OD1	7.08	124.67	118.30
3	G	59	ARG	NE-CZ-NH2	6.99	123.80	120.30
3	G	100	LEU	CB-CG-CD1	6.98	122.87	111.00
4	H	63	ARG	NE-CZ-NH2	6.96	123.78	120.30
2	B	133	ARG	NE-CZ-NH1	6.89	123.75	120.30
2	E	161	LEU	CA-CB-CG	6.78	130.89	115.30
2	E	94	ARG	NE-CZ-NH2	-6.72	116.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	91	CYS	CA-CB-SG	-6.71	101.93	114.00
3	I	35	ARG	CG-CD-NE	-6.69	97.74	111.80
2	B	41	ASP	CB-CG-OD1	6.69	124.32	118.30
2	E	-9	LEU	CB-CG-CD1	-6.68	99.65	111.00
4	J	217	ASP	CB-CG-OD1	-6.67	112.30	118.30
2	E	39	ARG	NE-CZ-NH1	6.67	123.63	120.30
3	I	35	ARG	NE-CZ-NH2	-6.64	116.98	120.30
3	G	53	ARG	NE-CZ-NH2	-6.63	116.98	120.30
4	J	55	ARG	NE-CZ-NH1	6.61	123.60	120.30
2	B	-15	CYS	CA-CB-SG	-6.55	102.20	114.00
3	I	164	MET	CG-SD-CE	6.48	110.57	100.20
4	J	91	CYS	CA-CB-SG	-6.48	102.34	114.00
4	J	223	ARG	NE-CZ-NH1	6.48	123.54	120.30
2	E	48	ARG	NE-CZ-NH2	6.47	123.53	120.30
4	J	181	ASP	N-CA-CB	-6.41	99.06	110.60
3	I	100	LEU	CB-CG-CD1	6.36	121.81	111.00
1	A	179	GLU	OE1-CD-OE2	-6.32	115.71	123.30
2	B	43	ASP	CB-CG-OD2	-6.28	112.65	118.30
4	J	238	ARG	NE-CZ-NH1	6.26	123.43	120.30
3	G	53	ARG	CG-CD-NE	-6.24	98.69	111.80
3	I	39	GLY	N-CA-C	-6.23	97.52	113.10
1	A	156	SER	N-CA-CB	6.17	119.76	110.50
1	A	162	ASP	CB-CG-OD2	6.16	123.85	118.30
3	G	88	CYS	N-CA-CB	-6.13	99.56	110.60
2	E	34	ARG	CG-CD-NE	-6.10	98.99	111.80
2	E	94	ARG	NE-CZ-NH1	6.05	123.33	120.30
4	J	73	ARG	NE-CZ-NH2	-6.02	117.29	120.30
3	G	53	ARG	NE-CZ-NH1	5.88	123.24	120.30
2	B	39	ARG	NE-CZ-NH2	-5.82	117.39	120.30
4	H	222	ASN	N-CA-CB	-5.73	100.28	110.60
3	I	61	ARG	NE-CZ-NH2	5.73	123.17	120.30
2	E	41	ASP	CB-CG-OD1	5.73	123.45	118.30
4	J	9	ARG	NE-CZ-NH1	-5.69	117.45	120.30
4	J	171	GLN	CB-CA-C	-5.68	99.04	110.40
4	J	166	VAL	CA-CB-CG1	5.67	119.41	110.90
4	J	79	SER	CB-CA-C	-5.64	99.38	110.10
4	H	70	SER	CB-CA-C	-5.62	99.43	110.10
4	H	207	ARG	NE-CZ-NH1	5.58	123.09	120.30
1	A	175	LEU	CA-CB-CG	5.58	128.12	115.30
4	J	198	GLN	CB-CA-C	5.57	121.53	110.40
2	B	6	ASP	CB-CG-OD1	5.56	123.31	118.30
2	B	39	ARG	NE-CZ-NH1	5.54	123.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	6	ASP	CB-CG-OD1	5.51	123.26	118.30
4	J	222	ASP	CB-CG-OD1	5.50	123.25	118.30
1	A	50	ARG	NE-CZ-NH2	-5.50	117.55	120.30
3	G	158	ASP	CB-CG-OD1	5.49	123.24	118.30
3	G	61	ARG	NE-CZ-NH2	-5.48	117.56	120.30
2	E	-9	LEU	CB-CG-CD2	5.47	120.30	111.00
4	H	9	ARG	NE-CZ-NH2	-5.47	117.56	120.30
3	G	35	ARG	NE-CZ-NH1	5.47	123.03	120.30
4	J	88	LEU	CA-CB-CG	5.45	127.84	115.30
1	D	80	THR	N-CA-C	-5.44	96.30	111.00
2	B	160	MET	CA-CB-CG	5.43	122.53	113.30
3	G	162	LEU	CB-CG-CD2	5.41	120.19	111.00
4	J	11	LEU	CB-CG-CD2	-5.41	101.81	111.00
1	A	30	GLU	OE1-CD-OE2	-5.40	116.82	123.30
4	H	179	LEU	CA-CB-CG	5.39	127.70	115.30
4	H	140	THR	N-CA-C	-5.37	96.51	111.00
3	I	40	ARG	NE-CZ-NH1	5.36	122.98	120.30
2	E	43	ASP	CB-CG-OD2	-5.36	113.48	118.30
2	E	94	ARG	CA-CB-CG	-5.36	101.61	113.40
3	I	53	ARG	NE-CZ-NH1	-5.34	117.63	120.30
3	I	139	ASP	CB-CG-OD1	-5.32	113.51	118.30
2	B	-11	GLY	N-CA-C	-5.31	99.82	113.10
4	J	198	GLN	CA-CB-CG	5.29	125.04	113.40
2	E	39	ARG	NE-CZ-NH2	-5.29	117.66	120.30
3	G	52	GLU	CG-CD-OE2	-5.29	107.73	118.30
4	J	63	ARG	N-CA-CB	-5.28	101.09	110.60
2	E	80	ARG	NE-CZ-NH1	-5.28	117.66	120.30
2	E	189	ARG	CD-NE-CZ	5.26	130.97	123.60
2	B	36	GLU	OE1-CD-OE2	-5.24	117.01	123.30
1	D	29	ASP	CB-CG-OD2	-5.24	113.58	118.30
2	B	29	ARG	NE-CZ-NH1	5.21	122.91	120.30
4	H	48	GLU	OE1-CD-OE2	-5.18	117.09	123.30
2	B	22	GLU	OE1-CD-OE2	-5.17	117.09	123.30
3	I	124	LEU	CA-CB-CG	5.16	127.17	115.30
4	J	113	LEU	CB-CG-CD2	5.15	119.75	111.00
3	I	141	ASP	CB-CG-OD1	5.14	122.92	118.30
2	E	6	ASP	CB-CG-OD2	-5.13	113.68	118.30
2	B	121	ASP	CB-CG-OD1	5.13	122.92	118.30
4	J	88	LEU	CB-CG-CD2	5.11	119.69	111.00
3	I	69	LYS	CD-CE-NZ	-5.07	100.03	111.70
2	E	173	CYS	CA-CB-SG	-5.07	104.87	114.00
4	J	67	ARG	NE-CZ-NH2	-5.07	117.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	38	ARG	NE-CZ-NH2	-5.07	117.77	120.30
4	H	99	ILE	C-N-CA	5.05	134.32	121.70
3	I	197	ASP	N-CA-CB	-5.03	101.55	110.60
1	A	179	GLU	CG-CD-OE2	5.02	128.35	118.30

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	E	-14	GLY	Peptide
2	E	149	ARG	Sidechain
2	E	167	ARG	Peptide
2	E	188	TRP	Peptide
2	E	189	ARG	Peptide
2	E	94	ARG	Sidechain
3	G	149	SER	Peptide
3	G	166	SER	Peptide
3	G	181	SER	Peptide
3	I	185	CYS	Peptide
3	I	38	SER	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1455	0	1392	9	0
1	D	1455	0	1392	11	0
2	B	1623	0	1568	16	0
2	E	1610	0	1547	25	0
3	G	1506	0	1450	20	0
3	I	1453	0	1392	22	0
4	H	1885	0	1785	27	0
4	J	1885	0	1786	24	0
5	C	28	0	25	0	0
6	A	4	0	6	0	0
7	D	14	0	13	0	0
8	A	116	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	146	0	0	1	0
8	D	96	0	0	1	0
8	E	84	0	0	2	0
8	G	57	0	0	0	0
8	H	131	0	0	4	0
8	I	46	0	0	0	0
8	J	99	0	0	1	0
All	All	13693	0	12356	132	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 (132) 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)
3:G:126:ASP:HA	3:G:127:SER:HB2	1.24	1.09
3:G:126:ASP:HB3	4:H:129:VAL:O	1.69	0.92
4:J:51:SER:O	4:J:52:GLU:HB2	1.70	0.90
3:G:126:ASP:HA	3:G:127:SER:CB	2.08	0.83
2:E:189:ARG:HB3	2:E:190:ALA:HB3	1.59	0.82
2:E:19:ASN:HB2	8:E:213:HOH:O	1.78	0.82
3:I:36:GLN:HE22	4:J:37:GLN:HE22	1.26	0.81
1:D:53:ARG:HH11	1:D:53:ARG:HB2	1.50	0.77
3:G:35:ARG:HH21	3:G:37:ASN:HD21	1.33	0.76
4:H:51:SER:O	4:H:52:GLU:CB	2.36	0.73
1:A:74:ILE:HG23	1:A:79:SER:HB2	1.70	0.73
3:I:35:ARG:HH21	3:I:37:ASN:HD21	1.37	0.71
3:G:126:ASP:CA	3:G:127:SER:HB2	2.13	0.69
3:G:179:ASN:O	3:G:180:LYS:C	2.34	0.65
1:D:53:ARG:HB2	1:D:53:ARG:NH1	2.12	0.64
2:E:188:TRP:HA	2:E:189:ARG:HB2	1.80	0.63
1:D:53:ARG:HH11	1:D:53:ARG:CB	2.11	0.62
2:E:93:ARG:NH1	8:E:202:HOH:O	2.32	0.61
3:G:14:GLU:OE2	3:G:170:LYS:HE2	1.99	0.61
2:B:19:ASN:ND2	2:B:22:GLU:OE2	2.33	0.61
1:A:99:LEU:HD22	1:A:156:SER:HB3	1.83	0.61
4:H:51:SER:O	4:H:52:GLU:HB2	2.01	0.60
2:E:169:ASP:OD1	3:G:68:LYS:NZ	2.34	0.60
3:G:38:SER:OG	4:H:177:GLN:NE2	2.32	0.60
2:E:189:ARG:CB	2:E:190:ALA:HB3	2.30	0.60
4:H:155:ASP:CG	4:H:178:PRO:HG2	2.21	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:90:THR:HG23	3:I:92:ALA:H	1.67	0.59
4:J:189:ARG:HD3	4:J:189:ARG:N	2.17	0.59
4:J:134:THR:HG22	4:J:136:LYS:H	1.66	0.59
2:B:-15:CYS:CB	2:B:-14:GLY:HA2	2.33	0.58
2:B:177:HIS:HD2	2:B:179:SER:OG	1.86	0.58
4:H:22:SER:HB3	8:H:340:HOH:O	2.04	0.57
4:J:134:THR:CG2	4:J:136:LYS:HB2	2.35	0.57
4:H:38:THR:HG23	4:H:41:GLN:H	1.69	0.57
4:H:11:LEU:HD22	4:H:19:VAL:HG21	1.87	0.57
4:H:14:THR:H	4:H:17:GLN:HE21	1.53	0.56
1:D:98:THR:HB	1:D:101:GLN:HG2	1.87	0.56
2:B:-15:CYS:HB2	2:B:-14:GLY:HA2	1.87	0.55
4:H:73:ARG:HG3	8:H:340:HOH:O	2.06	0.55
2:E:189:ARG:HG2	2:E:190:ALA:HB3	1.89	0.55
3:G:125:ARG:HB3	3:G:127:SER:OG	2.06	0.55
3:I:148:GLN:HA	3:I:148:GLN:OE1	2.07	0.55
2:B:163:MET:HE3	2:B:171:TYR:CE1	2.43	0.54
2:E:189:ARG:HB3	2:E:190:ALA:CB	2.34	0.54
1:A:157:ALA:O	1:A:158:ASP:CB	2.52	0.54
3:I:100:LEU:HD22	4:J:99:ILE:CD1	2.37	0.54
2:B:174:HIS:CE1	2:B:185:ILE:HD12	2.43	0.54
3:I:90:THR:CG2	3:I:92:ALA:H	2.21	0.53
4:H:38:THR:CG2	4:H:41:GLN:H	2.20	0.53
3:I:13:GLN:HB3	3:I:113:ASN:HD21	1.74	0.53
1:D:143:HIS:HD2	2:E:12:LYS:NZ	2.07	0.53
2:E:94:ARG:HH11	2:E:94:ARG:HG3	1.74	0.52
2:E:189:ARG:HH21	2:E:189:ARG:HA	1.74	0.52
4:J:115:ASN:ND2	8:J:302:HOH:O	2.42	0.52
2:B:124:PRO:O	2:B:177:HIS:HE1	1.92	0.52
4:H:29:HIS:HE1	8:H:420:HOH:O	1.93	0.51
4:J:51:SER:O	4:J:52:GLU:CB	2.46	0.51
4:H:52:GLU:H	4:H:68:GLN:HE21	1.58	0.50
4:J:144:THR:HG22	4:J:185:CYS:SG	2.51	0.50
3:G:123:GLN:O	4:H:133:SER:HB2	2.12	0.50
2:B:19:ASN:ND2	8:B:206:HOH:O	2.45	0.49
4:H:150:THR:HG22	4:H:191:CYS:SG	2.53	0.49
2:B:163:MET:CE	2:B:171:TYR:CE1	2.96	0.48
2:B:163:MET:HE3	2:B:171:TYR:CD1	2.47	0.48
4:J:188:SER:C	4:J:189:ARG:HD3	2.32	0.48
4:H:132:PRO:HD2	4:H:203:TRP:CZ2	2.48	0.48
2:E:189:ARG:CG	2:E:190:ALA:HB3	2.43	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:I:100:LEU:HD22	4:J:99:ILE:HD13	1.96	0.48
2:E:133:ARG:NH1	2:E:138:GLU:OE1	2.47	0.48
3:G:126:ASP:CA	3:G:127:SER:CB	2.83	0.48
1:D:35:ASP:OD2	1:D:38:ARG:HD3	2.13	0.48
4:J:187:SER:OG	4:J:189:ARG:NH1	2.46	0.48
3:G:32:GLN:HG3	3:G:46:ILE:O	2.14	0.47
1:A:14:GLN:NE2	2:B:6:ASP:OD2	2.47	0.47
4:J:140:VAL:HG22	4:J:189:ARG:HG3	1.95	0.47
2:E:177:HIS:CD2	2:E:178:PRO:HD2	2.49	0.47
4:H:52:GLU:H	4:H:68:GLN:NE2	2.12	0.47
4:J:134:THR:HG23	4:J:136:LYS:HB2	1.97	0.47
1:A:157:ALA:O	1:A:158:ASP:HB3	2.14	0.47
3:G:162:LEU:HD22	3:G:171:SER:OG	2.15	0.47
4:J:71:ASN:HD21	4:J:73:ARG:HB3	1.80	0.47
2:E:66:GLU:OE2	4:J:98:THR:OG1	2.22	0.46
3:G:86:TYR:O	3:G:105:GLY:HA2	2.15	0.46
3:I:152:SER:O	3:I:153:ASP:CB	2.63	0.46
4:H:137:ILE:O	4:H:140:THR:O	2.34	0.45
3:G:42:LEU:HD12	3:G:42:LEU:N	2.32	0.45
3:I:123:GLN:HG3	3:I:124:LEU:N	2.31	0.45
3:I:49:ARG:NH2	4:J:97:ASN:OD1	2.42	0.45
1:D:79:SER:O	8:D:301:HOH:O	2.21	0.45
4:H:14:THR:H	4:H:17:GLN:NE2	2.15	0.45
3:I:179:ASN:OD1	3:I:179:ASN:N	2.49	0.45
1:A:156:SER:OG	1:A:157:ALA:N	2.48	0.44
1:D:73:VAL:HG13	2:E:53:LEU:HD11	1.99	0.44
3:I:95:ASN:ND2	4:J:97:ASN:HD21	2.16	0.44
2:E:69:GLU:CG	3:I:49:ARG:HE	2.30	0.44
3:I:152:SER:O	3:I:153:ASP:HB2	2.18	0.44
4:J:185:CYS:SG	4:J:186:LEU:N	2.90	0.44
2:E:10:GLN:HB2	2:E:31:ILE:HB	1.99	0.44
4:H:6:GLN:NE2	4:H:91:CYS:H	2.15	0.44
3:G:125:ARG:O	3:G:126:ASP:HB2	2.18	0.44
2:E:174:HIS:CE1	2:E:185:ILE:HD12	2.53	0.44
3:I:35:ARG:HB2	3:I:45:LEU:HD11	1.98	0.44
2:B:-14:GLY:N	2:B:-13:GLY:O	2.51	0.44
4:H:29:HIS:HD2	4:H:93:SER:OG	2.02	0.43
2:E:66:GLU:OE2	4:J:98:THR:CB	2.66	0.43
2:E:117:CYS:HB2	2:E:131:TRP:CZ2	2.53	0.43
3:I:37:ASN:O	3:I:40:ARG:N	2.51	0.43
3:G:156:ILE:CD1	3:G:189:PHE:CE1	3.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:14:GLN:NE2	2:E:6:ASP:OD2	2.51	0.43
4:H:51:SER:O	4:H:52:GLU:HB3	2.14	0.43
2:B:-14:GLY:N	2:B:-13:GLY:C	2.72	0.43
1:A:52:ARG:HH21	2:B:-25:GLU:CD	2.21	0.43
4:J:125:GLU:OE1	4:J:238:ARG:NH1	2.51	0.43
2:E:177:HIS:CG	2:E:178:PRO:HD2	2.54	0.43
4:H:155:ASP:OD2	4:H:178:PRO:HG2	2.19	0.42
4:H:221:GLU:HB3	8:H:423:HOH:O	2.20	0.42
3:I:86:TYR:O	3:I:105:GLY:HA2	2.18	0.42
1:D:53:ARG:HH11	1:D:53:ARG:CG	2.33	0.42
3:I:40:ARG:HD3	4:J:103:GLU:OE1	2.19	0.42
4:H:46:LEU:HD23	4:H:60:PHE:CD1	2.55	0.42
3:I:160:CYS:SG	4:J:167:CYS:CB	3.07	0.42
3:G:95:ASN:ND2	4:H:97:ASN:HD21	2.18	0.42
1:A:105:LEU:HG	1:A:153:PHE:CE1	2.55	0.41
3:G:125:ARG:HD2	3:G:125:ARG:HA	1.84	0.41
4:H:29:HIS:CD2	4:H:93:SER:OG	2.73	0.41
1:A:43:TRP:CE3	1:A:48:PHE:HB3	2.56	0.41
3:I:60:LEU:HD22	3:I:75:ILE:HG12	2.02	0.41
3:I:60:LEU:CD2	3:I:75:ILE:HG12	2.51	0.41
4:J:14:THR:HG23	4:J:113:LEU:HD13	2.02	0.41
1:D:143:HIS:HD2	2:E:12:LYS:HZ2	1.68	0.41
2:B:177:HIS:CD2	2:B:179:SER:H	2.39	0.40
2:B:181:GLN:HA	2:E:94:ARG:O	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	178/188 (95%)	169 (95%)	8 (4%)	1 (1%)	22 16

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	178/188 (95%)	173 (97%)	5 (3%)	0	100	100
2	B	194/221 (88%)	187 (96%)	6 (3%)	1 (0%)	25	20
2	E	193/221 (87%)	182 (94%)	9 (5%)	2 (1%)	13	8
3	G	192/207 (93%)	174 (91%)	12 (6%)	6 (3%)	3	1
3	I	184/207 (89%)	176 (96%)	5 (3%)	3 (2%)	8	3
4	H	235/238 (99%)	228 (97%)	7 (3%)	0	100	100
4	J	235/238 (99%)	226 (96%)	9 (4%)	0	100	100
All	All	1589/1708 (93%)	1515 (95%)	61 (4%)	13 (1%)	16	11

All (13) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	157	ALA
3	G	127	SER
3	G	149	SER
3	G	150	LYS
3	I	180	LYS
3	I	186	ALA
2	B	-14	GLY
3	I	151	ASP
2	E	103	PRO
2	E	189	ARG
3	G	125	ARG
3	G	151	ASP
3	G	186	ALA

### 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	165/171 (96%)	157 (95%)	8 (5%)	21	18
1	D	165/171 (96%)	157 (95%)	8 (5%)	21	18

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B	178/192 (93%)	169 (95%)	9 (5%)	20	16
2	E	177/192 (92%)	161 (91%)	16 (9%)	8	4
3	G	171/183 (93%)	154 (90%)	17 (10%)	6	3
3	I	163/183 (89%)	150 (92%)	13 (8%)	10	6
4	H	207/208 (100%)	197 (95%)	10 (5%)	21	18
4	J	207/208 (100%)	193 (93%)	14 (7%)	13	9
All	All	1433/1508 (95%)	1338 (93%)	95 (7%)	14	10

All (95) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	49	ARG
1	A	53	ARG
1	A	79	SER
1	A	130	GLU
1	A	154	LEU
1	A	156	SER
1	A	159	GLU
1	A	175	LEU
2	B	133	ARG
2	B	139	THR
2	B	143	VAL
2	B	147	LEU
2	B	163	MET
2	B	164	THR
2	B	167	ARG
2	B	187	GLU
2	B	189	ARG
1	D	39	LYS
1	D	53	ARG
1	D	66	LEU
1	D	80	THR
1	D	105	LEU
1	D	128	VAL
1	D	130	GLU
1	D	154	LEU
2	E	-9	LEU
2	E	23	ARG
2	E	68	LEU
2	E	69	GLU

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Mol	Chain	Res	Type
2	E	113	ASN
2	E	126	GLN
2	E	133	ARG
2	E	135	ASP
2	E	136	GLN
2	E	140	THR
2	E	143	VAL
2	E	149	ARG
2	E	161	LEU
2	E	163	MET
2	E	166	GLN
2	E	189	ARG
3	G	8	GLN
3	G	30	ASN
3	G	60	LEU
3	G	66	THR
3	G	95	ASN
3	G	100	LEU
3	G	125	ARG
3	G	127	SER
3	G	130	SER
3	G	147	SER
3	G	150	LYS
3	G	156	ILE
3	G	162	LEU
3	G	165	ARG
3	G	179	ASN
3	G	180	LYS
3	G	196	GLU
4	H	22	SER
4	H	27	SER
4	H	29	HIS
4	H	38	THR
4	H	43	LEU
4	H	47	PHE
4	H	73	ARG
4	H	81	LEU
4	H	145	LEU
4	H	207	ARG
3	I	25	LYS
3	I	30	ASN
3	I	90	THR

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Mol	Chain	Res	Type
3	I	95	ASN
3	I	100	LEU
3	I	104	GLN
3	I	115	GLN
3	I	123	GLN
3	I	124	LEU
3	I	147	SER
3	I	148	GLN
3	I	180	LYS
3	I	187	ASN
4	J	47	PHE
4	J	52	GLU
4	J	67	ARG
4	J	71	ASN
4	J	73	ARG
4	J	79	SER
4	J	88	LEU
4	J	113	LEU
4	J	134	THR
4	J	139	LEU
4	J	189	ARG
4	J	218	GLU
4	J	227	VAL
4	J	238	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	177	HIS
1	D	124	ASN
1	D	143	HIS
2	E	19	ASN
2	E	84	GLN
2	E	92	GLN
2	E	113	ASN
2	E	181	GLN
3	G	13	GLN
3	G	21	ASN
3	G	29	ASN
3	G	30	ASN
3	G	36	GLN
3	G	37	ASN

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Mol	Chain	Res	Type
3	G	95	ASN
3	G	148	GLN
3	G	179	ASN
4	H	6	GLN
4	H	17	GLN
4	H	29	HIS
4	H	37	GLN
4	H	44	GLN
4	H	68	GLN
4	H	177	GLN
4	H	182	GLN
4	H	209	HIS
3	I	29	ASN
3	I	30	ASN
3	I	36	GLN
3	I	37	ASN
3	I	44	HIS
3	I	95	ASN
3	I	113	ASN
4	J	18	GLN
4	J	71	ASN
4	J	77	ASN
4	J	203	HIS
4	J	216	ASN

### 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](#)

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	$\# Z  > 2$
5	NAG	C	1	5,1	14,14,15	1.09	1 (7%)	17,19,21	1.56	6 (35%)
5	NAG	C	2	5	14,14,15	1.62	5 (35%)	17,19,21	2.33	9 (52%)

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
5	NAG	C	1	5,1	-	0/6/23/26	0/1/1/1
5	NAG	C	2	5	-	2/6/23/26	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	2	NAG	C2-N2	2.96	1.51	1.46
5	C	2	NAG	O4-C4	2.81	1.49	1.43
5	C	2	NAG	C1-C2	2.61	1.55	1.52
5	C	1	NAG	C1-C2	2.26	1.55	1.52
5	C	2	NAG	C4-C5	2.08	1.57	1.53
5	C	2	NAG	C4-C3	2.01	1.57	1.52

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	2	NAG	C8-C7-N2	4.59	123.73	116.12
5	C	2	NAG	C4-C3-C2	3.50	116.14	111.02
5	C	2	NAG	O7-C7-C8	-3.22	116.32	122.05
5	C	1	NAG	O5-C1-C2	-3.08	106.52	111.29
5	C	2	NAG	O5-C1-C2	2.78	115.60	111.29
5	C	2	NAG	O6-C6-C5	-2.66	102.26	111.33
5	C	2	NAG	O5-C5-C6	-2.44	102.91	107.66
5	C	1	NAG	C2-N2-C7	2.25	125.92	122.90
5	C	1	NAG	O5-C5-C4	-2.24	105.37	110.83
5	C	1	NAG	C1-C2-N2	-2.23	106.92	110.43
5	C	1	NAG	O6-C6-C5	-2.19	103.89	111.33
5	C	2	NAG	O4-C4-C5	2.14	114.59	109.32
5	C	2	NAG	C1-O5-C5	2.13	115.04	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	1	NAG	C8-C7-N2	-2.07	112.69	116.12
5	C	2	NAG	O3-C3-C2	-2.05	105.13	109.40

There are no chirality outliers.

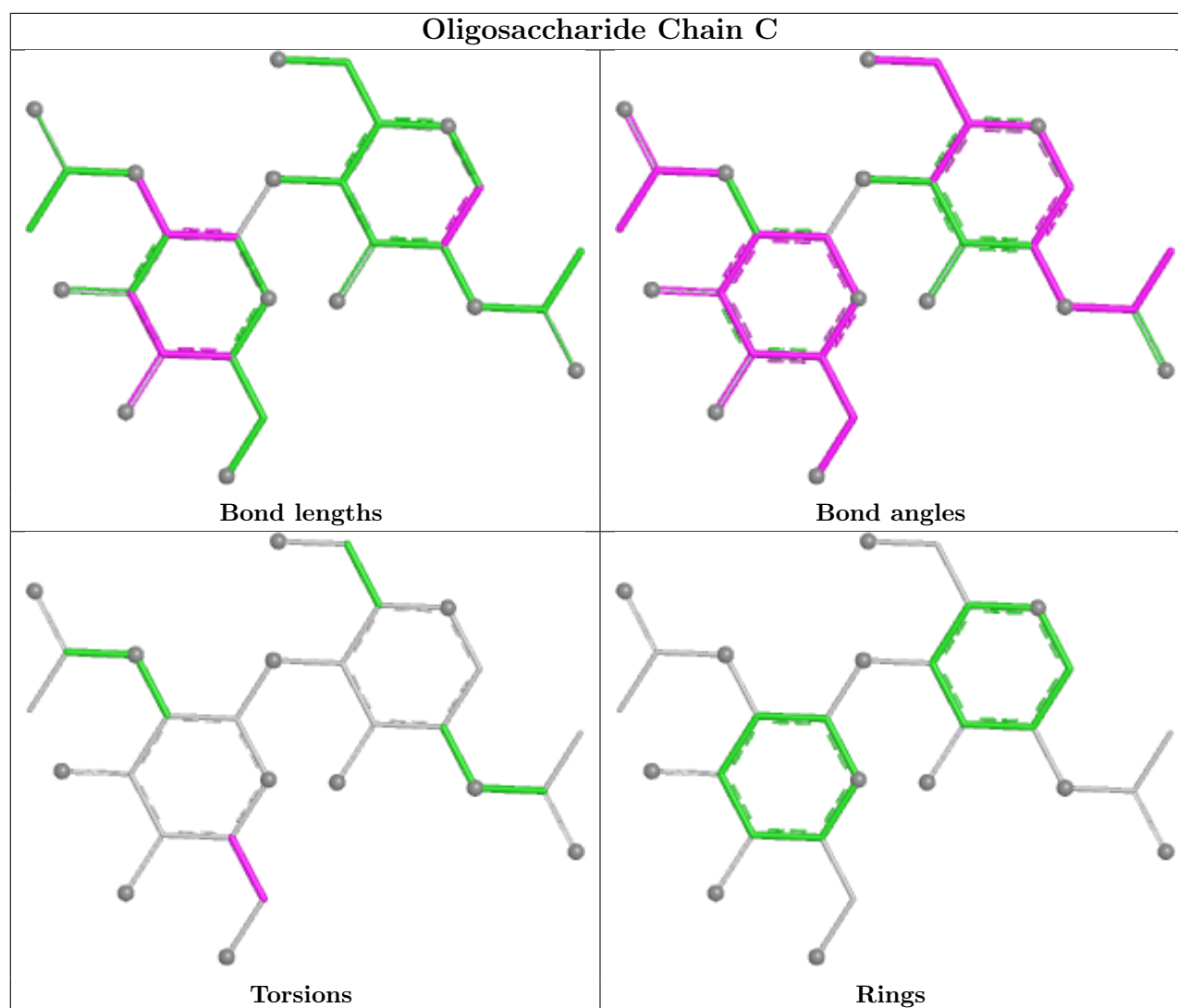
All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	C	2	NAG	O5-C5-C6-O6
5	C	2	NAG	C4-C5-C6-O6

There are no ring outliers.

No monomer is involved in short contacts.

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](#)

2 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	$\# Z  > 2$
7	NAG	D	201	1	14,14,15	2.69	5 (35%)	17,19,21	3.60	8 (47%)
6	EDO	A	203	-	3,3,3	0.79	0	2,2,2	0.47	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
7	NAG	D	201	1	-	0/6/23/26	0/1/1/1
6	EDO	A	203	-	-	1/1/1/1	-

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	D	201	NAG	C3-C2	5.80	1.64	1.52
7	D	201	NAG	O4-C4	4.77	1.54	1.43
7	D	201	NAG	O5-C5	4.69	1.52	1.43
7	D	201	NAG	C1-C2	3.10	1.56	1.52
7	D	201	NAG	C4-C3	2.39	1.58	1.52

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	D	201	NAG	C3-C4-C5	-7.12	97.31	110.23
7	D	201	NAG	O4-C4-C3	6.77	126.33	110.38
7	D	201	NAG	O5-C1-C2	-5.62	102.59	111.29
7	D	201	NAG	C1-C2-N2	-5.49	101.78	110.43
7	D	201	NAG	O3-C3-C4	4.50	120.97	110.38
7	D	201	NAG	O4-C4-C5	3.63	118.27	109.32
7	D	201	NAG	O6-C6-C5	-3.22	100.36	111.33
7	D	201	NAG	C2-N2-C7	2.06	125.67	122.90

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	A	203	EDO	O1-C1-C2-O2

There are no ring outliers.

No monomer is involved in short contacts.

## 5.7 Other polymers ⓘ

There are no such residues in this entry.

## 5.8 Polymer linkage issues ⓘ

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	180/188 (95%)	-0.29	3 (1%) 69 68	25, 40, 71, 82	0
1	D	180/188 (95%)	-0.19	1 (0%) 85 85	31, 44, 71, 87	0
2	B	200/221 (90%)	-0.10	6 (3%) 52 51	26, 39, 86, 109	0
2	E	199/221 (90%)	-0.05	6 (3%) 52 51	32, 45, 78, 96	0
3	G	194/207 (93%)	0.24	9 (4%) 38 37	28, 58, 89, 109	0
3	I	188/207 (90%)	0.40	7 (3%) 45 44	37, 59, 88, 100	0
4	H	237/238 (99%)	-0.20	3 (1%) 74 74	30, 42, 69, 77	0
4	J	237/238 (99%)	-0.18	3 (1%) 74 74	34, 44, 68, 79	0
All	All	1615/1708 (94%)	-0.05	38 (2%) 59 59	25, 46, 80, 109	0

All (38) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	190	ALA	5.1
1	A	157	ALA	4.4
4	J	185	CYS	4.2
2	E	-9	LEU	4.1
2	E	190	ALA	3.6
2	E	-13	GLY	3.5
4	H	191	CYS	3.1
3	I	125	ARG	3.0
1	D	79	SER	2.9
1	A	158	ASP	2.8
3	G	126	ASP	2.8
2	E	-10	SER	2.6
3	I	132	LYS	2.6
3	I	22	CYS	2.6
3	G	181	SER	2.6
1	A	178	TRP	2.6

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Mol	Chain	Res	Type	RSRZ
2	B	168	GLY	2.5
3	G	182	ASP	2.5
4	J	52	GLU	2.5
3	G	185	CYS	2.5
3	I	76	THR	2.5
2	E	167	ARG	2.5
2	B	-9	LEU	2.4
3	I	185	CYS	2.4
3	I	56	HIS	2.4
2	B	-13	GLY	2.3
2	B	-15	CYS	2.3
4	H	52	GLU	2.2
2	B	114	LEU	2.2
3	G	135	CYS	2.2
4	H	221	GLU	2.1
3	I	26	THR	2.1
3	G	167	MET	2.1
3	G	166	SER	2.1
4	J	179	LEU	2.1
3	G	193	ILE	2.1
3	G	186	ALA	2.0
2	E	3	SER	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](#)

SUGAR-RSR INFOmissingINFO

## 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
6	EDO	A	203	4/4	0.71	0.16	61,65,66,67	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors( $\text{\AA}^2$ )	Q<0.9
7	NAG	D	201	14/15	0.82	0.12	47,53,57,58	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.