



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:04 PM UTC

PDB ID : 6DFX / pdb_00006dfx
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

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>.

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

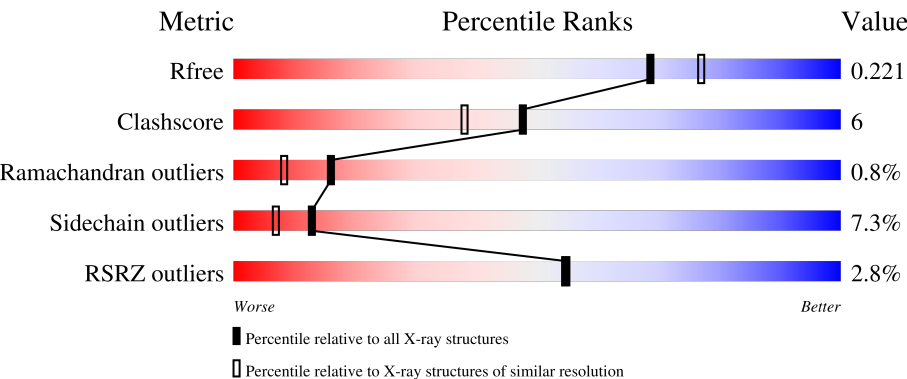
MolProbity : 4-5-2 with Phenix2.0
Mogul : 2022.3.0, CSD as543be (2022)
Xtriage (Phenix) : 2.0
EDS : 3.0
Percentile statistics : 20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4 : 9.0.010 (Gargrove)
Density-Fitness : 1.0.12
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.49

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_{free}	180053	13299 (2.04-2.00)
Clashscore	190562	1022 (2.02-2.02)
Ramachandran outliers	187476	1014 (2.02-2.02)
Sidechain outliers	187428	1014 (2.02-2.02)
RSRZ outliers	180081	13314 (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 ≥ 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	2% 74% 18% • • •
1	D	188	% 77% 17% • •
2	B	221	4% 65% 22% • 10%
2	E	221	3% 63% 22% • • 10%
3	G	207	4% 61% 25% 6% • 6%

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Mol	Chain	Length	Quality of chain
3	I	207	4% 70% 16% • • 9%
4	H	238	2% 73% 22% 5%
4	J	238	% 75% 19% • •
5	C	2	100%

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.

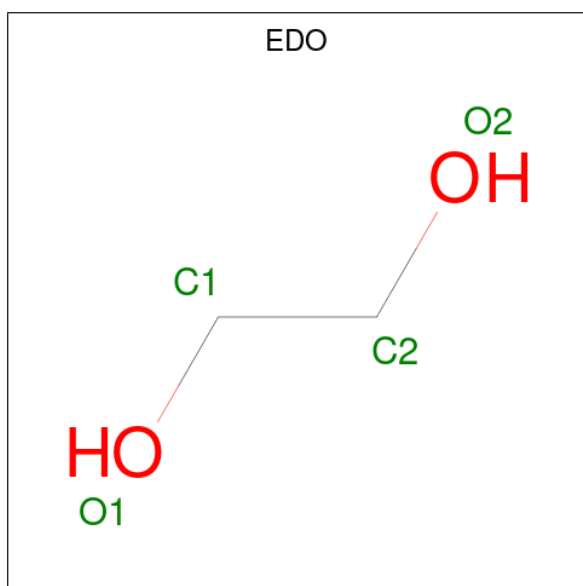
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
4	H	237	Total	C	N	O	S	0	0	0
			1885	1187	331	360	7			
4	J	237	Total	C	N	O	S	0	0	0
			1885	1187	331	360	7			

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



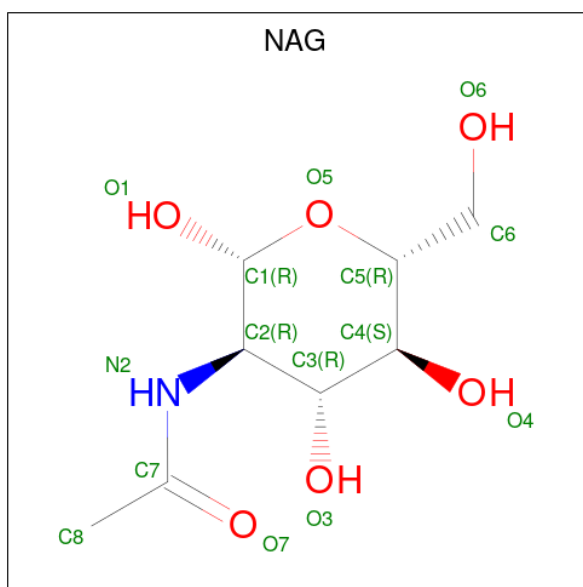
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
5	C	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 6 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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 (CCD ID: NAG) (formula: C₈H₁₅NO₆).



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

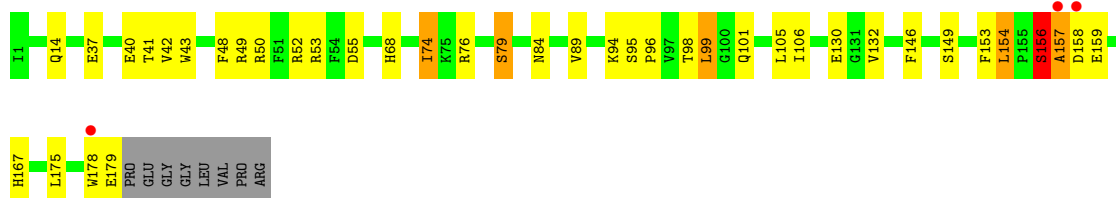
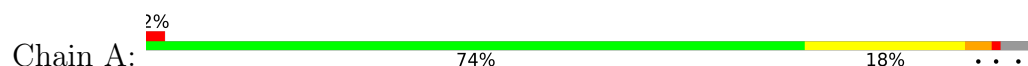
- Molecule 8 is water.

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		

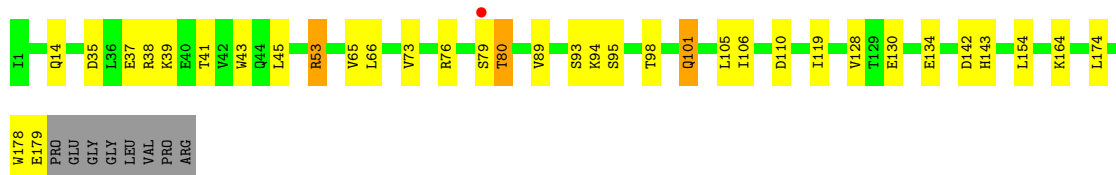
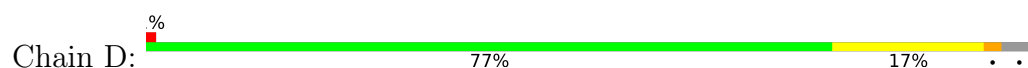
3 Residue-property plots [i](#)

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.

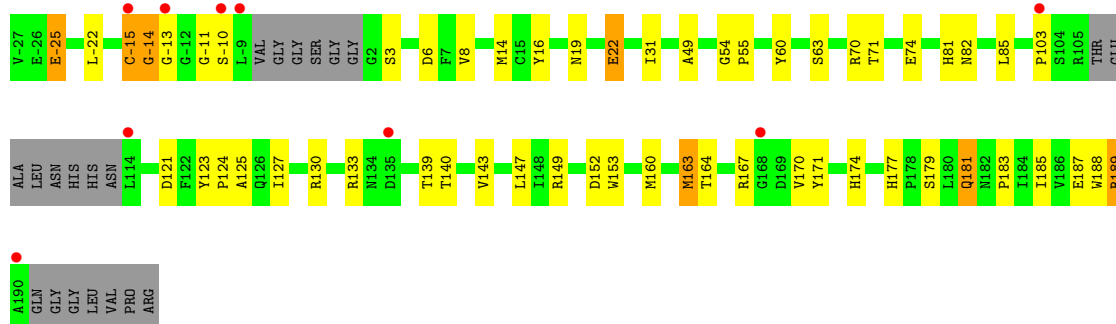
- Molecule 1: MHC class II HLA-DQ-alpha chain



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

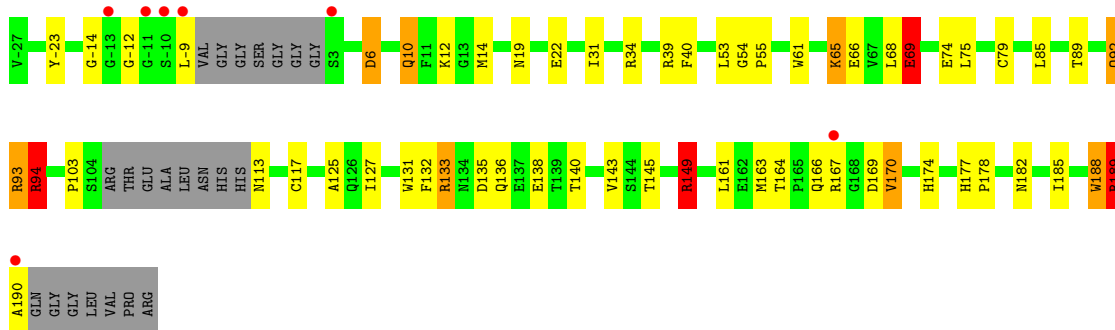


- Molecule 2: MHC class II antigen

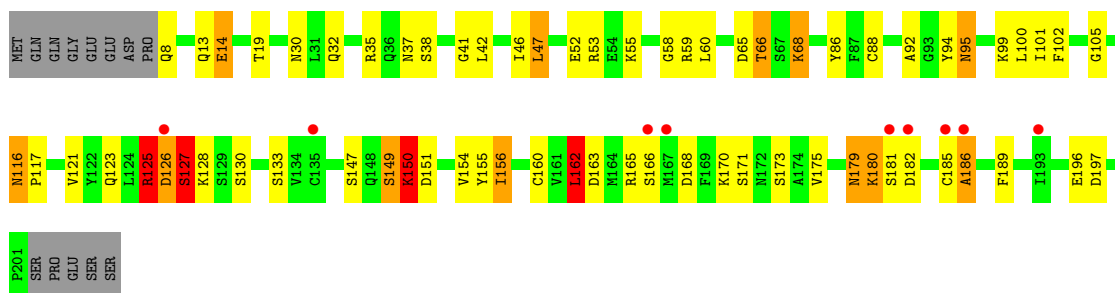


- Molecule 2: MHC class II antigen

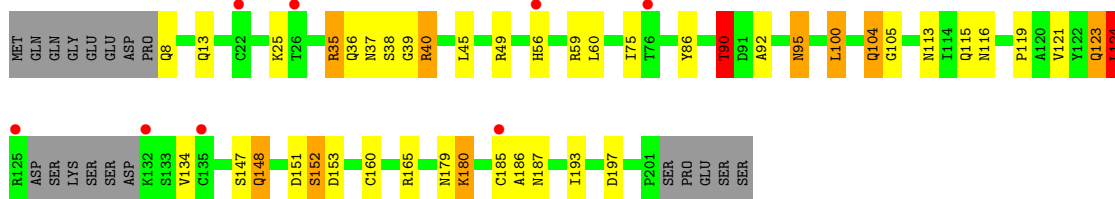




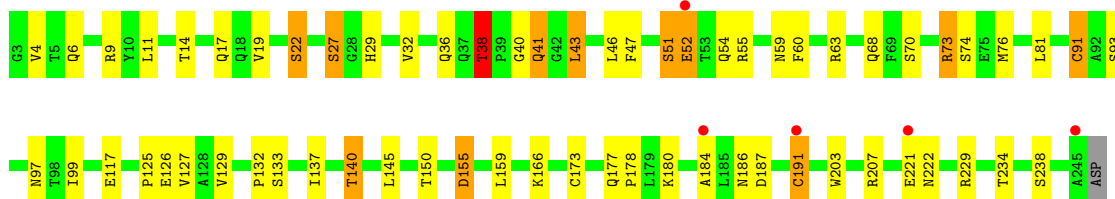
• Molecule 3: T1D3 alpha chain



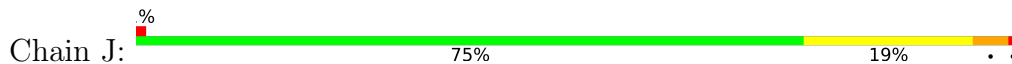
• Molecule 3: T1D3 alpha chain

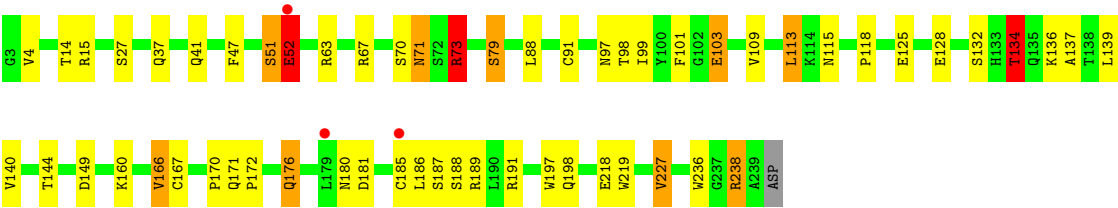


• Molecule 4: T1D3 beta chain

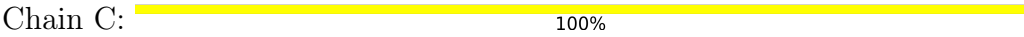


• Molecule 4: T1D3 beta chain





● 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, α , β , γ	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
$\langle I/\sigma(I) \rangle$ ¹	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	7241 reflections (5.08%)	wwPDB-VP
Wilson B-factor (Å ²)	40.5	Xtriage
Anisotropy	0.133	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.33 , 39.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

¹Intensities estimated from amplitudes.

²Theoretical 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: NAG, EDO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.81	26/1498 (1.7%)	1.35	5/2044 (0.2%)
1	D	1.69	17/1498 (1.1%)	1.31	6/2044 (0.3%)
2	B	1.83	29/1660 (1.7%)	1.44	16/2257 (0.7%)
2	E	1.72	22/1647 (1.3%)	1.52	24/2242 (1.1%)
3	G	1.76	27/1531 (1.8%)	1.48	18/2068 (0.9%)
3	I	1.57	8/1477 (0.5%)	1.40	12/1997 (0.6%)
4	H	1.78	32/1937 (1.7%)	1.45	24/2635 (0.9%)
4	J	1.69	23/1937 (1.2%)	1.41	20/2635 (0.8%)
All	All	1.74	184/13185 (1.4%)	1.42	125/17922 (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 (184) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	G	126	ASP	N-CA	10.20	1.59	1.46
2	B	189	ARG	CA-C	9.85	1.64	1.52
4	J	70	SER	C-O	-8.87	1.12	1.24
2	B	-10	SER	N-CA	8.72	1.56	1.46
3	I	40	ARG	C-O	-8.71	1.14	1.23
1	A	95	SER	CA-C	8.56	1.60	1.52
4	H	155	ASP	CA-C	8.22	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	H	52	GLU	CA-CB	7.94	1.63	1.54
4	J	103	GLU	CD-OE1	7.94	1.40	1.25
4	H	126	GLU	CD-OE2	7.80	1.40	1.25
3	G	19	THR	C-O	-7.73	1.15	1.24
4	J	118	PRO	C-O	-7.69	1.15	1.24
2	E	149	ARG	CD-NE	-7.55	1.35	1.46
1	D	41	THR	C-O	-7.50	1.14	1.24
3	I	197	ASP	CA-C	7.47	1.62	1.52
1	D	94	LYS	CA-C	7.36	1.62	1.52
2	E	22	GLU	C-O	-7.34	1.14	1.24
1	A	89	VAL	C-O	-7.28	1.16	1.24
4	H	99	ILE	C-N	7.21	1.43	1.33
4	J	79	SER	N-CA	6.94	1.53	1.45
2	E	14	MET	N-CA	6.81	1.54	1.46
2	B	8	VAL	N-CA	-6.80	1.38	1.46
4	H	186	ASN	CA-C	6.79	1.61	1.52
3	G	125	ARG	CA-C	6.78	1.61	1.52
2	B	70	ARG	N-CA	-6.77	1.38	1.46
2	B	74	GLU	CD-OE1	6.75	1.38	1.25
1	A	101	GLN	CA-C	6.72	1.59	1.52
4	H	63	ARG	CA-C	6.71	1.62	1.52
3	G	55	LYS	N-CA	-6.67	1.37	1.46
1	D	89	VAL	C-O	-6.66	1.16	1.24
1	A	84	ASN	C-O	-6.64	1.15	1.24
1	A	96	PRO	CA-C	6.57	1.60	1.52
2	B	183	PRO	CA-C	6.55	1.60	1.52
4	J	109	VAL	C-O	-6.50	1.17	1.24
3	G	30	ASN	N-CA	-6.46	1.37	1.45
1	A	179	GLU	N-CA	6.45	1.58	1.46
1	A	76	ARG	C-O	-6.45	1.15	1.23
3	G	58	GLY	C-O	-6.42	1.14	1.24
1	A	154	LEU	C-O	-6.39	1.17	1.24
4	J	197	TRP	C-O	-6.38	1.16	1.24
2	B	63	SER	C-O	-6.37	1.15	1.24
1	D	95	SER	CA-C	6.33	1.58	1.52
4	H	159	LEU	N-CA	-6.32	1.38	1.46
3	G	99	LYS	CA-CB	-6.29	1.44	1.53
4	J	52	GLU	N-CA	-6.24	1.38	1.46
2	B	-15	CYS	CA-C	6.23	1.61	1.53
2	B	22	GLU	C-O	-6.18	1.16	1.24
4	H	222	ASN	CA-C	6.18	1.61	1.52
1	D	80	THR	N-CA	6.16	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	121	VAL	C-O	-6.13	1.17	1.24
3	G	168	ASP	CA-C	6.06	1.61	1.53
1	D	134	GLU	C-O	-6.05	1.16	1.23
2	E	182	ASN	CA-C	-6.05	1.46	1.52
2	B	49	ALA	C-O	-6.04	1.16	1.23
2	B	-25	GLU	N-CA	-6.04	1.38	1.45
2	B	71	THR	N-CA	-6.02	1.39	1.46
2	B	152	ASP	C-O	-5.99	1.16	1.23
1	A	68	HIS	C-O	-5.99	1.17	1.24
4	J	101	PHE	C-O	-5.99	1.16	1.23
3	I	119	PRO	C-O	-5.98	1.16	1.23
1	D	106	ILE	N-CA	-5.94	1.39	1.46
1	D	142	ASP	CA-C	5.94	1.61	1.52
4	J	4	VAL	N-CA	-5.94	1.39	1.46
4	H	4	VAL	N-CA	-5.93	1.39	1.46
2	B	85	LEU	CA-C	-5.93	1.44	1.52
2	B	121	ASP	CA-C	-5.88	1.46	1.53
1	D	101	GLN	CA-C	5.87	1.58	1.52
1	A	41	THR	C-O	-5.86	1.16	1.24
2	E	132	PHE	CA-C	-5.85	1.45	1.52
2	E	39	ARG	N-CA	-5.83	1.38	1.45
2	B	16	TYR	CA-C	5.82	1.59	1.52
4	H	74	SER	N-CA	-5.82	1.38	1.45
2	E	74	GLU	CD-OE2	5.81	1.36	1.25
4	H	54	GLN	N-CA	-5.80	1.39	1.46
4	H	125	PRO	C-O	-5.79	1.17	1.23
2	B	82	ASN	CA-C	5.79	1.60	1.52
2	B	-22	LEU	N-CA	-5.75	1.38	1.46
3	G	186	ALA	N-CA	5.75	1.53	1.46
1	A	99	LEU	C-O	-5.75	1.17	1.23
3	G	197	ASP	CA-C	5.71	1.62	1.52
2	B	8	VAL	C-O	-5.70	1.18	1.24
1	D	179	GLU	N-CA	5.70	1.57	1.46
1	A	106	ILE	N-CA	-5.70	1.39	1.46
3	G	175	VAL	C-O	-5.69	1.18	1.24
2	B	31	ILE	N-CA	-5.67	1.39	1.46
2	B	14	MET	N-CA	5.67	1.52	1.46
2	E	92	GLN	CG-CD	-5.66	1.37	1.52
4	H	127	VAL	C-O	-5.65	1.18	1.24
4	H	173	CYS	C-O	-5.63	1.17	1.24
1	A	89	VAL	CA-C	5.61	1.59	1.52
4	H	229	ARG	C-O	-5.60	1.17	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	153	TRP	CA-C	5.58	1.60	1.53
1	D	164	LYS	N-CA	5.57	1.53	1.46
1	A	149	SER	CA-C	5.57	1.59	1.52
1	D	119	ILE	CA-C	-5.55	1.45	1.52
3	G	155	TYR	CA-C	-5.54	1.46	1.52
3	G	121	VAL	C-O	-5.54	1.18	1.24
4	H	180	LYS	C-O	-5.54	1.17	1.24
1	A	167	HIS	C-O	-5.54	1.17	1.23
4	H	43	LEU	C-O	-5.53	1.17	1.24
1	A	146	PHE	CA-C	-5.53	1.45	1.52
1	A	95	SER	N-CA	5.52	1.50	1.45
2	E	61	TRP	N-CA	-5.52	1.39	1.46
1	D	76	ARG	C-O	-5.52	1.16	1.24
3	G	173	SER	C-O	-5.51	1.17	1.23
3	I	165	ARG	C-O	-5.51	1.16	1.24
1	D	45	LEU	C-O	-5.49	1.18	1.24
4	H	173	CYS	CA-CB	5.46	1.62	1.53
1	A	94	LYS	CA-C	5.46	1.59	1.52
2	B	181	GLN	N-CA	-5.43	1.39	1.46
1	A	98	THR	N-CA	-5.43	1.39	1.46
2	E	40	PHE	N-CA	-5.43	1.39	1.46
2	B	160	MET	CA-C	5.43	1.59	1.52
4	J	236	TRP	C-O	-5.42	1.17	1.23
4	J	51	SER	N-CA	5.41	1.54	1.46
4	J	134	THR	CA-C	5.40	1.59	1.52
4	J	27	SER	CA-C	5.39	1.59	1.52
1	D	93	SER	CA-C	5.38	1.59	1.52
2	E	6	ASP	N-CA	5.38	1.52	1.46
3	G	182	ASP	CA-C	5.38	1.60	1.52
4	J	219	TRP	CA-C	-5.38	1.46	1.52
4	H	40	GLY	N-CA	5.38	1.52	1.45
2	E	94	ARG	CG-CD	-5.37	1.36	1.52
3	G	52	GLU	CD-OE2	5.36	1.35	1.25
4	J	103	GLU	CG-CD	5.36	1.65	1.52
3	G	66	THR	CB-CG2	-5.35	1.34	1.52
3	G	162	LEU	N-CA	-5.35	1.39	1.45
3	G	52	GLU	CD-OE1	5.34	1.35	1.25
4	J	52	GLU	CA-CB	5.33	1.60	1.54
3	G	150	LYS	N-CA	5.32	1.53	1.46
4	H	184	ALA	N-CA	5.30	1.52	1.46
4	H	70	SER	C-O	-5.29	1.18	1.24
2	E	65	LYS	C-O	-5.29	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	-23	TYR	CA-CB	5.29	1.63	1.53
4	H	54	GLN	C-O	-5.29	1.17	1.23
2	E	22	GLU	CA-CB	5.28	1.62	1.53
4	H	91	CYS	N-CA	-5.27	1.39	1.46
4	H	126	GLU	CG-CD	5.26	1.65	1.52
4	H	234	THR	C-O	-5.26	1.17	1.23
1	A	178	TRP	CA-C	5.26	1.59	1.52
2	B	189	ARG	N-CA	5.25	1.52	1.46
2	E	10	GLN	CA-C	-5.25	1.46	1.52
3	G	41	GLY	CA-C	5.25	1.59	1.51
2	E	182	ASN	C-O	-5.24	1.17	1.24
3	G	126	ASP	C-O	5.24	1.30	1.24
3	I	193	ILE	CA-CB	5.24	1.58	1.53
1	A	74	ILE	C-O	-5.23	1.18	1.24
4	H	51	SER	N-CA	5.23	1.54	1.46
3	G	92	ALA	CA-C	5.23	1.60	1.53
3	G	133	SER	CA-C	-5.23	1.46	1.52
2	B	81	HIS	CA-CB	5.22	1.61	1.53
1	A	50	ARG	CA-C	-5.22	1.46	1.52
4	J	170	PRO	N-CA	5.22	1.54	1.47
1	A	37	GLU	CD-OE2	5.20	1.35	1.25
4	J	176	GLN	N-CA	5.19	1.51	1.46
3	I	104	GLN	CA-C	5.19	1.59	1.52
4	H	59	ASN	C-O	-5.18	1.17	1.24
4	H	55	ARG	N-CA	-5.17	1.39	1.46
3	I	193	ILE	CA-C	5.17	1.58	1.53
4	J	15	ARG	CA-C	-5.16	1.46	1.52
2	E	89	THR	CA-CB	5.16	1.62	1.53
2	B	123	TYR	CA-CB	5.15	1.61	1.53
1	D	110	ASP	CA-C	5.15	1.59	1.52
1	A	132	VAL	C-O	-5.14	1.17	1.24
4	J	73	ARG	N-CA	-5.14	1.39	1.46
2	B	60	TYR	C-O	-5.13	1.18	1.24
3	G	102	PHE	C-O	-5.13	1.17	1.24
4	H	36	GLN	N-CA	-5.13	1.40	1.46
2	E	93	ARG	NE-CZ	-5.12	1.27	1.33
3	G	47	LEU	C-O	-5.11	1.17	1.24
3	G	94	TYR	CA-C	-5.10	1.46	1.52
1	A	55	ASP	CB-CG	5.09	1.64	1.52
4	J	103	GLU	CD-OE2	5.09	1.35	1.25
1	A	42	VAL	CA-C	5.07	1.58	1.52
2	E	79	CYS	N-CA	5.06	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	85	LEU	C-O	-5.06	1.17	1.24
4	H	187	ASP	CB-CG	5.05	1.64	1.52
1	D	43	TRP	C-O	-5.04	1.17	1.23
4	J	137	ALA	N-CA	-5.03	1.39	1.46
4	H	32	VAL	N-CA	-5.03	1.40	1.46
4	J	191	ARG	C-O	-5.02	1.18	1.24
2	E	75	LEU	CA-C	5.02	1.59	1.52
2	B	-22	LEU	CA-C	5.01	1.58	1.52
4	H	54	GLN	CD-NE2	-5.01	1.22	1.33

All (125) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	164	THR	CB-CA-C	10.30	120.83	110.33
4	H	140	THR	N-CA-C	-9.28	96.51	110.14
3	I	165	ARG	NE-CZ-NH2	9.05	127.34	119.20
2	E	149	ARG	NE-CZ-NH2	8.96	127.26	119.20
2	E	149	ARG	NE-CZ-NH1	-8.95	112.55	121.50
4	H	52	GLU	CB-CA-C	-8.76	101.15	109.83
2	E	149	ARG	CG-CD-NE	-8.46	93.38	112.00
3	I	152	SER	N-CA-C	-8.46	99.13	110.55
3	I	124	LEU	N-CA-C	8.32	123.37	112.72
4	H	99	ILE	CA-C-N	8.05	134.32	123.05
4	H	99	ILE	C-N-CA	8.05	134.32	123.05
4	H	41	GLN	CB-CG-CD	-8.02	98.96	112.60
1	D	80	THR	N-CA-C	-7.93	96.30	109.07
3	I	35	ARG	N-CA-CB	-7.65	97.15	111.00
4	H	173	CYS	CA-CB-SG	-7.53	97.09	114.40
4	H	99	ILE	O-C-N	-7.49	115.50	123.14
2	B	170	VAL	N-CA-C	-7.28	97.91	108.11
2	E	149	ARG	CD-NE-CZ	7.20	134.48	124.40
2	E	170	VAL	N-CA-C	-7.11	98.16	108.11
4	J	171	GLN	CB-CA-C	-7.05	99.04	109.97
4	H	191	CYS	CB-CA-C	-7.03	94.61	110.07
3	G	88	CYS	N-CA-CB	-7.01	99.56	110.57
4	J	149	ASP	N-CA-C	6.95	120.71	112.93
2	B	149	ARG	NE-CZ-NH2	6.84	125.36	119.20
4	H	70	SER	CB-CA-C	-6.84	99.43	110.79
3	G	127	SER	N-CA-CB	6.62	121.76	110.50
1	D	178	TRP	CA-C-N	6.53	133.46	121.70
1	D	178	TRP	C-N-CA	6.53	133.46	121.70
2	B	130	ARG	NE-CZ-NH2	6.51	125.06	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	222	ASN	N-CA-CB	-6.51	100.28	110.30
3	I	35	ARG	CG-CD-NE	-6.48	97.74	112.00
3	I	165	ARG	NE-CZ-NH1	-6.45	115.05	121.50
4	H	191	CYS	CA-CB-SG	-6.42	99.63	114.40
2	E	22	GLU	CB-CG-CD	6.40	123.49	112.60
4	J	79	SER	CB-CA-C	-6.40	99.38	110.45
2	B	55	PRO	N-CA-C	6.31	118.39	110.70
2	B	149	ARG	NE-CZ-NH1	-6.29	115.21	121.50
3	I	90	THR	N-CA-CB	-6.25	101.23	110.85
2	E	94	ARG	CA-CB-CG	-6.24	101.61	114.10
4	H	51	SER	CB-CA-C	-6.20	102.74	111.80
4	J	181	ASP	N-CA-CB	-6.19	99.06	110.32
4	J	180	ASN	CA-C-N	6.17	132.47	120.99
4	J	180	ASN	C-N-CA	6.17	132.47	120.99
1	A	37	GLU	CB-CG-CD	6.10	122.98	112.60
3	G	88	CYS	CB-CA-C	6.08	120.24	109.72
3	G	53	ARG	CG-CD-NE	-6.05	98.69	112.00
3	G	14	GLU	N-CA-CB	6.05	119.53	109.56
2	B	-10	SER	N-CA-C	6.03	118.02	108.79
3	G	163	ASP	N-CA-C	6.02	118.23	108.41
2	E	34	ARG	NE-CZ-NH2	-5.99	113.81	119.20
3	I	116	ASN	CA-C-N	-5.98	113.60	119.76
3	I	116	ASN	C-N-CA	-5.98	113.60	119.76
2	B	3	SER	N-CA-C	5.97	117.41	109.83
2	E	34	ARG	CG-CD-NE	-5.91	98.99	112.00
3	G	186	ALA	N-CA-C	-5.88	98.27	110.80
2	E	54	GLY	N-CA-C	5.79	124.15	112.34
3	G	128	LYS	N-CA-C	-5.75	104.38	111.40
4	J	63	ARG	N-CA-CB	-5.73	101.09	110.14
2	E	189	ARG	CA-C-N	5.72	131.99	121.70
2	E	189	ARG	C-N-CA	5.72	131.99	121.70
3	G	162	LEU	N-CA-CB	-5.71	101.31	111.08
4	H	38	THR	N-CA-CB	-5.70	100.94	111.19
4	H	27	SER	CB-CA-C	5.64	118.92	109.89
2	B	-11	GLY	N-CA-C	-5.64	99.82	113.18
4	J	51	SER	CB-CA-C	-5.59	103.63	111.80
2	E	22	GLU	N-CA-C	-5.57	105.35	111.82
4	J	198	GLN	CB-CA-C	5.57	121.53	110.17
2	B	188	TRP	CA-C-N	5.55	131.29	122.74
2	B	188	TRP	C-N-CA	5.55	131.29	122.74
4	J	128	GLU	CB-CG-CD	5.54	122.01	112.60
3	G	65	ASP	CA-C-N	5.50	129.40	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	G	65	ASP	C-N-CA	5.50	129.40	120.60
3	G	116	ASN	CA-C-N	-5.48	114.12	119.76
3	G	116	ASN	C-N-CA	-5.48	114.12	119.76
4	H	238	SER	N-CA-C	5.48	117.30	109.14
4	J	198	GLN	CA-CB-CG	5.47	125.04	114.10
1	D	65	VAL	N-CA-C	5.46	115.67	110.42
1	A	156	SER	N-CA-CB	5.45	119.76	110.50
3	I	39	GLY	N-CA-C	-5.44	97.52	113.30
3	G	162	LEU	CA-CB-CG	5.44	135.33	116.30
4	H	166	LYS	CG-CD-CE	5.43	123.80	111.30
4	H	91	CYS	CA-CB-SG	-5.42	101.93	114.40
3	I	59	ARG	NE-CZ-NH2	5.42	124.08	119.20
2	E	55	PRO	N-CA-C	5.39	117.28	110.70
2	E	125	ALA	N-CA-C	5.37	118.05	111.82
2	B	31	ILE	N-CA-C	5.37	116.01	108.17
4	H	117	GLU	CB-CG-CD	5.35	121.69	112.60
4	H	222	ASN	N-CA-C	5.34	118.96	112.23
4	H	9	ARG	N-CA-C	5.33	117.17	111.36
4	H	191	CYS	N-CA-C	5.32	117.28	109.24
2	E	65	LYS	CB-CA-C	-5.31	101.97	110.79
2	E	189	ARG	NE-CZ-NH2	5.31	123.98	119.20
4	J	132	SER	CB-CA-C	-5.31	102.55	110.88
2	B	-15	CYS	CA-CB-SG	-5.30	102.20	114.40
2	E	54	GLY	CA-C-N	-5.30	114.92	120.38
2	E	54	GLY	C-N-CA	-5.30	114.92	120.38
4	J	166	VAL	CA-CB-CG1	5.30	119.41	110.40
3	I	197	ASP	N-CA-CB	-5.29	101.55	110.49
4	J	166	VAL	N-CA-CB	5.26	119.28	110.86
1	A	40	GLU	N-CA-C	5.25	117.23	108.99
4	J	91	CYS	CA-CB-SG	-5.24	102.34	114.40
4	J	227	VAL	N-CA-CB	-5.23	101.87	111.91
2	B	103	PRO	CA-C-N	-5.22	114.13	122.53
2	B	103	PRO	C-N-CA	-5.22	114.13	122.53
3	G	160	CYS	N-CA-CB	-5.22	101.82	111.52
2	E	-12	GLY	N-CA-C	-5.21	103.32	110.20
1	A	179	GLU	CB-CG-CD	5.15	121.36	112.60
4	J	227	VAL	CB-CA-C	5.14	118.59	111.49
1	D	37	GLU	CB-CG-CD	-5.12	103.89	112.60
3	G	66	THR	N-CA-CB	-5.11	101.63	110.32
3	G	185	CYS	N-CA-C	-5.11	102.12	110.20
4	H	38	THR	CB-CA-C	5.11	117.34	108.91
3	G	59	ARG	NE-CZ-NH2	5.11	123.80	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	H	63	ARG	NE-CZ-NH2	5.09	123.78	119.20
2	B	125	ALA	N-CA-C	5.08	117.71	111.82
4	J	51	SER	CA-C-N	-5.07	118.90	126.86
4	J	51	SER	C-N-CA	-5.07	118.90	126.86
4	H	155	ASP	O-C-N	-5.07	115.92	122.61
4	J	172	PRO	CA-C-O	-5.05	115.70	121.56
2	E	69	GLU	CB-CG-CD	5.03	121.15	112.60
1	D	80	THR	N-CA-CB	5.03	118.47	110.57
1	A	49	ARG	CB-CG-CD	5.02	122.86	111.30
2	E	145	THR	CA-C-N	-5.02	114.48	120.11
2	E	145	THR	C-N-CA	-5.02	114.48	120.11
2	B	54	GLY	N-CA-C	5.00	122.55	112.34

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	17	0
2	E	1610	0	1547	25	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	G	1506	0	1450	24	0
3	I	1453	0	1392	23	0
4	H	1885	0	1785	28	0
4	J	1885	0	1786	25	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
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	140	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 6.

All (140) 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:179:ASN:O	3:G:180:LYS:C	2.34	0.69
3:G:126:ASP:CA	3:G:127:SER:HB2	2.13	0.69
4:H:155:ASP:CG	4:H:178:PRO:HG2	2.21	0.64
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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
4:J:188:SER:C	4:J:189:ARG:HD3	2.32	0.55
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:E:66:GLU:OE2	4:J:98:THR:OG1	2.22	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:HE3	2:B:171:TYR:CD1	2.47	0.49
2:B:163:MET:CE	2:B:171:TYR:CE1	2.96	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
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
2:B:-14:GLY:N	2:B:-13:GLY:C	2.72	0.48
1:A:52:ARG:HH21	2:B:-25:GLU:CD	2.21	0.47
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
2:B:163:MET:HE3	2:B:171:TYR:CE1	2.50	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
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:G:13:GLN:O	3:G:14:GLU:C	2.60	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
3:G:47:LEU:HD23	3:G:47:LEU:C	2.43	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
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
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: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
2:E:69:GLU:CD	3:I:49:ARG:HE	2.27	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
2:B:-14:GLY:CA	2:B:-13:GLY:C	2.93	0.41
3:G:116:ASN:O	3:G:117:PRO:C	2.62	0.41
4:H:29:HIS:CD2	4:H:93:SER:OG	2.73	0.41
4:H:155:ASP:OD2	4:H:178:PRO:HG2	2.19	0.41
3:G:179:ASN:C	3:G:179:ASN:HD22	2.28	0.41
1:A:43:TRP:CE3	1:A:48:PHE:HB3	2.56	0.41
1:D:174:LEU:HD23	1:D:174:LEU:C	2.46	0.41
4:H:76:MET:HE3	4:H:76:MET:HB2	2.00	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
2:B:177:HIS:CD2	2:B:179:SER:H	2.39	0.40
4:J:71:ASN:C	4:J:71:ASN:HD22	2.29	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 ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	178/188 (95%)	169 (95%)	8 (4%)	1 (1%)	21	12
1	D	178/188 (95%)	173 (97%)	5 (3%)	0	100	100
2	B	194/221 (88%)	187 (96%)	6 (3%)	1 (0%)	24	17
2	E	193/221 (87%)	182 (94%)	9 (5%)	2 (1%)	12	5
3	G	192/207 (93%)	174 (91%)	12 (6%)	6 (3%)	3	0
3	I	184/207 (89%)	176 (96%)	5 (3%)	3 (2%)	7	2
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	8

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%)	158 (96%)	7 (4%)	26	20
1	D	165/171 (96%)	157 (95%)	8 (5%)	23	15
2	B	178/192 (93%)	167 (94%)	11 (6%)	16	9
2	E	177/192 (92%)	158 (89%)	19 (11%)	6	2
3	G	171/183 (93%)	152 (89%)	19 (11%)	6	1
3	I	163/183 (89%)	148 (91%)	15 (9%)	8	3
4	H	207/208 (100%)	198 (96%)	9 (4%)	26	19
4	J	207/208 (100%)	190 (92%)	17 (8%)	10	5
All	All	1433/1508 (95%)	1328 (93%)	105 (7%)	13	7

All (105) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
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	127	ILE
2	B	133	ARG
2	B	139	THR
2	B	140	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

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Mol	Chain	Res	Type
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	65	LYS
2	E	68	LEU
2	E	69	GLU
2	E	92	GLN
2	E	94	ARG
2	E	113	ASN
2	E	127	ILE
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	170	VAL
2	E	189	ARG
3	G	8	GLN
3	G	60	LEU
3	G	66	THR
3	G	68	LYS
3	G	95	ASN
3	G	100	LEU
3	G	101	ILE
3	G	125	ARG
3	G	127	SER
3	G	130	SER
3	G	147	SER
3	G	150	LYS
3	G	154	VAL
3	G	156	ILE
3	G	162	LEU
3	G	165	ARG

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Mol	Chain	Res	Type
3	G	179	ASN
3	G	180	LYS
3	G	196	GLU
4	H	22	SER
4	H	27	SER
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	8	GLN
3	I	25	LYS
3	I	56	HIS
3	I	90	THR
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	134	VAL
3	I	147	SER
3	I	148	GLN
3	I	180	LYS
3	I	187	ASN
4	J	41	GLN
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	160	LYS
4	J	166	VAL
4	J	176	GLN
4	J	218	GLU

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Mol	Chain	Res	Type
4	J	227	VAL
4	J	238	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
2	B	64	GLN
2	B	150	ASN
2	B	156	GLN
2	B	177	HIS
2	B	182	ASN
1	D	124	ASN
1	D	126	HIS
1	D	143	HIS
2	E	19	ASN
2	E	64	GLN
2	E	92	GLN
2	E	150	ASN
2	E	156	GLN
2	E	166	GLN
2	E	181	GLN
3	G	21	ASN
3	G	29	ASN
3	G	30	ASN
3	G	36	GLN
3	G	37	ASN
3	G	95	ASN
3	G	148	GLN
3	G	179	ASN
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	204	GLN
4	H	209	HIS
4	H	213	GLN
4	H	215	GLN
3	I	8	GLN
3	I	29	ASN
3	I	30	ASN

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Mol	Chain	Res	Type
3	I	36	GLN
3	I	37	ASN
3	I	95	ASN
3	I	113	ASN
4	J	18	GLN
4	J	36	GLN
4	J	71	ASN
4	J	203	HIS

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

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
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
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.

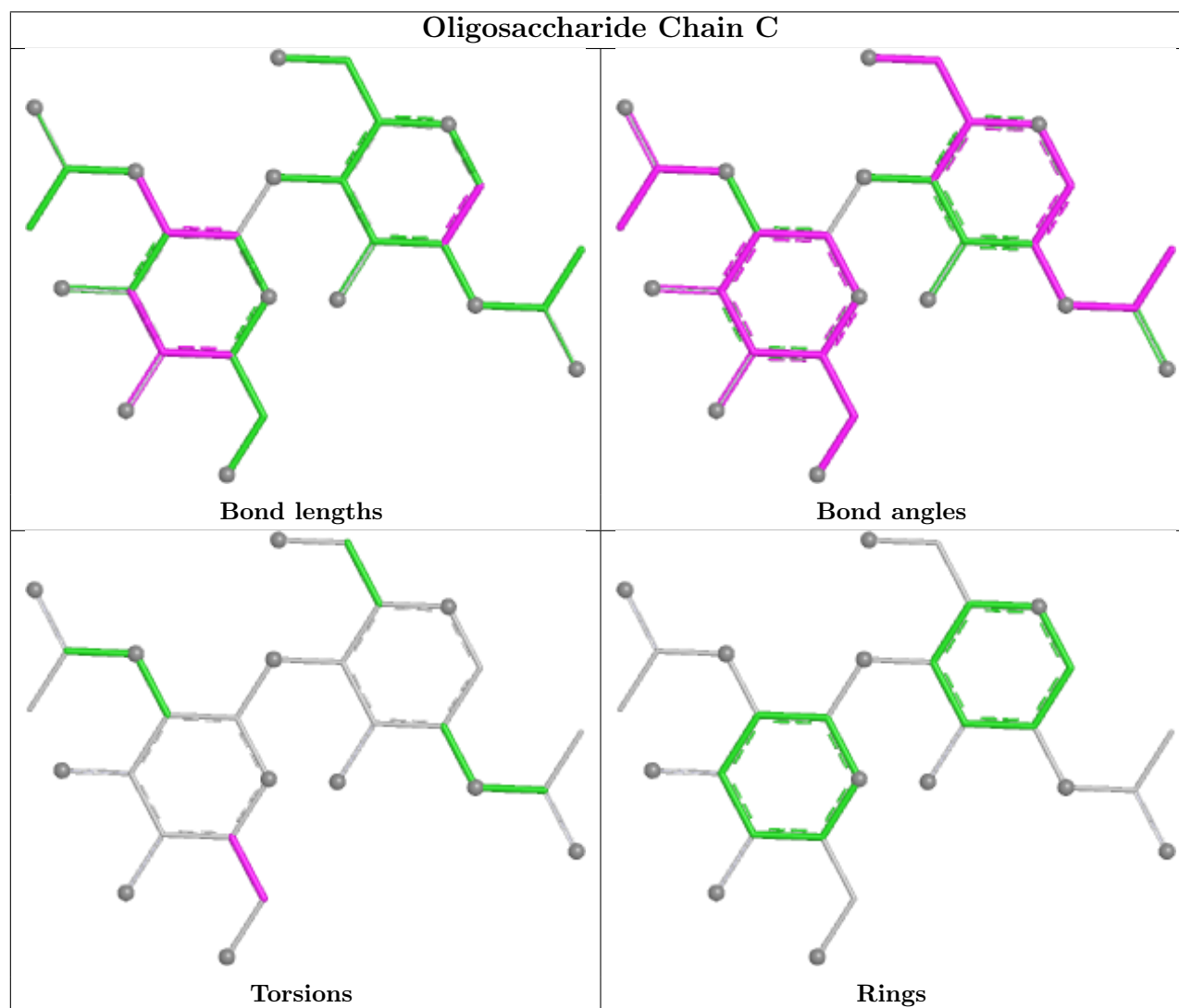
All (2) torsion outliers are listed below:

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%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
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 [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, 95th 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 ²)	Q < 0.9
1	A	180/188 (95%)	-0.18	3 (1%) 69 69	25, 40, 71, 82	0
1	D	180/188 (95%)	-0.09	1 (0%) 85 86	31, 44, 71, 87	0
2	B	200/221 (90%)	0.01	9 (4%) 38 37	26, 39, 86, 109	0
2	E	199/221 (90%)	0.06	7 (3%) 47 46	32, 45, 78, 96	0
3	G	194/207 (93%)	0.34	9 (4%) 37 36	28, 58, 89, 109	0
3	I	188/207 (90%)	0.50	8 (4%) 40 39	37, 59, 88, 100	0
4	H	237/238 (99%)	-0.10	5 (2%) 63 63	30, 42, 69, 77	0
4	J	237/238 (99%)	-0.08	3 (1%) 75 75	34, 44, 68, 79	0
All	All	1615/1708 (94%)	0.05	45 (2%) 55 54	25, 46, 80, 109	0

All (45) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	190	ALA	5.3
1	A	157	ALA	4.6
4	J	185	CYS	4.4
2	E	-9	LEU	4.2
2	E	190	ALA	3.8
2	E	-13	GLY	3.6
4	H	191	CYS	3.2
3	I	125	ARG	3.0
1	D	79	SER	3.0
1	A	158	ASP	2.9
3	G	126	ASP	2.9
3	I	22	CYS	2.8
1	A	178	TRP	2.8
2	E	-10	SER	2.7
3	G	181	SER	2.7
2	B	168	GLY	2.7

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Mol	Chain	Res	Type	RSRZ
3	G	182	ASP	2.7
3	I	132	LYS	2.7
3	I	76	THR	2.6
3	G	185	CYS	2.6
4	J	52	GLU	2.6
2	E	167	ARG	2.6
2	B	-9	LEU	2.6
3	I	185	CYS	2.5
3	I	56	HIS	2.5
2	B	-13	GLY	2.4
2	B	-15	CYS	2.4
2	B	114	LEU	2.3
4	H	52	GLU	2.3
3	G	135	CYS	2.3
3	I	26	THR	2.2
3	G	167	MET	2.2
3	G	186	ALA	2.2
4	J	179	LEU	2.2
3	G	193	ILE	2.2
4	H	221	GLU	2.2
2	E	3	SER	2.2
3	G	166	SER	2.2
4	H	245	ALA	2.1
2	B	135	ASP	2.1
3	I	135	CYS	2.0
2	E	-11	GLY	2.0
2	B	-10	SER	2.0
4	H	184	ALA	2.0
2	B	103	PRO	2.0

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

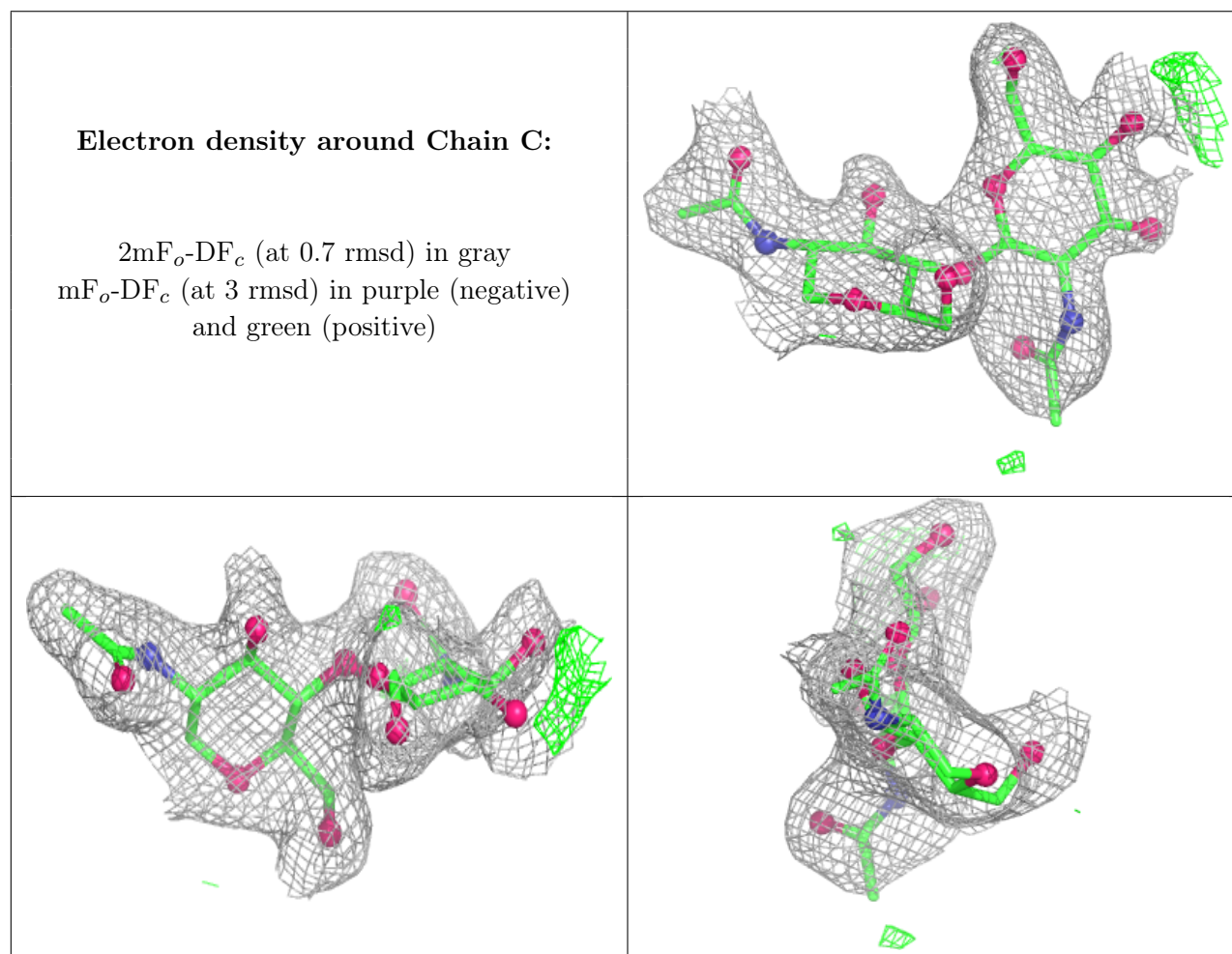
There are no non-standard protein/DNA/RNA residues in this entry.

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, 95th 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
5	NAG	C	1	14/15	-	-	47,56,60,65	0
5	NAG	C	2	14/15	-	-	70,75,83,83	0

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, 95th 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
6	EDO	A	203	4/4	0.71	0.16	61,65,66,67	0
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.