



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 04:21 AM UTC

PDB ID : 4ZFM / pdb_00004zfm
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

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
Buster-report : wwPDB partial adaption of 1.1.7 (2018)
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

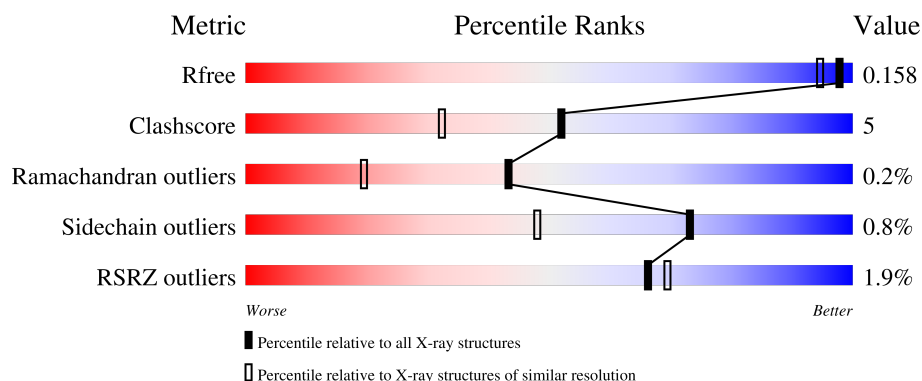
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

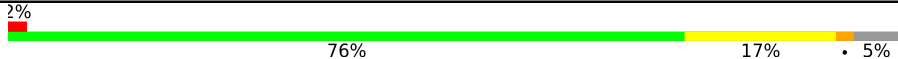
The reported resolution of this entry is 1.40 Å.

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}	180053	2563 (1.40-1.40)
Clashscore	190562	2660 (1.40-1.40)
Ramachandran outliers	187476	2611 (1.40-1.40)
Sidechain outliers	187428	2610 (1.40-1.40)
RSRZ outliers	180081	2561 (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 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	485	
1	B	485	
1	C	485	
1	D	485	
2	E	2	

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:

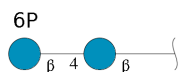
Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	MET	-	initiating methionine	UNP W8QF82
A	-5	ILE	-	expression tag	UNP W8QF82
A	-4	HIS	-	expression tag	UNP W8QF82
A	-3	HIS	-	expression tag	UNP W8QF82
A	-2	HIS	-	expression tag	UNP W8QF82
A	-1	HIS	-	expression tag	UNP W8QF82
A	0	HIS	-	expression tag	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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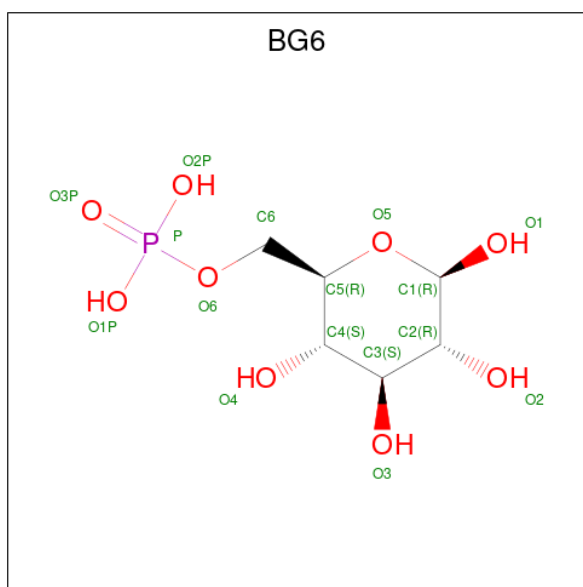
Chain	Residue	Modelled	Actual	Comment	Reference
C	-3	HIS	-	expression tag	UNP W8QF82
C	-2	HIS	-	expression tag	UNP W8QF82
C	-1	HIS	-	expression tag	UNP W8QF82
C	0	HIS	-	expression tag	UNP W8QF82
C	1	HIS	-	expression tag	UNP W8QF82
C	170	GLN	GLU	engineered mutation	UNP W8QF82
D	-6	MET	-	initiating methionine	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 (CCD ID: BG6) (formula: C₆H₁₃O₉P).



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 (CCD ID: GOL) (formula: $C_3H_8O_3$).



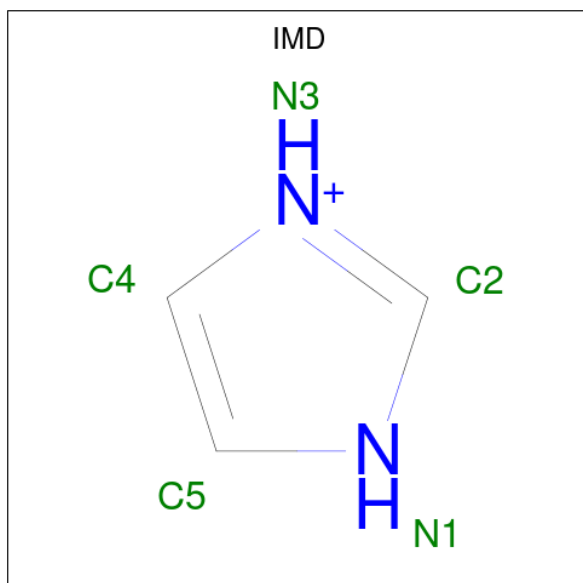
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	C	O	0	0
			6	3	3		
4	A	1	Total	C	O	0	0
			6	3	3		

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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	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 (CCD ID: IMD) (formula: $C_3H_5N_2$).



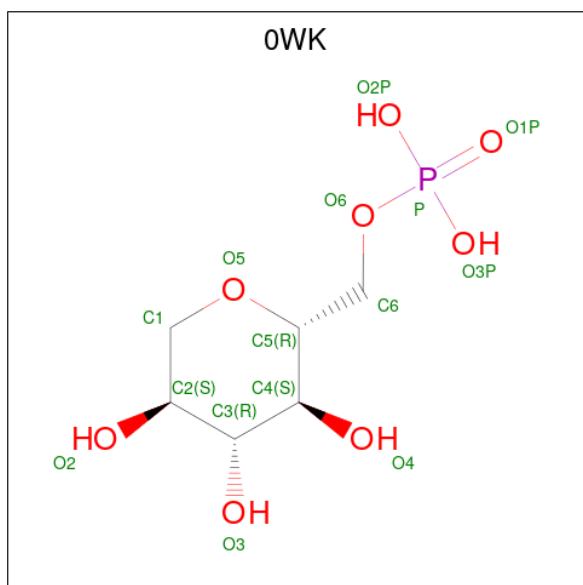
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	A	1	Total	C	N	0	0
			5	3	2		

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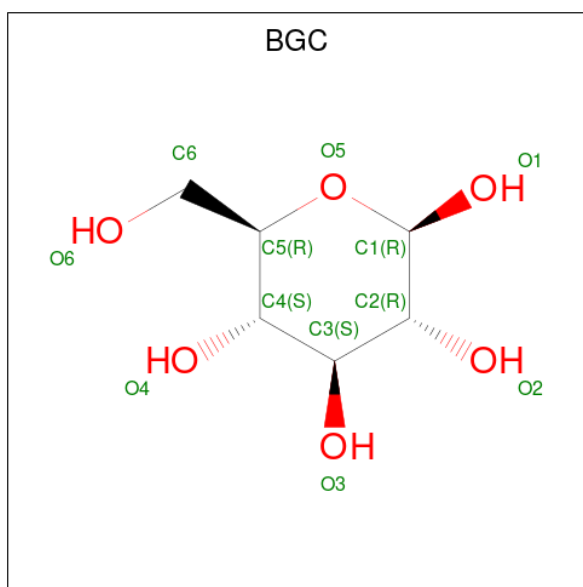
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
5	C	1	Total	C	N	0	0
			5	3	2		
5	D	1	Total	C	N	0	0
			5	3	2		

- Molecule 6 is 1,5-anhydro-6-O-phosphono-D-glucitol (CCD ID: 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 (CCD ID: BGC) (formula: $C_6H_{12}O_6$).



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

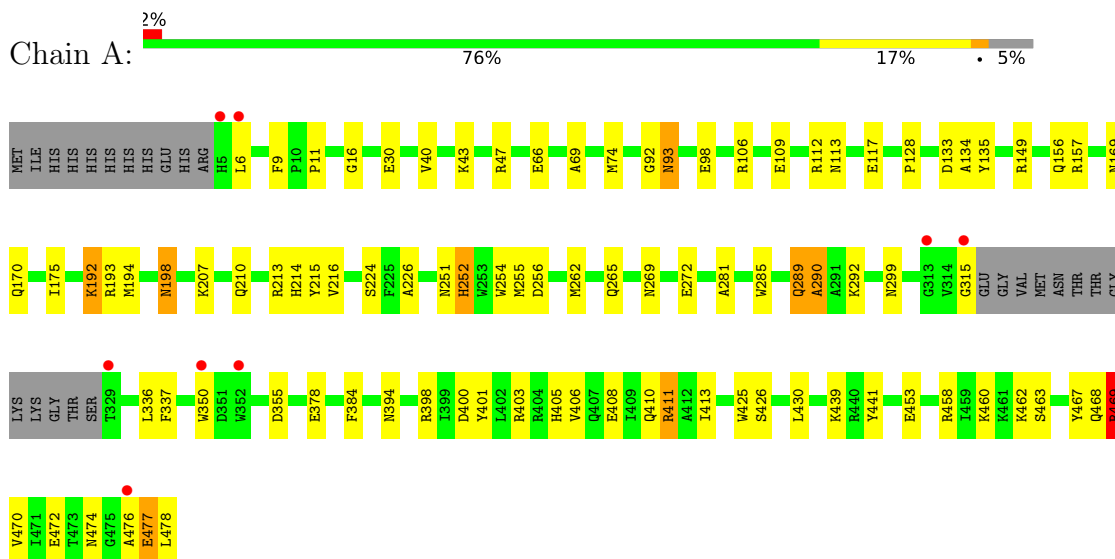
- Molecule 8 is water.

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		

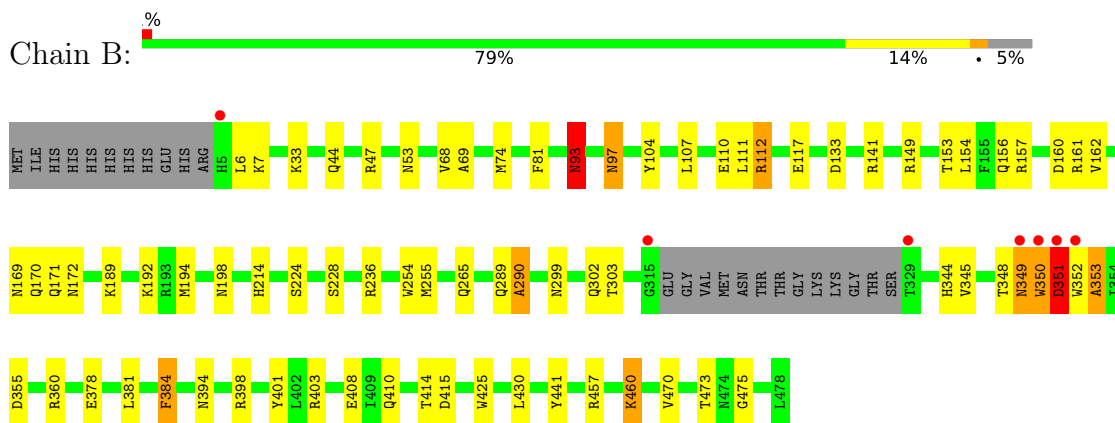
3 Residue-property plots [i](#)

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.

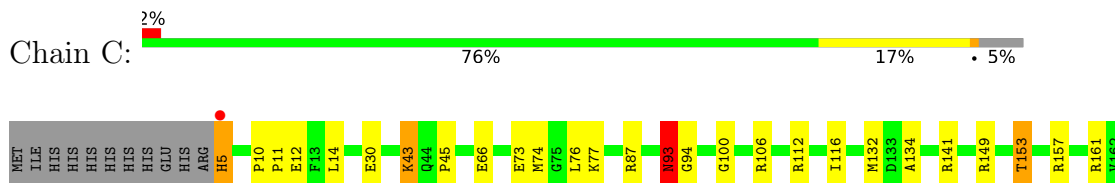
- Molecule 1: Putative 6-phospho-beta-galactobiosidase

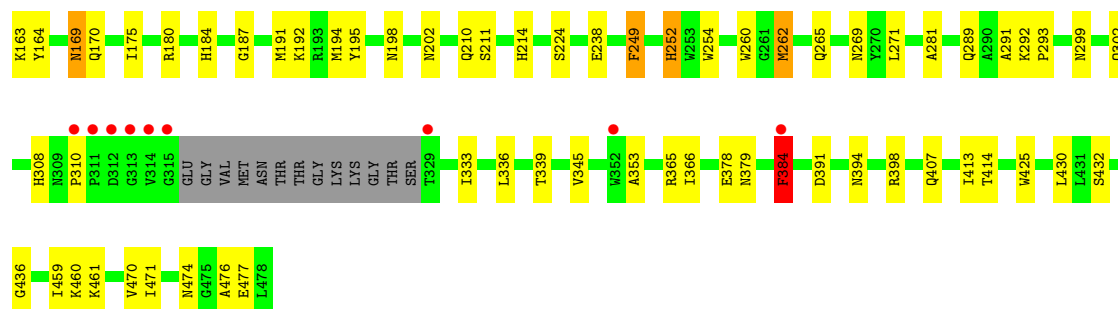


- Molecule 1: Putative 6-phospho-beta-galactobiosidase

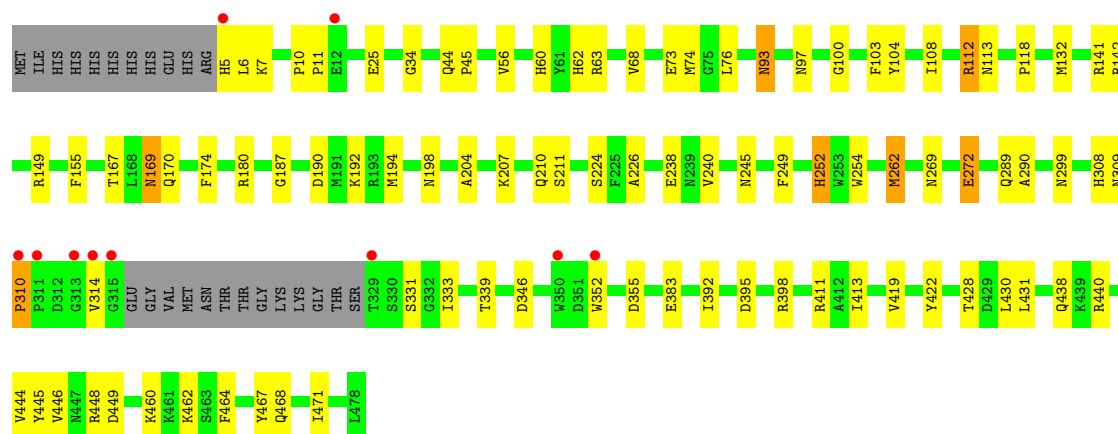
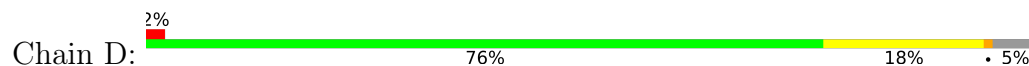


- Molecule 1: Putative 6-phospho-beta-galactobiosidase





- 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, α , β , γ	101.59Å 97.47Å 105.27Å 90.00° 97.66° 90.00°	Depositor
Resolution (Å)	22.37 – 1.40 22.37 – 1.40	Depositor EDS
% Data completeness (in resolution range)	98.7 (22.37-1.40) 98.7 (22.37-1.40)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.22 (at 1.40Å)	Xtriage
Refinement program	REFMAC 5.7.0032	Depositor
R, R_{free}	0.130 , 0.158 0.131 , 0.158	Depositor DCC
R_{free} test set	19771 reflections (4.96%)	wwPDB-VP
Wilson B-factor (Å ²)	10.1	Xtriage
Anisotropy	0.500	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	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 ²)	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.*

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: GOL, BG6, IMD, BGC, OWK

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	1.75	48/4146 (1.2%)	1.49	26/5630 (0.5%)
1	B	1.72	37/4087 (0.9%)	1.53	30/5558 (0.5%)
1	C	1.69	41/4107 (1.0%)	1.51	27/5581 (0.5%)
1	D	1.78	46/4050 (1.1%)	1.59	43/5509 (0.8%)
All	All	1.73	172/16390 (1.0%)	1.53	126/22278 (0.6%)

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 (172) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	384	PHE	C-O	9.80	1.35	1.24
1	C	74	MET	SD-CE	-9.03	1.56	1.79
1	D	60	HIS	CA-C	8.50	1.64	1.52
1	D	76	LEU	CA-C	-8.39	1.42	1.52
1	A	468	GLN	CA-C	8.08	1.63	1.52
1	D	398	ARG	CA-C	-7.98	1.42	1.52
1	A	9	PHE	CA-C	-7.92	1.45	1.53
1	A	476	ALA	N-CA	7.90	1.56	1.46
1	D	74	MET	SD-CE	-7.65	1.60	1.79
1	C	10	PRO	CA-CB	-7.60	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	398	ARG	C-O	7.59	1.33	1.24
1	B	110	GLU	N-CA	-7.59	1.37	1.46
1	D	398	ARG	CD-NE	-7.40	1.35	1.46
1	A	430	LEU	C-O	-7.38	1.14	1.23
1	A	106	ARG	CZ-NH2	-7.22	1.24	1.33
1	B	156	GLN	CA-CB	-7.17	1.41	1.53
1	C	45	PRO	CA-C	-7.06	1.43	1.52
1	B	381	LEU	C-N	-7.05	1.28	1.33
1	B	74	MET	SD-CE	-7.00	1.62	1.79
1	D	56	VAL	CA-C	6.92	1.59	1.52
1	C	470	VAL	CA-C	-6.91	1.44	1.52
1	A	405	HIS	CA-C	-6.82	1.44	1.52
1	A	474	ASN	CA-C	-6.74	1.44	1.53
1	A	469[A]	ARG	CA-C	6.68	1.62	1.52
1	A	469[B]	ARG	CA-C	6.68	1.62	1.52
1	C	293	PRO	CA-C	-6.57	1.46	1.52
1	A	337	PHE	C-N	-6.55	1.25	1.33
1	A	265	GLN	CA-C	-6.50	1.44	1.52
1	A	290	ALA	C-O	6.50	1.33	1.24
1	B	47	ARG	CD-NE	-6.50	1.37	1.46
1	C	476	ALA	C-O	6.45	1.32	1.24
1	B	473	THR	CB-OG1	6.42	1.54	1.43
1	D	422	TYR	CA-C	-6.40	1.45	1.52
1	A	135	TYR	C-N	-6.35	1.25	1.33
1	D	45	PRO	CA-C	-6.33	1.44	1.52
1	A	290	ALA	C-N	-6.32	1.25	1.33
1	C	87	ARG	CA-C	-6.29	1.44	1.52
1	C	384	PHE	C-N	-6.28	1.24	1.33
1	D	272	GLU	C-O	6.28	1.31	1.24
1	D	310	PRO	CA-C	6.24	1.57	1.52
1	A	384	PHE	C-O	6.24	1.31	1.24
1	D	392	ILE	C-O	-6.23	1.17	1.24
1	C	265	GLN	CA-C	-6.23	1.44	1.52
1	A	134	ALA	CA-CB	-6.20	1.43	1.53
1	A	213	ARG	N-CA	6.18	1.54	1.46
1	D	68	VAL	N-CA	-6.17	1.39	1.46
1	B	265	GLN	CA-C	-6.17	1.44	1.52
1	D	180[A]	ARG	CA-C	-6.16	1.46	1.52
1	D	180[B]	ARG	CA-C	-6.16	1.46	1.52
1	A	477	GLU	C-O	6.10	1.30	1.24
1	B	68	VAL	CA-CB	-6.09	1.46	1.54
1	B	47	ARG	N-CA	-6.06	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	401	TYR	CA-C	-6.02	1.45	1.52
1	D	269	ASN	CA-C	-5.99	1.45	1.52
1	B	44	GLN	CD-NE2	-5.98	1.20	1.33
1	B	133	ASP	CG-OD1	-5.97	1.14	1.25
1	A	462	LYS	CA-CB	-5.96	1.44	1.53
1	D	464	PHE	C-O	-5.93	1.17	1.24
1	D	419	VAL	C-O	5.93	1.30	1.24
1	D	240	VAL	CA-C	-5.86	1.45	1.52
1	D	34	GLY	N-CA	-5.85	1.38	1.45
1	D	103	PHE	N-CA	5.82	1.53	1.46
1	B	112	ARG	N-CA	5.80	1.53	1.46
1	D	210	GLN	CA-C	-5.77	1.45	1.52
1	B	430	LEU	C-O	-5.75	1.16	1.23
1	C	77	LYS	N-CA	-5.75	1.38	1.46
1	C	269	ASN	CG-ND2	-5.73	1.21	1.33
1	D	190	ASP	N-CA	-5.71	1.39	1.46
1	A	411	ARG	CA-CB	-5.68	1.44	1.53
1	A	472	GLU	C-N	-5.68	1.26	1.33
1	C	345	VAL	C-O	-5.68	1.18	1.24
1	B	6	LEU	C-O	-5.68	1.16	1.23
1	B	303	THR	CA-C	-5.68	1.45	1.53
1	B	172	ASN	N-CA	-5.67	1.39	1.46
1	A	74	MET	SD-CE	-5.66	1.65	1.79
1	A	467	TYR	CA-C	-5.63	1.45	1.52
1	C	106	ARG	CZ-NH2	-5.62	1.26	1.33
1	D	462	LYS	C-O	-5.61	1.17	1.24
1	B	475	GLY	CA-C	-5.61	1.44	1.51
1	C	459	ILE	CA-CB	-5.57	1.47	1.54
1	C	414	THR	CA-CB	-5.57	1.44	1.53
1	B	460	LYS	C-O	5.56	1.30	1.23
1	C	461	LYS	C-O	-5.54	1.16	1.23
1	C	141	ARG	CZ-NH2	-5.53	1.26	1.33
1	C	187	GLY	CA-C	-5.53	1.44	1.51
1	D	269	ASN	C-O	5.52	1.30	1.24
1	D	174	PHE	CA-C	-5.51	1.45	1.52
1	D	449	ASP	CA-C	-5.51	1.46	1.53
1	B	414	THR	N-CA	5.49	1.53	1.46
1	D	68	VAL	CA-C	5.46	1.59	1.52
1	C	116	ILE	CA-C	-5.45	1.46	1.52
1	D	44	GLN	CD-NE2	-5.45	1.21	1.33
1	D	192	LYS	N-CA	-5.45	1.39	1.46
1	B	47	ARG	CA-C	5.45	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	476	ALA	CA-CB	-5.43	1.44	1.53
1	B	53	ASN	C-O	-5.43	1.17	1.23
1	B	81	PHE	CA-C	-5.43	1.46	1.52
1	C	249	PHE	N-CA	-5.42	1.39	1.46
1	C	398	ARG	CD-NE	-5.39	1.38	1.46
1	B	344	HIS	N-CA	-5.39	1.39	1.46
1	B	160	ASP	CB-CG	5.38	1.65	1.52
1	C	202	ASN	CG-ND2	-5.38	1.22	1.33
1	B	154	LEU	C-O	-5.37	1.17	1.24
1	D	413	ILE	CA-C	5.37	1.59	1.52
1	A	406	VAL	N-CA	-5.36	1.40	1.46
1	D	113	ASN	N-CA	5.36	1.53	1.46
1	D	395	ASP	CA-C	-5.36	1.45	1.52
1	A	216	VAL	CA-CB	5.35	1.61	1.54
1	C	169	ASN	CG-ND2	-5.35	1.22	1.33
1	C	175	ILE	C-O	5.35	1.30	1.24
1	A	289[A]	GLN	C-O	5.34	1.30	1.24
1	A	289[B]	GLN	C-O	5.34	1.30	1.24
1	C	339	THR	C-N	-5.34	1.27	1.33
1	D	467	TYR	C-O	-5.33	1.17	1.24
1	A	69	ALA	CA-C	-5.33	1.45	1.52
1	C	76	LEU	CA-C	-5.33	1.46	1.52
1	A	255	MET	SD-CE	-5.33	1.66	1.79
1	A	458	ARG	CD-NE	5.33	1.53	1.46
1	B	161	ARG	CA-C	5.33	1.59	1.52
1	C	76	LEU	CB-CG	-5.32	1.42	1.53
1	D	62	HIS	CA-CB	-5.32	1.45	1.53
1	D	73	GLU	CA-CB	-5.32	1.45	1.53
1	B	345	VAL	C-O	-5.31	1.18	1.24
1	D	431	LEU	C-O	-5.31	1.17	1.24
1	D	448	ARG	CD-NE	-5.31	1.38	1.46
1	C	271	LEU	C-O	5.29	1.30	1.24
1	A	470	VAL	CA-C	-5.29	1.46	1.52
1	A	410	GLN	C-N	-5.28	1.27	1.33
1	D	471	ILE	CA-C	5.26	1.59	1.52
1	A	252	HIS	CD2-NE2	-5.25	1.32	1.37
1	B	160	ASP	CG-OD1	5.25	1.35	1.25
1	B	171	GLN	CA-C	-5.24	1.45	1.52
1	B	161	ARG	N-CA	-5.24	1.38	1.45
1	C	210	GLN	C-O	5.24	1.30	1.24
1	C	202	ASN	CG-OD1	5.24	1.33	1.23
1	A	175	ILE	C-O	5.23	1.29	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	169	ASN	CG-ND2	-5.21	1.22	1.33
1	A	269	ASN	CG-ND2	-5.20	1.22	1.33
1	B	290	ALA	C-N	-5.20	1.26	1.33
1	D	308	HIS	C-N	-5.19	1.28	1.33
1	C	43	LYS	N-CA	5.17	1.52	1.46
1	D	76	LEU	C-O	5.17	1.29	1.23
1	A	214	HIS	CA-C	-5.15	1.46	1.52
1	C	477	GLU	N-CA	-5.14	1.39	1.46
1	A	281	ALA	CA-C	-5.13	1.45	1.52
1	B	117	GLU	CD-OE1	5.13	1.35	1.25
1	D	309	ASN	C-O	-5.12	1.20	1.24
1	C	164	TYR	CA-CB	-5.11	1.46	1.53
1	D	468	GLN	N-CA	-5.11	1.40	1.46
1	A	43	LYS	CA-C	-5.11	1.45	1.52
1	C	163	LYS	C-O	-5.11	1.17	1.24
1	B	408	GLU	CA-C	-5.10	1.45	1.52
1	A	109	GLU	CA-C	-5.09	1.46	1.52
1	C	379	ASN	CG-OD1	5.08	1.33	1.23
1	C	14	LEU	CA-CB	-5.08	1.46	1.52
1	A	98	GLU	N-CA	-5.07	1.39	1.46
1	B	255	MET	SD-CE	-5.07	1.66	1.79
1	C	391	ASP	N-CA	5.07	1.53	1.46
1	D	10	PRO	CA-CB	-5.06	1.49	1.54
1	A	6	LEU	C-O	-5.06	1.17	1.23
1	B	33	LYS	CA-C	-5.05	1.46	1.52
1	A	251	ASN	CG-ND2	-5.04	1.22	1.33
1	A	216	VAL	N-CA	-5.03	1.40	1.46
1	D	444	VAL	CA-C	-5.03	1.46	1.52
1	A	40	VAL	C-O	5.02	1.29	1.24
1	A	441	TYR	CE2-CZ	-5.02	1.26	1.38
1	D	118	PRO	N-CD	5.01	1.54	1.47
1	A	113	ASN	N-CA	5.01	1.52	1.46
1	B	228	SER	CA-CB	-5.01	1.47	1.53
1	C	471	ILE	CA-C	5.01	1.59	1.52
1	C	398	ARG	CA-C	-5.01	1.46	1.52
1	C	30	GLU	CA-C	-5.00	1.46	1.52

All (126) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	398	ARG	NE-CZ-NH2	12.84	130.75	119.20
1	B	93	ASN	CA-C-N	-12.05	100.66	121.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	93	ASN	C-N-CA	-12.05	100.66	121.39
1	C	384	PHE	O-C-N	-10.84	108.14	122.77
1	B	141	ARG	NE-CZ-NH1	-10.43	111.07	121.50
1	C	11	PRO	CA-C-N	-9.93	107.67	122.86
1	C	11	PRO	C-N-CA	-9.93	107.67	122.86
1	B	47	ARG	CG-CD-NE	-9.40	91.31	112.00
1	A	133	ASP	CA-CB-CG	8.47	121.08	112.60
1	A	468	GLN	O-C-N	8.45	131.07	122.12
1	D	471	ILE	O-C-N	8.41	130.03	121.87
1	D	155	PHE	O-C-N	8.31	130.93	122.12
1	B	289	GLN	CB-CG-CD	8.06	126.31	112.60
1	C	398	ARG	NE-CZ-NH2	8.01	126.41	119.20
1	A	384	PHE	CB-CA-C	7.56	121.61	110.26
1	B	384	PHE	O-C-N	-7.38	112.68	122.57
1	B	398	ARG	NE-CZ-NH2	7.35	125.81	119.20
1	B	355	ASP	O-C-N	-7.24	115.36	121.23
1	D	194	MET	CG-SD-CE	-7.17	85.13	100.90
1	D	11	PRO	CA-C-N	-7.16	111.20	122.73
1	D	11	PRO	C-N-CA	-7.16	111.20	122.73
1	D	411	ARG	NE-CZ-NH2	-7.14	112.77	119.20
1	C	10	PRO	N-CA-CB	7.14	106.93	103.22
1	B	141	ARG	NH1-CZ-NH2	7.12	128.55	119.30
1	C	100	GLY	O-C-N	-7.09	115.38	122.19
1	D	10	PRO	N-CA-CB	6.97	106.84	103.22
1	D	289	GLN	CB-CG-CD	6.92	124.36	112.60
1	A	401	TYR	O-C-N	-6.80	114.74	122.09
1	C	413	ILE	O-C-N	6.74	128.41	121.87
1	C	289	GLN	CB-CG-CD	6.67	123.95	112.60
1	A	193	ARG	NE-CZ-NH1	-6.64	114.86	121.50
1	D	398	ARG	O-C-N	-6.64	114.57	122.15
1	B	162	VAL	O-C-N	6.64	130.08	123.18
1	A	355	ASP	O-C-N	-6.59	115.57	121.17
1	D	112	ARG	CA-CB-CG	-6.57	100.96	114.10
1	A	476	ALA	O-C-N	-6.49	113.51	122.46
1	A	460	LYS	O-C-N	-6.47	114.93	122.95
1	D	413	ILE	O-C-N	6.43	128.11	121.87
1	A	384	PHE	O-C-N	-6.35	114.96	122.96
1	A	117	GLU	O-C-N	6.11	126.50	121.31
1	C	66	GLU	CG-CD-OE2	-6.10	104.36	118.40
1	B	410	GLN	O-C-N	6.09	128.58	122.12
1	A	252	HIS	CB-CG-CD2	-6.03	123.37	131.20
1	B	457	ARG	CA-CB-CG	6.01	126.12	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	16	GLY	CA-C-O	6.01	126.94	121.47
1	A	66	GLU	CG-CD-OE2	-6.00	104.59	118.40
1	C	471	ILE	O-C-N	5.99	128.00	121.83
1	C	384	PHE	N-CA-C	-5.95	100.59	109.15
1	D	252	HIS	CB-CG-CD2	-5.93	123.50	131.20
1	D	112	ARG	O-C-N	5.92	128.39	122.12
1	D	141	ARG	NE-CZ-NH1	-5.92	115.58	121.50
1	B	93	ASN	CB-CA-C	5.91	122.18	110.42
1	C	291	ALA	O-C-N	-5.91	114.60	122.28
1	C	413	ILE	CA-C-O	-5.90	114.81	120.95
1	A	384	PHE	N-CA-C	-5.90	100.92	109.59
1	D	445	TYR	CA-C-O	-5.86	114.60	121.16
1	B	97	ASN	CA-C-O	5.83	126.60	120.54
1	D	438	GLN	N-CA-C	5.81	118.56	111.82
1	B	104	TYR	O-C-N	5.78	129.38	122.27
1	A	265	GLN	N-CA-C	5.73	117.61	111.36
1	D	440	ARG	O-C-N	-5.70	116.54	123.16
1	D	60	HIS	O-C-N	5.70	128.88	122.22
1	D	187	GLY	O-C-N	-5.63	116.80	122.54
1	C	252	HIS	CB-CG-CD2	-5.61	123.91	131.20
1	A	198	ASN	OD1-CG-ND2	5.61	128.21	122.60
1	C	366	ILE	O-C-N	5.60	127.59	121.83
1	C	93	ASN	CA-C-N	-5.59	112.04	120.65
1	C	93	ASN	C-N-CA	-5.59	112.04	120.65
1	D	142	ARG	NH1-CZ-NH2	5.58	126.56	119.30
1	A	413	ILE	O-C-N	5.58	127.28	121.87
1	C	260	TRP	O-C-N	-5.57	115.80	122.27
1	D	355	ASP	O-C-N	-5.54	116.46	121.17
1	B	360	ARG	NE-CZ-NH2	-5.54	114.22	119.20
1	B	97	ASN	O-C-N	-5.54	116.46	123.05
1	D	97[A]	ASN	O-C-N	-5.53	116.06	122.87
1	D	97[B]	ASN	O-C-N	-5.53	116.06	122.87
1	D	63	ARG	NE-CZ-NH1	-5.51	115.99	121.50
1	A	401	TYR	CA-C-N	5.49	127.57	120.44
1	A	401	TYR	C-N-CA	5.49	127.57	120.44
1	A	463	SER	O-C-N	-5.49	115.80	122.22
1	B	398	ARG	CD-NE-CZ	5.47	132.05	124.40
1	C	175	ILE	O-C-N	-5.44	116.25	121.90
1	D	428	THR	N-CA-CB	5.38	118.95	110.56
1	D	108	ILE	O-C-N	5.37	127.08	121.87
1	B	111	LEU	O-C-N	5.34	127.57	122.07
1	D	446	VAL	CA-C-O	5.33	126.13	120.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	314	VAL	N-CA-C	5.32	116.27	109.30
1	D	104	TYR	CA-C-O	5.32	126.08	119.97
1	D	398	ARG	CD-NE-CZ	5.32	131.84	124.40
1	D	25	GLU	CA-C-O	-5.29	114.81	120.42
1	B	69	ALA	O-C-N	-5.29	116.03	122.22
1	A	272	GLU	N-CA-C	-5.29	105.69	111.82
1	A	66	GLU	CG-CD-OE1	5.28	130.55	118.40
1	D	211	SER	O-C-N	-5.28	116.52	122.12
1	D	413	ILE	CA-C-O	-5.28	115.46	120.95
1	D	238	GLU	CG-CD-OE1	-5.27	106.28	118.40
1	C	43	LYS	CA-CB-CG	-5.25	103.60	114.10
1	A	337	PHE	CA-C-O	-5.24	115.67	121.28
1	B	107	LEU	O-C-N	5.24	127.47	122.07
1	B	154	LEU	N-CA-C	5.23	116.98	111.28
1	D	204	ALA	CA-C-O	5.22	126.08	120.55
1	A	192	LYS	CB-CG-CD	5.20	123.27	111.30
1	B	415	ASP	CA-CB-CG	5.19	117.79	112.60
1	C	134	ALA	O-C-N	-5.18	116.50	122.09
1	B	403	ARG	NE-CZ-NH1	5.16	126.66	121.50
1	D	398	ARG	CA-C-N	5.14	127.04	120.56
1	D	398	ARG	C-N-CA	5.14	127.04	120.56
1	C	474	ASN	OD1-CG-ND2	-5.14	117.46	122.60
1	C	365	ARG	NE-CZ-NH2	-5.14	114.58	119.20
1	C	153	THR	CA-C-O	5.14	126.21	120.82
1	B	398	ARG	NE-CZ-NH1	-5.13	116.37	121.50
1	B	384	PHE	CB-CA-C	5.12	119.70	111.05
1	D	398	ARG	NE-CZ-NH1	-5.12	116.38	121.50
1	D	100	GLY	O-C-N	-5.09	117.29	122.18
1	C	184	HIS	ND1-CE1-NE2	5.09	113.49	108.40
1	B	470	VAL	O-C-N	-5.08	116.93	121.91
1	B	441	TYR	OH-CZ-CE2	-5.08	104.68	119.90
1	D	174	PHE	CA-CB-CG	5.07	118.87	113.80
1	A	215	TYR	CA-C-O	5.06	124.71	119.14
1	A	256	ASP	CA-CB-CG	5.05	117.65	112.60
1	D	269	ASN	CB-CG-ND2	5.05	123.97	116.40
1	B	384	PHE	N-CA-C	-5.03	99.58	108.23
1	C	281	ALA	CA-C-O	5.02	125.81	120.63
1	C	211	SER	O-C-N	-5.02	116.80	122.12
1	D	238	GLU	CB-CG-CD	5.02	121.13	112.60
1	B	353	ALA	N-CA-C	-5.00	103.45	110.50

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	43	0
1	B	3911	0	3750	34	0
1	C	3914	0	3770	50	0
1	D	3875	0	3706	31	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	18	0
8	B	638	0	0	14	0
8	C	692	0	0	21	0
8	D	608	0	0	17	0
All	All	18396	0	15229	157	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 (157) 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:C:132[A]:MET:HE3	8:C:1116:HOH:O	1.58	1.01
1:C:191[B]:MET:HE1	8:C:1242:HOH:O	1.66	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:D:132[A]:MET:HE3	8:D:1075:HOH:O	1.68	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:D:249:PHE:CE2	1:D:333:ILE:HD11	2.13	0.83
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:C:93:ASN:HD22	1:C:93:ASN:C	2.07	0.63
1:C:262[B]:MET:HE2	8:C:877:HOH:O	1.99	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:93:ASN:C	1:A:93:ASN:HD22	2.09	0.60
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: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
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: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:192:LYS:NZ	8:B:608:HOH:O	2.37	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:C:73:GLU:CD	1:C:460[B]:LYS:HE2	2.32	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:A:198:ASN:HD21	1:A:254:TRP:NE1	2.05	0.52
1:D:460:LYS:HE2	8:D:1109:HOH:O	2.09	0.52
1:B:93:ASN:C	1:B:93:ASN:HD22	2.16	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:C:198:ASN:HD21	1:C:254:TRP:NE1	2.07	0.51
1:A:403[B]:ARG:HD3	1:A:478:LEU:C	2.36	0.51
1:B:112:ARG:HG2	8:B:612:HOH:O	2.09	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:192:LYS:HD2	8:C:865:HOH:O	2.10	0.50
1:D:272:GLU:CD	8:D:639:HOH:O	2.54	0.50
1:B:198:ASN:HD21	1:B:254:TRP:NE1	2.07	0.50
1:D:132[A]:MET:HE1	8:D:742:HOH:O	2.10	0.50
1:D:331:SER:O	1:D:339[B]:THR:HG22	2.11	0.50
1:D:93:ASN:HD22	1:D:93:ASN:C	2.20	0.49
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: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:D:198:ASN:HD21	1:D:254:TRP:NE1	2.08	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:A:469[A]:ARG:HE	1:A:477:GLU:CD	2.19	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
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:O	1:C:5:HIS:CG	2.68	0.46
1:A:350:TRP:CD1	1:A:439:LYS:HD2	2.50	0.46
1:D:132[A]:MET:CE	8:D:1075:HOH:O	2.42	0.46
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:A:210[B]:GLN:NE2	8:A:621:HOH:O	2.50	0.45
1:A:453:GLU:OE1	5:A:507:IMD:N1	2.37	0.45
1:D:430:LEU:C	1:D:430:LEU:HD12	2.42	0.45
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:156:GLN:HE22	1:B:349[A]:ASN:HD22	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:350[A]:TRP:O	1:B:351[A]:ASP:CG	2.61	0.43
1:A:194[B]:MET:HB3	1:A:194[B]:MET:HE2	1.64	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:C:194[B]:MET:HE2	1:C:195:TYR:CE2	2.54	0.43
1:C:460[B]:LYS:NZ	8:C:610: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:C:132[A]:MET:HE1	8:C:739:HOH:O	2.18	0.42
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:170:GLN:HE21	1:D:226:ALA:HB2	1.84	0.42
1:B:194[B]:MET:HE2	1:B:194[B]:MET:HB3	1.89	0.42
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:94:GLY:O	1:C:149:ARG:NH2	2.39	0.41
1:C:214:HIS:HE1	1:D:383[A]:GLU:CG	2.28	0.41
1:A:262[B]:MET:HE2	8:A:850:HOH:O	2.20	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:378:GLU:HG3	1:C:425:TRP:HB2	2.02	0.41
1:C:394:ASN:ND2	8:C:618:HOH:O	2.46	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:C:153:THR:O	1:C:157[B]:ARG:HG2	2.21	0.40
1:C:430:LEU:C	1:C:430:LEU:HD12	2.46	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	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%)	43	19
1	D	475/485 (98%)	457 (96%)	16 (3%)	2 (0%)	30	10
All	All	1918/1940 (99%)	1849 (96%)	66 (3%)	3 (0%)	43	19

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%)	81	61
1	B	412/412 (100%)	406 (98%)	6 (2%)	57	26
1	C	415/412 (101%)	410 (99%)	5 (1%)	63	34
1	D	409/412 (99%)	403 (98%)	6 (2%)	57	26
All	All	1654/1648 (100%)	1635 (99%)	19 (1%)	73	37

All (19) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	93	ASN
1	A	192	LYS
1	B	7	LYS
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	C	262[A]	MET
1	C	262[B]	MET
1	C	262[C]	MET
1	D	6	LEU
1	D	7	LYS
1	D	93	ASN
1	D	262[A]	MET
1	D	262[B]	MET
1	D	262[C]	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (62) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	5	HIS
1	A	93	ASN
1	A	169	ASN
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	274	GLN
1	A	344	HIS
1	A	394	ASN
1	A	410	GLN
1	B	65	GLN
1	B	93	ASN
1	B	129	GLN
1	B	169	ASN
1	B	170	GLN

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Mol	Chain	Res	Type
1	B	171	GLN
1	B	198	ASN
1	B	202	ASN
1	B	205	ASN
1	B	214	HIS
1	B	265	GLN
1	B	269	ASN
1	B	274	GLN
1	B	289	GLN
1	B	468	GLN
1	C	5	HIS
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	252	HIS
1	C	265	GLN
1	C	269	ASN
1	C	274	GLN
1	C	468	GLN
1	D	93	ASN
1	D	129	GLN
1	D	169	ASN
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	274	GLN
1	D	349	ASN
1	D	394	ASN
1	D	410	GLN
1	D	468	GLN

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	0.72	0	17,17,17	2.10	6 (35%)
2	0WK	E	2	2	15,15,15	1.98	4 (26%)	21,22,22	2.79	7 (33%)

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	-4.66	1.33	1.43
2	E	2	0WK	P-O3P	-3.75	1.40	1.54
2	E	2	0WK	O3-C3	3.39	1.51	1.43
2	E	2	0WK	C4-C3	2.00	1.57	1.52

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	2	0WK	O3-C3-C4	7.23	127.41	110.38
2	E	2	0WK	C1-C2-C3	5.42	117.54	109.64
2	E	2	0WK	O3-C3-C2	-5.24	99.35	110.05
2	E	2	0WK	O2-C2-C1	-4.67	98.52	109.22
2	E	1	BGC	C1-C2-C3	-3.64	102.93	110.36
2	E	2	0WK	O2P-P-O1P	3.23	123.43	110.83
2	E	1	BGC	O2-C2-C3	3.11	117.72	110.38
2	E	1	BGC	O5-C1-C2	-3.07	104.90	110.30
2	E	1	BGC	O5-C5-C6	-2.97	99.08	106.44
2	E	1	BGC	O3-C3-C4	-2.86	103.64	110.38
2	E	2	0WK	O2-C2-C3	-2.82	104.30	110.15
2	E	1	BGC	O2-C2-C1	2.42	114.83	109.25
2	E	2	0WK	O4-C4-C5	-2.30	103.67	109.32

There are no chirality outliers.

All (2) torsion outliers are listed below:

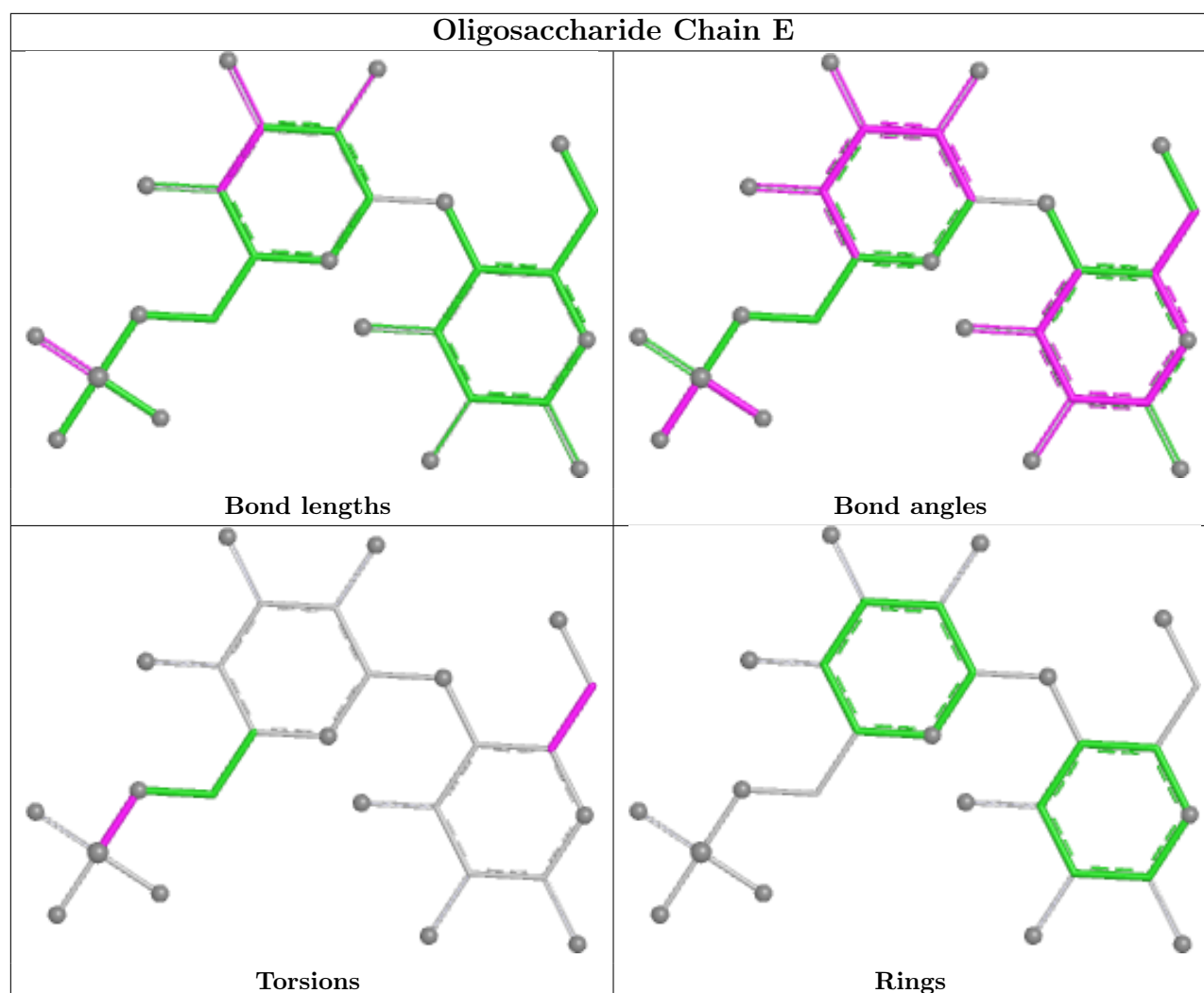
Mol	Chain	Res	Type	Atoms
2	E	1	BGC	O5-C5-C6-O6
2	E	2	0WK	C6-O6-P-O2P

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	2.11	4 (25%)	23,24,24	3.44	12 (52%)
4	GOL	C	503	-	5,5,5	0.73	0	5,5,5	1.03	0
4	GOL	A	506	-	5,5,5	0.31	0	5,5,5	1.25	0
6	0WK	C	506	-	15,15,15	2.13	4 (26%)	21,22,22	4.20	9 (42%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	GOL	A	503	-	5,5,5	0.29	0	5,5,5	1.63	1 (20%)
4	GOL	A	504	-	5,5,5	1.04	0	5,5,5	1.60	1 (20%)
4	GOL	D	501	-	5,5,5	0.34	0	5,5,5	0.79	0
4	GOL	B	502	-	5,5,5	0.79	0	5,5,5	1.12	0
4	GOL	C	501	-	5,5,5	0.98	0	5,5,5	1.84	2 (40%)
4	GOL	A	505	-	5,5,5	0.90	0	5,5,5	1.49	1 (20%)
5	IMD	A	507	-	5,5,5	0.97	0	5,5,5	1.26	0
7	BGC	C	507	-	12,12,12	1.26	1 (8%)	17,17,17	3.37	12 (70%)
4	GOL	A	502	-	5,5,5	0.39	0	5,5,5	1.04	0
5	IMD	C	505	-	5,5,5	0.91	0	5,5,5	0.47	0
4	GOL	C	504	-	5,5,5	0.80	0	5,5,5	1.53	1 (20%)
4	GOL	C	502	-	5,5,5	1.08	1 (20%)	5,5,5	1.29	1 (20%)
5	IMD	D	502	-	5,5,5	0.74	0	5,5,5	0.60	0
3	BG6	A	501	-	16,16,16	2.18	4 (25%)	23,24,24	3.08	7 (30%)
4	GOL	B	503	-	5,5,5	0.42	0	5,5,5	1.10	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	C	503	-	-	0/4/4/4	-
4	GOL	A	506	-	-	4/4/4/4	-
6	0WK	C	506	-	-	1/6/23/23	0/1/1/1
4	GOL	A	503	-	-	0/4/4/4	-
4	GOL	A	504	-	-	0/4/4/4	-
4	GOL	D	501	-	-	1/4/4/4	-
4	GOL	B	502	-	-	0/4/4/4	-
4	GOL	C	501	-	-	0/4/4/4	-
4	GOL	A	505	-	-	0/4/4/4	-
5	IMD	A	507	-	-	-	0/1/1/1
7	BGC	C	507	-	-	2/2/22/22	0/1/1/1
4	GOL	A	502	-	-	0/4/4/4	-
5	IMD	C	505	-	-	-	0/1/1/1
4	GOL	C	504	-	-	2/4/4/4	-
4	GOL	C	502	-	-	0/4/4/4	-
5	IMD	D	502	-	-	-	0/1/1/1
3	BG6	A	501	-	-	1/6/26/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	GOL	B	503	-	-	2/4/4/4	-

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	501	BG6	O2-C2	-5.14	1.30	1.43
6	C	506	0WK	O2-C2	-4.88	1.33	1.43
3	B	501	BG6	O2-C2	-4.74	1.31	1.43
3	A	501	BG6	O3-C3	4.58	1.54	1.43
3	B	501	BG6	O3-C3	4.29	1.53	1.43
6	C	506	0WK	O3-C3	3.99	1.52	1.43
3	B	501	BG6	C4-C3	3.39	1.61	1.52
6	C	506	0WK	C4-C3	3.05	1.60	1.52
3	A	501	BG6	P-O1P	-2.94	1.43	1.54
7	C	507	BGC	O5-C1	2.80	1.49	1.42
6	C	506	0WK	P-O3P	2.68	1.64	1.54
3	A	501	BG6	C4-C3	2.63	1.59	1.52
3	B	501	BG6	P-O2P	-2.27	1.46	1.54
4	C	502	GOL	O2-C2	2.18	1.49	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	-11.71	76.14	106.67
3	A	501	BG6	O3-C3-C4	9.70	133.24	110.38
3	B	501	BG6	O3-C3-C4	9.00	131.59	110.38
6	C	506	0WK	O3-C3-C4	8.26	129.84	110.38
6	C	506	0WK	C1-C2-C3	8.04	121.36	109.64
3	B	501	BG6	O2-C2-C1	-6.75	93.67	109.25
6	C	506	0WK	O3-C3-C2	-6.21	97.38	110.05
7	C	507	BGC	O2-C2-C1	6.13	123.40	109.25
3	A	501	BG6	O2-C2-C1	-5.75	95.96	109.25
7	C	507	BGC	C1-C2-C3	-5.57	99.00	110.36
3	B	501	BG6	O3-C3-C2	-5.53	97.35	110.38
7	C	507	BGC	O5-C5-C6	5.33	119.64	106.44
3	A	501	BG6	O3-C3-C2	-5.21	98.09	110.38
3	B	501	BG6	C1-C2-C3	5.21	120.97	110.36
6	C	506	0WK	O3P-P-O2P	5.06	126.79	107.80
3	A	501	BG6	C1-C2-C3	4.89	120.34	110.36
7	C	507	BGC	O3-C3-C4	4.28	120.46	110.38
3	B	501	BG6	O2-C2-C3	-3.71	101.63	110.38
3	B	501	BG6	O2P-P-O6	3.46	115.70	106.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	C	507	BGC	O1-C1-O5	3.42	120.56	110.41
7	C	507	BGC	C3-C4-C5	-3.36	104.15	110.23
7	C	507	BGC	C1-O5-C5	-3.34	107.19	113.65
3	B	501	BG6	O4-C4-C3	3.33	118.23	110.38
4	A	503	GOL	O3-C3-C2	3.30	125.25	110.38
7	C	507	BGC	O5-C1-C2	-3.18	104.70	110.30
7	C	507	BGC	C4-C3-C2	-3.16	105.27	110.83
3	B	501	BG6	O4-C4-C5	-3.14	101.59	109.32
3	B	501	BG6	C6-C5-C4	3.12	118.61	112.07
4	C	501	GOL	O3-C3-C2	3.11	124.38	110.38
6	C	506	0WK	O2-C2-C1	-2.95	102.46	109.22
4	A	504	GOL	O3-C3-C2	2.95	123.65	110.38
3	B	501	BG6	O2P-P-O3P	-2.89	99.58	110.83
3	A	501	BG6	O4-C4-C5	-2.72	102.63	109.32
3	A	501	BG6	O2P-P-O3P	2.70	121.35	110.83
6	C	506	0WK	O3P-P-O1P	2.67	121.25	110.83
7	C	507	BGC	O4-C4-C5	-2.63	102.84	109.32
4	A	505	GOL	O3-C3-C2	2.54	121.81	110.38
3	B	501	BG6	O1P-P-O3P	2.53	120.69	110.83
3	A	501	BG6	O4-C4-C3	2.51	116.28	110.38
3	B	501	BG6	O1P-P-O6	-2.50	100.16	106.67
7	C	507	BGC	O6-C6-C5	2.44	119.66	111.33
7	C	507	BGC	O4-C4-C3	2.34	115.89	110.38
4	C	504	GOL	C3-C2-C1	2.33	120.34	111.80
4	C	501	GOL	C3-C2-C1	-2.30	103.36	111.80
6	C	506	0WK	O4-C4-C3	2.18	115.50	110.38
6	C	506	0WK	O2-C2-C3	-2.15	105.70	110.15
4	C	502	GOL	O3-C3-C2	2.08	119.73	110.38

There are no chirality outliers.

All (14) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	506	GOL	C1-C2-C3-O3
4	B	503	GOL	O1-C1-C2-C3
4	C	504	GOL	C1-C2-C3-O3
4	C	504	GOL	O2-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

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

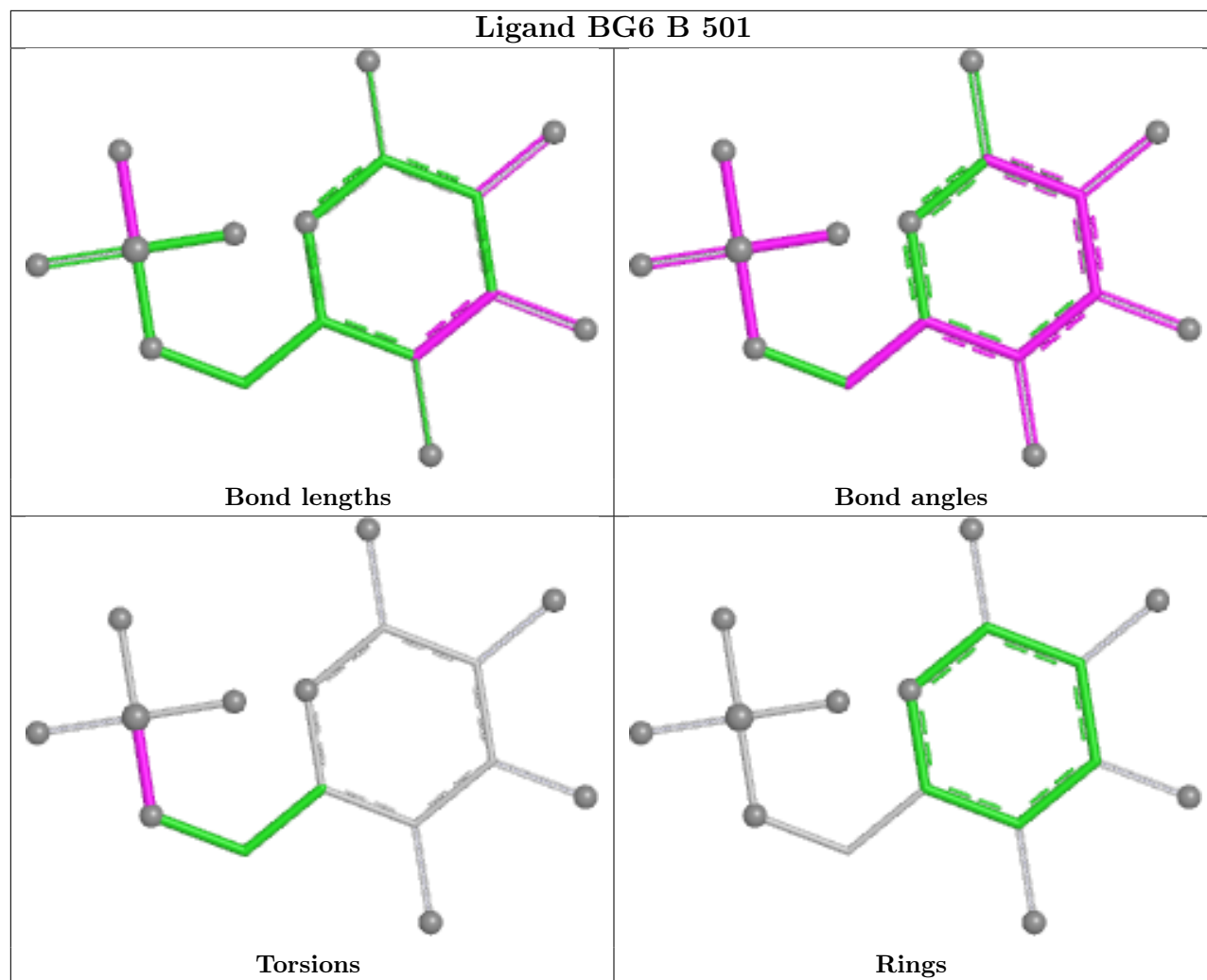
There are no ring outliers.

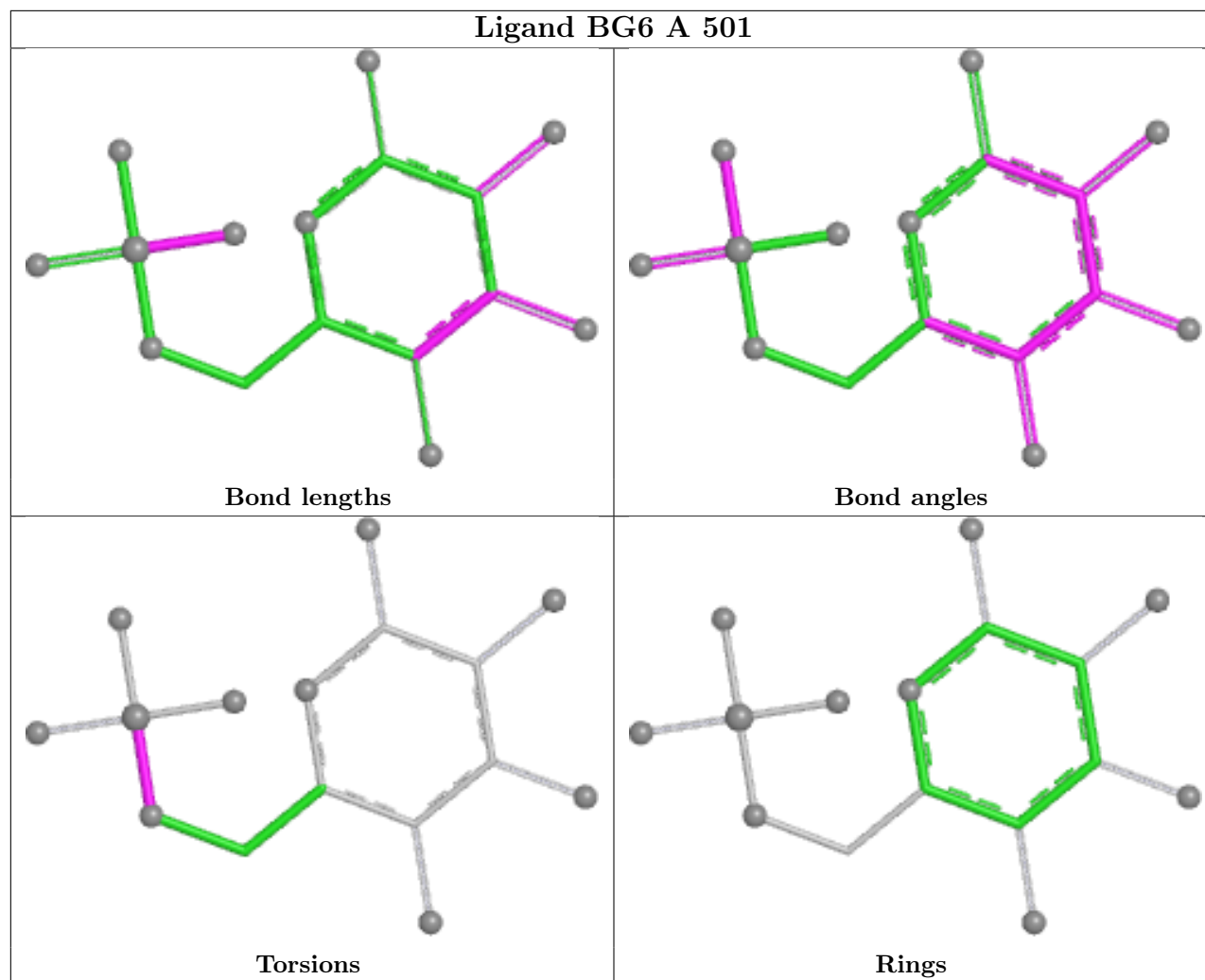
7 monomers are involved in 11 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	506	GOL	2	0
6	C	506	0WK	1	0
4	A	505	GOL	1	0
5	A	507	IMD	1	0
7	C	507	BGC	4	0
4	C	504	GOL	1	0
5	D	502	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, 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	461/485 (95%)	-0.37	8 (1%) 69 72	4, 10, 27, 74	27 (5%)
1	B	461/485 (95%)	-0.42	7 (1%) 72 75	5, 10, 24, 61	20 (4%)
1	C	461/485 (95%)	-0.51	10 (2%) 62 65	4, 9, 22, 68	22 (4%)
1	D	461/485 (95%)	-0.39	10 (2%) 62 65	5, 11, 25, 76	17 (3%)
All	All	1844/1940 (95%)	-0.42	35 (1%) 66 69	4, 10, 25, 76	86 (4%)

All (35) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	350	TRP	7.8
1	B	350[A]	TRP	7.5
1	A	329	THR	5.3
1	B	329	THR	4.4
1	D	5	HIS	4.2
1	A	5	HIS	3.6
1	B	352	TRP	3.6
1	D	310	PRO	3.6
1	C	5	HIS	3.6
1	A	352	TRP	3.5
1	D	313	GLY	3.5
1	C	311	PRO	3.5
1	C	315	GLY	3.4
1	D	315	GLY	3.4
1	B	5	HIS	3.3
1	D	329	THR	3.1
1	B	349[A]	ASN	3.1
1	B	315	GLY	3.1
1	B	351[A]	ASP	3.0
1	D	352	TRP	3.0
1	C	310	PRO	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	314	VAL	2.8
1	D	350	TRP	2.8
1	D	314	VAL	2.6
1	C	352	TRP	2.6
1	A	315	GLY	2.6
1	C	312	ASP	2.6
1	C	329	THR	2.5
1	C	313	GLY	2.5
1	A	313	GLY	2.3
1	A	476	ALA	2.2
1	D	311	PRO	2.2
1	A	6	LEU	2.1
1	D	12	GLU	2.1
1	C	384	PHE	2.0

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

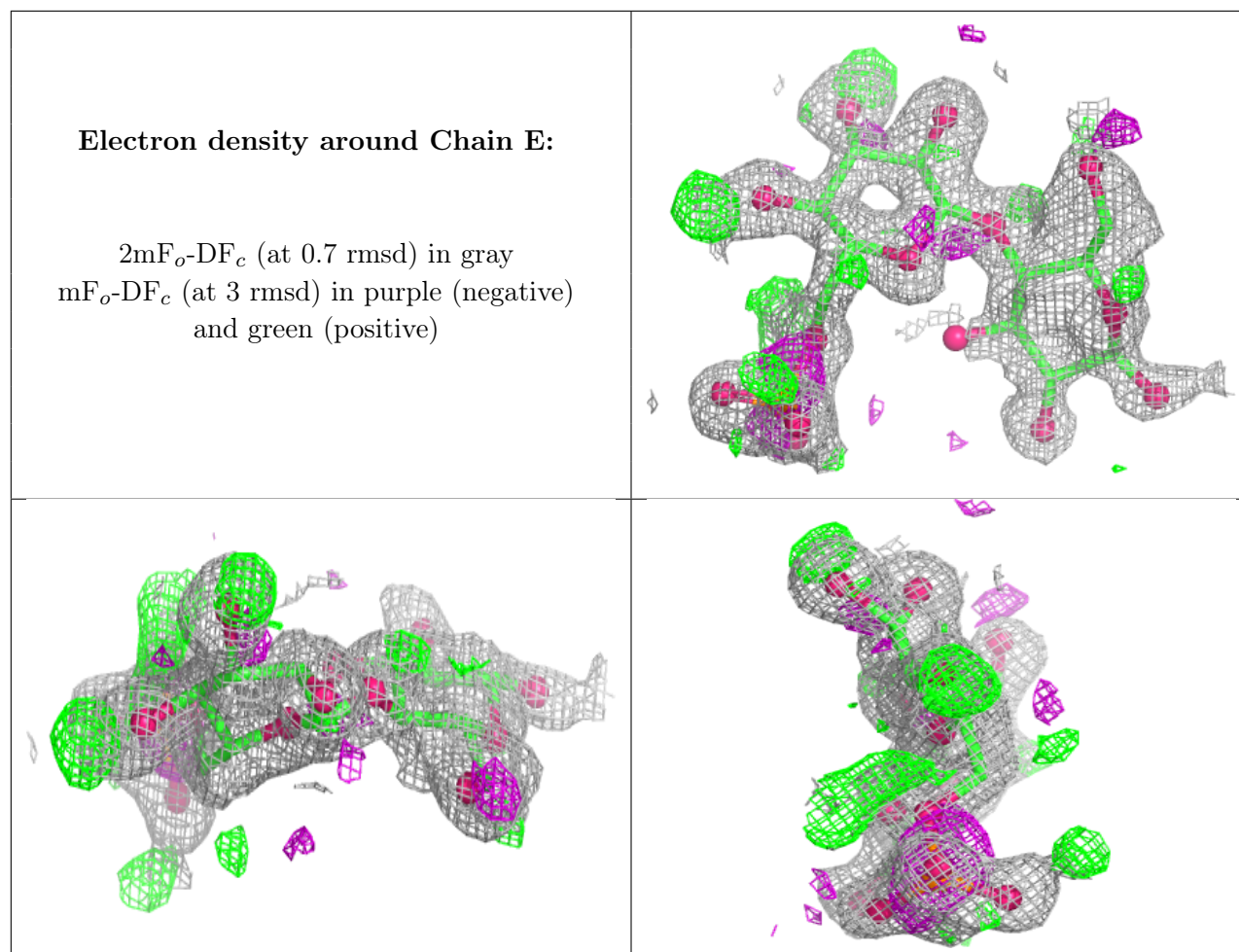
There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

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
2	BGC	E	1	12/12	0.81	0.12	21,36,42,50	12
2	0WK	E	2	15/15	0.91	0.10	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, 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
7	BGC	C	507	12/12	0.68	0.18	24,42,54,60	12
4	GOL	D	501	6/6	0.76	0.13	39,40,43,50	0
4	GOL	B	503	6/6	0.79	0.16	31,40,44,47	0
4	GOL	A	505	6/6	0.80	0.14	31,42,49,50	0
4	GOL	A	502	6/6	0.81	0.14	36,36,40,42	0
4	GOL	C	503	6/6	0.81	0.13	30,38,43,54	0
4	GOL	B	502	6/6	0.84	0.13	25,41,43,46	0
5	IMD	D	502	5/5	0.84	0.12	17,21,23,25	5
4	GOL	C	504	6/6	0.84	0.14	37,44,46,59	0
5	IMD	A	507	5/5	0.85	0.10	25,28,32,32	0
3	BG6	B	501	16/16	0.85	0.13	9,26,41,43	16

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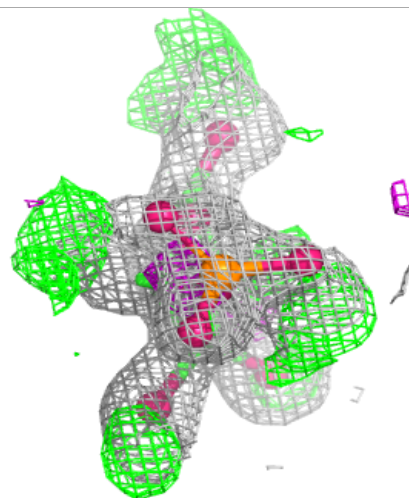
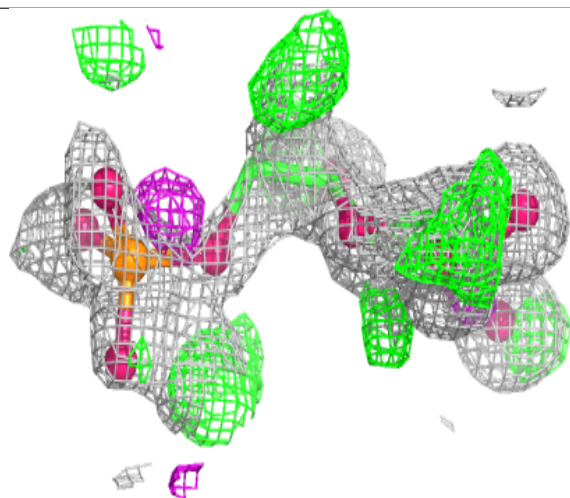
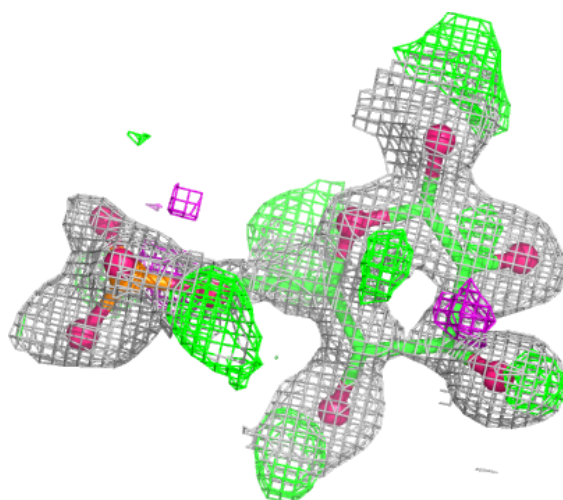
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
6	0WK	C	506	15/15	0.85	0.14	10,20,39,42	15
3	BG6	A	501	16/16	0.85	0.14	8,28,41,44	16
5	IMD	C	505	5/5	0.89	0.12	23,29,30,32	0
4	GOL	A	506	6/6	0.91	0.10	36,40,44,45	0
4	GOL	A	504	6/6	0.94	0.07	13,19,24,26	0
4	GOL	C	502	6/6	0.95	0.07	15,18,21,26	0
4	GOL	C	501	6/6	0.96	0.07	13,17,24,27	0
4	GOL	A	503	6/6	0.96	0.06	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.

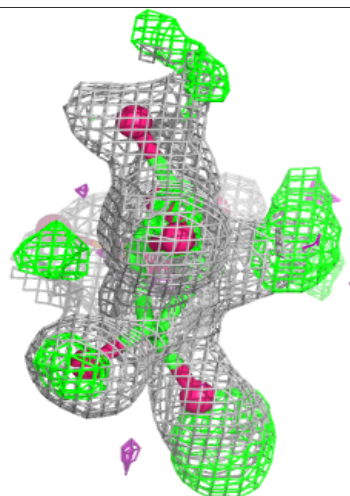
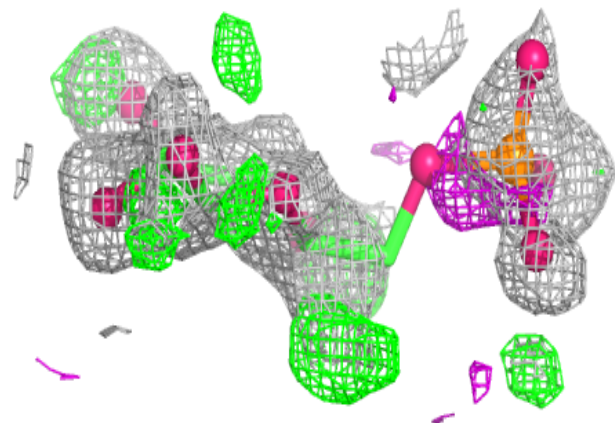
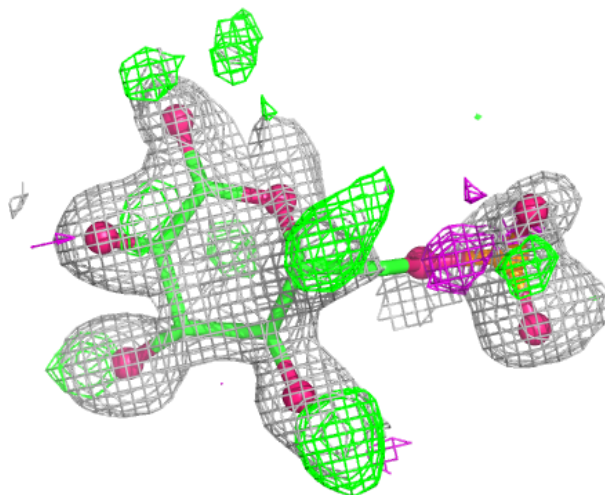
Electron density around BG6 B 501:

2mF_o-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (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 ⓘ

There are no such residues in this entry.