Full wwPDB X-ray Structure Validation Report (i)

Nov 13, 2023 – 07:03 PM JST

PDB ID	:	5XQG
Title	:	Crystal structure of a PL 26 exo-rhamnogalacturonan lyase from Penicillium chrysogenum complexed with unsaturated galacturonosyl rhamnose
Authors	:	Kunishige, Y.; Iwai, M.; Tada, T.; Nishimura, S.; Sakamoto, T.
Deposited on	:	2017-06-07
Resolution	:	2.74 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 (i) 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 (i)) were used in the production of this report:

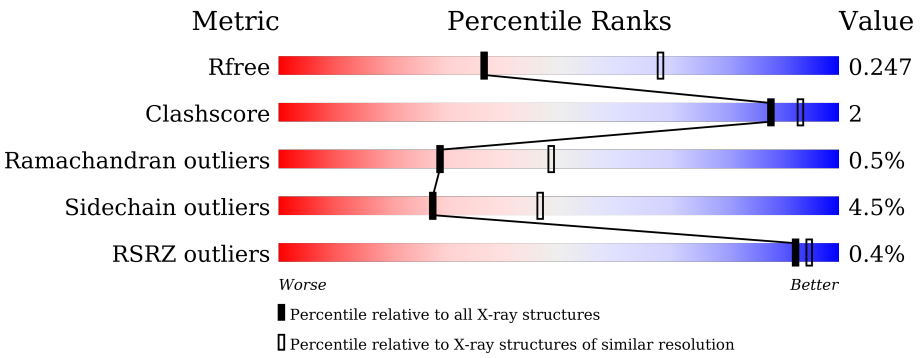
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

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 2.74 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1271 (2.76-2.72)
Clashscore	141614	1322 (2.76-2.72)
Ramachandran outliers	138981	1297 (2.76-2.72)
Sidechain outliers	138945	1298 (2.76-2.72)
RSRZ outliers	127900	1243 (2.76-2.72)

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 <=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	906	89% 9% ••
1	B	906	90% 8% ••
1	C	906	89% 8% ••
1	D	906	89% 8% ••
1	E	906	90% 8% ••
1	F	906	92% 7% ••

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Mol	Chain	Length	Quality of chain
1	G	906	% 88% 8%
1	H	906	% 88% 9%
2	I	2	100%
2	J	2	100%
2	K	2	100%
2	L	2	50% 50%
2	M	2	100%
2	N	2	50% 50%
2	O	2	50% 50%
2	P	2	100%

2 Entry composition (i)

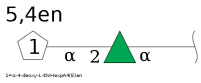
There are 4 unique types of molecules in this entry. The entry contains 57208 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Pcrglx protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	896	7025	4479	1178	1362	6	0	1	0
1	B	896	7052	4492	1182	1372	6	0	2	0
1	C	885	7007	4473	1176	1352	6	0	5	0
1	D	884	6994	4464	1174	1350	6	0	6	0
1	E	899	7054	4493	1183	1372	6	0	1	0
1	F	900	7040	4487	1183	1364	6	0	0	0
1	G	888	6989	4460	1170	1353	6	0	1	0
1	H	888	6997	4462	1174	1355	6	0	1	0

- Molecule 2 is an oligosaccharide called 2,6-anhydro-3-deoxy-L-threo-hex-2-enonic acid-(1-2)-alpha-L-rhamnopyranose.



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf	Trace
			Total	C	O			
2	I	2	22	12	10	0	0	0
2	J	2	22	12	10	0	0	0
2	K	2	22	12	10	0	0	0
2	L	2	22	12	10	0	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	M	2	Total C O 22 12 10	0	0	0
2	N	2	Total C O 22 12 10	0	0	0
2	O	2	Total C O 22 12 10	0	0	0
2	P	2	Total C O 22 12 10	0	0	0

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total Ca 1 1	0	0
3	B	1	Total Ca 1 1	0	0
3	C	1	Total Ca 1 1	0	0
3	D	1	Total Ca 1 1	0	0
3	E	1	Total Ca 1 1	0	0
3	F	1	Total Ca 1 1	0	0
3	G	1	Total Ca 1 1	0	0
3	H	1	Total Ca 1 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	122	Total O 122 122	0	0
4	B	128	Total O 128 128	0	0
4	C	122	Total O 122 122	0	0
4	D	95	Total O 95 95	0	0
4	E	122	Total O 122 122	0	0

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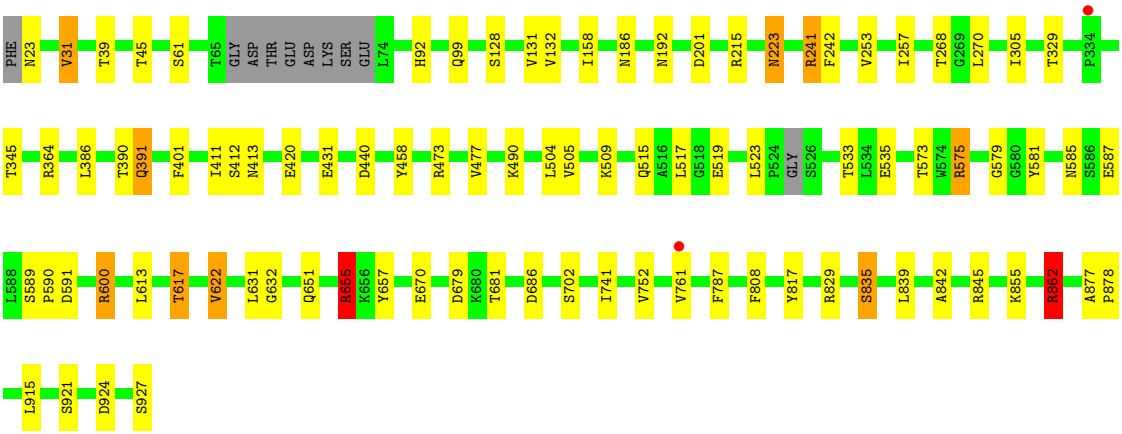
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	O		
4	F	116	116	116	0	0
			Total	O		
4	G	72	72	72	0	0
			Total	O		
4	H	89	89	89	0	0

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.

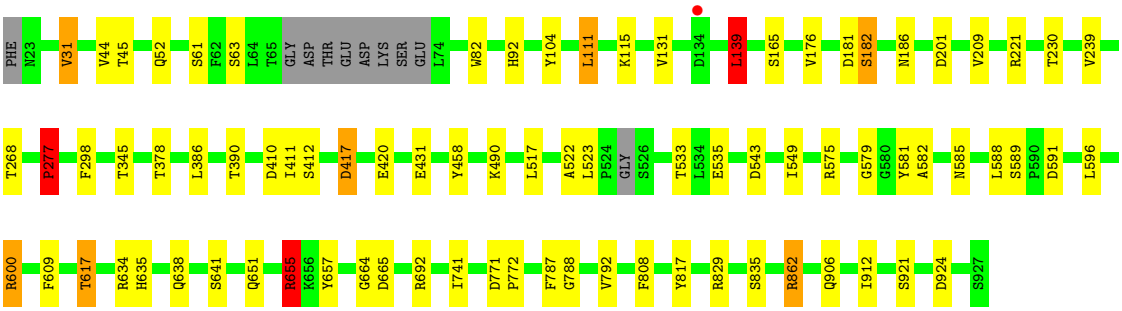
• Molecule 1: Pcrglx protein

Chain A: 89% 9% ••



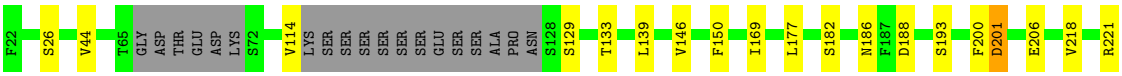
• Molecule 1: Pcrglx protein

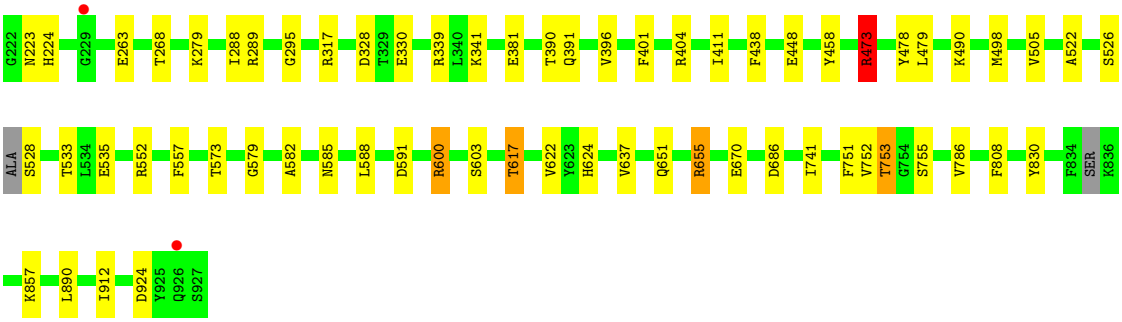
Chain B: 90% 8% ••



• Molecule 1: Pcrglx protein

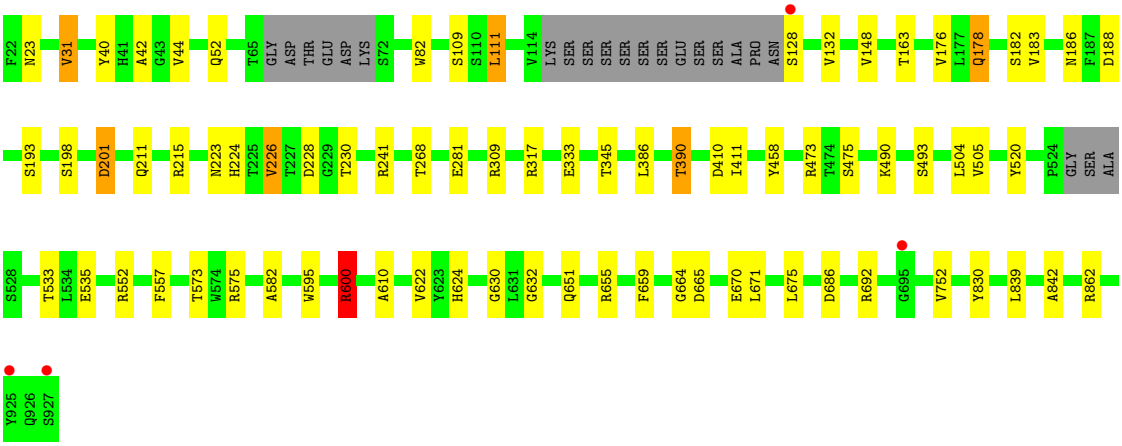
Chain C: 89% 8% ••





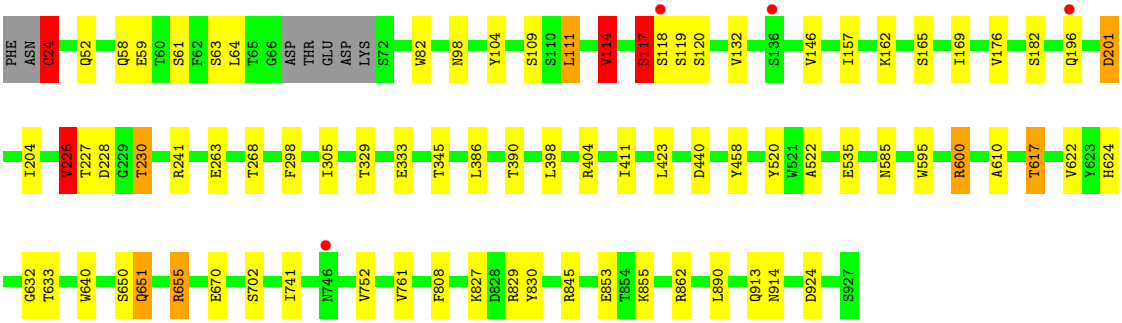
• Molecule 1: Pcrglx protein

Chain D:



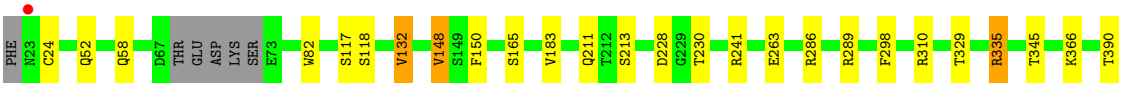
• Molecule 1: Pcrglx protein

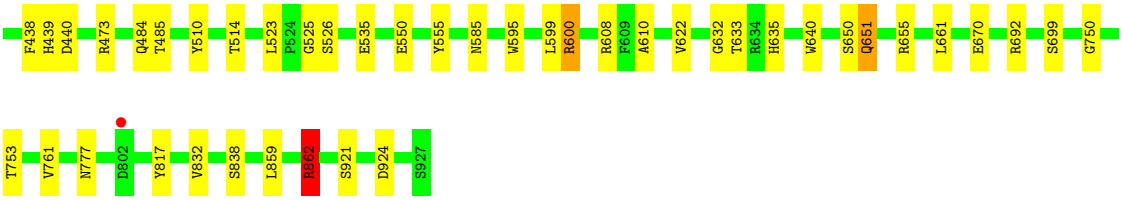
Chain E:



• Molecule 1: Pcrglx protein

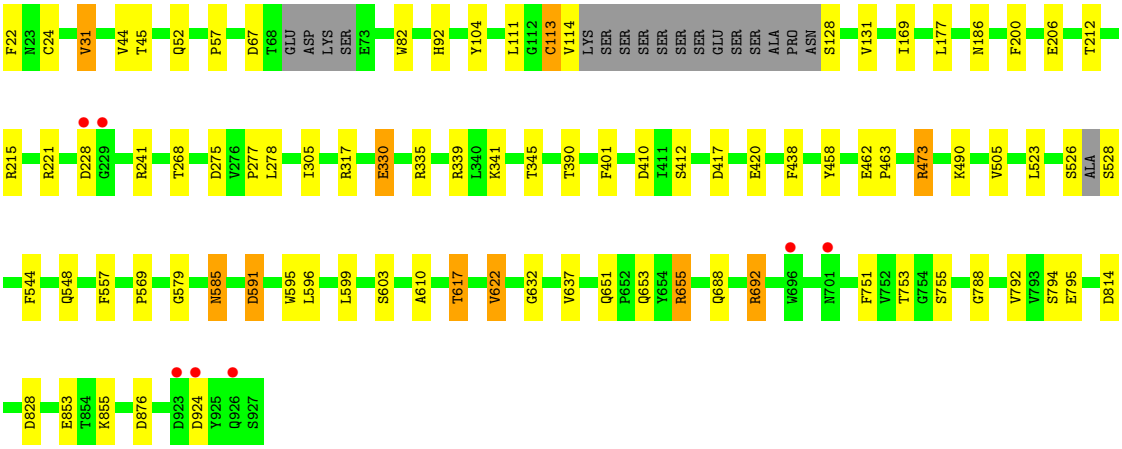
Chain F:





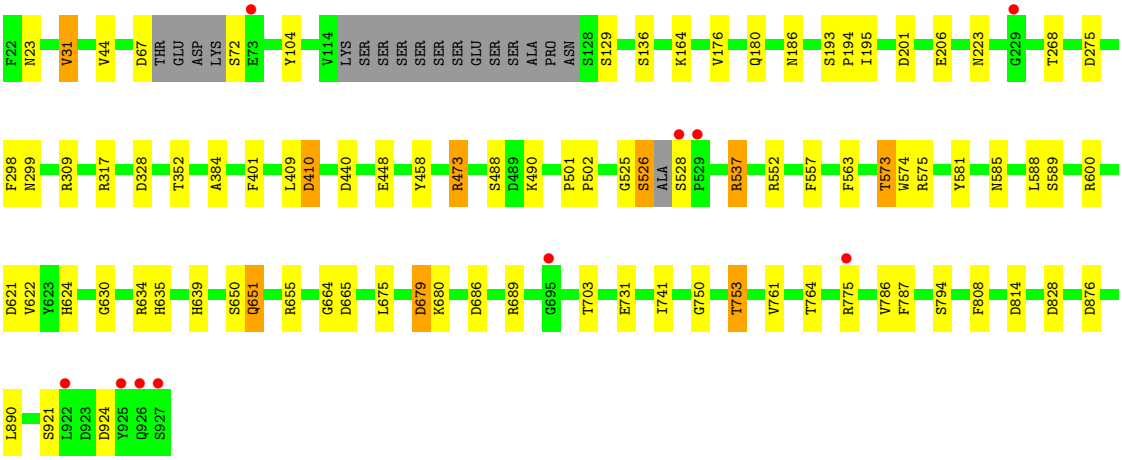
• Molecule 1: Pcrglx protein

Chain G:



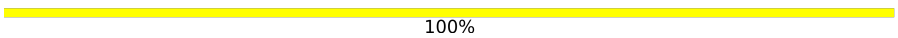
• Molecule 1: Pcrglx protein

Chain H:



• Molecule 2: 2,6-anhydro-3-deoxy-L-threo-hex-2-enonic acid-(1-2)-alpha-L-rhamnopyranose

Chain I:



• Molecule 2: 2,6-anhydro-3-deoxy-L-threo-hex-2-enonic acid-(1-2)-alpha-L-rhamnopyranose

Chain J: 100%

RAM1 GAD2

• Molecule 2: 2,6-anhydro-3-deoxy-L-threo-hex-2-enonic acid-(1-2)-alpha-L-rhamnopyranose

Chain K: 100%

RAM1 GAD2

• Molecule 2: 2,6-anhydro-3-deoxy-L-threo-hex-2-enonic acid-(1-2)-alpha-L-rhamnopyranose

Chain L: 50% 50%

RAM1 GAD2

• Molecule 2: 2,6-anhydro-3-deoxy-L-threo-hex-2-enonic acid-(1-2)-alpha-L-rhamnopyranose

Chain M: 100%

RAM1 GAD2

• Molecule 2: 2,6-anhydro-3-deoxy-L-threo-hex-2-enonic acid-(1-2)-alpha-L-rhamnopyranose

Chain N: 50% 50%

RAM1 GAD2

• Molecule 2: 2,6-anhydro-3-deoxy-L-threo-hex-2-enonic acid-(1-2)-alpha-L-rhamnopyranose

Chain O: 50% 50%

RAM1 GAD2

• Molecule 2: 2,6-anhydro-3-deoxy-L-threo-hex-2-enonic acid-(1-2)-alpha-L-rhamnopyranose

Chain P: 100%

RAM1
GAD2

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	167.88Å 171.94Å 342.38Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	171.19 – 2.74 49.16 – 2.74	Depositor EDS
% Data completeness (in resolution range)	99.7 (171.19-2.74) 99.7 (49.16-2.74)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	6.08 (at 2.73Å)	Xtriage
Refinement program	REFMAC 5.8.0151	Depositor
R, R_{free}	0.188 , 0.247 0.192 , 0.247	Depositor DCC
R_{free} test set	12767 reflections (4.94%)	wwPDB-VP
Wilson B-factor (Å^2)	32.3	Xtriage
Anisotropy	0.007	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.32 , 25.5	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	0.019 for k,h,-l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	57208	wwPDB-VP
Average B, all atoms (Å^2)	30.0	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 46.86 % 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 1.0780e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

Bond lengths and bond angles in the following residue types are not validated in this section: CA, RAM, GAD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
1	A	0.73	1/7232 (0.0%)	0.89	17/9878 (0.2%)
1	B	0.76	4/7256 (0.1%)	0.88	16/9907 (0.2%)
1	C	0.72	0/7223	0.86	8/9857 (0.1%)
1	D	0.71	0/7218	0.87	13/9854 (0.1%)
1	E	0.74	1/7262 (0.0%)	0.89	11/9914 (0.1%)
1	F	0.72	0/7245	0.89	9/9892 (0.1%)
1	G	0.70	0/7196	0.88	12/9822 (0.1%)
1	H	0.73	0/7204	0.89	17/9833 (0.2%)
All	All	0.73	6/57836 (0.0%)	0.88	103/78957 (0.1%)

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	E	0	1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	24	CYS	C-N	10.18	1.57	1.34
1	B	201[A]	ASP	CB-CG	6.94	1.66	1.51
1	B	201[B]	ASP	CB-CG	6.94	1.66	1.51
1	B	431	GLU	CG-CD	5.55	1.60	1.51
1	B	431	GLU	CD-OE2	5.49	1.31	1.25
1	A	431	GLU	CG-CD	5.06	1.59	1.51

All (103) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	24	CYS	O-C-N	-21.61	88.12	122.70
1	A	600	ARG	NE-CZ-NH1	9.32	124.96	120.30
1	E	600	ARG	NE-CZ-NH1	8.72	124.66	120.30
1	A	655	ARG	NE-CZ-NH2	8.25	124.42	120.30
1	F	600	ARG	NE-CZ-NH1	7.79	124.20	120.30
1	G	317	ARG	NE-CZ-NH2	-7.65	116.48	120.30
1	H	600	ARG	NE-CZ-NH2	-7.40	116.60	120.30
1	F	608	ARG	NE-CZ-NH1	7.21	123.90	120.30
1	A	600	ARG	NE-CZ-NH2	-7.18	116.71	120.30
1	H	317	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	H	473	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	G	241	ARG	NE-CZ-NH2	-7.08	116.76	120.30
1	H	473	ARG	NE-CZ-NH1	7.06	123.83	120.30
1	D	600	ARG	NE-CZ-NH1	7.04	123.82	120.30
1	G	221	ARG	NE-CZ-NH2	-6.99	116.81	120.30
1	A	473	ARG	NE-CZ-NH1	6.96	123.78	120.30
1	B	862	ARG	NE-CZ-NH1	6.85	123.72	120.30
1	B	181	ASP	CB-CG-OD1	6.83	124.45	118.30
1	B	600	ARG	NE-CZ-NH2	-6.77	116.91	120.30
1	B	692	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	D	23	ASN	CB-CA-C	-6.71	96.97	110.40
1	G	317	ARG	NE-CZ-NH1	6.65	123.62	120.30
1	D	600	ARG	NE-CZ-NH2	-6.51	117.04	120.30
1	D	317	ARG	NE-CZ-NH1	6.48	123.54	120.30
1	B	600	ARG	NE-CZ-NH1	6.44	123.52	120.30
1	D	552	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	B	655	ARG	NE-CZ-NH2	6.39	123.50	120.30
1	B	181	ASP	CB-CG-OD2	-6.29	112.64	118.30
1	E	829	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	C	600	ARG	NE-CZ-NH2	-6.20	117.20	120.30
1	A	829	ARG	NE-CZ-NH1	6.19	123.40	120.30
1	E	404	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	C	339	ARG	NE-CZ-NH1	6.14	123.37	120.30
1	E	924	ASP	CB-CG-OD1	6.12	123.81	118.30
1	C	686	ASP	CB-CG-OD1	6.11	123.80	118.30
1	B	139	LEU	CA-CB-CG	6.10	129.33	115.30
1	G	814	ASP	CB-CG-OD2	-6.10	112.81	118.30
1	H	317	ARG	NE-CZ-NH2	-6.07	117.26	120.30
1	H	600	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	C	404	ARG	NE-CZ-NH1	6.05	123.32	120.30
1	B	862	ARG	NE-CZ-NH2	-6.01	117.29	120.30
1	A	473	ARG	NE-CZ-NH2	-5.96	117.32	120.30
1	E	114	VAL	CB-CA-C	-5.94	100.12	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	814	ASP	CB-CG-OD1	5.91	123.62	118.30
1	H	309	ARG	NE-CZ-NH1	5.89	123.24	120.30
1	E	226	VAL	CB-CA-C	-5.85	100.28	111.40
1	G	113	CYS	CA-CB-SG	5.85	124.52	114.00
1	F	600	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	C	552	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	H	679	ASP	CB-CG-OD1	5.82	123.53	118.30
1	D	317	ARG	NE-CZ-NH2	-5.81	117.39	120.30
1	H	410	ASP	CB-CG-OD1	5.81	123.53	118.30
1	A	223	ASN	CB-CA-C	-5.79	98.83	110.40
1	H	537	ARG	NE-CZ-NH1	5.77	123.18	120.30
1	A	862	ARG	NE-CZ-NH1	5.76	123.18	120.30
1	H	814	ASP	CB-CG-OD1	5.76	123.49	118.30
1	A	440	ASP	CB-CG-OD1	5.76	123.48	118.30
1	G	221	ARG	NE-CZ-NH1	5.74	123.17	120.30
1	E	862	ARG	NE-CZ-NH2	-5.73	117.44	120.30
1	F	473	ARG	NE-CZ-NH1	5.67	123.14	120.30
1	B	221	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	440	ASP	CB-CG-OD2	-5.66	113.21	118.30
1	C	317	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	D	575	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	A	364	ARG	NE-CZ-NH1	5.60	123.10	120.30
1	A	862	ARG	NE-CZ-NH2	-5.59	117.50	120.30
1	A	845	ARG	NE-CZ-NH1	5.59	123.09	120.30
1	G	275	ASP	CB-CG-OD1	5.55	123.30	118.30
1	F	473	ARG	NE-CZ-NH2	-5.53	117.54	120.30
1	B	417	ASP	CB-CG-OD2	-5.49	113.36	118.30
1	E	24	CYS	N-CA-CB	5.48	120.47	110.60
1	A	679	ASP	CB-CG-OD1	5.47	123.22	118.30
1	F	440	ASP	CB-CG-OD1	5.46	123.21	118.30
1	E	440	ASP	CB-CG-OD1	5.45	123.21	118.30
1	A	575	ARG	NE-CZ-NH1	5.44	123.02	120.30
1	F	286	ARG	NE-CZ-NH2	-5.43	117.58	120.30
1	C	473	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	H	634	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	B	829	ARG	NE-CZ-NH1	5.34	122.97	120.30
1	F	608	ARG	NE-CZ-NH2	-5.33	117.63	120.30
1	A	686	ASP	CB-CG-OD1	5.33	123.10	118.30
1	B	221	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	G	114	VAL	N-CA-CB	5.28	123.12	111.50
1	C	223	ASN	CB-CA-C	-5.26	99.87	110.40
1	F	862	ARG	NE-CZ-NH1	5.26	122.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	328	ASP	CB-CG-OD1	5.26	123.03	118.30
1	G	692	ARG	NE-CZ-NH1	5.25	122.92	120.30
1	H	552	ARG	NE-CZ-NH2	-5.25	117.68	120.30
1	D	686	ASP	CB-CG-OD1	5.24	123.01	118.30
1	D	226	VAL	CB-CA-C	-5.23	101.47	111.40
1	H	440	ASP	CB-CG-OD1	5.23	123.00	118.30
1	E	600	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	B	692	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	H	275	ASP	CB-CG-OD1	5.16	122.95	118.30
1	D	309	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	241	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	D	552	ARG	NE-CZ-NH2	-5.11	117.75	120.30
1	D	692	ARG	NE-CZ-NH1	5.09	122.84	120.30
1	B	543	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	D	862	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	H	814	ASP	CB-CG-OD2	-5.06	113.75	118.30
1	B	410	ASP	CB-CG-OD1	5.03	122.83	118.30
1	G	473	ARG	NE-CZ-NH1	5.02	122.81	120.30

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	E	24	CYS	Mainchain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	7025	0	6584	31	0
1	B	7052	0	6618	30	0
1	C	7007	0	6587	27	0
1	D	6994	0	6572	21	1
1	E	7054	0	6633	34	1
1	F	7040	0	6601	21	0
1	G	6989	0	6553	31	0
1	H	6997	0	6567	26	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	I	22	0	17	0	0
2	J	22	0	17	0	0
2	K	22	0	16	0	0
2	L	22	0	17	0	0
2	M	22	0	17	0	0
2	N	22	0	17	0	0
2	O	22	0	17	2	0
2	P	22	0	17	0	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
3	C	1	0	0	0	0
3	D	1	0	0	0	0
3	E	1	0	0	0	0
3	F	1	0	0	0	0
3	G	1	0	0	0	0
3	H	1	0	0	0	0
4	A	122	0	0	2	0
4	B	128	0	0	1	0
4	C	122	0	0	1	0
4	D	95	0	0	0	0
4	E	122	0	0	2	0
4	F	116	0	0	0	0
4	G	72	0	0	1	0
4	H	89	0	0	1	0
All	All	57208	0	52850	217	1

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 2.

All (217) 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:G:24:CYS:CB	1:G:113:CYS:SG	2.14	1.34
1:G:526:SER:HG	1:G:528:SER:N	1.56	1.04
1:E:201:ASP:OD2	1:E:227:THR:HG21	1.73	0.88
1:G:24:CYS:HG	1:G:113:CYS:CB	1.95	0.78
1:E:119:SER:O	1:E:120:SER:C	2.23	0.76
1:G:24:CYS:HB2	1:G:113:CYS:SG	2.28	0.72
1:G:688:GLN:HE22	2:O:1:RAM:H62	1.57	0.69
1:G:526:SER:OG	1:G:528:SER:N	2.26	0.69
1:H:526:SER:O	1:H:528:SER:N	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:31:VAL:HG12	1:G:104:TYR:HB2	1.77	0.66
1:G:277:PRO:O	1:G:417:ASP:O	2.13	0.66
1:E:241:ARG:NH2	1:E:670:GLU:OE2	2.28	0.65
1:G:473:ARG:HD3	1:G:557:PHE:O	1.96	0.65
1:C:391:GLN:HG2	4:C:1214:HOH:O	1.97	0.65
1:E:196:GLN:NE2	1:E:230:THR:HG21	2.12	0.65
1:D:281:GLU:OE1	1:D:390:THR:HB	1.97	0.64
1:E:59:GLU:HA	1:E:111:LEU:HD22	1.79	0.63
1:A:591:ASP:OD2	1:A:617:THR:HG21	2.00	0.62
1:A:192:ASN:ND2	1:D:228:ASP:OD2	2.32	0.62
1:G:591:ASP:OD2	1:G:617:THR:HG21	2.00	0.61
1:B:591:ASP:OD2	1:B:617:THR:HG21	2.01	0.60
1:G:111:LEU:HD12	1:G:111:LEU:O	2.00	0.60
1:E:617:THR:HG23	1:E:655:ARG:NH1	2.17	0.60
1:E:752:VAL:HG21	1:E:830:TYR:CZ	2.35	0.59
1:F:753:THR:HG22	1:F:777:ASN:HB3	1.84	0.59
1:B:617:THR:HG23	1:B:655:ARG:NH1	2.18	0.59
1:B:817:TYR:O	1:B:862:ARG:NH2	2.36	0.59
1:H:750:GLY:O	1:H:753:THR:HG23	2.02	0.59
1:D:31:VAL:HG13	1:D:504:LEU:HB3	1.85	0.59
1:B:600:ARG:HD3	1:B:912:ILE:HG23	1.85	0.58
1:D:178[A]:GLN:HG2	1:D:268:THR:HG22	1.85	0.58
1:D:386:LEU:HD22	1:D:411:ILE:HG23	1.85	0.58
1:G:688:GLN:NE2	2:O:1:RAM:H62	2.18	0.58
1:D:111:LEU:O	1:D:111:LEU:HD12	2.03	0.57
1:A:617:THR:CG2	1:A:655:ARG:NH1	2.68	0.57
1:C:288:ILE:HG23	1:C:411:ILE:CD1	2.35	0.56
1:D:473:ARG:HD3	1:D:557:PHE:O	2.07	0.55
1:G:595:TRP:CE2	1:G:610:ALA:HB1	2.43	0.54
1:H:195:ILE:HG23	1:H:195:ILE:O	2.07	0.54
1:A:631:LEU:HG	1:A:681:THR:HG21	1.89	0.54
1:B:522:ALA:O	1:B:600:ARG:HD2	2.07	0.54
1:C:751:PHE:O	1:C:753:THR:O	2.26	0.54
1:A:535:GLU:OE1	1:A:600:ARG:NH2	2.40	0.54
1:G:412:SER:HB3	1:G:420:GLU:HB2	1.90	0.54
1:C:535:GLU:OE1	1:C:600:ARG:NH2	2.40	0.54
1:G:751:PHE:O	1:G:753:THR:O	2.26	0.53
1:C:201:ASP:O	1:C:224:HIS:HA	2.09	0.53
1:F:599:LEU:HD21	1:F:661:LEU:HD11	1.89	0.53
1:C:522:ALA:O	1:C:600:ARG:HD2	2.08	0.53
1:B:664:GLY:O	1:B:665:ASP:C	2.46	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:575:ARG:HD2	1:H:581:TYR:HB3	1.91	0.52
1:F:750:GLY:O	1:F:753:THR:OG1	2.27	0.52
1:B:139:LEU:HD11	1:B:209:VAL:HG21	1.91	0.52
1:E:196:GLN:HE21	1:E:230:THR:HG21	1.71	0.52
1:D:198:SER:OG	1:D:230:THR:HG22	2.10	0.52
1:E:741:ILE:HG23	1:E:808:PHE:CG	2.45	0.51
1:C:221:ARG:NH2	1:C:670:GLU:OE1	2.38	0.51
1:C:288:ILE:HG23	1:C:411:ILE:HD13	1.93	0.51
1:C:473:ARG:HD3	1:C:557:PHE:O	2.11	0.51
1:B:277:PRO:O	1:B:417:ASP:O	2.28	0.51
1:E:114:VAL:O	1:E:117:SER:OG	2.21	0.51
1:F:535:GLU:OE1	1:F:600:ARG:NH2	2.43	0.51
1:A:535:GLU:CD	1:A:600:ARG:HH22	2.14	0.51
1:B:517:LEU:HG	1:B:657:TYR:HD1	1.76	0.51
1:B:549:ILE:HD11	1:B:609:PHE:CE1	2.46	0.50
1:H:473:ARG:HD3	1:H:557:PHE:O	2.10	0.50
1:E:622:VAL:HA	1:E:632:GLY:HA2	1.93	0.49
1:F:241:ARG:NH2	1:F:670:GLU:OE2	2.45	0.49
1:F:622:VAL:HA	1:F:632:GLY:HA2	1.94	0.49
1:H:741:ILE:HG23	1:H:808:PHE:CD1	2.47	0.49
1:A:741:ILE:HG23	1:A:808:PHE:CD1	2.47	0.49
1:F:650:SER:O	1:F:651:GLN:C	2.51	0.49
1:C:752:VAL:HG21	1:C:830:TYR:CZ	2.47	0.49
1:G:596:LEU:HD23	1:G:599:LEU:HD12	1.95	0.49
1:B:617:THR:CG2	1:B:655:ARG:NH1	2.75	0.49
1:H:31:VAL:HG12	1:H:104:TYR:HB2	1.95	0.49
1:H:630:GLY:HA2	1:H:675:LEU:HD23	1.95	0.49
1:E:157:ILE:HA	1:E:204:ILE:HD11	1.95	0.48
1:A:617:THR:HG23	4:A:1123:HOH:O	2.13	0.48
1:A:817:TYR:O	1:A:862:ARG:NH2	2.46	0.48
1:B:589:SER:OG	1:B:787:PHE:HA	2.14	0.48
1:E:535:GLU:OE1	1:E:600:ARG:NH2	2.47	0.48
1:E:52:GLN:HA	1:E:82:TRP:CD1	2.48	0.48
1:G:622:VAL:HA	1:G:632:GLY:HA2	1.95	0.48
1:C:526:SER:O	1:C:528:SER:N	2.47	0.48
1:A:253:VAL:HB	1:A:477:VAL:HB	1.96	0.48
1:B:741:ILE:HG23	1:B:808:PHE:CD1	2.48	0.48
1:B:45:THR:HA	1:B:92:HIS:O	2.14	0.47
1:F:148:VAL:HG22	1:F:150:PHE:CE2	2.49	0.47
1:F:550:GLU:HG3	1:F:555:TYR:OH	2.15	0.47
1:A:31:VAL:HG13	1:A:504:LEU:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:386:LEU:HD22	1:B:411:ILE:HG23	1.94	0.47
1:E:226:VAL:HG22	4:E:1142:HOH:O	2.13	0.47
1:B:412:SER:HB3	1:B:420:GLU:HB2	1.96	0.47
1:D:241:ARG:NH2	1:D:670:GLU:OE2	2.48	0.47
1:D:624:HIS:CE1	1:D:671:LEU:HD22	2.49	0.47
1:G:335:ARG:O	1:G:339:ARG:HD2	2.14	0.47
1:E:650:SER:O	1:E:651:GLN:C	2.53	0.47
1:F:595:TRP:CE2	1:F:610:ALA:HB1	2.49	0.46
1:H:180:GLN:NE2	1:H:195:ILE:HD11	2.30	0.46
1:E:169:ILE:C	1:E:169:ILE:HD12	2.35	0.46
1:B:182:SER:HB2	4:B:1217:HOH:O	2.14	0.46
1:D:630:GLY:HA2	1:D:675:LEU:HD23	1.97	0.46
1:F:438:PHE:CZ	1:F:439:HIS:HD2	2.34	0.46
1:B:298:PHE:HB2	1:C:890:LEU:HD13	1.97	0.46
1:G:169:ILE:C	1:G:169:ILE:HD12	2.36	0.46
1:C:741:ILE:HG23	1:C:808:PHE:CD1	2.50	0.46
1:C:588:LEU:HD22	1:C:786:VAL:CG2	2.46	0.46
1:E:520:TYR:O	1:E:913:GLN:HG2	2.17	0.46
1:F:132:VAL:HG13	1:F:211:GLN:NE2	2.30	0.46
1:C:857:LYS:NZ	1:C:924:ASP:OD2	2.45	0.45
1:E:114:VAL:O	1:E:117:SER:CB	2.64	0.45
1:E:633:THR:HG21	1:E:640:TRP:HA	1.97	0.45
1:B:31:VAL:HG12	1:B:104:TYR:HB2	1.98	0.45
1:G:462:GLU:HG3	1:G:463:PRO:HD2	1.97	0.45
1:F:310:ARG:HG3	1:F:335:ARG:HB3	1.99	0.45
1:G:52:GLN:HA	1:G:82:TRP:CD1	2.51	0.45
1:D:664:GLY:O	1:D:665:ASP:C	2.55	0.45
1:H:589:SER:HG	1:H:787:PHE:HA	1.82	0.45
1:A:158:ILE:HD11	1:A:242:PHE:CE2	2.52	0.45
1:C:396:VAL:HG23	1:C:479:LEU:HD23	1.99	0.45
1:C:478:TYR:CD2	1:C:498:MET:HG3	2.51	0.45
1:E:111:LEU:HD12	1:E:111:LEU:HA	1.63	0.45
1:B:111:LEU:HD23	1:B:115:LYS:HE3	1.99	0.45
1:C:591:ASP:OD2	1:C:617:THR:HG21	2.17	0.45
1:G:585:ASN:N	1:G:585:ASN:HD22	2.15	0.45
1:A:517:LEU:HG	1:A:657:TYR:HD1	1.81	0.44
1:B:588:LEU:HD13	1:B:906:GLN:HG3	1.99	0.44
1:A:589:SER:OG	1:A:787:PHE:HA	2.18	0.44
1:D:839:LEU:HB3	1:D:842:ALA:HB3	1.98	0.44
1:E:845:ARG:HA	1:E:914:ASN:OD1	2.17	0.44
1:H:384:ALA:HB2	1:H:409:LEU:HD13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:634:ARG:HG3	1:B:635:HIS:CD2	2.52	0.44
1:F:510:TYR:O	1:F:514:THR:HG23	2.18	0.44
1:A:413:ASN:ND2	1:A:420:GLU:OE1	2.42	0.44
1:A:839:LEU:HB3	1:A:842:ALA:HB3	1.99	0.44
1:F:817:TYR:O	1:F:862:ARG:NH2	2.51	0.44
1:H:589:SER:OG	1:H:787:PHE:HA	2.17	0.44
1:E:298:PHE:HB2	1:H:890:LEU:HD13	2.00	0.44
1:F:633:THR:HG21	1:F:640:TRP:HA	1.99	0.44
1:A:752:VAL:HG12	1:A:752:VAL:O	2.18	0.43
1:H:621:ASP:OD1	1:H:639:HIS:HB3	2.19	0.43
1:A:509:LYS:HB3	4:A:1207:HOH:O	2.18	0.43
1:F:484:GLN:O	1:F:485:THR:C	2.56	0.43
1:C:438:PHE:CE1	1:C:637:VAL:HB	2.54	0.43
1:G:438:PHE:CE1	1:G:637:VAL:HB	2.54	0.43
1:D:40:TYR:OH	1:D:42:ALA:HB2	2.19	0.43
1:E:595:TRP:CE2	1:E:610:ALA:HB1	2.54	0.43
1:B:549:ILE:HD11	1:B:609:PHE:HE1	1.84	0.43
1:E:398:LEU:HB2	1:E:423:LEU:HD21	2.00	0.43
1:H:664:GLY:O	1:H:665:ASP:C	2.57	0.43
1:A:45:THR:HA	1:A:92:HIS:O	2.19	0.43
1:A:915:LEU:HD23	1:A:915:LEU:HA	1.93	0.43
1:E:622:VAL:HG22	1:E:624:HIS:CE1	2.54	0.43
1:D:535:GLU:OE1	1:D:600:ARG:NH2	2.47	0.42
1:E:117:SER:HB3	1:E:118:SER:H	1.35	0.42
1:G:653:GLN:NE2	1:G:795:GLU:OE1	2.48	0.42
1:H:299:ASN:OD1	1:H:488:SER:OG	2.35	0.42
1:H:588:LEU:HD22	1:H:786:VAL:HG21	2.01	0.42
1:B:596:LEU:O	1:B:600:ARG:HG3	2.18	0.42
1:F:535:GLU:CD	1:F:600:ARG:HH22	2.22	0.42
1:G:569:PRO:HD2	4:G:1120:HOH:O	2.20	0.42
1:H:622:VAL:HG22	1:H:624:HIS:CE1	2.54	0.42
1:A:515:GLN:HE21	1:A:519:GLU:HG2	1.84	0.42
1:A:587:GLU:O	1:A:590:PRO:HD3	2.18	0.42
1:G:45:THR:HA	1:G:92:HIS:O	2.19	0.42
1:H:679:ASP:OD1	1:H:680:LYS:N	2.53	0.42
1:A:257:ILE:HD13	1:A:270:LEU:HD21	2.02	0.42
1:A:613:LEU:O	1:A:617:THR:HB	2.19	0.42
1:B:638:GLN:HB2	1:B:641:SER:HB3	2.01	0.42
1:F:52:GLN:HA	1:F:82:TRP:CD1	2.54	0.42
1:F:289:ARG:HA	1:F:298:PHE:O	2.20	0.42
1:A:877:ALA:O	1:A:878:PRO:C	2.56	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:617:THR:CG2	1:C:655:ARG:NH1	2.83	0.42
1:H:501:PRO:HA	1:H:502:PRO:HD3	1.97	0.42
1:H:741:ILE:HG23	1:H:808:PHE:CG	2.55	0.42
1:B:788:GLY:O	1:B:792:VAL:HG23	2.19	0.42
1:D:622:VAL:HA	1:D:632:GLY:HA2	2.00	0.42
1:D:752:VAL:HG21	1:D:830:TYR:CZ	2.55	0.42
1:G:24:CYS:CA	1:G:113:CYS:SG	3.01	0.42
1:A:617:THR:HG23	1:A:655:ARG:NH1	2.35	0.42
1:C:600:ARG:HD3	1:C:912:ILE:HG23	2.01	0.42
1:D:659:PHE:CE1	1:D:664:GLY:HA2	2.54	0.42
1:G:617:THR:HG23	1:G:655:ARG:NH1	2.35	0.42
1:G:544:PHE:O	1:G:548:GLN:HG2	2.20	0.41
1:B:575:ARG:HD2	1:B:581:TYR:HB3	2.02	0.41
1:E:24:CYS:O	1:E:24:CYS:SG	2.78	0.41
1:D:595:TRP:CE2	1:D:610:ALA:HB1	2.56	0.41
1:E:386:LEU:HB2	1:E:411:ILE:HD12	2.01	0.41
1:A:622:VAL:HA	1:A:632:GLY:HA2	2.03	0.41
1:C:150:PHE:CE2	1:C:218:VAL:HG21	2.55	0.41
1:A:241:ARG:NH2	1:A:670:GLU:OE2	2.53	0.41
1:C:295:GLY:H	1:C:381[A]:GLU:CD	2.23	0.41
1:E:241:ARG:NH1	4:E:1115:HOH:O	2.54	0.41
1:H:573:THR:HB	1:H:574:TRP:O	2.20	0.41
1:E:146:VAL:HA	1:E:162:LYS:O	2.20	0.41
1:B:535:GLU:CD	1:B:600:ARG:HH22	2.24	0.41
1:C:169:ILE:C	1:C:169:ILE:HD12	2.40	0.41
1:A:575:ARG:HD2	1:A:581:TYR:HB3	2.03	0.41
1:C:622:VAL:HG22	1:C:624:HIS:CE1	2.55	0.41
1:E:522:ALA:O	1:E:600:ARG:HG2	2.21	0.41
1:F:859:LEU:O	1:F:862:ARG:HB3	2.20	0.41
1:H:525:GLY:N	4:H:1105:HOH:O	2.53	0.41
1:A:386:LEU:HD22	1:A:411:ILE:HG23	2.02	0.41
1:C:617:THR:CG2	1:C:655:ARG:HH11	2.34	0.41
1:D:52:GLN:HA	1:D:82:TRP:CD1	2.56	0.41
1:E:64:LEU:HD11	1:E:104:TYR:HB3	2.02	0.41
1:E:890:LEU:HD13	1:H:298:PHE:HB2	2.02	0.41
1:G:177:LEU:HB3	1:G:200:PHE:HB2	2.03	0.41
1:A:390:THR:HG22	1:A:391[B]:GLN:OE1	2.20	0.40
1:H:686:ASP:HB3	1:H:689:ARG:HB3	2.02	0.40
1:H:650:SER:O	1:H:651:GLN:C	2.59	0.40
1:D:201:ASP:O	1:D:224:HIS:HA	2.22	0.40
1:B:52:GLN:HA	1:B:82:TRP:CD1	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:771:ASP:N	1:B:772:PRO:CD	2.84	0.40
1:C:177:LEU:HB3	1:C:200:PHE:HB2	2.02	0.40
1:G:788:GLY:O	1:G:792:VAL:HG23	2.21	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:211:GLN:O	1:E:117:SER:CB[3_644]	2.15	0.05

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	891/906 (98%)	850 (95%)	37 (4%)	4 (0%)	34	55
1	B	892/906 (98%)	856 (96%)	31 (4%)	5 (1%)	25	44
1	C	880/906 (97%)	842 (96%)	34 (4%)	4 (0%)	29	48
1	D	882/906 (97%)	830 (94%)	50 (6%)	2 (0%)	47	69
1	E	896/906 (99%)	851 (95%)	41 (5%)	4 (0%)	34	55
1	F	896/906 (99%)	849 (95%)	39 (4%)	8 (1%)	17	32
1	G	881/906 (97%)	839 (95%)	35 (4%)	7 (1%)	19	36
1	H	881/906 (97%)	841 (96%)	37 (4%)	3 (0%)	41	61
All	All	7099/7248 (98%)	6758 (95%)	304 (4%)	37 (0%)	29	48

All (37) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	E	117	SER
1	E	263	GLU

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Mol	Chain	Res	Type
1	F	526	SER
1	A	401	PHE
1	F	24	CYS
1	H	401	PHE
1	A	835	SER
1	B	582	ALA
1	C	582	ALA
1	F	117	SER
1	G	401	PHE
1	A	579	GLY
1	A	651	GLN
1	B	165	SER
1	B	277	PRO
1	B	579	GLY
1	B	651	GLN
1	C	579	GLY
1	D	582	ALA
1	F	635	HIS
1	F	651	GLN
1	F	692	ARG
1	G	67	ASP
1	G	330	GLU
1	G	828	ASP
1	H	651	GLN
1	C	401	PHE
1	C	651	GLN
1	E	329	THR
1	E	651	GLN
1	F	263	GLU
1	F	525	GLY
1	G	278	LEU
1	G	651	GLN
1	H	635	HIS
1	D	651	GLN
1	G	579	GLY

5.3.2 Protein sidechains (i)

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	724/745 (97%)	687 (95%)	37 (5%)	24	41
1	B	731/745 (98%)	704 (96%)	27 (4%)	34	54
1	C	726/745 (97%)	692 (95%)	34 (5%)	26	45
1	D	724/745 (97%)	689 (95%)	35 (5%)	25	44
1	E	732/745 (98%)	700 (96%)	32 (4%)	28	47
1	F	724/745 (97%)	700 (97%)	24 (3%)	38	59
1	G	721/745 (97%)	686 (95%)	35 (5%)	25	43
1	H	724/745 (97%)	686 (95%)	38 (5%)	23	39
All	All	5806/5960 (97%)	5544 (96%)	262 (4%)	27	47

All (262) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	23	ASN
1	A	31	VAL
1	A	39	THR
1	A	61	SER
1	A	99	GLN
1	A	128	SER
1	A	131	VAL
1	A	132	VAL
1	A	186	ASN
1	A	201	ASP
1	A	215	ARG
1	A	223	ASN
1	A	268	THR
1	A	305	ILE
1	A	329	THR
1	A	345	THR
1	A	391[A]	GLN
1	A	391[B]	GLN
1	A	412	SER
1	A	458	TYR
1	A	490	LYS
1	A	505	VAL
1	A	523	LEU
1	A	533	THR
1	A	573	THR

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Mol	Chain	Res	Type
1	A	585	ASN
1	A	617	THR
1	A	622	VAL
1	A	655	ARG
1	A	702	SER
1	A	761	VAL
1	A	835	SER
1	A	855	LYS
1	A	862	ARG
1	A	921	SER
1	A	924	ASP
1	A	927	SER
1	B	31	VAL
1	B	44	VAL
1	B	61	SER
1	B	63	SER
1	B	111	LEU
1	B	131	VAL
1	B	139	LEU
1	B	176	VAL
1	B	182	SER
1	B	186	ASN
1	B	230	THR
1	B	239	VAL
1	B	268	THR
1	B	277	PRO
1	B	345	THR
1	B	378	THR
1	B	390	THR
1	B	458	TYR
1	B	490	LYS
1	B	523	LEU
1	B	533	THR
1	B	585	ASN
1	B	617	THR
1	B	655	ARG
1	B	835	SER
1	B	921	SER
1	B	924	ASP
1	C	26	SER
1	C	44	VAL
1	C	114	VAL

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Mol	Chain	Res	Type
1	C	129	SER
1	C	133	THR
1	C	139	LEU
1	C	146	VAL
1	C	182	SER
1	C	186	ASN
1	C	188	ASP
1	C	193	SER
1	C	201	ASP
1	C	206	GLU
1	C	263	GLU
1	C	268	THR
1	C	279	LYS
1	C	289	ARG
1	C	328	ASP
1	C	330	GLU
1	C	341	LYS
1	C	390	THR
1	C	448	GLU
1	C	458	TYR
1	C	473	ARG
1	C	490	LYS
1	C	505	VAL
1	C	533	THR
1	C	573	THR
1	C	585	ASN
1	C	603	SER
1	C	617	THR
1	C	655	ARG
1	C	753	THR
1	C	755	SER
1	D	31	VAL
1	D	44	VAL
1	D	109	SER
1	D	111	LEU
1	D	128	SER
1	D	132	VAL
1	D	148	VAL
1	D	163	THR
1	D	176	VAL
1	D	178[A]	GLN
1	D	178[B]	GLN

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Mol	Chain	Res	Type
1	D	182	SER
1	D	183	VAL
1	D	186	ASN
1	D	188	ASP
1	D	193	SER
1	D	201	ASP
1	D	215	ARG
1	D	223[A]	ASN
1	D	223[B]	ASN
1	D	226	VAL
1	D	333	GLU
1	D	345	THR
1	D	390	THR
1	D	410	ASP
1	D	458	TYR
1	D	475	SER
1	D	490	LYS
1	D	493	SER
1	D	505	VAL
1	D	520	TYR
1	D	533	THR
1	D	573	THR
1	D	600	ARG
1	D	655	ARG
1	E	24	CYS
1	E	58[A]	GLN
1	E	58[B]	GLN
1	E	61	SER
1	E	63	SER
1	E	98	ASN
1	E	109	SER
1	E	111	LEU
1	E	114	VAL
1	E	117	SER
1	E	132	VAL
1	E	165	SER
1	E	176	VAL
1	E	182	SER
1	E	201	ASP
1	E	226	VAL
1	E	228	ASP
1	E	230	THR

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Mol	Chain	Res	Type
1	E	268	THR
1	E	305	ILE
1	E	333	GLU
1	E	345	THR
1	E	390	THR
1	E	458	TYR
1	E	585	ASN
1	E	617	THR
1	E	655	ARG
1	E	702	SER
1	E	761	VAL
1	E	827	LYS
1	E	853	GLU
1	E	855	LYS
1	F	58	GLN
1	F	118	SER
1	F	132	VAL
1	F	148	VAL
1	F	165	SER
1	F	183	VAL
1	F	213	SER
1	F	228	ASP
1	F	230	THR
1	F	329	THR
1	F	335	ARG
1	F	345	THR
1	F	366	LYS
1	F	390	THR
1	F	523	LEU
1	F	585	ASN
1	F	655	ARG
1	F	699	SER
1	F	761	VAL
1	F	832	VAL
1	F	838	SER
1	F	862	ARG
1	F	921	SER
1	F	924	ASP
1	G	22	PHE
1	G	31	VAL
1	G	44	VAL
1	G	57	PRO

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Mol	Chain	Res	Type
1	G	128	SER
1	G	131	VAL
1	G	186	ASN
1	G	206	GLU
1	G	212	THR
1	G	215	ARG
1	G	228	ASP
1	G	268	THR
1	G	305	ILE
1	G	330	GLU
1	G	341	LYS
1	G	345	THR
1	G	390	THR
1	G	410	ASP
1	G	458	TYR
1	G	490	LYS
1	G	505	VAL
1	G	523	LEU
1	G	585	ASN
1	G	591	ASP
1	G	603	SER
1	G	617	THR
1	G	622	VAL
1	G	655	ARG
1	G	692	ARG
1	G	755	SER
1	G	794	SER
1	G	853	GLU
1	G	855	LYS
1	G	876	ASP
1	G	924	ASP
1	H	23	ASN
1	H	31	VAL
1	H	44	VAL
1	H	67	ASP
1	H	72	SER
1	H	129	SER
1	H	136	SER
1	H	164	LYS
1	H	176	VAL
1	H	186	ASN
1	H	193	SER

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Mol	Chain	Res	Type
1	H	194	PRO
1	H	201	ASP
1	H	206	GLU
1	H	223	ASN
1	H	268	THR
1	H	352	THR
1	H	410	ASP
1	H	448	GLU
1	H	458	TYR
1	H	490	LYS
1	H	526	SER
1	H	537	ARG
1	H	563	PHE
1	H	573	THR
1	H	585	ASN
1	H	655	ARG
1	H	703	THR
1	H	731	GLU
1	H	753	THR
1	H	761	VAL
1	H	764	THR
1	H	775	ARG
1	H	794	SER
1	H	828	ASP
1	H	876	ASP
1	H	921	SER
1	H	924	ASP

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

Mol	Chain	Res	Type
1	A	32	HIS
1	A	75	GLN
1	A	155	ASN
1	A	178	GLN
1	A	186	ASN
1	A	223	ASN
1	A	515	GLN
1	A	585	ASN
1	A	810	GLN
1	B	23	ASN
1	B	99	GLN

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Mol	Chain	Res	Type
1	B	178	GLN
1	B	186	ASN
1	B	210	ASN
1	B	223	ASN
1	B	324	GLN
1	B	369	GLN
1	B	585	ASN
1	B	746	ASN
1	B	810	GLN
1	C	75	GLN
1	C	186	ASN
1	C	324	GLN
1	C	391	GLN
1	D	324	GLN
1	D	391	GLN
1	D	515	GLN
1	D	585	ASN
1	E	98	ASN
1	E	178	GLN
1	E	196	GLN
1	E	324	GLN
1	E	515	GLN
1	E	585	ASN
1	E	810	GLN
1	F	32	HIS
1	F	58	GLN
1	F	210	ASN
1	F	223	ASN
1	F	324	GLN
1	F	515	GLN
1	G	75	GLN
1	G	178	GLN
1	G	180	GLN
1	G	189	ASN
1	G	324	GLN
1	G	369	GLN
1	G	391	GLN
1	G	512	HIS
1	G	515	GLN
1	G	688	GLN
1	H	23	ASN
1	H	98	ASN

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Mol	Chain	Res	Type
1	H	180	GLN
1	H	186	ASN
1	H	324	GLN
1	H	585	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

16 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	RAM	I	1	2	11,11,11	0.53	0	15,16,16	1.41	2 (13%)
2	GAD	I	2	2	10,11,11	2.00	3 (30%)	13,15,15	1.88	3 (23%)
2	RAM	J	1	2	11,11,11	0.42	0	15,16,16	1.18	2 (13%)
2	GAD	J	2	2	10,11,11	2.06	3 (30%)	13,15,15	1.94	3 (23%)
2	RAM	K	1	2	11,11,11	0.55	0	15,16,16	1.26	2 (13%)
2	GAD	K	2	2	10,11,11	2.19	2 (20%)	13,15,15	2.47	5 (38%)
2	RAM	L	1	2	11,11,11	0.54	0	15,16,16	0.87	0
2	GAD	L	2	2	10,11,11	2.03	3 (30%)	13,15,15	2.10	5 (38%)
2	RAM	M	1	2	11,11,11	0.51	0	15,16,16	1.19	2 (13%)
2	GAD	M	2	2	10,11,11	2.20	1 (10%)	13,15,15	2.00	3 (23%)
2	RAM	N	1	2	11,11,11	0.84	0	15,16,16	1.28	0
2	GAD	N	2	2	10,11,11	2.20	1 (10%)	13,15,15	2.63	5 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	RAM	O	1	2	11,11,11	0.70	0	15,16,16	1.72	5 (33%)
2	GAD	O	2	2	10,11,11	2.14	1 (10%)	13,15,15	1.57	5 (38%)
2	RAM	P	1	2	11,11,11	0.43	0	15,16,16	1.32	3 (20%)
2	GAD	P	2	2	10,11,11	2.01	1 (10%)	13,15,15	2.25	3 (23%)

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	RAM	I	1	2	-	-	0/1/1/1
2	GAD	I	2	2	-	0/4/17/17	0/1/1/1
2	RAM	J	1	2	-	-	0/1/1/1
2	GAD	J	2	2	-	0/4/17/17	0/1/1/1
2	RAM	K	1	2	-	-	0/1/1/1
2	GAD	K	2	2	-	2/4/17/17	0/1/1/1
2	RAM	L	1	2	-	-	0/1/1/1
2	GAD	L	2	2	-	0/4/17/17	0/1/1/1
2	RAM	M	1	2	-	-	0/1/1/1
2	GAD	M	2	2	-	0/4/17/17	0/1/1/1
2	RAM	N	1	2	-	-	0/1/1/1
2	GAD	N	2	2	-	0/4/17/17	0/1/1/1
2	RAM	O	1	2	-	-	0/1/1/1
2	GAD	O	2	2	-	0/4/17/17	0/1/1/1
2	RAM	P	1	2	-	-	0/1/1/1
2	GAD	P	2	2	-	0/4/17/17	0/1/1/1

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	M	2	GAD	O5-C5	5.93	1.45	1.37
2	N	2	GAD	O5-C5	5.89	1.45	1.37
2	K	2	GAD	O5-C5	5.89	1.45	1.37
2	O	2	GAD	O5-C5	5.67	1.45	1.37
2	P	2	GAD	O5-C5	5.10	1.44	1.37
2	J	2	GAD	O5-C5	4.95	1.44	1.37
2	L	2	GAD	O5-C5	4.91	1.44	1.37
2	I	2	GAD	O5-C5	4.90	1.44	1.37
2	I	2	GAD	O6B-C6	-2.32	1.23	1.30
2	L	2	GAD	O5-C1	-2.29	1.41	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	I	2	GAD	C5-C6	-2.28	1.43	1.48
2	J	2	GAD	C3-C4	2.27	1.53	1.50
2	J	2	GAD	O6B-C6	-2.26	1.24	1.30
2	L	2	GAD	C4-C5	2.09	1.36	1.33
2	K	2	GAD	C4-C5	2.06	1.36	1.33

All (48) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	K	2	GAD	O5-C5-C4	-6.18	119.59	124.81
2	P	2	GAD	O5-C5-C4	-5.89	119.84	124.81
2	N	2	GAD	O5-C5-C4	-5.77	119.94	124.81
2	J	2	GAD	O5-C5-C4	-5.22	120.40	124.81
2	N	2	GAD	O5-C5-C6	5.09	119.17	111.52
2	I	2	GAD	O5-C5-C4	-4.79	120.76	124.81
2	L	2	GAD	O5-C5-C4	-4.46	121.05	124.81
2	M	2	GAD	O5-C5-C4	-4.40	121.10	124.81
2	K	2	GAD	O5-C5-C6	4.33	118.02	111.52
2	M	2	GAD	O5-C5-C6	4.12	117.70	111.52
2	P	2	GAD	O5-C5-C6	3.99	117.51	111.52
2	O	1	RAM	O5-C1-C2	3.98	117.38	110.28
2	I	1	RAM	O4-C4-C5	3.50	117.43	109.67
2	J	2	GAD	C1-O5-C5	3.00	121.88	115.58
2	O	2	GAD	O5-C5-C4	-2.90	122.36	124.81
2	O	1	RAM	O5-C5-C4	2.89	114.71	109.52
2	L	2	GAD	C1-C2-C3	-2.87	106.14	109.67
2	L	2	GAD	C2-C3-C4	-2.85	108.42	112.32
2	P	1	RAM	C6-C5-C4	-2.81	107.88	113.07
2	I	2	GAD	C1-O5-C5	2.78	121.42	115.58
2	M	2	GAD	C2-C3-C4	-2.65	108.70	112.32
2	L	2	GAD	O5-C5-C6	2.61	115.44	111.52
2	P	1	RAM	O5-C5-C4	2.59	114.17	109.52
2	K	2	GAD	C2-C3-C4	-2.54	108.85	112.32
2	P	1	RAM	C1-C2-C3	2.48	115.45	110.31
2	L	2	GAD	O3-C3-C2	2.48	113.71	109.42
2	P	2	GAD	C1-C2-C3	-2.47	106.63	109.67
2	N	2	GAD	O3-C3-C2	2.41	113.60	109.42
2	O	2	GAD	C2-C3-C4	-2.41	109.02	112.32
2	K	2	GAD	C1-C2-C3	-2.40	106.71	109.67
2	I	2	GAD	O5-C5-C6	2.35	115.04	111.52
2	J	2	GAD	O5-C5-C6	2.34	115.03	111.52
2	M	1	RAM	C6-C5-C4	-2.29	108.84	113.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	O	1	RAM	C1-C2-C3	2.28	115.05	110.31
2	O	2	GAD	O3-C3-C2	2.27	113.36	109.42
2	I	1	RAM	O4-C4-C3	-2.25	105.15	110.35
2	K	1	RAM	O4-C4-C3	-2.24	105.17	110.35
2	M	1	RAM	O1-C1-C2	-2.23	102.76	109.03
2	N	2	GAD	O6B-C6-C5	2.19	119.67	114.20
2	J	1	RAM	O5-C1-C2	-2.13	106.48	110.28
2	N	2	GAD	C2-C3-C4	-2.13	109.41	112.32
2	K	1	RAM	O2-C2-C3	-2.13	105.42	110.35
2	O	2	GAD	C1-O5-C5	2.12	120.04	115.58
2	O	1	RAM	O5-C5-C6	-2.10	102.17	106.70
2	J	1	RAM	C4-C3-C2	2.09	114.46	110.82
2	K	2	GAD	O3-C3-C4	-2.07	104.66	109.31
2	O	1	RAM	C6-C5-C4	-2.03	109.32	113.07
2	O	2	GAD	O5-C5-C6	2.01	114.53	111.52

There are no chirality outliers.

All (2) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	2	GAD	O5-C5-C6-O6A
2	K	2	GAD	C4-C5-C6-O6A

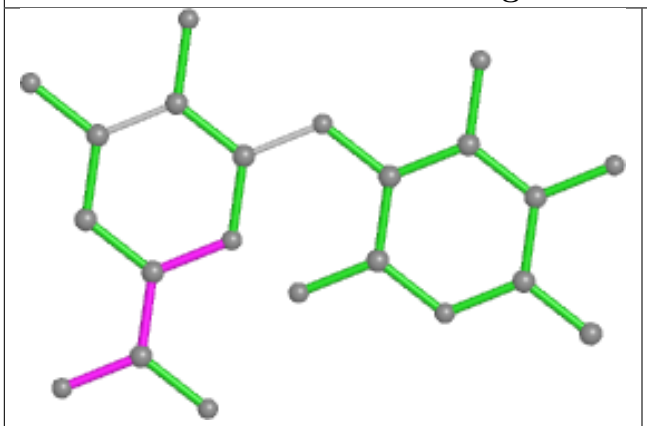
There are no ring outliers.

1 monomer is involved in 2 short contacts:

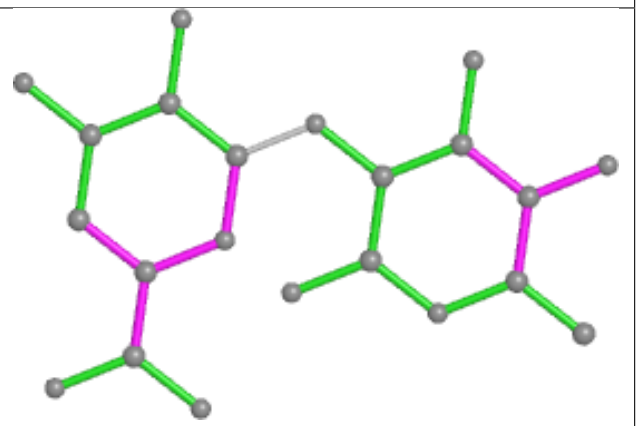
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	O	1	RAM	2	0

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

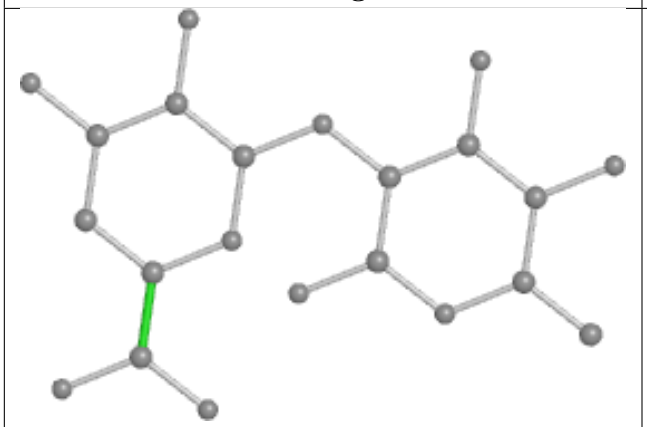
Oligosaccharide Chain I



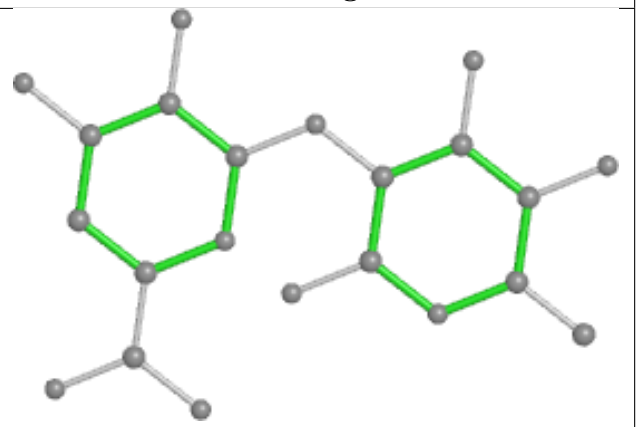
Bond lengths



Bond angles

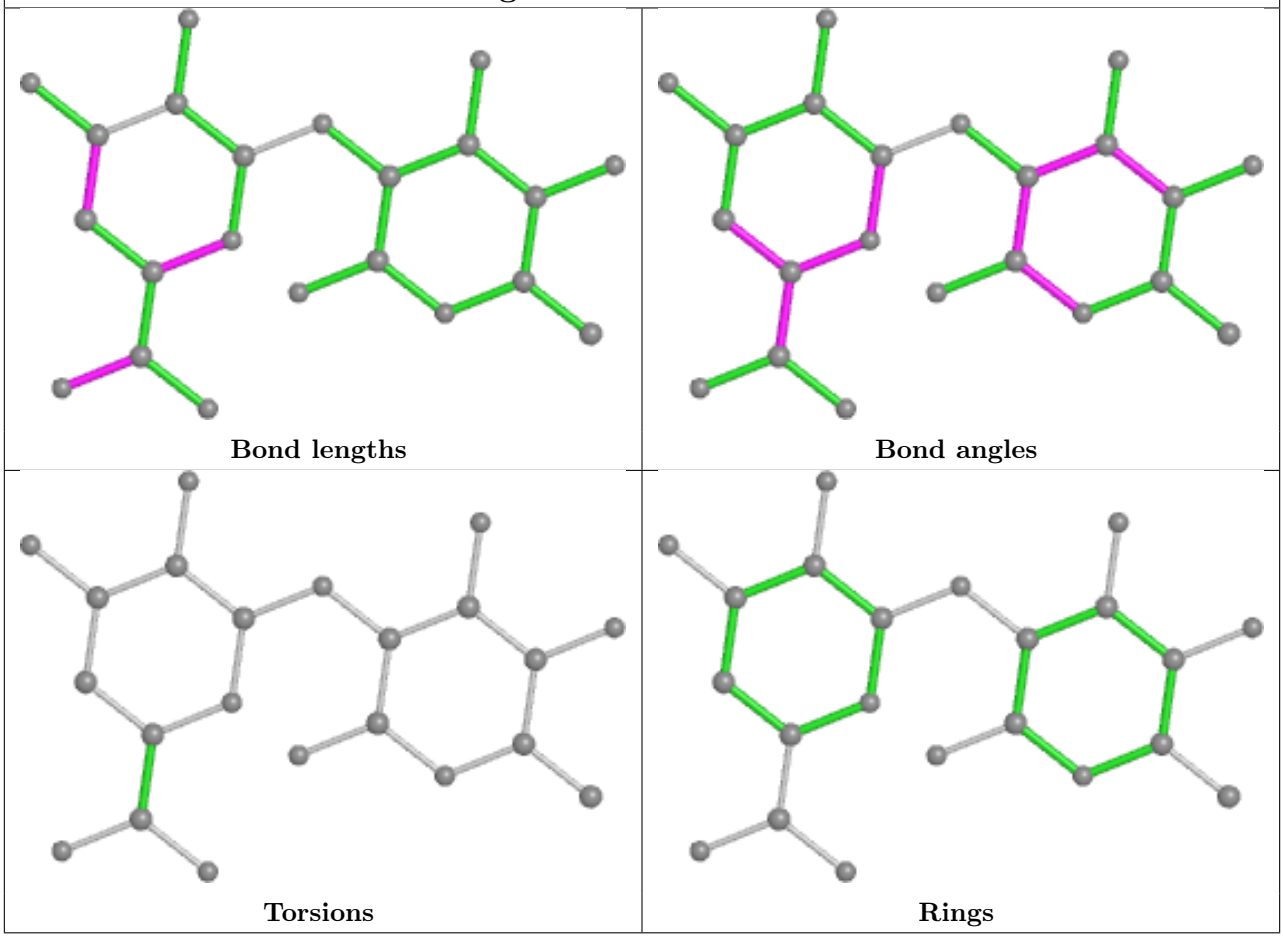


Torsions

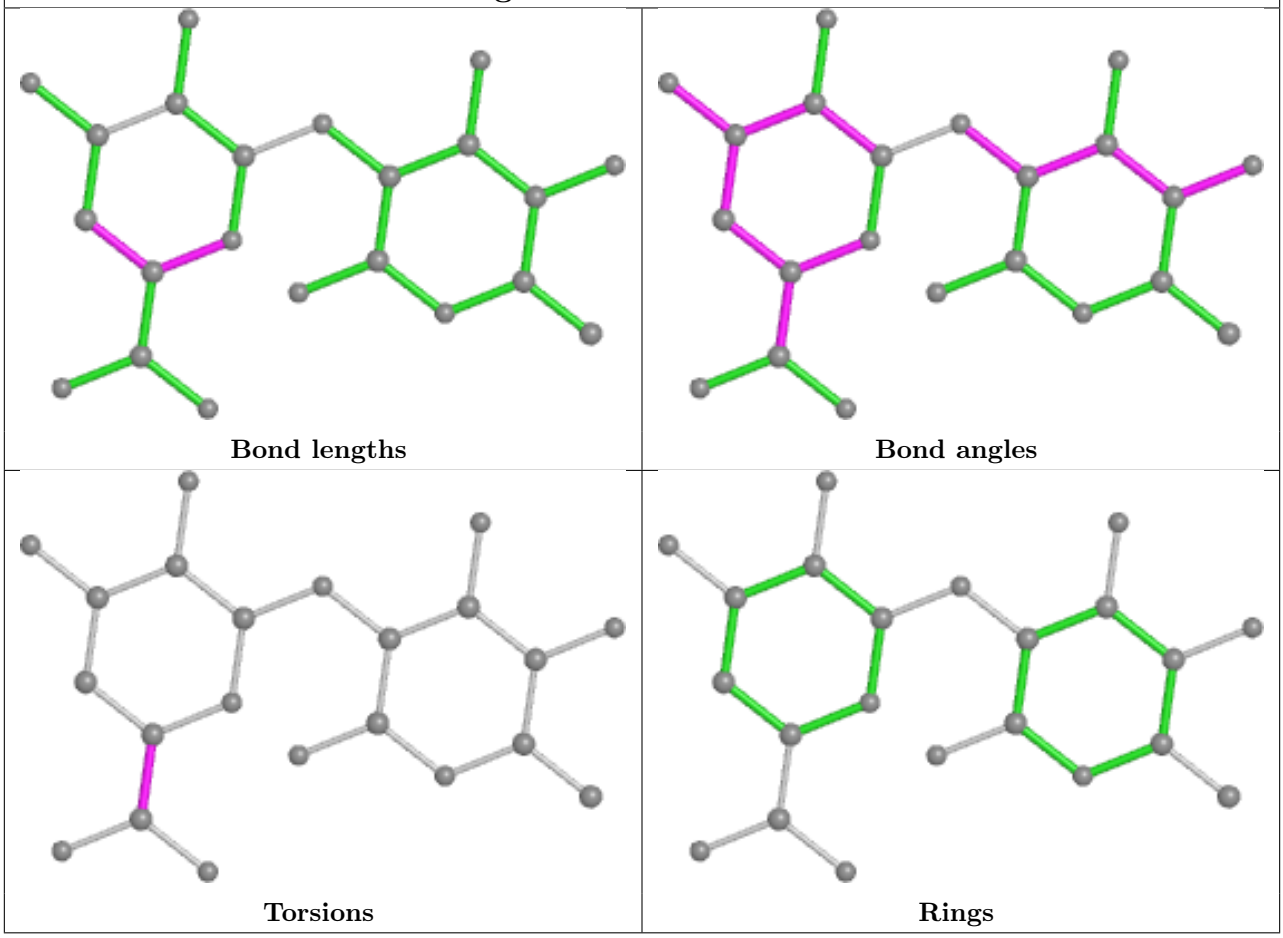


Rings

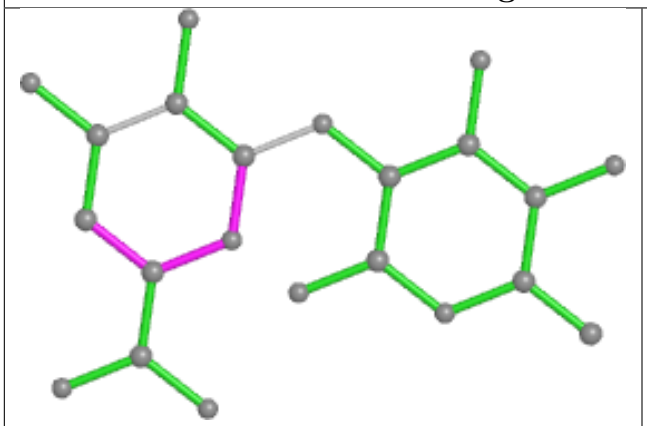
Oligosaccharide Chain J



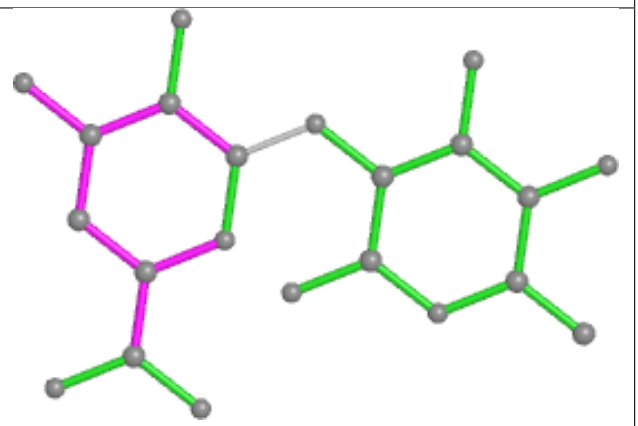
Oligosaccharide Chain K



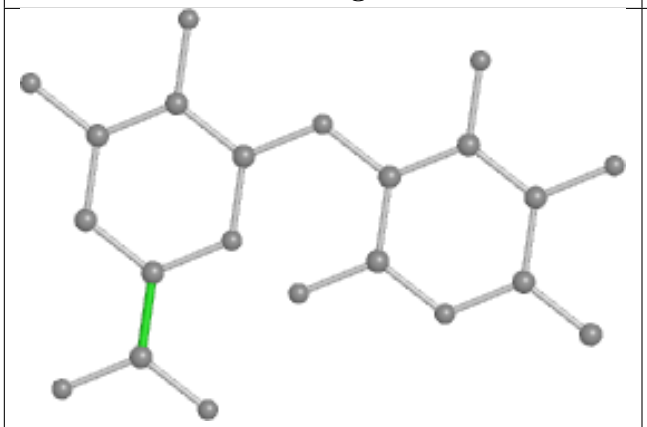
Oligosaccharide Chain L



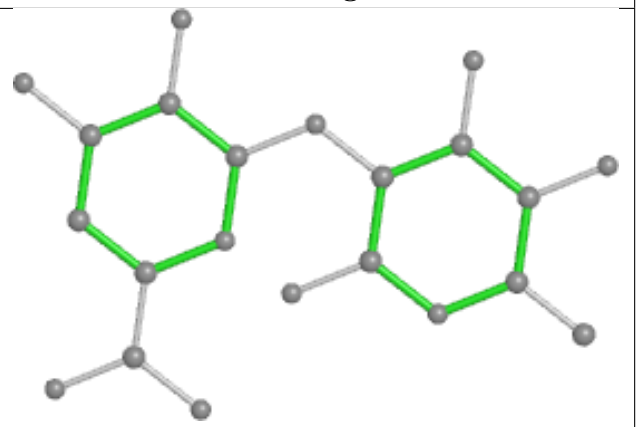
Bond lengths



Bond angles

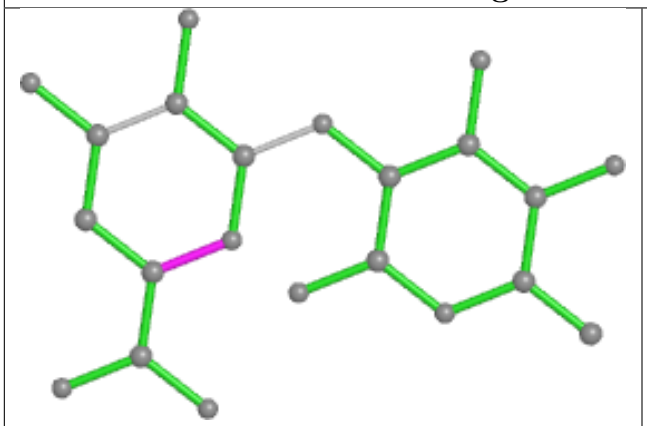


Torsions

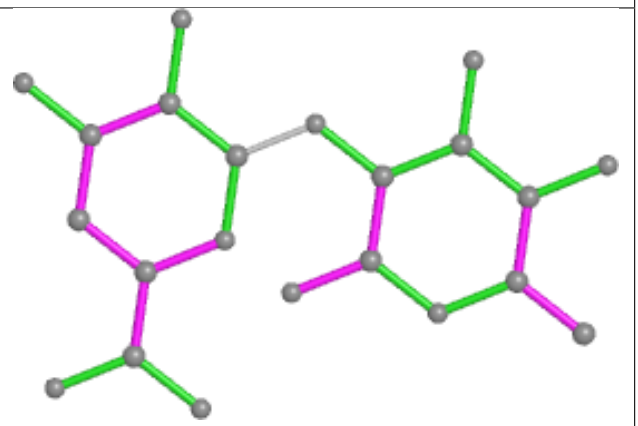


Rings

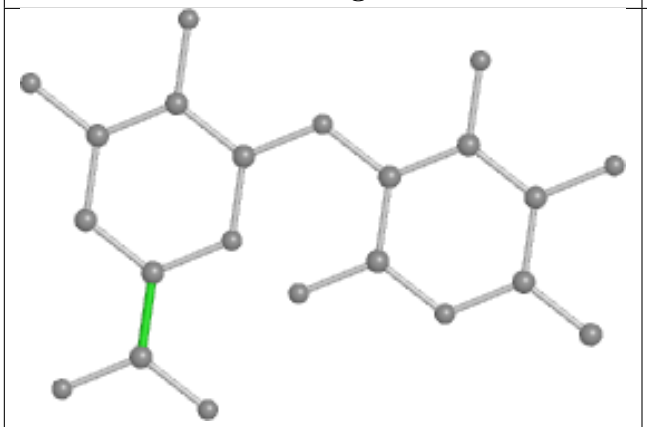
Oligosaccharide Chain M



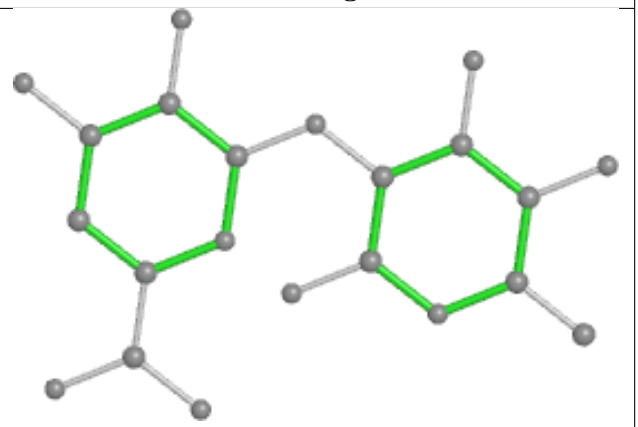
Bond lengths



Bond angles

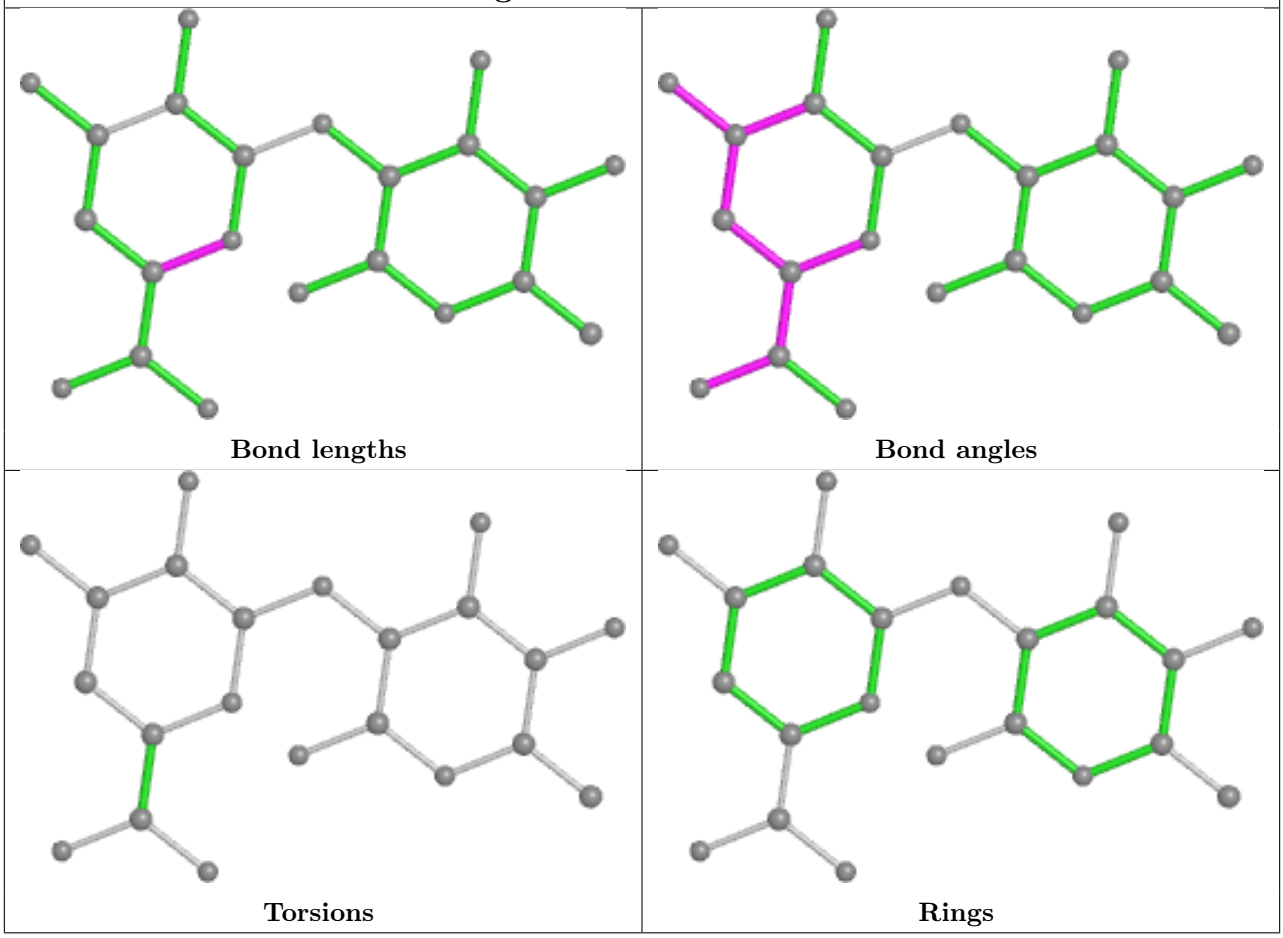


Torsions

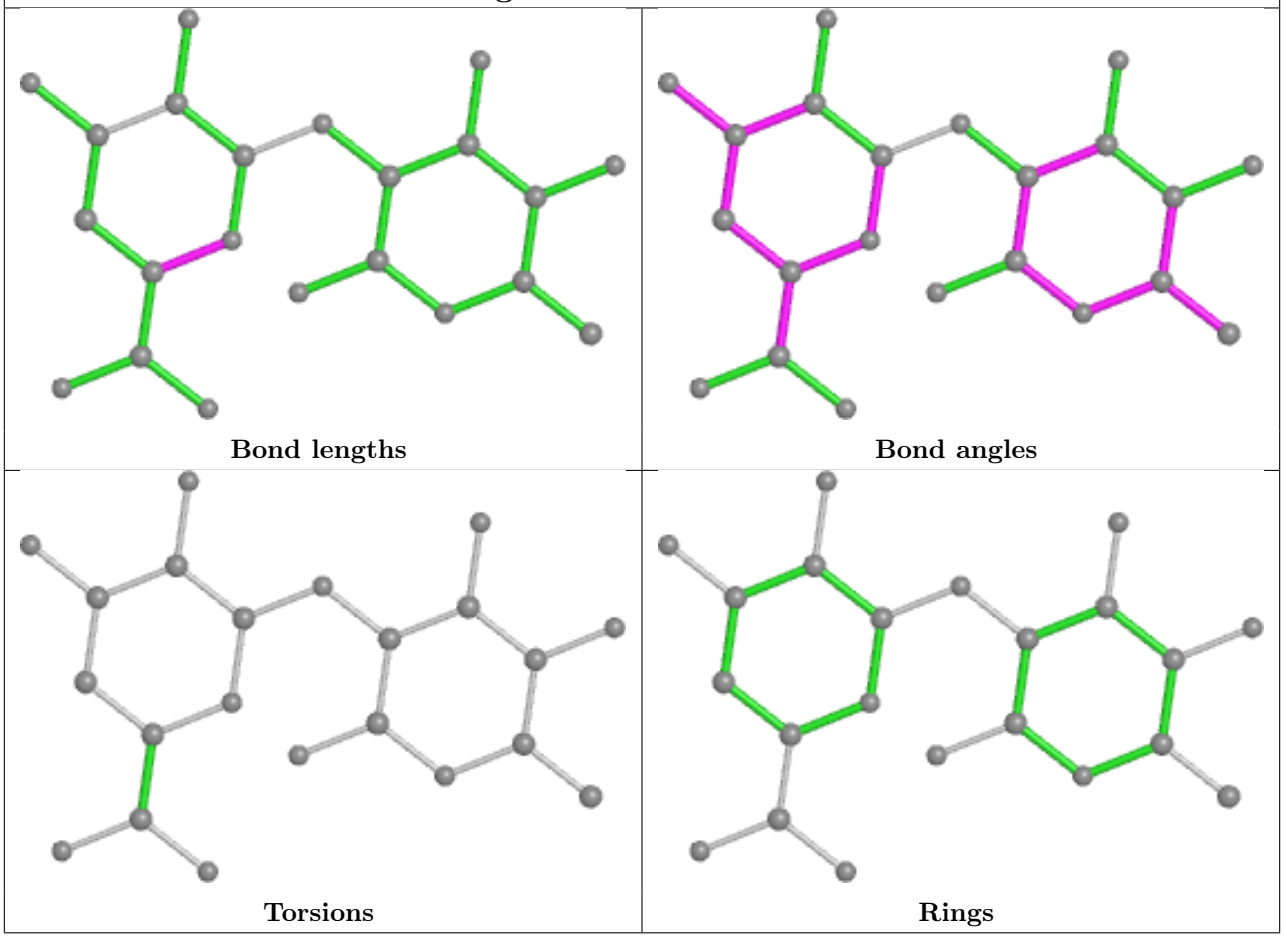


Rings

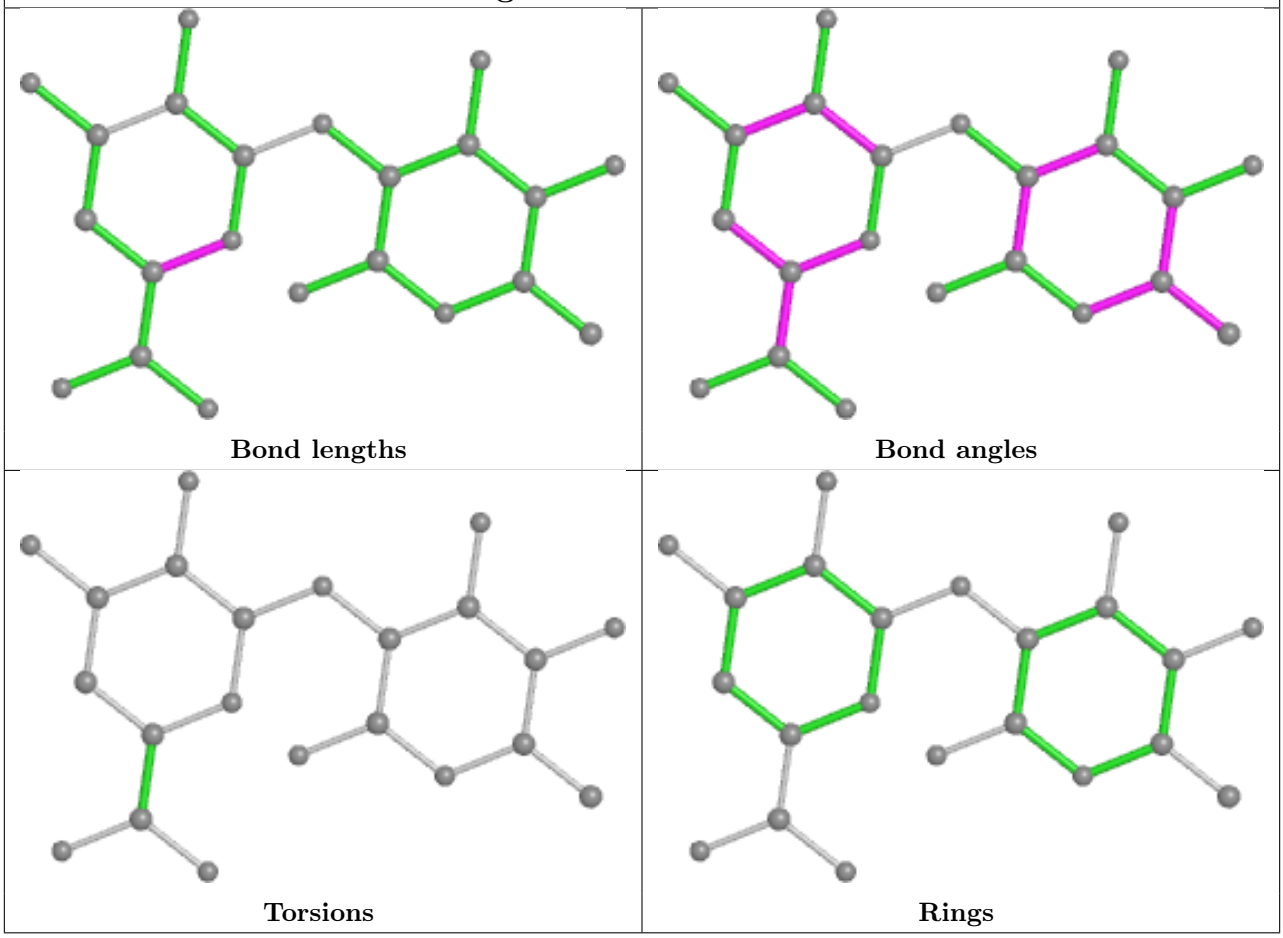
Oligosaccharide Chain N



Oligosaccharide Chain O



Oligosaccharide Chain P



5.6 Ligand geometry (i)

Of 8 ligands modelled in this entry, 8 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data (i)

6.1 Protein, DNA and RNA chains (i)

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	896/906 (98%)	-0.47	2 (0%)	95	97	16, 26, 45, 71	0
1	B	896/906 (98%)	-0.47	1 (0%)	95	97	14, 26, 45, 68	0
1	C	885/906 (97%)	-0.44	2 (0%)	95	97	15, 28, 47, 74	0
1	D	884/906 (97%)	-0.42	4 (0%)	91	93	17, 30, 49, 71	0
1	E	899/906 (99%)	-0.38	4 (0%)	92	95	16, 28, 49, 72	0
1	F	900/906 (99%)	-0.42	2 (0%)	95	97	16, 28, 49, 75	0
1	G	888/906 (98%)	-0.30	7 (0%)	86	89	16, 32, 56, 84	0
1	H	888/906 (98%)	-0.30	10 (1%)	80	85	16, 32, 55, 79	0
All	All	7136/7248 (98%)	-0.40	32 (0%)	92	95	14, 29, 50, 84	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	G	923	ASP	4.4
1	G	926	GLN	3.4
1	H	528	SER	3.2
1	F	23	ASN	3.0
1	E	118	SER	3.0
1	E	136	SER	3.0
1	H	922	LEU	2.9
1	C	229	GLY	2.8
1	H	529	PRO	2.5
1	C	926	GLN	2.5
1	A	761	VAL	2.5
1	D	927	SER	2.5
1	D	925	TYR	2.5
1	G	229	GLY	2.5
1	D	128	SER	2.4
1	H	927	SER	2.4

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Mol	Chain	Res	Type	RSRZ
1	E	196	GLN	2.3
1	H	229	GLY	2.3
1	G	696	TRP	2.3
1	B	134	ASP	2.3
1	G	924	ASP	2.3
1	H	695	GLY	2.2
1	H	925	TYR	2.2
1	A	334	PRO	2.1
1	D	695	GLY	2.1
1	E	746	ASN	2.1
1	G	701	ASN	2.1
1	F	802	ASP	2.1
1	G	228	ASP	2.1
1	H	775	ARG	2.1
1	H	73	GLU	2.1
1	H	926	GLN	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(Å^2)	Q<0.9
2	GAD	K	2	11/11	0.96	0.10	29,32,34,36	0
2	GAD	L	2	11/11	0.96	0.12	27,30,32,34	0
2	GAD	M	2	11/11	0.96	0.12	29,31,33,33	0
2	GAD	N	2	11/11	0.96	0.11	25,29,30,30	0
2	RAM	O	1	11/11	0.96	0.11	40,44,46,50	0
2	GAD	O	2	11/11	0.96	0.12	30,38,42,45	0
2	RAM	K	1	11/11	0.97	0.12	31,34,36,41	0
2	RAM	M	1	11/11	0.97	0.14	26,27,30,34	0
2	RAM	P	1	11/11	0.97	0.12	31,34,36,38	0
2	GAD	P	2	11/11	0.97	0.11	30,35,38,39	0
2	RAM	N	1	11/11	0.98	0.12	23,24,26,29	0
2	GAD	I	2	11/11	0.98	0.12	19,23,24,26	0

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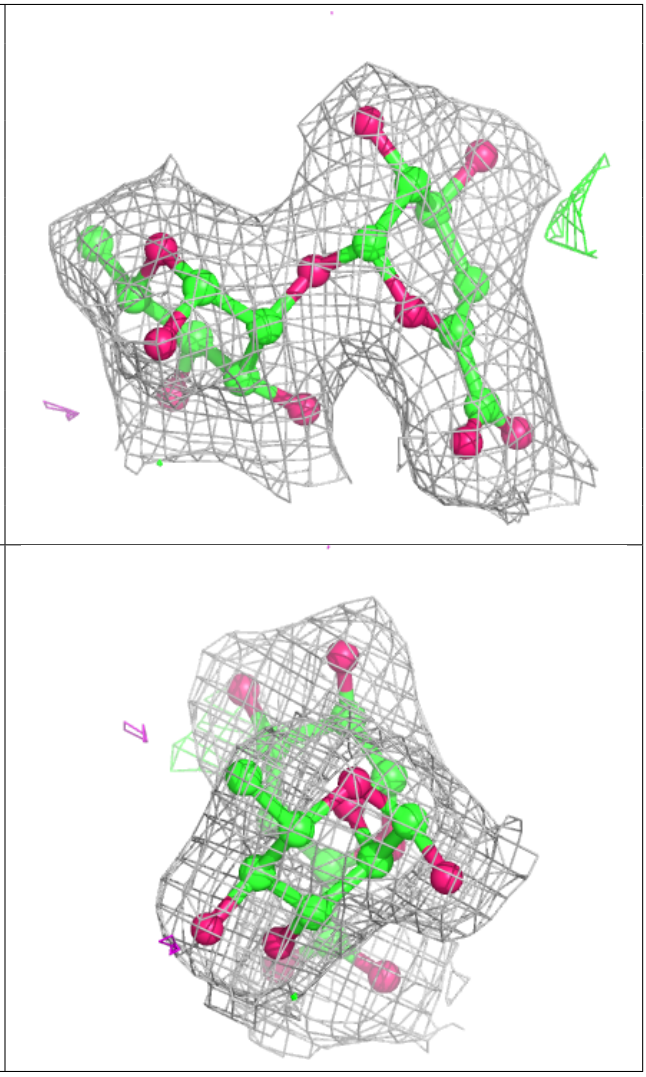
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	RAM	L	1	11/11	0.98	0.11	28,32,34,37	0
2	RAM	J	1	11/11	0.98	0.12	21,23,24,25	0
2	GAD	J	2	11/11	0.98	0.10	22,25,26,29	0
2	RAM	I	1	11/11	0.98	0.11	21,23,24,24	0

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.

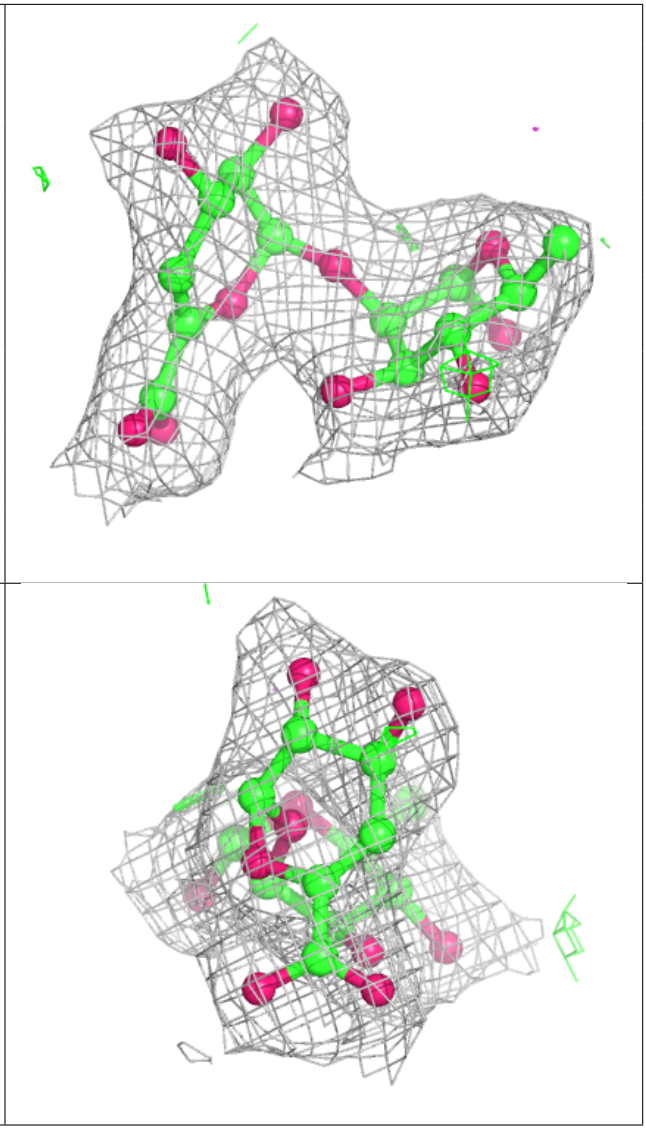
Electron density around Chain I:

2mF$_o$-DF$_c$ (at 0.7 rmsd) in gray
mF$_o$-DF$_c$ (at 3 rmsd) in purple (negative) and green (positive)



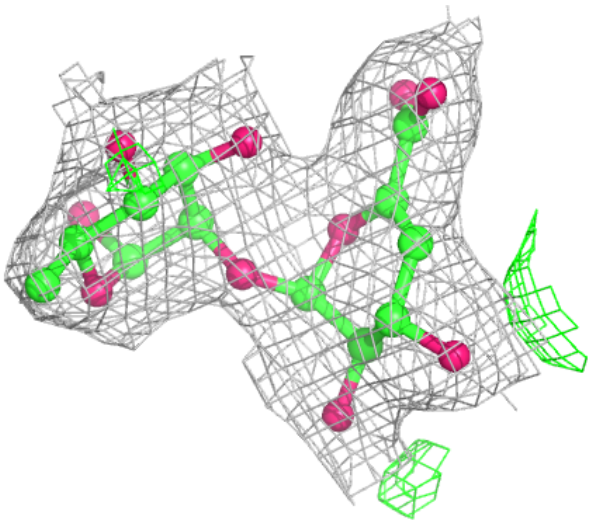
Electron density around Chain J:

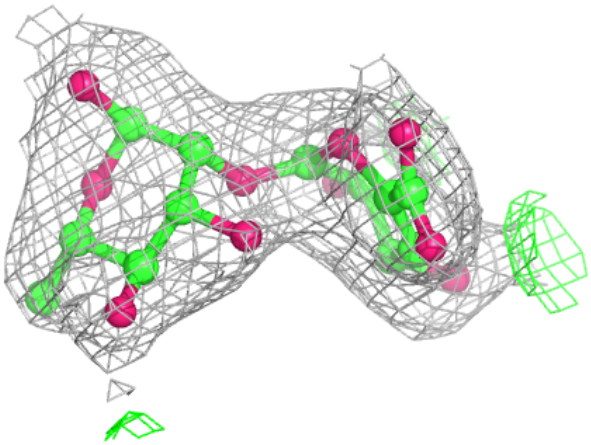
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

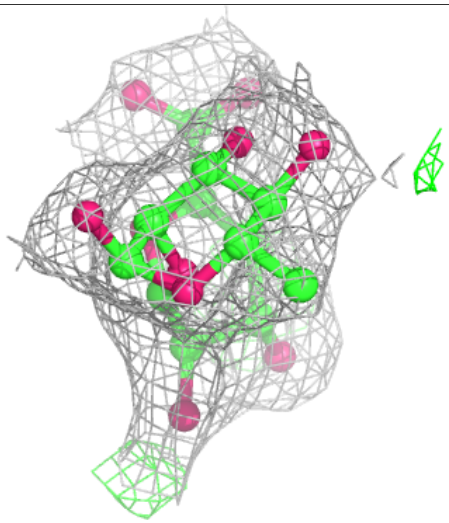


Electron density around Chain K:

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

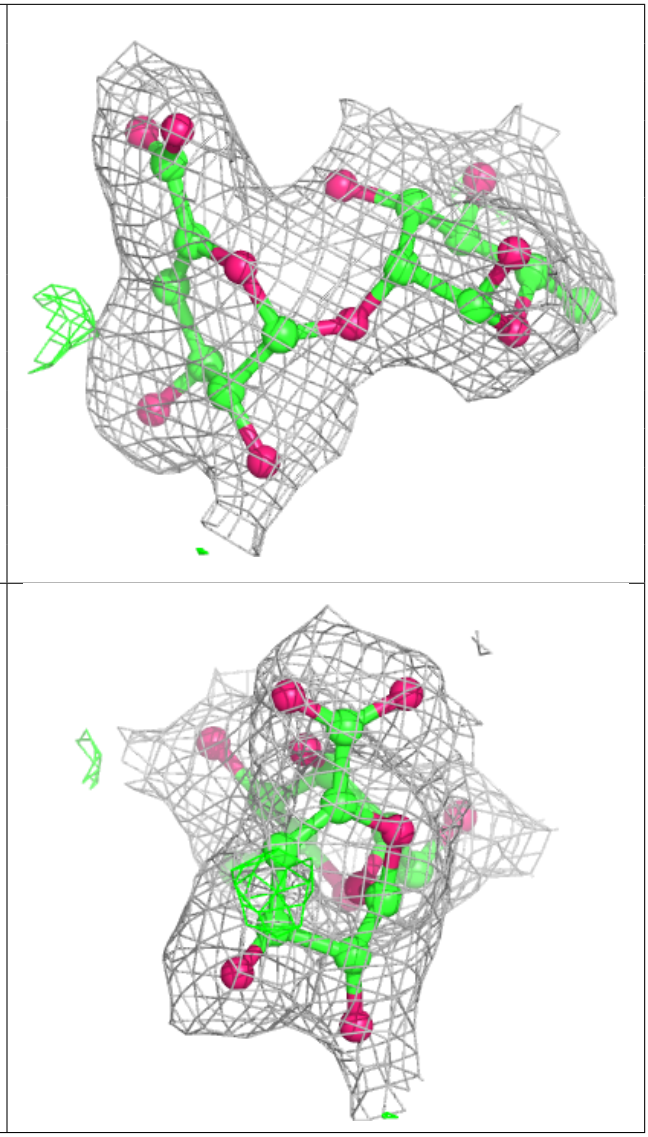






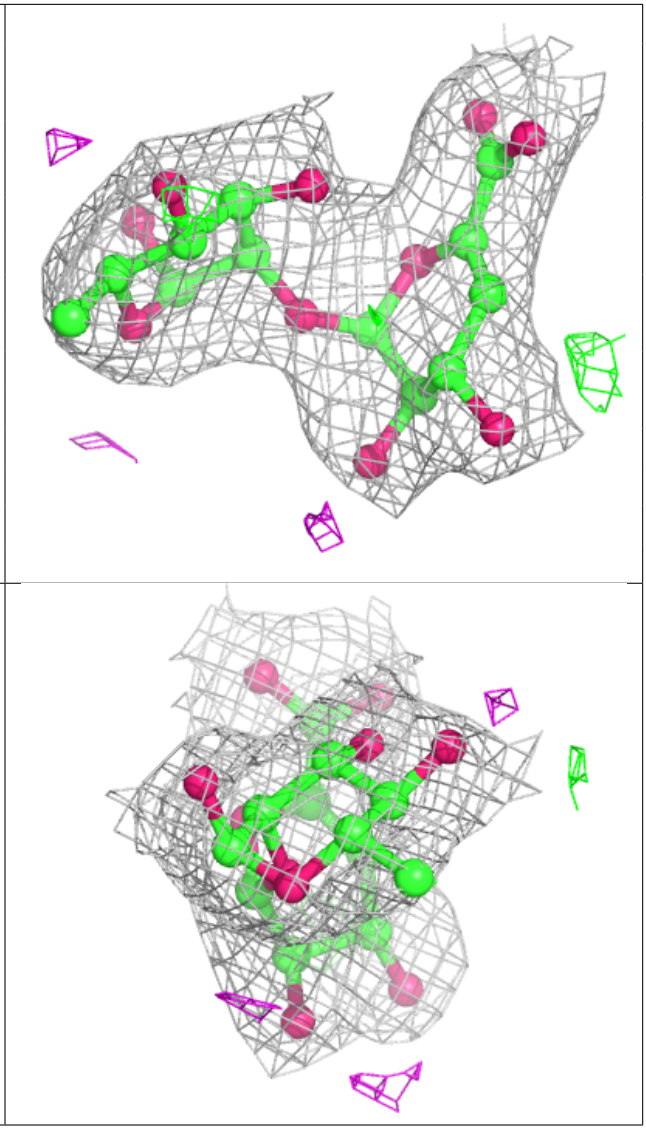
Electron density around Chain L:

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



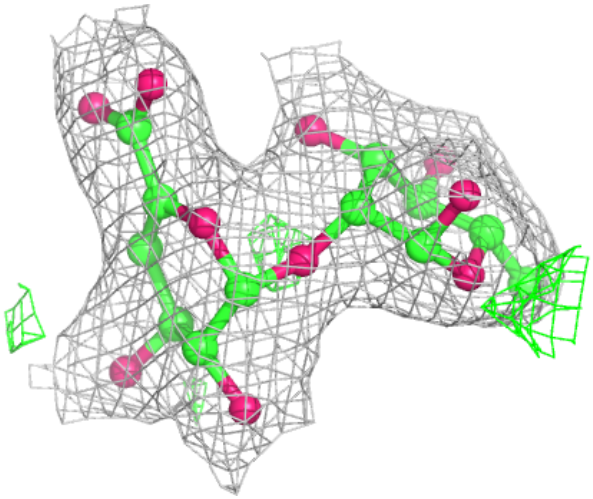
Electron density around Chain M:

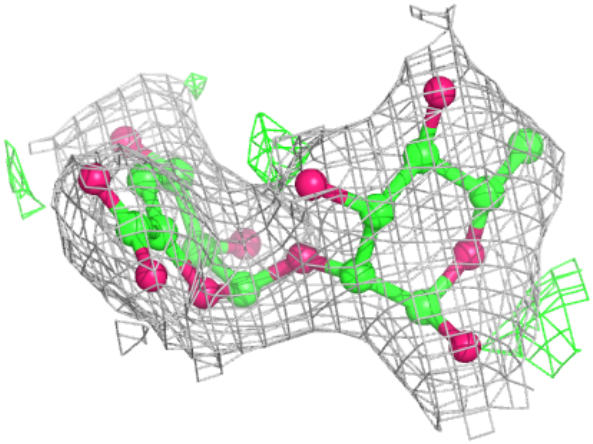
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

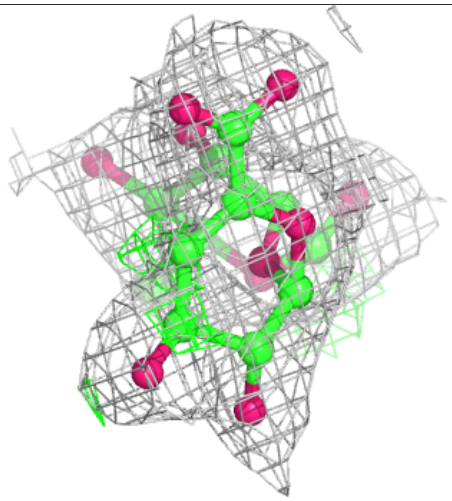


Electron density around Chain N:

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

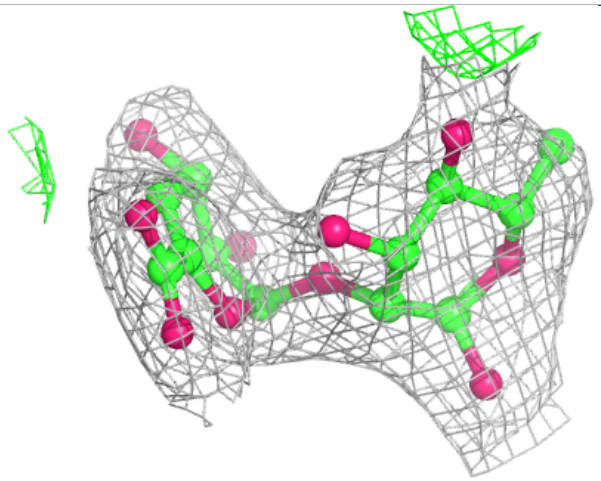


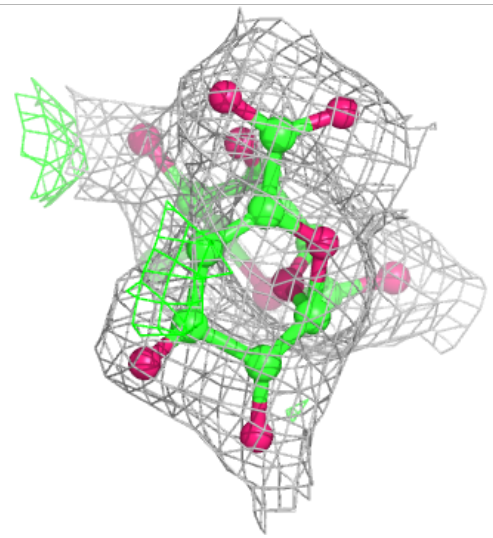




Electron density around Chain O:

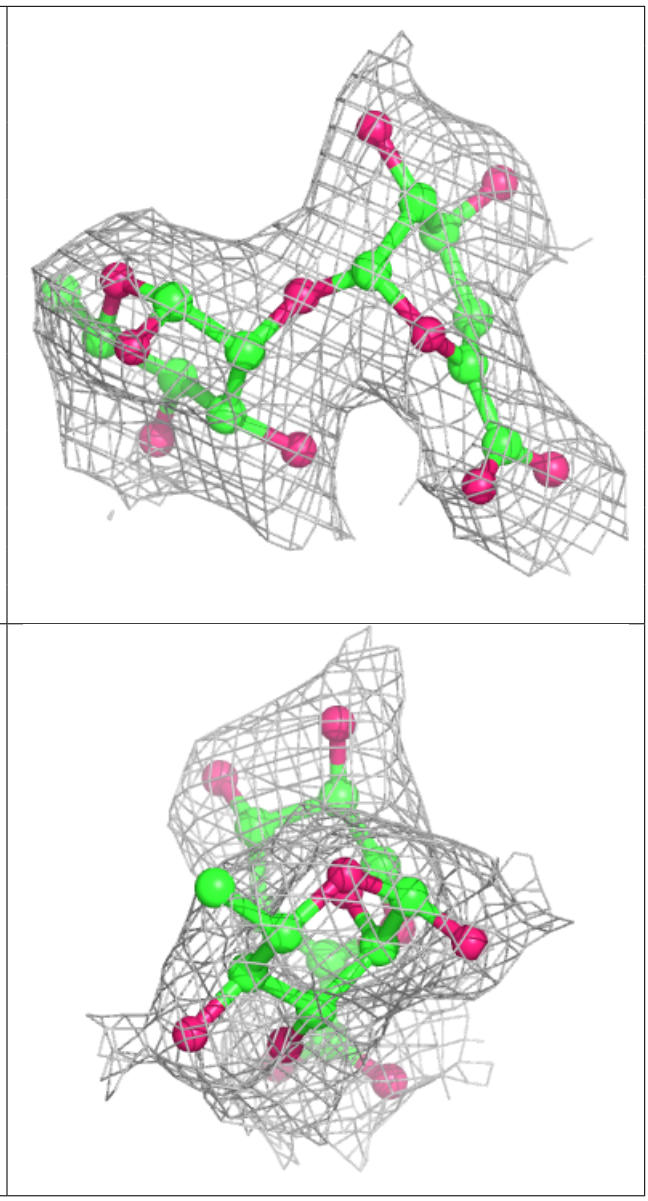
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)





Electron density around Chain P:

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



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(Å^2)	Q<0.9
3	CA	H	1003	1/1	0.96	0.17	19,19,19,19	0
3	CA	B	1003	1/1	0.98	0.15	11,11,11,11	0
3	CA	C	1003	1/1	0.99	0.15	9,9,9,9	0
3	CA	E	1003	1/1	0.99	0.15	12,12,12,12	0
3	CA	F	1003	1/1	0.99	0.13	11,11,11,11	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	CA	G	1003	1/1	0.99	0.17	18,18,18,18	0
3	CA	A	1003	1/1	0.99	0.16	11,11,11,11	0
3	CA	D	1003	1/1	1.00	0.17	12,12,12,12	0

6.5 Other polymers (i)

There are no such residues in this entry.