Full wwPDB X-ray Structure Validation Report (i)

Oct 17, 2021 – 05:07 AM EDT

PDB ID	:	1JYN
Title	:	E. COLI (lacZ) BETA-GALACTOSIDASE (E537Q) IN COMPLEX WITH LACTOSE
Authors	:	Juers, D.H.; Matthews, B.W.
Deposited on	:	2001-09-13
Resolution	:	1.80 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 following versions of software and data (see references (1)) were used in the production of this report:

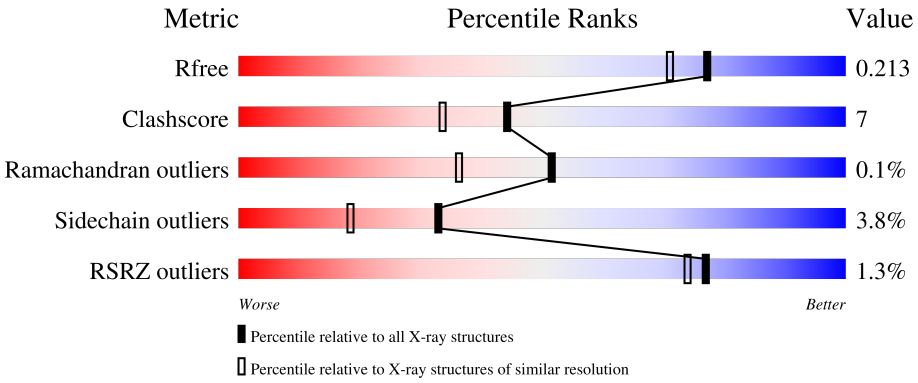
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

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 1.80 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	5950 (1.80-1.80)
Clashscore	141614	6793 (1.80-1.80)
Ramachandran outliers	138981	6697 (1.80-1.80)
Sidechain outliers	138945	6696 (1.80-1.80)
RSRZ outliers	127900	5850 (1.80-1.80)

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	1023	74% 21%
1	B	1023	75% 21%
1	C	1023	74% 21%
1	D	1023	74% 21%
2	E	2	100%

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Mol	Chain	Length	Quality of chain
2	F	2	100%
2	G	2	100%
2	H	2	100%

2 Entry composition (i)

There are 6 unique types of molecules in this entry. The entry contains 37546 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 Beta-Galactosidase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1011	Total	C	N	O	S	0	2	0
			8128	5139	1442	1509	38			
1	B	1011	Total	C	N	O	S	0	2	0
			8128	5139	1442	1509	38			
1	C	1011	Total	C	N	O	S	0	2	0
			8128	5139	1442	1509	38			
1	D	1011	Total	C	N	O	S	0	2	0
			8128	5139	1442	1509	38			

There are 36 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	GLY	THR	cloning artifact	? P00722
A	2	SER	MET	cloning artifact	? P00722
A	3	HIS	ILE	cloning artifact	? P00722
A	4	MET	THR	cloning artifact	? P00722
A	5	LEU	ASP	cloning artifact	? P00722
A	6	GLU	SER	cloning artifact	? P00722
A	7	ASP	LEU	cloning artifact	? P00722
A	8	PRO	ALA	cloning artifact	? P00722
A	537	GLN	GLU	engineered mutation	? P00722
B	1	GLY	THR	cloning artifact	? P00722
B	2	SER	MET	cloning artifact	? P00722
B	3	HIS	ILE	cloning artifact	? P00722
B	4	MET	THR	cloning artifact	? P00722
B	5	LEU	ASP	cloning artifact	? P00722
B	6	GLU	SER	cloning artifact	? P00722
B	7	ASP	LEU	cloning artifact	? P00722
B	8	PRO	ALA	cloning artifact	? P00722
B	537	GLN	GLU	engineered mutation	? P00722
C	1	GLY	THR	cloning artifact	? P00722
C	2	SER	MET	cloning artifact	? P00722
C	3	HIS	ILE	cloning artifact	? P00722

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Chain	Residue	Modelled	Actual	Comment	Reference
C	4	MET	THR	cloning artifact	? P00722
C	5	LEU	ASP	cloning artifact	? P00722
C	6	GLU	SER	cloning artifact	? P00722
C	7	ASP	LEU	cloning artifact	? P00722
C	8	PRO	ALA	cloning artifact	? P00722
C	537	GLN	GLU	engineered mutation	? P00722
D	1	GLY	THR	cloning artifact	? P00722
D	2	SER	MET	cloning artifact	? P00722
D	3	HIS	ILE	cloning artifact	? P00722
D	4	MET	THR	cloning artifact	? P00722
D	5	LEU	ASP	cloning artifact	? P00722
D	6	GLU	SER	cloning artifact	? P00722
D	7	ASP	LEU	cloning artifact	? P00722
D	8	PRO	ALA	cloning artifact	? P00722
D	537	GLN	GLU	engineered mutation	? P00722

- Molecule 2 is an oligosaccharide called beta-D-galactopyranose-(1-4)-beta-D-glucopyranose.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf	Trace
2	E	2	Total C O 23 12 11	0	0	0
2	F	2	Total C O 23 12 11	0	0	0
2	G	2	Total C O 23 12 11	0	0	0
2	H	2	Total C O 23 12 11	0	0	0

- Molecule 3 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	4	Total Mg 4 4	0	0
3	B	2	Total Mg 2 2	0	0
3	C	4	Total Mg 4 4	0	0

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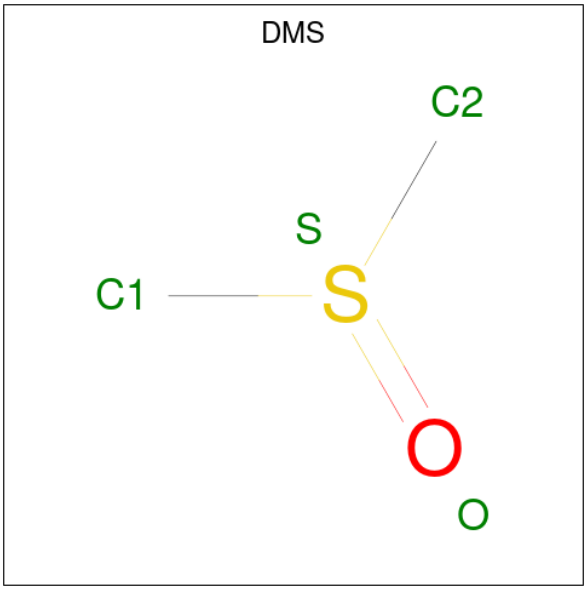
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	D	4	Total Mg 4 4	0	0

- Molecule 4 is SODIUM ION (three-letter code: NA) (formula: Na).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	4	Total Na 4 4	0	0
4	B	4	Total Na 4 4	0	0
4	C	4	Total Na 4 4	0	0
4	D	3	Total Na 3 3	0	0

- Molecule 5 is DIMETHYL SULFOXIDE (three-letter code: DMS) (formula: C_2H_6OS).



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

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	1	Total C O S 4 2 1 1	0	0
5	A	1	Total C O S 4 2 1 1	0	0
5	A	1	Total C O S 4 2 1 1	0	0
5	A	1	Total C O S 4 2 1 1	0	0
5	A	1	Total C O S 4 2 1 1	0	0
5	A	1	Total C O S 4 2 1 1	0	0
5	A	1	Total C O S 4 2 1 1	0	0
5	A	1	Total C O S 4 2 1 1	0	0
5	A	1	Total C O S 4 2 1 1	0	0
5	A	1	Total C O S 4 2 1 1	0	0
5	A	1	Total C O S 4 2 1 1	0	0
5	A	1	Total C O S 4 2 1 1	0	0
5	A	1	Total C O S 4 2 1 1	0	0
5	A	1	Total C O S 4 2 1 1	0	0
5	A	1	Total C O S 4 2 1 1	0	0
5	A	1	Total C O S 4 2 1 1	0	0
5	A	1	Total C O S 4 2 1 1	0	0
5	A	1	Total C O S 4 2 1 1	0	0
5	A	1	Total C O S 4 2 1 1	0	0
5	B	1	Total C O S 4 2 1 1	0	0
5	B	1	Total C O S 4 2 1 1	0	0

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	B	1	Total	C	O	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	B	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		
5	C	1	Total	C	O	S	0	0
			4	2	1	1		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	C	1	Total C O S 4 2 1 1	0	0
5	C	1	Total C O S 4 2 1 1	0	0
5	C	1	Total C O S 4 2 1 1	0	0
5	C	1	Total C O S 4 2 1 1	0	0
5	C	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0
5	D	1	Total C O S 4 2 1 1	0	0

- Molecule 6 is water.

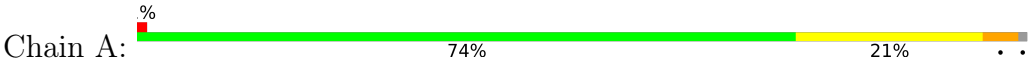
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
6	A	1136	Total O 1136 1136	0	0
6	B	1151	Total O 1151 1151	0	0
6	C	1133	Total O 1133 1133	0	0
6	D	1109	Total O 1109 1109	0	0

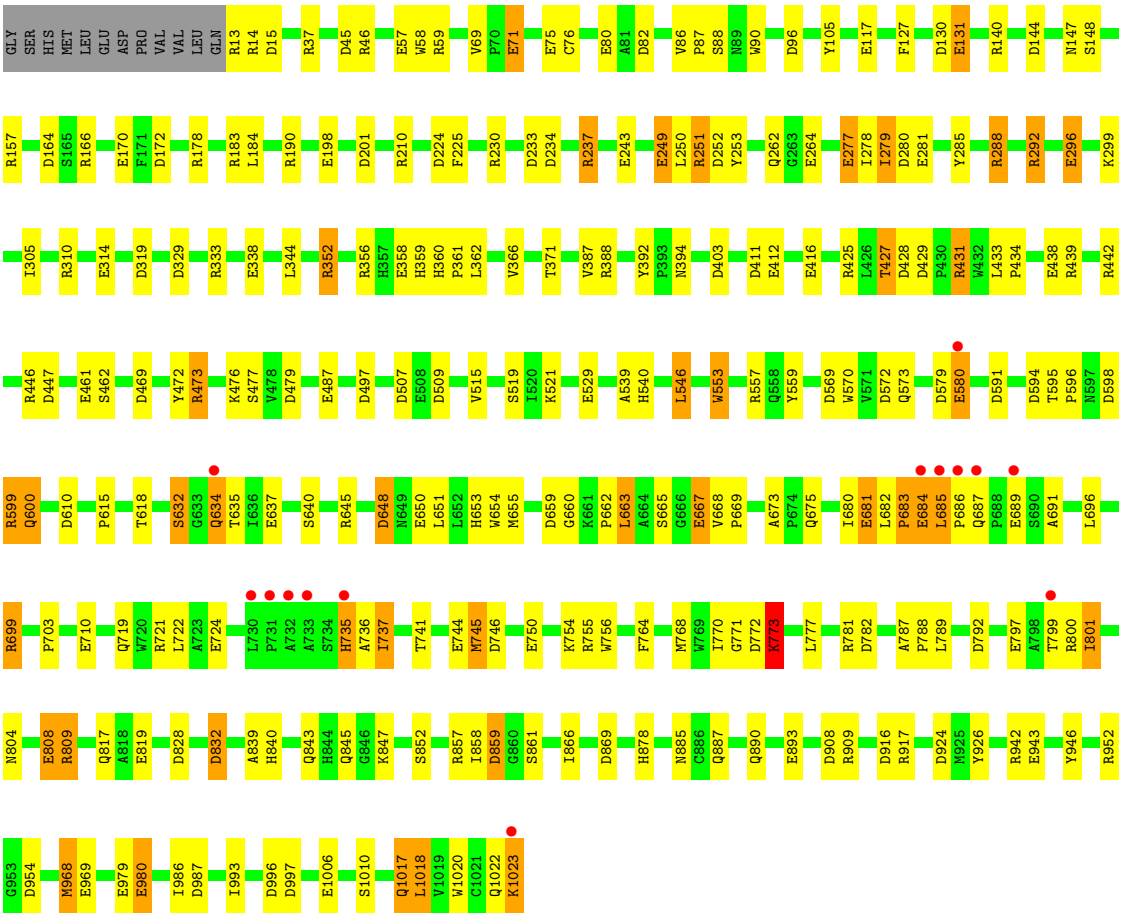
3 Residue-property plots (i)

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: Beta-Galactosidase

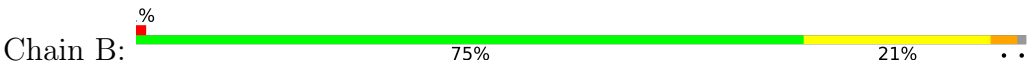
Chain A:

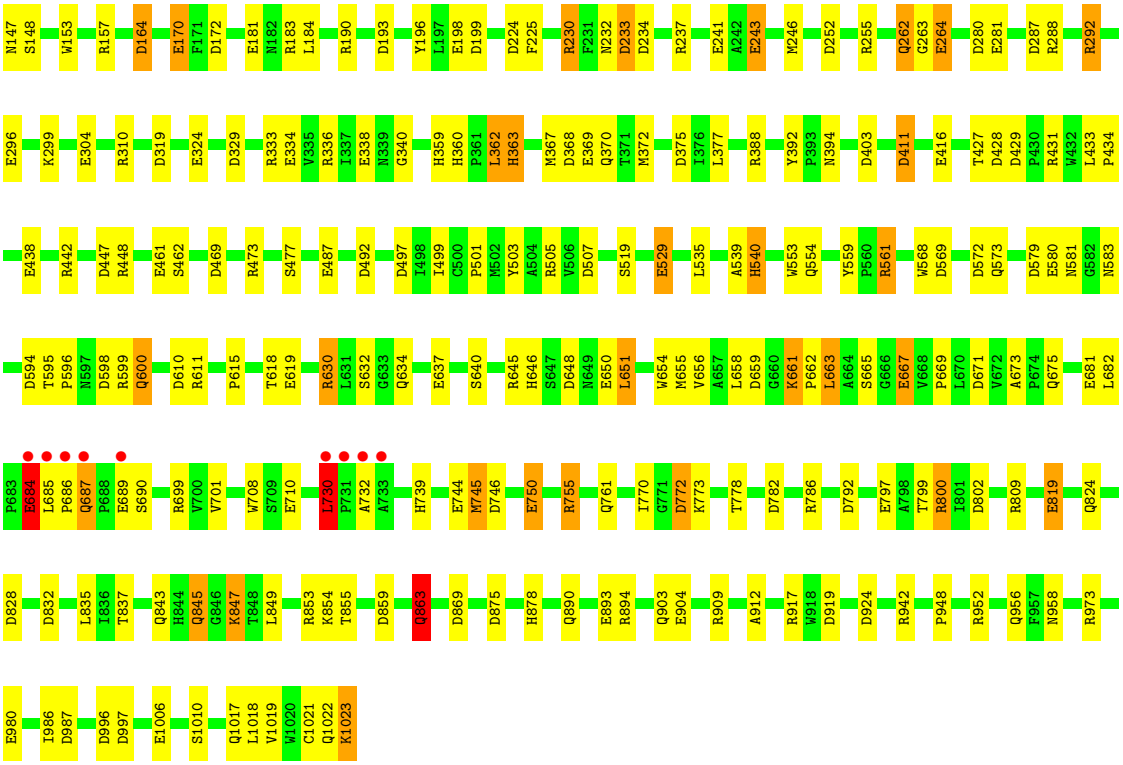




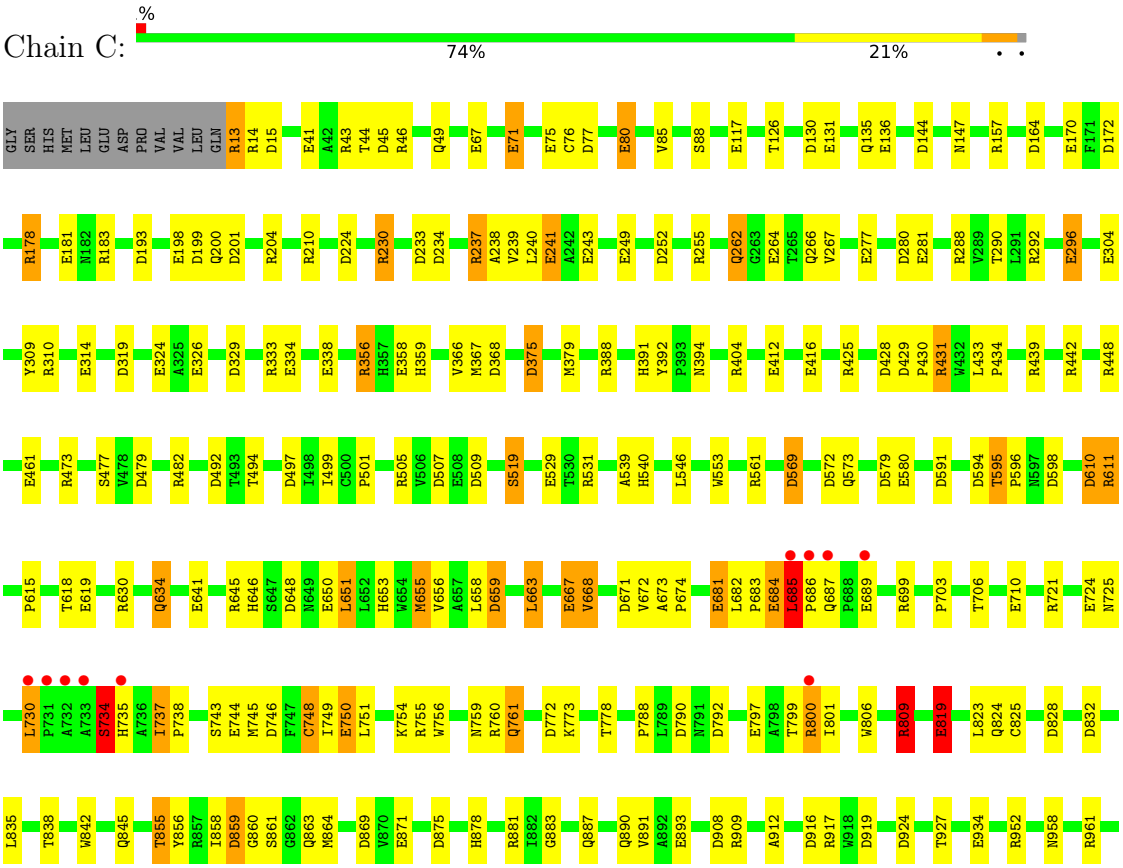
• Molecule 1: Beta-Galactosidase

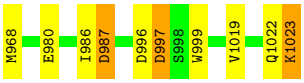
Chain B:





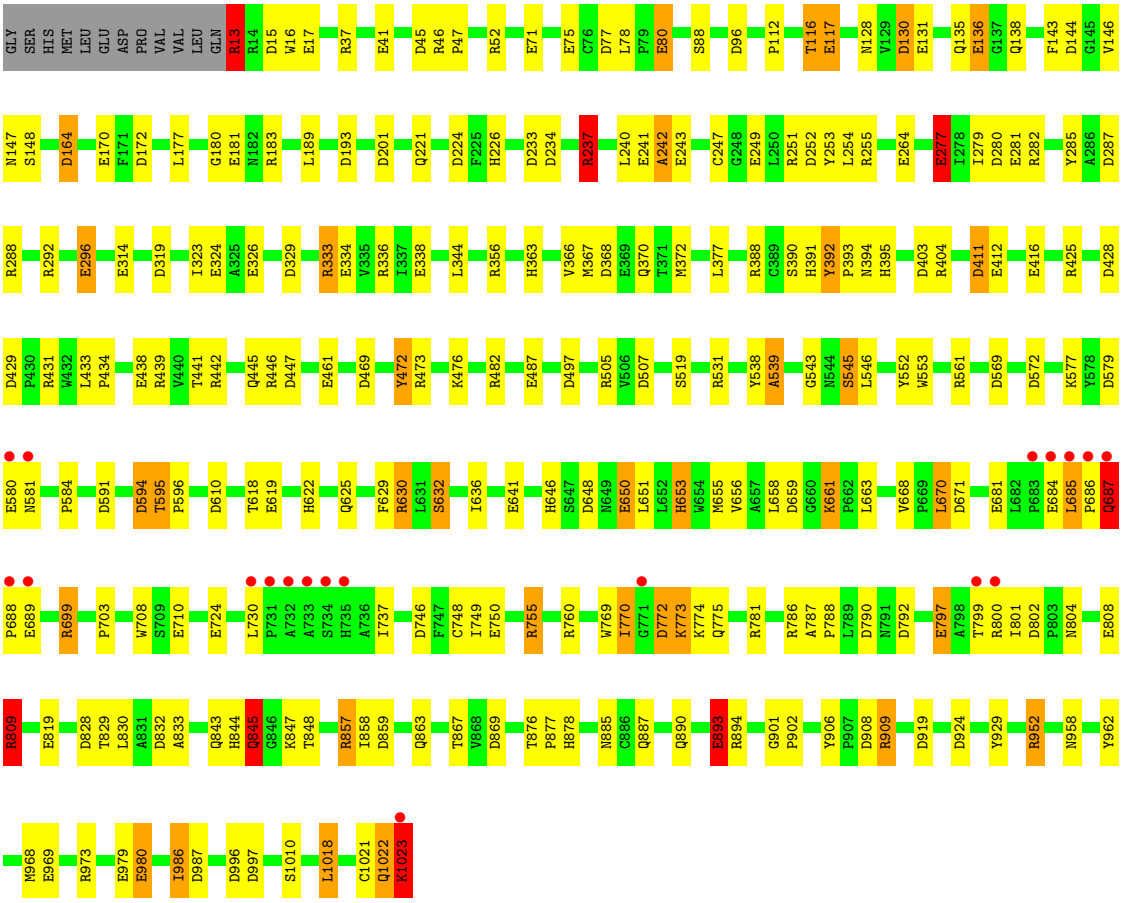
• Molecule 1: Beta-Galactosidase





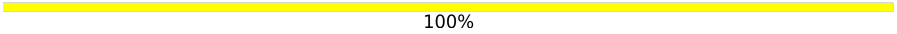
• Molecule 1: Beta-Galactosidase

Chain D:



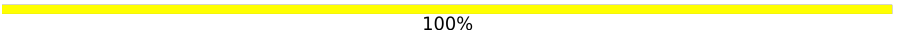
• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain E:



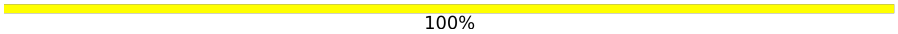
• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain F:



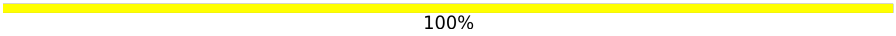
• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain G:



• Molecule 2: beta-D-galactopyranose-(1-4)-beta-D-glucopyranose

Chain H:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α, β, γ	149.55Å 168.63Å 200.88Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	17.00 – 1.80 16.99 – 1.80	Depositor EDS
% Data completeness (in resolution range)	92.0 (17.00-1.80) 93.5 (16.99-1.80)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.98 (at 1.80Å)	Xtriage
Refinement program	TNT	Depositor
R, R_{free}	0.155 , 0.219 0.153 , 0.213	Depositor DCC
R_{free} test set	6261 reflections (1.44%)	wwPDB-VP
Wilson B-factor (Å^2)	10.7	Xtriage
Anisotropy	0.262	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.35 , 90.7	EDS
L-test for twinning[2]	$< \|L\| > = 0.50$, $< L^2 > = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.96	EDS
Total number of atoms	37546	wwPDB-VP
Average B, all atoms (Å^2)	18.0	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 35.20 % 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 6.0529e-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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: MG, DMS, GAL, BGC, NA

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	1.13	43/8383 (0.5%)	1.66	175/11437 (1.5%)
1	B	1.15	42/8383 (0.5%)	1.64	159/11437 (1.4%)
1	C	1.13	46/8383 (0.5%)	1.66	171/11437 (1.5%)
1	D	1.13	41/8383 (0.5%)	1.64	173/11437 (1.5%)
All	All	1.14	172/33532 (0.5%)	1.65	678/45748 (1.5%)

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	D	1	0

All (172) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	71	GLU	CD-OE2	10.67	1.37	1.25
1	B	71	GLU	CD-OE2	9.89	1.36	1.25
1	B	487	GLU	CD-OE2	9.46	1.36	1.25
1	D	243	GLU	CD-OE2	9.36	1.35	1.25
1	A	296	GLU	CD-OE2	9.25	1.35	1.25
1	D	650	GLU	CD-OE2	9.15	1.35	1.25
1	A	249	GLU	CD-OE2	9.03	1.35	1.25
1	A	487	GLU	CD-OE2	8.86	1.35	1.25
1	C	529	GLU	CD-OE2	8.79	1.35	1.25
1	D	277	GLU	CD-OE2	8.76	1.35	1.25
1	D	334	GLU	CD-OE2	8.75	1.35	1.25
1	C	80	GLU	CD-OE2	8.64	1.35	1.25
1	D	75	GLU	CD-OE2	8.34	1.34	1.25
1	A	277	GLU	CD-OE2	8.14	1.34	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	181	GLU	CD-OE2	8.13	1.34	1.25
1	A	243	GLU	CD-OE2	8.07	1.34	1.25
1	B	650	GLU	CD-OE2	8.02	1.34	1.25
1	C	684	GLU	CD-OE2	7.91	1.34	1.25
1	C	304	GLU	CD-OE2	7.87	1.34	1.25
1	A	170	GLU	CD-OE2	7.83	1.34	1.25
1	A	529	GLU	CD-OE2	7.75	1.34	1.25
1	D	893	GLU	CD-OE2	7.67	1.34	1.25
1	D	170	GLU	CD-OE2	7.64	1.34	1.25
1	C	580	GLU	CD-OE2	7.64	1.34	1.25
1	C	314	GLU	CD-OE1	-7.62	1.17	1.25
1	C	934	GLU	CD-OE2	7.56	1.33	1.25
1	B	80	GLU	CD-OE2	7.50	1.33	1.25
1	B	819	GLU	CD-OE2	7.49	1.33	1.25
1	A	314	GLU	CD-OE1	-7.46	1.17	1.25
1	B	170	GLU	CD-OE2	7.45	1.33	1.25
1	D	980	GLU	CD-OE2	7.45	1.33	1.25
1	B	1006	GLU	CD-OE2	7.41	1.33	1.25
1	A	264	GLU	CD-OE2	7.33	1.33	1.25
1	D	681	GLU	CD-OE2	7.27	1.33	1.25
1	A	1006	GLU	CD-OE2	7.24	1.33	1.25
1	B	980	GLU	CD-OE2	7.24	1.33	1.25
1	A	681	GLU	CD-OE2	7.23	1.33	1.25
1	D	979	GLU	CD-OE2	7.23	1.33	1.25
1	A	281	GLU	CD-OE2	7.21	1.33	1.25
1	D	80	GLU	CD-OE2	7.00	1.33	1.25
1	C	416	GLU	CD-OE2	6.99	1.33	1.25
1	D	41	GLU	CD-OE1	-6.95	1.18	1.25
1	C	334	GLU	CD-OE2	6.88	1.33	1.25
1	C	281	GLU	CD-OE2	6.88	1.33	1.25
1	B	689	GLU	CD-OE2	6.87	1.33	1.25
1	D	797	GLU	CD-OE2	6.87	1.33	1.25
1	A	580	GLU	CD-OE2	6.85	1.33	1.25
1	D	684	GLU	CD-OE2	6.83	1.33	1.25
1	A	689	GLU	CD-OE2	6.80	1.33	1.25
1	B	580	GLU	CD-OE2	6.80	1.33	1.25
1	A	684	GLU	CD-OE2	6.79	1.33	1.25
1	D	461	GLU	CD-OE2	6.77	1.33	1.25
1	D	750	GLU	CD-OE2	6.73	1.33	1.25
1	A	416	GLU	CD-OE2	6.73	1.33	1.25
1	C	324	GLU	CD-OE2	6.72	1.33	1.25
1	C	461	GLU	CD-OE2	6.72	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	710	GLU	CD-OE2	6.70	1.33	1.25
1	C	71	GLU	CD-OE2	6.69	1.33	1.25
1	A	969	GLU	CD-OE2	6.68	1.32	1.25
1	C	198	GLU	CD-OE2	6.66	1.32	1.25
1	B	181	GLU	CD-OE2	6.65	1.32	1.25
1	D	136	GLU	CD-OE2	6.65	1.32	1.25
1	D	580	GLU	CD-OE2	6.63	1.32	1.25
1	D	710	GLU	CD-OE2	6.63	1.32	1.25
1	D	689	GLU	CD-OE2	6.58	1.32	1.25
1	A	71	GLU	CD-OE2	6.58	1.32	1.25
1	B	416	GLU	CD-OE2	6.57	1.32	1.25
1	C	296	GLU	CD-OE2	6.57	1.32	1.25
1	A	461	GLU	CD-OE2	6.55	1.32	1.25
1	B	684	GLU	CD-OE2	6.55	1.32	1.25
1	C	641	GLU	CD-OE1	-6.54	1.18	1.25
1	A	117	GLU	CD-OE2	6.50	1.32	1.25
1	C	744	GLU	CD-OE2	6.48	1.32	1.25
1	C	667	GLU	CD-OE2	6.48	1.32	1.25
1	D	249	GLU	CD-OE2	6.38	1.32	1.25
1	D	619	GLU	CD-OE2	6.38	1.32	1.25
1	B	893	GLU	CD-OE2	6.33	1.32	1.25
1	A	979	GLU	CD-OE2	6.32	1.32	1.25
1	D	819	GLU	CD-OE2	6.30	1.32	1.25
1	B	296	GLU	CD-OE2	6.29	1.32	1.25
1	C	338	GLU	CD-OE2	6.29	1.32	1.25
1	A	80	GLU	CD-OE2	6.28	1.32	1.25
1	C	277	GLU	CD-OE2	6.28	1.32	1.25
1	B	438	GLU	CD-OE2	6.24	1.32	1.25
1	A	131	GLU	CD-OE2	6.24	1.32	1.25
1	B	529	GLU	CD-OE2	6.22	1.32	1.25
1	B	243	GLU	CD-OE2	6.20	1.32	1.25
1	B	281	GLU	CD-OE2	6.19	1.32	1.25
1	A	57	GLU	CD-OE2	6.17	1.32	1.25
1	C	689	GLU	CD-OE2	6.17	1.32	1.25
1	A	650	GLU	CD-OE2	6.17	1.32	1.25
1	B	67	GLU	CD-OE1	-6.15	1.18	1.25
1	A	412	GLU	CD-OE2	6.15	1.32	1.25
1	B	667	GLU	CD-OE2	6.12	1.32	1.25
1	A	338	GLU	CD-OE2	6.08	1.32	1.25
1	C	980	GLU	CD-OE2	6.07	1.32	1.25
1	B	681	GLU	CD-OE2	6.07	1.32	1.25
1	B	904	GLU	CD-OE2	6.04	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	819	GLU	CD-OE2	6.03	1.32	1.25
1	B	710	GLU	CD-OE2	6.02	1.32	1.25
1	D	131	GLU	CD-OE2	6.01	1.32	1.25
1	B	338	GLU	CD-OE2	6.00	1.32	1.25
1	C	893	GLU	CD-OE2	5.99	1.32	1.25
1	C	681	GLU	CD-OE2	5.99	1.32	1.25
1	A	808	GLU	CD-OE2	5.97	1.32	1.25
1	D	641	GLU	CD-OE1	-5.96	1.19	1.25
1	D	314	GLU	CD-OE1	-5.93	1.19	1.25
1	C	170	GLU	CD-OE2	5.92	1.32	1.25
1	A	75	GLU	CD-OE2	5.91	1.32	1.25
1	A	438	GLU	CD-OE2	5.90	1.32	1.25
1	B	17	GLU	CD-OE1	-5.87	1.19	1.25
1	B	117	GLU	CD-OE2	5.86	1.32	1.25
1	D	117	GLU	CD-OE2	5.86	1.32	1.25
1	C	249	GLU	CD-OE2	5.83	1.32	1.25
1	B	744	GLU	CD-OE2	5.83	1.32	1.25
1	C	241	GLU	CD-OE2	5.83	1.32	1.25
1	C	75	GLU	CD-OE2	5.79	1.32	1.25
1	A	980	GLU	CD-OE2	5.78	1.32	1.25
1	C	650	GLU	CD-OE2	5.76	1.31	1.25
1	A	667	GLU	CD-OE2	5.73	1.31	1.25
1	A	893	GLU	CD-OE2	5.73	1.31	1.25
1	D	181	GLU	CD-OE2	5.72	1.31	1.25
1	D	487	GLU	CD-OE2	5.67	1.31	1.25
1	C	326	GLU	CD-OE1	-5.66	1.19	1.25
1	D	17	GLU	CD-OE2	5.65	1.31	1.25
1	D	264	GLU	CD-OE2	5.63	1.31	1.25
1	B	904	GLU	CD-OE1	-5.62	1.19	1.25
1	A	819	GLU	CD-OE2	5.62	1.31	1.25
1	C	136	GLU	CD-OE2	5.62	1.31	1.25
1	B	264	GLU	CD-OE2	5.58	1.31	1.25
1	B	304	GLU	CD-OE2	5.55	1.31	1.25
1	D	326	GLU	CD-OE2	5.53	1.31	1.25
1	A	637	GLU	CD-OE2	5.49	1.31	1.25
1	D	281	GLU	CD-OE1	-5.48	1.19	1.25
1	C	243	GLU	CD-OE2	5.47	1.31	1.25
1	C	117	GLU	CD-OE2	5.46	1.31	1.25
1	A	724	GLU	CD-OE2	5.46	1.31	1.25
1	C	710	GLU	CD-OE2	5.44	1.31	1.25
1	D	438	GLU	CD-OE2	5.42	1.31	1.25
1	D	296	GLU	CD-OE2	5.42	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	324	GLU	CD-OE2	5.42	1.31	1.25
1	A	744	GLU	CD-OE2	5.41	1.31	1.25
1	C	412	GLU	CD-OE2	5.39	1.31	1.25
1	C	264	GLU	CD-OE2	5.39	1.31	1.25
1	B	136	GLU	CD-OE2	5.38	1.31	1.25
1	C	724	GLU	CD-OE2	5.36	1.31	1.25
1	B	797	GLU	CD-OE2	5.35	1.31	1.25
1	C	67	GLU	CD-OE2	5.33	1.31	1.25
1	B	334	GLU	CD-OE1	-5.33	1.19	1.25
1	B	57	GLU	CD-OE2	5.32	1.31	1.25
1	D	241	GLU	CD-OE2	5.32	1.31	1.25
1	B	461	GLU	CD-OE2	5.31	1.31	1.25
1	D	338	GLU	CD-OE2	5.31	1.31	1.25
1	B	750	GLU	CD-OE1	-5.31	1.19	1.25
1	C	41	GLU	CD-OE2	5.29	1.31	1.25
1	C	750	GLU	CD-OE2	5.28	1.31	1.25
1	A	310	ARG	CZ-NH2	5.26	1.39	1.33
1	A	570	TRP	CG-CD1	5.26	1.44	1.36
1	B	198	GLU	CD-OE2	5.24	1.31	1.25
1	C	243	GLU	CD-OE1	-5.22	1.20	1.25
1	C	619	GLU	CD-OE2	5.21	1.31	1.25
1	B	75	GLU	CD-OE2	5.18	1.31	1.25
1	C	131	GLU	CD-OE2	5.17	1.31	1.25
1	A	943	GLU	CD-OE2	5.16	1.31	1.25
1	A	750	GLU	CD-OE2	5.15	1.31	1.25
1	D	41	GLU	CD-OE2	5.15	1.31	1.25
1	A	198	GLU	CD-OE2	5.12	1.31	1.25
1	B	131	GLU	CD-OE2	5.11	1.31	1.25
1	D	808	GLU	CD-OE1	-5.09	1.20	1.25
1	D	724	GLU	CD-OE2	5.08	1.31	1.25
1	C	358	GLU	CD-OE2	5.03	1.31	1.25
1	B	369	GLU	CD-OE2	5.02	1.31	1.25

All (678) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	442	ARG	NE-CZ-NH2	-20.09	110.26	120.30
1	D	183	ARG	NE-CZ-NH1	-15.78	112.41	120.30
1	A	755	ARG	NE-CZ-NH1	13.86	127.23	120.30
1	B	809	ARG	NE-CZ-NH2	-13.62	113.49	120.30
1	C	178	ARG	NE-CZ-NH1	13.44	127.02	120.30
1	A	166	ARG	NE-CZ-NH2	-12.83	113.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	224	ASP	CB-CG-OD2	-12.25	107.28	118.30
1	B	442	ARG	NE-CZ-NH1	12.23	126.42	120.30
1	C	442	ARG	NE-CZ-NH1	11.85	126.23	120.30
1	C	448	ARG	NE-CZ-NH2	-11.80	114.40	120.30
1	A	917	ARG	NE-CZ-NH1	-11.73	114.44	120.30
1	A	234	ASP	CB-CG-OD1	11.46	128.61	118.30
1	A	224	ASP	CB-CG-OD1	11.25	128.42	118.30
1	B	671	ASP	CB-CG-OD2	-10.95	108.44	118.30
1	C	869	ASP	CB-CG-OD2	-10.90	108.49	118.30
1	C	869	ASP	CB-CG-OD1	10.87	128.08	118.30
1	D	473	ARG	NE-CZ-NH1	10.78	125.69	120.30
1	B	507	ASP	CB-CG-OD2	-10.76	108.62	118.30
1	D	781	ARG	NE-CZ-NH1	10.76	125.68	120.30
1	B	246	MET	CG-SD-CE	-10.67	83.12	100.20
1	A	659	ASP	CB-CG-OD2	-10.64	108.72	118.30
1	C	645	ARG	NE-CZ-NH2	-10.54	115.03	120.30
1	B	442	ARG	NE-CZ-NH2	-10.53	115.03	120.30
1	A	96	ASP	CB-CG-OD1	10.51	127.76	118.30
1	A	234	ASP	CB-CG-OD2	-10.49	108.86	118.30
1	B	853	ARG	NE-CZ-NH1	10.47	125.54	120.30
1	C	431	ARG	NE-CZ-NH2	-10.45	115.08	120.30
1	A	431	ARG	NE-CZ-NH2	-10.38	115.11	120.30
1	D	987	ASP	CB-CG-OD1	10.38	127.64	118.30
1	D	561	ARG	NE-CZ-NH1	10.35	125.48	120.30
1	B	252	ASP	CB-CG-OD2	-10.30	109.03	118.30
1	B	388	ARG	NE-CZ-NH2	-10.30	115.15	120.30
1	B	772	ASP	CB-CG-OD2	-10.26	109.06	118.30
1	C	917	ARG	NE-CZ-NH2	10.26	125.43	120.30
1	D	859	ASP	CB-CG-OD2	-10.25	109.08	118.30
1	D	699	ARG	NE-CZ-NH1	10.20	125.40	120.30
1	A	46	ARG	NE-CZ-NH1	10.18	125.39	120.30
1	D	172	ASP	CB-CG-OD2	-10.17	109.15	118.30
1	B	336	ARG	NE-CZ-NH1	10.07	125.33	120.30
1	D	648	ASP	CB-CG-OD2	-10.05	109.26	118.30
1	A	610	ASP	CB-CG-OD1	10.04	127.33	118.30
1	A	144	ASP	CB-CG-OD1	10.04	127.33	118.30
1	A	952	ARG	NE-CZ-NH1	9.99	125.29	120.30
1	C	721	ARG	NE-CZ-NH1	9.94	125.27	120.30
1	D	439	ARG	NE-CZ-NH2	-9.93	115.34	120.30
1	C	199	ASP	CB-CG-OD1	9.90	127.21	118.30
1	D	172	ASP	CB-CG-OD1	9.89	127.20	118.30
1	B	648	ASP	CB-CG-OD1	9.86	127.17	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	439	ARG	NE-CZ-NH2	-9.84	115.38	120.30
1	B	469	ASP	CB-CG-OD2	-9.84	109.44	118.30
1	C	792	ASP	CB-CG-OD1	9.80	127.12	118.30
1	D	446	ARG	NE-CZ-NH2	-9.80	115.40	120.30
1	A	509	ASP	CB-CG-OD1	9.78	127.10	118.30
1	C	909	ARG	NE-CZ-NH1	9.76	125.18	120.30
1	C	505	ARG	NE-CZ-NH2	-9.74	115.43	120.30
1	B	368	ASP	CB-CG-OD1	9.70	127.03	118.30
1	A	746	ASP	CB-CG-OD2	-9.60	109.67	118.30
1	B	368	ASP	CB-CG-OD2	-9.56	109.70	118.30
1	B	96	ASP	CB-CG-OD2	-9.53	109.72	118.30
1	D	183	ARG	NE-CZ-NH2	9.53	125.06	120.30
1	B	853	ARG	NE-CZ-NH2	-9.50	115.55	120.30
1	D	224	ASP	CB-CG-OD1	9.50	126.85	118.30
1	B	772	ASP	CB-CG-OD1	9.49	126.84	118.30
1	C	204	ARG	NE-CZ-NH1	9.49	125.05	120.30
1	B	469	ASP	CB-CG-OD1	9.45	126.80	118.30
1	C	875	ASP	CB-CG-OD1	9.43	126.78	118.30
1	D	579	ASP	CB-CG-OD2	-9.43	109.82	118.30
1	B	594	ASP	CB-CG-OD2	-9.42	109.82	118.30
1	A	37	ARG	NE-CZ-NH1	9.40	125.00	120.30
1	C	224	ASP	CB-CG-OD1	9.39	126.75	118.30
1	D	329	ASP	CB-CG-OD1	9.38	126.74	118.30
1	A	473	ARG	NE-CZ-NH2	-9.38	115.61	120.30
1	A	233	ASP	CB-CG-OD1	9.36	126.72	118.30
1	B	648	ASP	CB-CG-OD2	-9.35	109.89	118.30
1	D	431	ARG	NE-CZ-NH2	-9.32	115.64	120.30
1	C	473	ARG	NE-CZ-NH1	9.31	124.96	120.30
1	D	255	ARG	NE-CZ-NH1	9.28	124.94	120.30
1	D	594	ASP	CB-CG-OD1	9.27	126.64	118.30
1	D	869	ASP	CB-CG-OD1	9.23	126.61	118.30
1	C	721	ARG	NE-CZ-NH2	-9.15	115.72	120.30
1	B	610	ASP	CB-CG-OD2	-9.14	110.07	118.30
1	D	802	ASP	CB-CG-OD2	-9.08	110.13	118.30
1	B	869	ASP	CB-CG-OD1	9.07	126.47	118.30
1	B	594	ASP	CB-CG-OD1	9.07	126.46	118.30
1	B	539[A]	ALA	CB-CA-C	-9.06	96.52	110.10
1	B	539[B]	ALA	CB-CA-C	-9.06	96.52	110.10
1	C	828	ASP	CB-CG-OD2	-9.00	110.20	118.30
1	C	280	ASP	CB-CG-OD2	-8.90	110.29	118.30
1	D	183	ARG	CD-NE-CZ	-8.84	111.23	123.60
1	A	172	ASP	CB-CG-OD2	-8.72	110.45	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	671	ASP	CB-CG-OD1	8.67	126.10	118.30
1	D	234	ASP	CB-CG-OD1	8.67	126.10	118.30
1	A	13	ARG	NE-CZ-NH2	-8.63	115.98	120.30
1	D	193	ASP	CB-CG-OD2	-8.62	110.54	118.30
1	A	599	ARG	NE-CZ-NH1	-8.60	116.00	120.30
1	A	771	GLY	C-N-CA	-8.58	100.25	121.70
1	C	492	ASP	CB-CG-OD2	-8.58	110.58	118.30
1	A	610	ASP	CB-CG-OD2	-8.57	110.59	118.30
1	B	875	ASP	CB-CG-OD1	8.54	125.99	118.30
1	C	579	ASP	CB-CG-OD2	-8.52	110.63	118.30
1	D	15	ASP	CB-CG-OD2	-8.51	110.64	118.30
1	A	411	ASP	CB-CG-OD2	-8.50	110.65	118.30
1	A	659	ASP	CB-CG-OD1	8.49	125.94	118.30
1	A	319	ASP	CB-CG-OD2	-8.49	110.66	118.30
1	A	233	ASP	CB-CG-OD2	-8.48	110.67	118.30
1	A	13	ARG	NE-CZ-NH1	8.45	124.52	120.30
1	D	919	ASP	CB-CG-OD2	-8.43	110.71	118.30
1	D	446	ARG	NE-CZ-NH1	8.39	124.50	120.30
1	B	919	ASP	CB-CG-OD2	-8.37	110.76	118.30
1	C	233	ASP	CB-CG-OD1	8.37	125.83	118.30
1	B	172	ASP	CB-CG-OD1	8.34	125.81	118.30
1	B	234	ASP	CB-CG-OD1	8.34	125.81	118.30
1	C	561	ARG	NE-CZ-NH2	-8.34	116.13	120.30
1	D	439	ARG	NE-CZ-NH1	8.26	124.43	120.30
1	D	280	ASP	CB-CG-OD1	8.24	125.72	118.30
1	B	572	ASP	CB-CG-OD2	-8.22	110.90	118.30
1	B	77	ASP	CB-CG-OD1	8.21	125.69	118.30
1	B	255	ARG	NE-CZ-NH1	8.21	124.40	120.30
1	B	611	ARG	NE-CZ-NH1	8.17	124.39	120.30
1	D	429	ASP	CB-CG-OD2	-8.16	110.96	118.30
1	D	482	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	A	164	ASP	CB-CG-OD1	8.11	125.59	118.30
1	B	193	ASP	CB-CG-OD1	8.08	125.57	118.30
1	C	144	ASP	CB-CG-OD1	8.08	125.57	118.30
1	B	319	ASP	CB-CG-OD1	8.07	125.57	118.30
1	D	193	ASP	CB-CG-OD1	8.04	125.53	118.30
1	D	591	ASP	CB-CG-OD1	8.03	125.53	118.30
1	D	130	ASP	CB-CG-OD2	-8.01	111.09	118.30
1	C	909	ARG	NE-CZ-NH2	-8.00	116.30	120.30
1	B	559	TYR	CB-CG-CD1	7.99	125.80	121.00
1	C	356	ARG	NE-CZ-NH1	7.99	124.29	120.30
1	C	428	ASP	CB-CG-OD1	7.99	125.49	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	45	ASP	CB-CG-OD1	7.98	125.48	118.30
1	B	828	ASP	CB-CG-OD1	7.93	125.44	118.30
1	C	996	ASP	CB-CG-OD1	7.92	125.43	118.30
1	D	201	ASP	CB-CG-OD2	-7.91	111.18	118.30
1	A	792	ASP	CB-CG-OD1	7.88	125.39	118.30
1	C	43	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	C	375	ASP	CB-CG-OD1	7.86	125.37	118.30
1	B	572	ASP	CB-CG-OD1	7.85	125.36	118.30
1	A	800	ARG	NE-CZ-NH1	7.83	124.21	120.30
1	A	428	ASP	CB-CG-OD1	7.82	125.34	118.30
1	B	497	ASP	CB-CG-OD1	7.82	125.34	118.30
1	D	802	ASP	CB-CG-OD1	7.81	125.33	118.30
1	A	909	ARG	NE-CZ-NH1	7.80	124.20	120.30
1	B	832	ASP	CB-CG-OD2	-7.80	111.28	118.30
1	A	251	ARG	NE-CZ-NH1	7.79	124.20	120.30
1	A	579	ASP	CB-CG-OD2	-7.78	111.30	118.30
1	A	997	ASP	CB-CG-OD2	-7.76	111.31	118.30
1	C	610	ASP	CB-CG-OD1	7.74	125.27	118.30
1	D	469	ASP	CB-CG-OD1	7.74	125.27	118.30
1	C	832	ASP	CB-CG-OD1	7.73	125.26	118.30
1	A	559	TYR	CB-CG-CD2	-7.72	116.37	121.00
1	D	252	ASP	CB-CG-OD2	-7.71	111.36	118.30
1	C	809	ARG	CG-CD-NE	7.69	127.96	111.80
1	A	691	ALA	CB-CA-C	-7.66	98.61	110.10
1	C	233	ASP	CB-CG-OD2	-7.65	111.42	118.30
1	D	287	ASP	CB-CG-OD1	7.64	125.18	118.30
1	B	319	ASP	CB-CG-OD2	-7.63	111.43	118.30
1	D	403	ASP	CB-CG-OD1	7.63	125.17	118.30
1	B	792	ASP	CB-CG-OD1	7.63	125.17	118.30
1	B	375	ASP	CB-CG-OD1	7.62	125.16	118.30
1	C	746	ASP	CB-CG-OD2	-7.62	111.44	118.30
1	C	77	ASP	CB-CG-OD1	7.60	125.14	118.30
1	B	1018	LEU	CB-CA-C	-7.59	95.78	110.20
1	A	800	ARG	NE-CZ-NH2	-7.58	116.51	120.30
1	B	610	ASP	CB-CG-OD1	7.57	125.11	118.30
1	C	507	ASP	CB-CG-OD2	-7.54	111.51	118.30
1	A	172	ASP	CB-CG-OD1	7.54	125.08	118.30
1	D	859	ASP	CB-CG-OD1	7.53	125.08	118.30
1	D	13	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	B	909	ARG	NE-CZ-NH2	-7.51	116.55	120.30
1	A	166	ARG	NE-CZ-NH1	7.51	124.05	120.30
1	C	772	ASP	CB-CG-OD2	-7.50	111.55	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	77	ASP	CB-CG-OD2	-7.50	111.55	118.30
1	B	233	ASP	CB-CG-OD2	-7.48	111.57	118.30
1	C	832	ASP	CB-CG-OD2	-7.46	111.58	118.30
1	C	234	ASP	CB-CG-OD1	7.45	125.00	118.30
1	A	648	ASP	CB-CG-OD1	7.45	125.00	118.30
1	C	645	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	A	594	ASP	CB-CG-OD1	7.44	125.00	118.30
1	A	477	SER	N-CA-CB	7.40	121.61	110.50
1	A	859	ASP	CB-CG-OD2	-7.40	111.64	118.30
1	A	439	ARG	NE-CZ-NH1	7.39	124.00	120.30
1	B	559	TYR	CB-CG-CD2	-7.39	116.57	121.00
1	C	77	ASP	CB-CG-OD2	-7.37	111.66	118.30
1	A	908	ASP	CB-CG-OD1	7.36	124.92	118.30
1	A	509	ASP	CB-CG-OD2	-7.35	111.68	118.30
1	C	280	ASP	CB-CG-OD1	7.35	124.92	118.30
1	B	598	ASP	CB-CG-OD1	7.34	124.91	118.30
1	D	908	ASP	CB-CG-OD2	-7.34	111.69	118.30
1	D	507	ASP	CB-CG-OD1	7.33	124.90	118.30
1	D	539[A]	ALA	CB-CA-C	-7.33	99.11	110.10
1	D	539[B]	ALA	CB-CA-C	-7.33	99.11	110.10
1	D	15	ASP	CB-CG-OD1	7.33	124.89	118.30
1	B	919	ASP	CB-CG-OD1	7.27	124.84	118.30
1	A	685	LEU	CB-CA-C	7.26	123.99	110.20
1	B	190	ARG	NE-CZ-NH1	-7.25	116.67	120.30
1	B	411	ASP	CB-CG-OD1	7.25	124.82	118.30
1	A	403	ASP	CB-CG-OD2	-7.23	111.79	118.30
1	C	15	ASP	CB-CG-OD2	-7.23	111.80	118.30
1	B	659	ASP	CB-CG-OD1	7.21	124.79	118.30
1	D	630	ARG	NE-CZ-NH1	7.21	123.91	120.30
1	B	172	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	C	13	ARG	NE-CZ-NH1	7.21	123.90	120.30
1	C	439	ARG	NE-CZ-NH2	-7.21	116.70	120.30
1	A	356	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	C	473	ARG	NE-CZ-NH2	-7.19	116.70	120.30
1	A	539[A]	ALA	CB-CA-C	-7.19	99.32	110.10
1	A	539[B]	ALA	CB-CA-C	-7.19	99.32	110.10
1	B	287	ASP	CB-CG-OD1	7.17	124.75	118.30
1	C	952	ARG	NE-CZ-NH1	7.15	123.88	120.30
1	B	428	ASP	CB-CG-OD1	7.13	124.72	118.30
1	D	828	ASP	CB-CG-OD2	-7.12	111.89	118.30
1	A	329	ASP	CB-CG-OD2	-7.10	111.91	118.30
1	A	144	ASP	CB-CG-OD2	-7.10	111.91	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	659	ASP	CB-CG-OD2	-7.10	111.91	118.30
1	D	428	ASP	CB-CG-OD1	7.10	124.69	118.30
1	D	497	ASP	CB-CG-OD2	-7.10	111.91	118.30
1	D	973	ARG	NE-CZ-NH1	-7.09	116.76	120.30
1	C	310	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	C	630	ARG	NE-CZ-NH1	7.08	123.84	120.30
1	D	996	ASP	CB-CG-OD1	7.08	124.67	118.30
1	D	987	ASP	CB-CG-OD2	-7.08	111.93	118.30
1	C	425	ARG	NE-CZ-NH1	7.07	123.83	120.30
1	D	368	ASP	CB-CG-OD2	-7.06	111.94	118.30
1	D	429	ASP	CB-CG-OD1	7.06	124.65	118.30
1	D	251	ARG	NE-CZ-NH2	-7.03	116.79	120.30
1	A	403	ASP	CB-CG-OD1	7.01	124.61	118.30
1	B	403	ASP	CB-CG-OD2	-7.01	111.99	118.30
1	C	996	ASP	CB-CG-OD2	-7.01	111.99	118.30
1	D	561	ARG	NE-CZ-NH2	-7.01	116.80	120.30
1	A	59	ARG	NE-CZ-NH1	-7.00	116.80	120.30
1	A	997	ASP	CB-CG-OD1	7.00	124.59	118.30
1	C	856	TYR	CB-CG-CD2	-6.98	116.81	121.00
1	C	210	ARG	NE-CZ-NH1	-6.97	116.81	120.30
1	C	482	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	B	792	ASP	CB-CG-OD2	-6.97	112.03	118.30
1	D	610	ASP	CB-CG-OD1	6.93	124.53	118.30
1	D	909	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	B	828	ASP	CB-CG-OD2	-6.92	112.07	118.30
1	A	388	ARG	NE-CZ-NH2	-6.90	116.85	120.30
1	A	442	ARG	NE-CZ-NH2	-6.89	116.85	120.30
1	A	782	ASP	CB-CG-OD2	-6.89	112.10	118.30
1	D	411	ASP	CB-CG-OD2	-6.89	112.10	118.30
1	D	809	ARG	NE-CZ-NH1	6.88	123.74	120.30
1	D	1018	LEU	CB-CA-C	-6.88	97.13	110.20
1	C	539[A]	ALA	CB-CA-C	-6.88	99.78	110.10
1	C	539[B]	ALA	CB-CA-C	-6.88	99.78	110.10
1	B	800	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	C	924	ASP	CB-CG-OD1	6.86	124.48	118.30
1	D	630	ARG	NE-CZ-NH2	-6.86	116.87	120.30
1	C	46	ARG	NE-CZ-NH1	-6.85	116.87	120.30
1	D	531	ARG	NE-CZ-NH1	-6.85	116.87	120.30
1	C	755	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	D	909	ARG	NE-CZ-NH2	-6.84	116.88	120.30
1	A	446	ARG	NE-CZ-NH1	6.83	123.71	120.30
1	A	594	ASP	CB-CG-OD2	-6.82	112.17	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	224	ASP	CB-CG-OD1	6.82	124.43	118.30
1	C	746	ASP	CB-CG-OD1	6.81	124.43	118.30
1	D	472	TYR	CB-CG-CD2	-6.81	116.91	121.00
1	B	611	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	C	952	ARG	NE-CZ-NH2	-6.80	116.90	120.30
1	A	431	ARG	NE-CZ-NH1	6.78	123.69	120.30
1	D	594	ASP	CB-CG-OD2	-6.78	112.20	118.30
1	A	987	ASP	CB-CG-OD2	-6.78	112.20	118.30
1	D	77	ASP	CB-CG-OD2	-6.78	112.20	118.30
1	A	442	ARG	NE-CZ-NH1	6.77	123.69	120.30
1	A	721	ARG	NE-CZ-NH2	-6.76	116.92	120.30
1	B	233	ASP	CB-CG-OD1	6.76	124.39	118.30
1	B	770	ILE	CA-CB-CG1	-6.76	98.15	111.00
1	C	553	TRP	CA-CB-CG	-6.76	100.86	113.70
1	D	869	ASP	CB-CG-OD2	-6.76	112.22	118.30
1	D	924	ASP	CB-CG-OD2	-6.76	112.22	118.30
1	D	832	ASP	CB-CG-OD2	-6.76	112.22	118.30
1	D	632	SER	N-CA-CB	6.75	120.63	110.50
1	A	746	ASP	CB-CA-C	-6.74	96.92	110.40
1	B	519	SER	N-CA-CB	-6.73	100.40	110.50
1	A	329	ASP	CB-CG-OD1	6.73	124.35	118.30
1	A	411	ASP	CB-CG-OD1	6.72	124.35	118.30
1	A	572	ASP	CB-CG-OD2	-6.72	112.25	118.30
1	B	411	ASP	CB-CG-OD2	-6.72	112.26	118.30
1	C	136	GLU	CB-CA-C	-6.71	96.98	110.40
1	D	52	ARG	NE-CZ-NH1	6.71	123.65	120.30
1	C	699	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	D	497	ASP	CB-CG-OD1	6.69	124.32	118.30
1	B	569	ASP	CB-CG-OD1	6.69	124.32	118.30
1	D	924	ASP	CB-CG-OD1	6.69	124.32	118.30
1	B	310	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	A	832	ASP	N-CA-CB	-6.67	98.59	110.60
1	C	85	VAL	CA-CB-CG2	-6.67	100.90	110.90
1	B	859	ASP	CB-CG-OD2	-6.65	112.31	118.30
1	D	324	GLU	N-CA-CB	6.65	122.58	110.60
1	D	329	ASP	CB-CG-OD2	-6.64	112.33	118.30
1	C	859	ASP	CB-CG-OD2	-6.61	112.35	118.30
1	C	792	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	C	748	CYS	CA-CB-SG	-6.59	102.13	114.00
1	D	659	ASP	CB-CG-OD2	-6.59	112.37	118.30
1	C	610	ASP	CB-CG-OD2	-6.59	112.37	118.30
1	D	130	ASP	CB-CG-OD1	6.59	124.23	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	507	ASP	CB-CG-OD2	-6.59	112.37	118.30
1	C	924	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	D	282	ARG	NE-CZ-NH1	6.57	123.58	120.30
1	B	505	ARG	NE-CZ-NH1	6.56	123.58	120.30
1	A	987	ASP	CB-CG-OD1	6.56	124.21	118.30
1	D	845	GLN	C-N-CA	-6.56	108.53	122.30
1	D	996	ASP	CB-CG-OD2	-6.56	112.40	118.30
1	B	832	ASP	CB-CG-OD1	6.55	124.20	118.30
1	C	193	ASP	CB-CG-OD1	6.54	124.18	118.30
1	C	448	ARG	NE-CZ-NH1	6.54	123.57	120.30
1	D	144	ASP	CB-CG-OD1	6.54	124.18	118.30
1	D	792	ASP	CB-CG-OD1	6.52	124.17	118.30
1	A	828	ASP	CB-CG-OD1	6.52	124.17	118.30
1	A	682	LEU	CB-CA-C	-6.52	97.82	110.20
1	A	632	SER	N-CA-CB	6.51	120.27	110.50
1	C	630	ARG	NE-CZ-NH2	-6.51	117.05	120.30
1	A	857	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	B	782	ASP	CB-CG-OD1	6.50	124.15	118.30
1	D	579	ASP	CB-CG-OD1	6.49	124.14	118.30
1	B	997	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	A	755	ARG	NE-CZ-NH2	-6.48	117.06	120.30
1	D	233	ASP	CB-CG-OD2	-6.47	112.47	118.30
1	A	890	GLN	N-CA-CB	-6.47	98.95	110.60
1	B	659	ASP	CB-CG-OD2	-6.47	112.48	118.30
1	B	280	ASP	CB-CG-OD1	6.46	124.12	118.30
1	C	519	SER	N-CA-CB	-6.46	100.80	110.50
1	D	253	TYR	CB-CG-CD1	-6.46	117.12	121.00
1	B	199	ASP	CB-CG-OD1	6.45	124.11	118.30
1	B	630	ARG	NE-CZ-NH1	6.45	123.53	120.30
1	C	772	ASP	CB-CG-OD1	6.44	124.09	118.30
1	D	890	GLN	N-CA-CB	-6.44	99.01	110.60
1	C	531	ARG	NE-CZ-NH1	6.43	123.51	120.30
1	A	140	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	A	469	ASP	CB-CG-OD1	6.42	124.08	118.30
1	A	553	TRP	CA-CB-CG	-6.41	101.52	113.70
1	C	255	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	C	509	ASP	CB-CG-OD2	-6.40	112.54	118.30
1	D	800	ARG	NE-CZ-NH1	6.40	123.50	120.30
1	B	507	ASP	CB-CG-OD1	6.39	124.05	118.30
1	A	507	ASP	CB-CG-OD2	-6.38	112.56	118.30
1	D	425	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	D	919	ASP	CB-CG-OD1	6.36	124.03	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	659	ASP	CB-CG-OD1	6.36	124.02	118.30
1	B	996	ASP	CB-CG-OD2	-6.36	112.58	118.30
1	C	917	ARG	NE-CZ-NH1	-6.35	117.12	120.30
1	A	130	ASP	CB-CG-OD2	-6.35	112.59	118.30
1	B	429	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	D	1023	LYS	N-CA-CB	6.34	122.01	110.60
1	A	82	ASP	CB-CG-OD1	6.33	124.00	118.30
1	D	96	ASP	CB-CG-OD1	6.33	124.00	118.30
1	D	648	ASP	CB-CG-OD1	6.33	123.99	118.30
1	C	987	ASP	CB-CG-OD1	6.33	123.99	118.30
1	D	656	VAL	CA-CB-CG2	-6.32	101.42	110.90
1	B	630	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	D	755	ARG	NE-CZ-NH2	-6.30	117.15	120.30
1	A	832	ASP	CB-CG-OD2	-6.30	112.63	118.30
1	A	699	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	B	952	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	C	439	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	B	632	SER	N-CA-CB	6.25	119.88	110.50
1	C	164	ASP	CB-CG-OD2	-6.25	112.68	118.30
1	A	164	ASP	CB-CG-OD2	-6.23	112.70	118.30
1	C	828	ASP	CB-CG-OD1	6.22	123.90	118.30
1	B	497	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	C	329	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	D	279	ILE	CA-CB-CG2	6.22	123.33	110.90
1	D	746	ASP	CB-CG-OD2	-6.22	112.70	118.30
1	D	781	ARG	CD-NE-CZ	6.21	132.30	123.60
1	C	76	CYS	N-CA-CB	-6.21	99.43	110.60
1	C	531	ARG	NE-CZ-NH2	-6.19	117.20	120.30
1	C	572	ASP	CB-CG-OD2	-6.19	112.73	118.30
1	C	594	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	A	942	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	D	699	ARG	NE-CZ-NH2	-6.17	117.22	120.30
1	B	43	ARG	NE-CZ-NH1	6.17	123.38	120.30
1	D	287	ASP	CB-CG-OD2	-6.17	112.75	118.30
1	B	942	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	D	772	ASP	CB-CG-OD2	-6.15	112.76	118.30
1	C	507	ASP	CB-CG-OD1	6.14	123.83	118.30
1	A	942	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	C	429	ASP	CB-CG-OD1	6.13	123.81	118.30
1	C	404	ARG	NE-CZ-NH2	-6.12	117.24	120.30
1	A	14	ARG	N-CA-CB	-6.12	99.59	110.60
1	D	569	ASP	CB-CG-OD2	-6.12	112.80	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	411	ASP	CB-CG-OD1	6.11	123.80	118.30
1	A	673	ALA	N-CA-CB	-6.10	101.56	110.10
1	B	252	ASP	CB-CG-OD1	6.09	123.78	118.30
1	A	280	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	C	431	ARG	CA-CB-CG	-6.08	100.03	113.40
1	A	96	ASP	CB-CG-OD2	-6.07	112.83	118.30
1	A	278	ILE	CA-CB-CG1	-6.07	99.46	111.00
1	C	431	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	A	540[A]	HIS	N-CA-CB	-6.06	99.70	110.60
1	A	540[B]	HIS	N-CA-CB	-6.06	99.70	110.60
1	C	648	ASP	CB-CG-OD2	-6.05	112.85	118.30
1	C	172	ASP	CB-CG-OD1	6.04	123.74	118.30
1	B	761	GLN	CA-CB-CG	-6.04	100.12	113.40
1	C	594	ASP	CB-CG-OD1	6.02	123.72	118.30
1	B	579	ASP	CB-CG-OD1	6.02	123.72	118.30
1	C	659	ASP	CB-CG-OD1	6.02	123.72	118.30
1	B	363	HIS	CA-CB-CG	-6.02	103.37	113.60
1	C	509	ASP	CB-CG-OD1	6.01	123.71	118.30
1	C	859	ASP	CB-CG-OD1	6.00	123.70	118.30
1	D	277	GLU	N-CA-CB	-6.00	99.79	110.60
1	B	802	ASP	CB-CG-OD1	6.00	123.70	118.30
1	B	431	ARG	NE-CZ-NH2	-6.00	117.30	120.30
1	A	428	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	C	790	ASP	CB-CG-OD1	5.99	123.69	118.30
1	C	881	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	B	996	ASP	CB-CG-OD1	5.98	123.69	118.30
1	A	69	VAL	CA-CB-CG2	-5.98	101.93	110.90
1	D	80	GLU	CG-CD-OE2	-5.98	106.34	118.30
1	A	425	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	C	252	ASP	CB-CG-OD2	-5.95	112.94	118.30
1	D	319	ASP	CB-CG-OD1	5.95	123.65	118.30
1	C	668	VAL	CA-CB-CG1	-5.95	101.98	110.90
1	D	252	ASP	CB-CG-OD1	5.94	123.65	118.30
1	A	924	ASP	CB-CG-OD1	5.94	123.65	118.30
1	A	832	ASP	CB-CG-OD1	5.94	123.64	118.30
1	C	671	ASP	CB-CG-OD1	5.94	123.64	118.30
1	D	980	GLU	C-N-CA	-5.94	109.83	122.30
1	B	973	ARG	NE-CZ-NH1	-5.93	117.33	120.30
1	A	469	ASP	CB-CG-OD2	-5.93	112.97	118.30
1	D	790	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	A	253	TYR	CB-CG-CD2	-5.92	117.45	121.00
1	A	908	ASP	CB-CG-OD2	-5.92	112.97	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	572	ASP	CB-CG-OD2	-5.92	112.97	118.30
1	C	267	VAL	CA-CB-CG2	-5.92	102.02	110.90
1	C	997	ASP	CB-CG-OD1	5.92	123.63	118.30
1	B	329	ASP	CB-CG-OD2	-5.92	112.98	118.30
1	D	356	ARG	NE-CZ-NH1	5.91	123.26	120.30
1	C	319	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	C	239	VAL	CG1-CB-CG2	-5.91	101.45	110.90
1	A	288	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	A	190	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	B	13	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	B	746	ASP	CB-CG-OD1	5.90	123.61	118.30
1	B	553	TRP	CA-CB-CG	-5.89	102.50	113.70
1	D	96	ASP	CB-CG-OD2	-5.89	112.99	118.30
1	D	505	ARG	NE-CZ-NH1	5.89	123.24	120.30
1	A	773	LYS	N-CA-CB	5.89	121.20	110.60
1	D	404	ARG	NE-CZ-NH1	5.87	123.23	120.30
1	A	105	TYR	CG-CD2-CE2	5.86	125.99	121.30
1	A	745	MET	CG-SD-CE	-5.85	90.84	100.20
1	B	561	ARG	NE-CZ-NH1	5.85	123.22	120.30
1	B	843	GLN	O-C-N	5.85	132.06	122.70
1	A	201	ASP	CB-CG-OD1	5.85	123.56	118.30
1	A	788	PRO	N-CA-CB	5.84	110.31	103.30
1	D	392	TYR	CB-CG-CD2	5.84	124.51	121.00
1	D	687	GLN	N-CA-CB	5.84	121.12	110.60
1	A	210	ARG	NE-CZ-NH2	-5.84	117.38	120.30
1	B	854	LYS	CB-CA-C	-5.84	98.72	110.40
1	D	45	ASP	CB-CG-OD2	-5.83	113.05	118.30
1	C	255	ARG	NE-CZ-NH2	-5.83	117.39	120.30
1	D	553	TRP	CA-CB-CG	-5.81	102.65	113.70
1	A	741	THR	CA-CB-CG2	-5.81	104.27	112.40
1	B	875	ASP	CB-CG-OD2	-5.81	113.07	118.30
1	A	809	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	B	164	ASP	CB-CG-OD2	-5.80	113.08	118.30
1	A	1017	GLN	CA-CB-CG	-5.79	100.66	113.40
1	A	280	ASP	CB-CG-OD1	5.79	123.51	118.30
1	A	579	ASP	CB-CG-OD1	5.79	123.51	118.30
1	B	540[A]	HIS	N-CA-CB	-5.79	100.18	110.60
1	B	540[B]	HIS	N-CA-CB	-5.79	100.18	110.60
1	D	472	TYR	CB-CG-CD1	5.79	124.47	121.00
1	A	569	ASP	CB-CG-OD1	5.78	123.50	118.30
1	C	13	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	B	746	ASP	CB-CG-OD2	-5.78	113.10	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	183	ARG	NE-CZ-NH2	-5.78	117.41	120.30
1	B	599	ARG	NE-CZ-NH2	5.77	123.19	120.30
1	B	863	GLN	CB-CA-C	-5.77	98.87	110.40
1	C	172	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	D	242	ALA	CB-CA-C	-5.76	101.46	110.10
1	D	1018	LEU	CB-CG-CD1	-5.76	101.20	111.00
1	D	969	GLU	CB-CA-C	-5.76	98.88	110.40
1	A	924	ASP	CB-CG-OD2	-5.76	113.12	118.30
1	C	630	ARG	N-CA-CB	5.76	120.96	110.60
1	B	367	MET	CG-SD-CE	5.75	109.40	100.20
1	C	126	THR	CA-CB-CG2	-5.75	104.36	112.40
1	D	116	THR	CA-CB-CG2	-5.74	104.36	112.40
1	D	336	ARG	NE-CZ-NH1	5.73	123.17	120.30
1	B	37	ARG	NE-CZ-NH1	5.73	123.16	120.30
1	B	116	THR	CA-CB-CG2	-5.71	104.40	112.40
1	B	234	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	A	916	ASP	CB-CG-OD1	5.71	123.44	118.30
1	D	958	ASN	N-CA-CB	5.69	120.84	110.60
1	A	598	ASP	CB-CG-OD1	5.67	123.41	118.30
1	A	446	ARG	NE-CZ-NH2	-5.67	117.47	120.30
1	A	479	ASP	CB-CG-OD2	-5.66	113.21	118.30
1	A	37	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	C	230	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	C	871	GLU	CB-CA-C	-5.63	99.13	110.40
1	D	755	ARG	NE-CZ-NH1	5.63	123.12	120.30
1	A	1018	LEU	CB-CA-C	-5.62	99.53	110.20
1	C	45	ASP	CB-CG-OD1	5.61	123.35	118.30
1	C	368	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	C	685	LEU	N-CA-CB	5.60	121.61	110.40
1	A	279	ILE	CA-CB-CG2	5.60	122.11	110.90
1	B	193	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	A	591	ASP	CB-CG-OD2	-5.60	113.26	118.30
1	B	190	ARG	NH1-CZ-NH2	5.60	125.56	119.40
1	B	755	ARG	N-CA-CB	-5.60	100.53	110.60
1	C	147	ASN	N-CA-CB	-5.59	100.54	110.60
1	A	719	GLN	CB-CA-C	-5.58	99.24	110.40
1	A	427	THR	CA-CB-CG2	-5.58	104.59	112.40
1	C	477	SER	N-CA-CB	-5.58	102.13	110.50
1	C	579	ASP	CB-CG-OD1	5.58	123.32	118.30
1	C	845	GLN	CA-CB-CG	-5.57	101.15	113.40
1	C	927	THR	CA-CB-CG2	-5.57	104.61	112.40
1	C	908	ASP	CB-CG-OD1	5.56	123.31	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	958	ASN	N-CA-CB	5.56	120.61	110.60
1	B	809	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	B	492	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	B	800	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	D	591	ASP	CB-CG-OD2	-5.56	113.30	118.30
1	A	746	ASP	CB-CG-OD1	5.56	123.30	118.30
1	D	251	ARG	NE-CZ-NH1	5.56	123.08	120.30
1	C	706	THR	CA-CB-CG2	-5.55	104.62	112.40
1	B	96	ASP	CB-CG-OD1	5.55	123.30	118.30
1	A	772	ASP	CB-CG-OD1	5.55	123.29	118.30
1	C	130	ASP	CB-CG-OD1	5.54	123.29	118.30
1	B	448	ARG	NE-CZ-NH2	-5.54	117.53	120.30
1	C	912	ALA	CB-CA-C	-5.54	101.80	110.10
1	A	546	LEU	N-CA-CB	5.53	121.45	110.40
1	D	77	ASP	CB-CG-OD1	5.52	123.27	118.30
1	B	71	GLU	CB-CA-C	5.52	121.43	110.40
1	C	136	GLU	C-N-CA	-5.52	110.72	122.30
1	A	845	GLN	CA-CB-CG	-5.51	101.28	113.40
1	A	771	GLY	N-CA-C	-5.51	99.33	113.10
1	B	778	THR	CA-CB-CG2	-5.51	104.69	112.40
1	D	786	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	B	288	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	C	1019	VAL	CG1-CB-CG2	-5.50	102.10	110.90
1	D	319	ASP	CB-CG-OD2	-5.50	113.35	118.30
1	B	164	ASP	CB-CG-OD1	5.49	123.24	118.30
1	D	237	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	A	46	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	B	958	ASN	N-CA-CB	5.48	120.46	110.60
1	B	392	TYR	CG-CD2-CE2	5.48	125.68	121.30
1	D	469	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	C	201	ASP	CB-CG-OD2	-5.46	113.38	118.30
1	C	916	ASP	CB-CG-OD1	5.45	123.21	118.30
1	D	906	TYR	CB-CG-CD2	5.45	124.27	121.00
1	C	375	ASP	CB-CG-OD2	-5.44	113.40	118.30
1	A	447	ASP	CB-CG-OD1	5.44	123.19	118.30
1	D	80	GLU	OE1-CD-OE2	5.43	129.82	123.30
1	C	540[A]	HIS	N-CA-CB	-5.43	100.83	110.60
1	C	540[B]	HIS	N-CA-CB	-5.43	100.83	110.60
1	C	252	ASP	CB-CG-OD1	5.42	123.18	118.30
1	C	505	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	A	292	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	D	431	ARG	NE-CZ-NH1	5.42	123.01	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	598	ASP	CB-CG-OD1	5.42	123.17	118.30
1	B	746	ASP	CB-CA-C	-5.41	99.58	110.40
1	A	96	ASP	N-CA-CB	5.41	120.34	110.60
1	A	954	ASP	CB-CG-OD1	5.41	123.17	118.30
1	A	828	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	C	611	ARG	NE-CZ-NH1	5.40	123.00	120.30
1	B	105	TYR	CZ-CE2-CD2	-5.38	114.96	119.80
1	C	234	ASP	CB-CG-OD2	-5.37	113.47	118.30
1	C	842	TRP	CA-CB-CG	-5.37	103.50	113.70
1	B	952	ARG	NE-CZ-NH1	5.36	122.98	120.30
1	B	123	TYR	CB-CA-C	-5.36	99.68	110.40
1	D	395	HIS	N-CA-CB	-5.35	100.96	110.60
1	D	770	ILE	N-CA-C	-5.35	96.55	111.00
1	A	479	ASP	CB-CG-OD1	5.35	123.12	118.30
1	B	105	TYR	CB-CG-CD2	-5.35	117.79	121.00
1	A	252	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	A	859	ASP	CB-CG-OD1	5.34	123.11	118.30
1	D	442	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	A	926	TYR	CB-CG-CD1	5.34	124.20	121.00
1	B	138	GLN	N-CA-CB	-5.33	101.00	110.60
1	B	924	ASP	CB-CG-OD1	5.33	123.10	118.30
1	A	253	TYR	CB-CG-CD1	5.33	124.20	121.00
1	C	961	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	D	552	TYR	CB-CG-CD2	-5.33	117.80	121.00
1	C	725	ASN	CA-CB-CG	-5.32	101.69	113.40
1	A	497	ASP	CB-CG-OD1	5.32	123.08	118.30
1	C	648	ASP	CB-CG-OD1	5.32	123.08	118.30
1	B	196	TYR	CB-CG-CD2	-5.31	117.81	121.00
1	C	199	ASP	CB-CG-OD2	-5.31	113.52	118.30
1	B	859	ASP	CB-CG-OD1	5.31	123.08	118.30
1	A	157	ARG	CG-CD-NE	5.30	122.92	111.80
1	B	786	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	D	221	GLN	N-CA-CB	-5.29	101.08	110.60
1	D	670	LEU	CB-CA-C	-5.28	100.17	110.20
1	C	224	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	A	230	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	B	292	ARG	NE-CZ-NH1	5.27	122.93	120.30
1	B	503	TYR	CB-CG-CD2	-5.26	117.84	121.00
1	A	507	ASP	CB-CG-OD1	5.25	123.03	118.30
1	A	438	GLU	CG-CD-OE2	-5.25	107.80	118.30
1	A	183	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	C	591	ASP	CB-CG-OD1	5.24	123.01	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	279	ILE	CB-CG1-CD1	-5.24	99.23	113.90
1	C	473	ARG	CG-CD-NE	5.24	122.80	111.80
1	B	894	ARG	CB-CA-C	-5.24	99.93	110.40
1	B	986	ILE	CB-CG1-CD1	-5.24	99.24	113.90
1	A	201	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	A	15	ASP	CB-CG-OD2	-5.23	113.59	118.30
1	B	640	SER	CB-CA-C	-5.23	100.16	110.10
1	D	388	ARG	NE-CZ-NH2	-5.23	117.69	120.30
1	D	52	ARG	CB-CA-C	-5.22	99.95	110.40
1	C	730	LEU	N-CA-CB	-5.22	99.96	110.40
1	A	130	ASP	CB-CG-OD1	5.21	122.99	118.30
1	A	840	HIS	CB-CA-C	-5.21	99.97	110.40
1	C	838	THR	CA-CB-CG2	-5.21	105.10	112.40
1	B	730	LEU	CB-CA-C	5.21	120.10	110.20
1	D	138	GLN	N-CA-CB	-5.21	101.22	110.60
1	D	280	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	D	760	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	A	429	ASP	CB-CG-OD1	5.20	122.98	118.30
1	D	247	CYS	CA-CB-SG	-5.19	104.65	114.00
1	A	344	LEU	CA-CB-CG	-5.19	103.36	115.30
1	D	952	ARG	NE-CZ-NH1	5.19	122.89	120.30
1	D	164	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	A	45	ASP	CB-CG-OD1	5.18	122.97	118.30
1	A	225	PHE	N-CA-CB	5.18	119.93	110.60
1	B	429	ASP	CB-CG-OD1	5.18	122.96	118.30
1	D	37	ARG	NE-CZ-NH2	-5.18	117.71	120.30
1	A	515	VAL	CA-CB-CG1	-5.18	103.13	110.90
1	D	997	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	C	569	ASP	CB-CG-OD1	5.18	122.96	118.30
1	D	177	LEU	CB-CA-C	-5.18	100.36	110.20
1	D	710	GLU	CB-CA-C	-5.18	100.05	110.40
1	B	917	ARG	CD-NE-CZ	-5.17	116.36	123.60
1	B	372	MET	CG-SD-CE	5.17	108.47	100.20
1	D	253	TYR	CB-CG-CD2	5.17	124.10	121.00
1	C	183	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	C	671	ASP	CB-CG-OD2	-5.15	113.66	118.30
1	D	234	ASP	CB-CG-OD2	-5.15	113.66	118.30
1	D	908	ASP	CB-CG-OD1	5.15	122.94	118.30
1	C	721	ARG	CD-NE-CZ	5.15	130.81	123.60
1	A	968	MET	CA-CB-CG	5.15	122.05	113.30
1	B	14	ARG	N-CA-CB	5.14	119.85	110.60
1	C	772	ASP	N-CA-CB	5.14	119.85	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	917	ARG	CD-NE-CZ	-5.14	116.41	123.60
1	A	952	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	C	997	ASP	CB-CG-OD2	-5.14	113.68	118.30
1	B	987	ASP	CB-CG-OD1	5.13	122.92	118.30
1	D	668	VAL	CB-CA-C	-5.13	101.64	111.40
1	C	368	ASP	CB-CG-OD1	5.13	122.92	118.30
1	D	687	GLN	CB-CA-C	5.13	120.66	110.40
1	B	144	ASP	CB-CG-OD1	5.12	122.91	118.30
1	D	857	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	B	13	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	A	954	ASP	CB-CG-OD2	-5.12	113.70	118.30
1	B	667	GLU	CB-CG-CD	-5.12	100.39	114.20
1	A	946	TYR	CB-CG-CD2	-5.11	117.94	121.00
1	B	80	GLU	CG-CD-OE2	-5.10	108.10	118.30
1	D	416	GLU	CG-CD-OE1	5.09	128.49	118.30
1	D	425	ARG	NH1-CZ-NH2	-5.09	113.80	119.40
1	A	685	LEU	CA-CB-CG	-5.09	103.59	115.30
1	D	867	THR	CA-CB-CG2	-5.09	105.28	112.40
1	C	497	ASP	CB-CG-OD1	5.08	122.87	118.30
1	D	595	THR	CA-CB-CG2	-5.08	105.29	112.40
1	B	52	ARG	CB-CA-C	-5.08	100.25	110.40
1	A	591	ASP	CB-CG-OD1	5.08	122.87	118.30
1	A	598	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	B	190	ARG	NE-CZ-NH2	-5.08	117.76	120.30
1	D	333	ARG	NE-CZ-NH2	5.07	122.83	120.30
1	A	352	ARG	CG-CD-NE	5.07	122.44	111.80
1	A	996	ASP	CB-CG-OD1	5.07	122.86	118.30
1	C	404	ARG	NE-CZ-NH1	5.07	122.83	120.30
1	C	479	ASP	CB-CG-OD1	5.05	122.85	118.30
1	B	645	ARG	NE-CZ-NH2	5.05	122.83	120.30
1	C	919	ASP	CB-CG-OD2	-5.04	113.76	118.30
1	D	545	SER	N-CA-CB	-5.04	102.94	110.50
1	C	855	THR	N-CA-CB	5.04	119.88	110.30
1	C	494	THR	CA-CB-CG2	-5.04	105.34	112.40
1	A	857	ARG	NE-CZ-NH1	5.03	122.81	120.30
1	C	288	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	A	358	GLU	CG-CD-OE2	-5.02	108.26	118.30
1	D	929	TYR	CB-CG-CD2	5.02	124.01	121.00
1	B	750	GLU	OE1-CD-OE2	-5.02	117.28	123.30
1	A	869	ASP	CB-CG-OD1	5.02	122.81	118.30
1	C	43	ARG	NE-CZ-NH2	-5.01	117.79	120.30
1	C	388	ARG	NE-CZ-NH1	5.00	122.80	120.30

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	D	687	GLN	CA

There are no planarity outliers.

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	8128	0	7712	106	0
1	B	8128	0	7712	102	0
1	C	8128	0	7712	97	0
1	D	8128	0	7712	110	0
2	E	23	0	20	0	0
2	F	23	0	20	0	0
2	G	23	0	20	0	0
2	H	23	0	20	0	0
3	A	4	0	0	1	0
3	B	2	0	0	0	0
3	C	4	0	0	0	0
3	D	4	0	0	0	0
4	A	4	0	0	0	0
4	B	4	0	0	0	0
4	C	4	0	0	0	0
4	D	3	0	0	0	0
5	A	92	0	138	6	0
5	B	96	0	144	5	0
5	C	100	0	150	5	0
5	D	96	0	144	5	0
6	A	1136	0	0	15	1
6	B	1151	0	0	19	0
6	C	1133	0	0	11	0
6	D	1109	0	0	9	1
All	All	37546	0	31504	425	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 7.

All (425) 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)
5:B:8508:DMS:C1	5:B:8508:DMS:S	2.01	1.46
1:A:634:GLN:H	1:A:634:GLN:NE2	1.41	1.18
1:D:804:ASN:HD22	1:D:809:ARG:NH2	1.43	1.16
1:B:655:MET:HE2	1:B:665:SER:HB3	1.16	1.12
1:C:237:ARG:HH11	1:C:237:ARG:HB3	1.24	1.02
1:A:685:LEU:HD23	1:A:686:PRO:CD	1.91	1.01
1:C:737:ILE:HD12	1:C:738:PRO:HD2	1.44	1.00
1:A:1022:GLN:HG2	1:A:1023:LYS:H	1.27	0.98
1:C:761:GLN:N	1:C:761:GLN:HE21	1.65	0.95
1:A:292:ARG:HH12	5:A:8412:DMS:H22	1.32	0.95
1:A:685:LEU:CD2	1:A:686:PRO:HD2	1.96	0.94
1:C:761:GLN:H	1:C:761:GLN:NE2	1.69	0.90
1:B:600:GLN:H	1:B:600:GLN:HE21	1.19	0.90
1:D:809:ARG:HH11	1:D:809:ARG:HG2	1.37	0.90
1:B:847:LYS:HD3	1:B:849:LEU:HD23	1.53	0.90
1:D:804:ASN:ND2	1:D:809:ARG:NH2	2.19	0.89
1:B:651:LEU:CD2	1:B:701:VAL:HB	2.04	0.88
1:A:634:GLN:NE2	1:A:634:GLN:N	2.22	0.87
1:A:809:ARG:HG2	1:A:809:ARG:HH11	1.38	0.87
1:B:262:GLN:HE21	1:B:263:GLY:N	1.73	0.87
1:A:685:LEU:HD23	1:A:686:PRO:HD3	1.56	0.87
1:B:655:MET:CE	1:B:665:SER:HB3	2.04	0.85
1:A:292:ARG:HH12	5:A:8412:DMS:C2	1.91	0.84
1:A:685:LEU:HD23	1:A:686:PRO:HD2	1.55	0.84
1:A:773:LYS:H	1:A:773:LYS:HD3	1.42	0.84
1:D:629:PHE:O	1:D:630:ARG:HD3	1.79	0.82
1:A:600:GLN:H	1:A:600:GLN:HE21	1.28	0.82
1:B:651:LEU:HD21	1:B:701:VAL:HB	1.62	0.82
5:B:8417:DMS:H11	6:B:9733:HOH:O	1.80	0.81
1:A:773:LYS:HD3	1:A:773:LYS:N	1.95	0.80
5:A:8420:DMS:H21	6:D:9525:HOH:O	1.82	0.80
1:C:237:ARG:HH11	1:C:237:ARG:CB	1.94	0.80
1:C:685:LEU:HB3	1:C:686:PRO:HD2	1.64	0.79
1:A:777:LEU:CD1	1:A:980:GLU:HG2	2.13	0.79
1:B:655:MET:HE2	1:B:665:SER:CB	2.08	0.78
1:D:658:LEU:O	1:D:661:LYS:HG3	1.83	0.78
1:D:292:ARG:HH12	5:D:8412:DMS:H22	1.47	0.78
1:C:367:MET:HE3	1:C:367:MET:HA	1.65	0.78
1:B:684:GLU:O	1:B:686:PRO:HD3	1.84	0.77
1:C:44:THR:HB	6:C:9688:HOH:O	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:863:GLN:HG2	1:B:1019:VAL:CG1	2.15	0.76
1:A:1017:GLN:HG2	1:A:1018:LEU:N	1.99	0.76
1:C:761:GLN:HE21	1:C:761:GLN:H	1.23	0.75
1:D:292:ARG:HH12	5:D:8412:DMS:C2	1.98	0.75
1:C:651:LEU:HD23	1:C:703:PRO:HG3	1.69	0.74
1:D:237:ARG:HH11	1:D:237:ARG:HB3	1.53	0.74
1:C:748:CYS:C	1:C:749:ILE:HD12	2.08	0.73
1:B:473:ARG:NH1	1:B:477:SER:HB2	2.02	0.73
1:B:687:GLN:HE21	1:B:687:GLN:N	1.85	0.73
1:A:797:GLU:O	1:A:801:ILE:HD13	1.89	0.73
1:C:737:ILE:HD12	1:C:738:PRO:CD	2.18	0.73
1:A:371:THR:HG22	6:A:9526:HOH:O	1.88	0.73
1:D:770:ILE:HD13	1:D:775:GLN:CD	2.10	0.72
1:B:634:GLN:HG3	1:B:682:LEU:HB2	1.72	0.72
1:D:237:ARG:NH1	6:D:9285:HOH:O	2.23	0.72
1:A:292:ARG:NH1	5:A:8412:DMS:H22	2.02	0.72
1:B:878:HIS:HD2	6:B:8695:HOH:O	1.71	0.72
1:D:804:ASN:ND2	1:D:809:ARG:HH21	1.89	0.71
1:C:878:HIS:HD2	6:C:8704:HOH:O	1.74	0.71
1:A:804:ASN:OD1	1:A:809:ARG:NH2	2.22	0.70
1:D:748:CYS:C	1:D:749:ILE:HD12	2.12	0.70
1:C:682:LEU:HB3	1:C:683:PRO:HD2	1.73	0.69
1:D:749:ILE:HD12	1:D:749:ILE:N	2.06	0.69
5:B:8410:DMS:H11	6:B:8982:HOH:O	1.91	0.69
1:D:857:ARG:NH1	1:D:857:ARG:HG2	2.07	0.68
1:C:634:GLN:H	1:C:634:GLN:NE2	1.92	0.68
1:A:878:HIS:HD2	6:A:8581:HOH:O	1.77	0.68
1:A:1022:GLN:CG	1:A:1023:LYS:H	2.02	0.68
1:A:809:ARG:HG2	1:A:809:ARG:NH1	2.06	0.67
1:C:651:LEU:HD11	1:C:653:HIS:CE1	2.29	0.67
1:D:687:GLN:HB3	1:D:688:PRO:HD2	1.76	0.67
1:D:857:ARG:HG2	1:D:857:ARG:HH11	1.60	0.67
1:B:241:GLU:HG3	1:B:292:ARG:HG2	1.75	0.67
1:D:809:ARG:HH11	1:D:809:ARG:CG	2.07	0.67
1:D:863:GLN:HG2	1:D:1021:CYS:HB3	1.78	0.66
1:A:654:TRP:CZ2	1:A:683:PRO:HG2	2.30	0.66
1:C:761:GLN:N	1:C:761:GLN:NE2	2.34	0.66
3:A:3105:MG:MG	6:A:9107:HOH:O	1.37	0.66
1:B:262:GLN:HE21	1:B:262:GLN:C	1.98	0.66
1:D:237:ARG:HH11	1:D:237:ARG:CG	2.08	0.66
1:B:847:LYS:NZ	6:B:9679:HOH:O	2.20	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:754:LYS:NZ	1:C:1022:GLN:OE1	2.29	0.66
1:C:237:ARG:HB3	1:C:237:ARG:NH1	2.05	0.66
1:C:651:LEU:HD11	1:C:653:HIS:HE1	1.61	0.66
1:A:634:GLN:H	1:A:634:GLN:HE21	1.38	0.65
1:A:431:ARG:HG3	6:A:9280:HOH:O	1.96	0.65
1:C:824:GLN:HG2	1:C:825:CYS:N	2.10	0.65
1:D:622:HIS:O	1:D:625:GLN:HG3	1.96	0.65
1:B:651:LEU:O	1:B:651:LEU:HD23	1.96	0.64
1:A:635:THR:OG1	1:A:681:GLU:HG3	1.97	0.64
1:B:772:ASP:OD1	1:B:773:LYS:HE3	1.97	0.64
1:C:797:GLU:O	1:C:801:ILE:HD13	1.97	0.64
1:D:829:THR:O	1:D:830:LEU:HD23	1.98	0.64
1:A:777:LEU:HD13	1:A:980:GLU:HG2	1.79	0.64
1:D:887:GLN:NE2	1:D:980:GLU:O	2.31	0.64
1:B:863:GLN:HG2	1:B:1019:VAL:HG13	1.80	0.63
1:D:847:LYS:HG3	1:D:848:THR:N	2.10	0.63
1:A:735:HIS:ND1	1:A:735:HIS:N	2.31	0.63
1:D:237:ARG:HH11	1:D:237:ARG:CB	2.11	0.63
1:A:277:GLU:H	1:A:277:GLU:CD	2.02	0.63
1:B:634:GLN:HE22	1:B:684:GLU:HA	1.64	0.62
5:B:8410:DMS:H12	6:B:9248:HOH:O	1.99	0.62
1:A:680:ILE:HG12	6:A:9152:HOH:O	2.00	0.62
1:D:1022:GLN:NE2	1:D:1023:LYS:HG3	2.12	0.62
1:A:262:GLN:NE2	1:A:299:LYS:HD3	2.16	0.61
1:A:685:LEU:CB	1:A:686:PRO:HD2	2.30	0.61
1:A:777:LEU:HD11	1:A:980:GLU:HG2	1.81	0.61
1:A:663:LEU:CD1	1:A:686:PRO:HG2	2.31	0.61
1:B:646:HIS:HB3	6:B:9486:HOH:O	2.01	0.61
1:C:595:THR:HA	1:C:596:PRO:C	2.21	0.61
1:C:806:TRP:HA	1:C:809:ARG:HD3	1.82	0.60
1:A:1022:GLN:HG2	1:A:1023:LYS:N	2.09	0.60
1:B:658:LEU:O	1:B:661:LYS:HE2	2.00	0.60
1:C:756:TRP:CE2	1:C:858:ILE:HD12	2.36	0.60
1:D:878:HIS:HD2	6:D:8819:HOH:O	1.83	0.60
1:C:673:ALA:HB1	1:C:674:PRO:HD2	1.83	0.60
1:D:773:LYS:HG3	1:D:775:GLN:HE21	1.64	0.60
1:D:651:LEU:HG	1:D:653:HIS:CE1	2.36	0.60
1:C:646:HIS:CE1	1:C:673:ALA:HB2	2.36	0.60
1:D:135:GLN:O	1:D:136:GLU:HG2	2.02	0.60
1:C:615:PRO:O	1:C:618:THR:HG22	2.01	0.60
1:A:648:ASP:OD2	6:A:9431:HOH:O	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:863:GLN:HG2	1:B:1019:VAL:HG11	1.82	0.59
1:C:1023:LYS:NZ	1:C:1023:LYS:HB3	2.16	0.59
1:D:1022:GLN:HE21	1:D:1023:LYS:HG3	1.67	0.59
1:D:367:MET:HB3	1:D:372:MET:CE	2.34	0.58
1:A:685:LEU:CD2	1:A:686:PRO:CD	2.64	0.58
1:D:367:MET:HB3	1:D:372:MET:HE3	1.85	0.58
1:D:651:LEU:CD2	1:D:653:HIS:HE1	2.17	0.58
1:C:749:ILE:HD12	1:C:749:ILE:N	2.18	0.58
1:B:75:GLU:HA	1:B:75:GLU:OE1	2.04	0.57
1:A:770:ILE:O	1:A:773:LYS:HD3	2.04	0.57
1:B:699:ARG:HD2	6:B:9661:HOH:O	2.05	0.57
1:B:1017:GLN:HB2	6:B:9588:HOH:O	2.03	0.57
1:A:832:ASP:OD1	1:A:832:ASP:N	2.32	0.57
1:A:685:LEU:HD22	1:A:686:PRO:HD2	1.86	0.57
1:B:730:LEU:H	1:B:730:LEU:CD1	2.11	0.57
1:D:363:HIS:HD2	6:D:9332:HOH:O	1.87	0.57
1:C:788:PRO:HD3	1:C:968:MET:HE3	1.86	0.56
1:C:200:GLN:HG2	1:C:391:HIS:HB2	1.87	0.56
1:D:646:HIS:NE2	1:D:671:ASP:OD1	2.35	0.56
1:C:634:GLN:H	1:C:634:GLN:CD	2.08	0.56
1:B:745:MET:SD	1:B:745:MET:N	2.78	0.56
1:A:387:VAL:HG22	6:A:9584:HOH:O	2.06	0.56
1:A:651:LEU:C	1:A:651:LEU:HD12	2.26	0.56
1:B:730:LEU:H	1:B:730:LEU:HD12	1.71	0.56
1:D:797:GLU:O	1:D:801:ILE:HD13	2.07	0.56
1:B:687:GLN:HE21	1:B:687:GLN:CA	2.19	0.55
1:C:667:GLU:C	1:C:668:VAL:HG23	2.27	0.55
1:C:237:ARG:NH1	1:C:296:GLU:OE2	2.38	0.55
1:D:618:THR:HG23	6:D:9075:HOH:O	2.05	0.55
1:A:654:TRP:HZ2	1:A:683:PRO:HG2	1.71	0.55
1:A:735:HIS:O	1:A:736:ALA:HB2	2.06	0.55
1:C:685:LEU:CB	1:C:686:PRO:HD2	2.26	0.55
1:B:634:GLN:NE2	1:B:684:GLU:HA	2.21	0.55
1:A:787:ALA:HA	1:A:968:MET:HG3	1.89	0.55
1:A:237:ARG:HH11	1:A:237:ARG:HB3	1.70	0.55
1:A:887:GLN:NE2	1:A:980:GLU:O	2.38	0.54
1:B:232:ASN:ND2	1:B:237:ARG:HG3	2.22	0.54
1:D:687:GLN:N	1:D:687:GLN:OE1	2.40	0.54
1:A:521:LYS:HE2	6:A:8938:HOH:O	2.07	0.54
1:B:127:PHE:CE1	1:B:184:LEU:HG	2.43	0.54
1:D:237:ARG:HH11	1:D:237:ARG:HG2	1.71	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:646:HIS:CE1	1:B:673:ALA:HA	2.42	0.54
1:B:630:ARG:HD3	1:B:637:GLU:OE1	2.07	0.54
1:B:615:PRO:O	1:B:618:THR:HG22	2.07	0.54
1:A:699:ARG:NH2	6:A:9373:HOH:O	2.41	0.54
1:D:577:LYS:O	1:D:584:PRO:HA	2.08	0.53
1:D:770:ILE:HD13	1:D:775:GLN:CG	2.38	0.53
1:A:595:THR:HA	1:A:596:PRO:C	2.29	0.53
1:B:157:ARG:HD3	6:B:9479:HOH:O	2.09	0.53
1:B:863:GLN:CG	1:B:1019:VAL:CG1	2.87	0.53
1:B:262:GLN:NE2	6:B:9167:HOH:O	2.40	0.53
1:C:756:TRP:CD2	1:C:858:ILE:HD12	2.43	0.53
1:A:615:PRO:O	1:A:618:THR:HG22	2.08	0.53
1:D:130:ASP:CG	5:D:8703:DMS:H22	2.29	0.53
1:B:634:GLN:HG2	1:B:682:LEU:O	2.09	0.53
1:A:88:SER:HA	1:A:366:VAL:HG21	1.91	0.53
1:B:360:HIS:CE1	1:B:362:LEU:HB2	2.44	0.53
1:B:655:MET:SD	1:B:656:VAL:N	2.83	0.53
1:C:266:GLN:O	5:C:8602:DMS:H22	2.09	0.53
1:B:363:HIS:HD2	6:B:9206:HOH:O	1.91	0.52
1:D:770:ILE:N	1:D:770:ILE:HD12	2.25	0.52
1:B:1022:GLN:HG3	1:B:1023:LYS:O	2.09	0.52
1:A:262:GLN:HE22	1:A:299:LYS:CD	2.22	0.52
1:C:356:ARG:HD2	1:C:379:MET:CE	2.40	0.52
1:C:760:ARG:N	1:C:761:GLN:NE2	2.57	0.52
1:A:764:PHE:CE2	1:A:781:ARG:NH1	2.77	0.52
1:A:878:HIS:CE1	1:A:1010:SER:HB3	2.45	0.52
1:B:377:LEU:HD22	1:B:708:TRP:HA	1.92	0.52
5:C:8420:DMS:O	6:C:8630:HOH:O	2.19	0.52
1:B:262:GLN:HE21	1:B:262:GLN:CA	2.21	0.52
1:D:595:THR:HA	1:D:596:PRO:C	2.29	0.52
1:B:845:GLN:OE1	1:B:845:GLN:HA	2.09	0.51
1:C:759:ASN:OD1	1:C:761:GLN:NE2	2.43	0.51
1:B:662:PRO:O	1:B:663:LEU:HD23	2.10	0.51
1:B:127:PHE:HE1	1:B:184:LEU:HG	1.74	0.51
1:C:569:ASP:HB2	6:C:9438:HOH:O	2.11	0.51
1:C:858:ILE:HD13	1:C:864:MET:HB2	1.90	0.51
1:A:737:ILE:C	1:A:737:ILE:HD13	2.30	0.51
1:A:866:ILE:O	1:A:1017:GLN:HG3	2.10	0.51
1:D:117:GLU:HG3	6:D:9155:HOH:O	2.11	0.51
1:A:249:GLU:OE2	1:A:251:ARG:NE	2.39	0.51
1:D:685:LEU:HD23	1:D:686:PRO:HD2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:230:ARG:HG3	1:C:230:ARG:NH1	2.26	0.50
1:C:743:SER:HB3	6:C:9612:HOH:O	2.11	0.50
1:C:230:ARG:HG3	1:C:230:ARG:HH11	1.76	0.50
1:D:749:ILE:N	1:D:749:ILE:CD1	2.72	0.50
1:A:756:TRP:CD2	1:A:858:ILE:HD13	2.46	0.50
1:B:262:GLN:NE2	1:B:262:GLN:HA	2.27	0.50
1:C:745:MET:O	1:C:761:GLN:NE2	2.44	0.50
1:A:305:ILE:HD11	1:A:645:ARG:HB3	1.94	0.50
1:A:178:ARG:HD2	6:A:9388:HOH:O	2.11	0.50
1:A:663:LEU:HD12	1:A:686:PRO:HG2	1.94	0.50
1:D:1022:GLN:O	1:D:1022:GLN:HG3	2.09	0.50
1:B:600:GLN:HE21	1:B:600:GLN:N	2.00	0.49
1:C:610:ASP:O	1:C:611:ARG:HB2	2.12	0.49
1:B:114:VAL:HB	1:B:115:PRO:HD2	1.93	0.49
1:A:86:VAL:HG13	1:A:87:PRO:HA	1.95	0.49
1:D:804:ASN:HA	1:D:809:ARG:CZ	2.42	0.49
1:D:809:ARG:HG2	1:D:809:ARG:NH1	2.12	0.49
1:A:651:LEU:HD23	1:A:703:PRO:HG3	1.94	0.49
1:A:801:ILE:HD12	1:A:808:GLU:OE2	2.13	0.49
1:B:669:PRO:CB	6:B:9509:HOH:O	2.60	0.49
1:B:662:PRO:C	1:B:663:LEU:HD23	2.33	0.49
1:D:857:ARG:HH11	1:D:857:ARG:CG	2.25	0.49
1:A:472:TYR:O	1:A:476:LYS:HG2	2.12	0.49
1:D:135:GLN:C	1:D:136:GLU:HG2	2.33	0.49
1:C:651:LEU:CD2	1:C:703:PRO:HG3	2.41	0.49
1:C:734:SER:CB	1:C:860:GLY:HA3	2.43	0.49
1:C:861:SER:OG	1:C:863:GLN:HG3	2.13	0.49
1:D:773:LYS:CG	1:D:775:GLN:NE2	2.76	0.48
1:C:88:SER:HA	1:C:366:VAL:HG21	1.95	0.48
1:D:80:GLU:OE1	1:D:80:GLU:N	2.39	0.48
1:C:1023:LYS:NZ	1:C:1023:LYS:CB	2.76	0.48
1:B:262:GLN:NE2	1:B:262:GLN:CA	2.76	0.48
1:D:952:ARG:NH2	1:D:1021:CYS:SG	2.86	0.48
1:C:835:LEU:HD11	1:C:855:THR:HB	1.95	0.48
1:D:844:HIS:O	1:D:845:GLN:HB2	2.13	0.48
1:A:687:GLN:HG3	6:A:9362:HOH:O	2.13	0.48
1:A:237:ARG:HD2	1:A:296:GLU:OE1	2.14	0.48
1:A:262:GLN:HE22	1:A:299:LYS:HD2	1.78	0.48
1:B:359:HIS:CD2	1:B:573:GLN:HA	2.49	0.48
1:C:367:MET:HE3	1:C:367:MET:CA	2.39	0.48
1:A:843:GLN:HA	1:A:847:LYS:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:A:8425:DMS:H21	6:A:9310:HOH:O	2.14	0.48
1:C:241:GLU:HG3	1:C:290:THR:CG2	2.44	0.48
1:A:660:GLY:O	1:A:662:PRO:HD3	2.14	0.47
1:C:655:MET:SD	1:C:656:VAL:N	2.87	0.47
1:B:78:LEU:HD23	6:B:9109:HOH:O	2.14	0.47
1:C:890:GLN:CG	1:C:891:VAL:N	2.78	0.47
1:D:237:ARG:NH1	1:D:237:ARG:HG2	2.29	0.47
1:D:277:GLU:CD	1:D:277:GLU:H	2.07	0.47
1:A:178:ARG:HG3	6:A:9388:HOH:O	2.14	0.47
1:A:754:LYS:NZ	6:A:9415:HOH:O	2.47	0.47
1:B:595:THR:HA	1:B:596:PRO:C	2.35	0.47
1:C:778:THR:HG23	1:C:887:GLN:OE1	2.14	0.47
1:D:377:LEU:HD22	1:D:708:TRP:HA	1.96	0.47
1:D:770:ILE:CD1	1:D:775:GLN:HG3	2.43	0.47
1:D:773:LYS:HG3	1:D:775:GLN:NE2	2.29	0.47
1:A:737:ILE:HD13	1:A:737:ILE:O	2.13	0.47
1:B:863:GLN:HG3	1:B:1021:CYS:HB3	1.96	0.47
1:D:285:TYR:HB3	1:D:288:ARG:HG3	1.96	0.47
1:C:684:GLU:O	1:C:684:GLU:HG2	2.06	0.47
1:C:651:LEU:CD1	1:C:653:HIS:CE1	2.97	0.47
1:A:352:ARG:HG2	1:A:553:TRP:CH2	2.50	0.46
1:D:804:ASN:HD22	1:D:809:ARG:CZ	2.19	0.46
1:D:147:ASN:HA	1:D:148:SER:HA	1.75	0.46
1:C:262:GLN:CG	1:C:309:TYR:CE2	2.98	0.46
1:A:237:ARG:HB3	1:A:237:ARG:NH1	2.31	0.46
1:B:230:ARG:HE	1:B:230:ARG:HB2	1.48	0.46
1:B:1023:LYS:HB3	1:B:1023:LYS:HE3	1.50	0.46
1:A:1022:GLN:CG	1:A:1023:LYS:N	2.74	0.46
1:C:292:ARG:HG3	1:C:292:ARG:HH11	1.81	0.46
1:D:843:GLN:HA	1:D:847:LYS:O	2.16	0.46
1:B:142:ILE:HG12	1:B:170:GLU:HG2	1.97	0.46
1:C:799:THR:O	1:C:800:ARG:HG2	2.16	0.46
1:C:367:MET:HE1	6:C:9629:HOH:O	2.15	0.46
1:D:876:THR:OG1	1:D:877:PRO:HD2	2.16	0.46
1:D:78:LEU:HA	1:D:78:LEU:HD23	1.81	0.45
1:D:830:LEU:N	1:D:833:ALA:O	2.40	0.45
1:B:654:TRP:CZ3	1:B:665:SER:HA	2.51	0.45
1:D:13:ARG:HD3	6:D:9806:HOH:O	2.15	0.45
1:A:600:GLN:HE21	1:A:600:GLN:N	2.06	0.45
1:B:262:GLN:HE21	1:B:263:GLY:H	1.60	0.45
1:B:473:ARG:NH1	1:B:477:SER:CB	2.78	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:557:ARG:HH11	1:A:557:ARG:HD2	1.62	0.45
1:A:433:LEU:N	1:A:434:PRO:CD	2.79	0.45
5:C:8408:DMS:C2	6:C:9354:HOH:O	2.64	0.45
1:D:393:PRO:HD3	1:D:412:GLU:O	2.16	0.45
1:D:411:ASP:OD2	1:D:447:ASP:OD2	2.34	0.45
1:A:279:ILE:HG21	1:A:279:ILE:HD13	1.70	0.45
1:A:768:MET:HE1	1:A:1020:TRP:CZ2	2.52	0.45
1:B:434:PRO:HB3	1:C:434:PRO:HB3	1.98	0.45
1:C:800:ARG:HE	1:C:800:ARG:HB3	1.59	0.45
1:A:262:GLN:NE2	1:A:299:LYS:CD	2.79	0.45
1:A:599:ARG:HH11	1:A:600:GLN:NE2	2.15	0.45
1:C:646:HIS:CE1	1:C:673:ALA:CB	2.99	0.45
1:D:433:LEU:HB3	1:D:434:PRO:HD3	1.98	0.45
1:A:668:VAL:HG12	1:A:669:PRO:O	2.17	0.45
1:B:675:GLN:NE2	6:B:9632:HOH:O	2.49	0.45
1:B:878:HIS:CE1	1:B:1010:SER:HB3	2.52	0.45
1:C:749:ILE:N	1:C:749:ILE:CD1	2.80	0.45
1:D:878:HIS:CE1	1:D:1010:SER:HB3	2.51	0.45
1:B:1022:GLN:CG	1:B:1023:LYS:N	2.80	0.44
1:C:367:MET:HA	1:C:367:MET:CE	2.42	0.44
1:C:890:GLN:HG3	1:C:891:VAL:N	2.32	0.44
1:D:893:GLU:HG2	1:D:894:ARG:HG2	2.00	0.44
1:D:787:ALA:HA	1:D:968:MET:HE2	1.98	0.44
1:D:1022:GLN:NE2	1:D:1023:LYS:CG	2.79	0.44
1:B:863:GLN:CG	1:B:1019:VAL:HG11	2.48	0.44
1:C:237:ARG:HH11	1:C:237:ARG:CG	2.30	0.44
1:C:430:PRO:HD3	5:C:8420:DMS:H23	1.98	0.44
1:D:962:TYR:CE2	5:D:8508:DMS:H21	2.52	0.44
1:C:751:LEU:HD21	1:C:860:GLY:O	2.18	0.44
1:C:997:ASP:HB2	1:C:999:TRP:CZ2	2.53	0.44
1:D:128:ASN:HB3	1:D:180:GLY:O	2.17	0.44
1:A:745:MET:HB3	1:A:745:MET:HE2	1.57	0.44
1:B:147:ASN:HA	1:B:148:SER:HA	1.66	0.44
1:B:835:LEU:HD11	1:B:855:THR:HB	1.99	0.44
1:C:658:LEU:O	1:C:659:ASP:C	2.54	0.43
1:D:472:TYR:O	1:D:476:LYS:HG2	2.17	0.43
1:A:147:ASN:HA	1:A:148:SER:HA	1.54	0.43
1:D:143:PHE:HB3	1:D:146:VAL:HG23	2.00	0.43
1:B:1022:GLN:HG3	1:B:1023:LYS:N	2.32	0.43
1:C:499:ILE:HG22	1:C:501:PRO:HD3	1.99	0.43
1:A:58:TRP:CD1	1:A:86:VAL:HB	2.54	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:789:LEU:HD11	1:A:993:ILE:HG22	1.99	0.43
1:B:225:PHE:HA	1:B:243:GLU:O	2.18	0.43
1:B:948:PRO:O	1:B:1023:LYS:N	2.40	0.43
1:B:824:GLN:OE1	1:B:837:THR:HG22	2.19	0.43
1:C:240:LEU:C	1:C:240:LEU:HD23	2.39	0.43
1:D:773:LYS:HD2	1:D:774:LYS:O	2.18	0.43
1:A:768:MET:CE	1:A:1020:TRP:CZ2	3.02	0.43
1:B:74:LEU:HD22	1:B:153:TRP:CG	2.54	0.43
1:C:356:ARG:NH2	6:C:9629:HOH:O	2.28	0.43
1:B:755:ARG:HD2	6:B:9670:HOH:O	2.17	0.43
1:D:769:TRP:C	1:D:770:ILE:HD12	2.39	0.43
1:D:773:LYS:HG3	1:D:773:LYS:O	2.11	0.43
1:A:640:SER:O	1:A:675:GLN:HA	2.18	0.43
1:C:883:GLY:HA3	1:C:987:ASP:HA	2.00	0.43
1:D:636:ILE:HG21	1:D:636:ILE:HD13	1.82	0.43
1:A:634:GLN:N	1:A:634:GLN:CD	2.68	0.43
1:B:646:HIS:ND1	6:B:9486:HOH:O	2.37	0.43
1:B:773:LYS:HA	1:B:773:LYS:HD3	1.75	0.43
1:B:890:GLN:HB2	6:B:9722:HOH:O	2.18	0.43
1:D:237:ARG:NH1	1:D:296:GLU:OE2	2.52	0.43
1:D:804:ASN:HA	1:D:809:ARG:NH1	2.34	0.43
1:A:685:LEU:HD23	1:A:685:LEU:HA	1.87	0.43
1:C:655:MET:SD	1:C:656:VAL:O	2.77	0.43
1:C:756:TRP:CE2	1:C:858:ILE:CD1	3.02	0.42
1:A:360:HIS:ND1	1:A:361:PRO:HD2	2.34	0.42
1:D:237:ARG:HB3	1:D:237:ARG:NH1	2.29	0.42
1:D:254:LEU:CD2	1:D:323:ILE:CD1	2.97	0.42
1:C:13:ARG:O	1:C:14:ARG:C	2.57	0.42
1:C:359:HIS:CD2	1:C:573:GLN:HA	2.54	0.42
1:D:226:HIS:O	1:D:242:ALA:HA	2.18	0.42
1:C:356:ARG:HD2	1:C:379:MET:HE3	2.02	0.42
1:A:237:ARG:NH1	1:A:296:GLU:OE2	2.52	0.42
1:D:545:SER:O	1:D:909:ARG:HD3	2.19	0.42
1:A:127:PHE:CE1	1:A:184:LEU:HG	2.54	0.42
1:A:359:HIS:CD2	1:A:573:GLN:HA	2.54	0.42
1:A:696:LEU:HB2	1:A:722:LEU:HD11	2.00	0.42
1:B:377:LEU:CD2	1:B:708:TRP:HA	2.49	0.42
1:B:847:LYS:HD3	1:B:849:LEU:CD2	2.37	0.42
1:C:433:LEU:HB3	1:C:434:PRO:HD3	2.01	0.42
1:A:427:THR:HG21	1:A:462:SER:HB3	2.01	0.42
1:B:233:ASP:HA	5:B:8417:DMS:C1	2.50	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:411:ASP:OD2	1:B:447:ASP:OD2	2.38	0.42
1:C:760:ARG:H	1:C:761:GLN:NE2	2.17	0.42
1:D:863:GLN:HG2	1:D:1021:CYS:CB	2.48	0.42
1:A:859:ASP:OD1	1:A:861:SER:OG	2.31	0.42
1:A:1022:GLN:C	1:A:1023:LYS:HG3	2.39	0.42
5:C:8408:DMS:H22	6:C:9354:HOH:O	2.20	0.41
1:D:687:GLN:HB3	1:D:688:PRO:CD	2.47	0.41
1:D:1022:GLN:HE21	1:D:1023:LYS:CG	2.33	0.41
1:D:833:ALA:HB1	1:D:858:ILE:O	2.20	0.41
1:D:901:GLY:HA3	1:D:902:PRO:HA	1.83	0.41
1:B:646:HIS:ND1	1:B:673:ALA:HA	2.35	0.41
1:B:684:GLU:HG2	1:B:685:LEU:N	2.34	0.41
1:D:46:ARG:HB3	1:D:47:PRO:HD2	2.03	0.41
1:D:240:LEU:HD23	1:D:240:LEU:C	2.40	0.41
1:D:538:TYR:C	1:D:539[B]:ALA:O	2.56	0.41
1:D:441:THR:O	1:D:445:GLN:HG3	2.20	0.41
1:D:650:GLU:HB3	1:D:670:LEU:HD12	2.02	0.41
1:A:285:TYR:HB3	1:A:288:ARG:HG3	2.02	0.41
1:B:596:PRO:HB3	6:B:9424:HOH:O	2.20	0.41
1:A:839:ALA:HA	1:A:852:SER:O	2.21	0.41
1:B:127:PHE:CD1	1:B:127:PHE:N	2.89	0.41
1:B:499:ILE:HD11	1:B:529:GLU:CG	2.51	0.41
1:B:619:GLU:HA	1:B:912:ALA:HB2	2.02	0.41
1:C:819:GLU:H	1:C:819:GLU:HG2	1.58	0.41
1:D:687:GLN:CB	1:D:688:PRO:HD2	2.47	0.41
1:A:127:PHE:CD1	1:A:127:PHE:N	2.88	0.41
1:B:433:LEU:HB3	1:B:434:PRO:HD3	2.03	0.41
1:A:770:ILE:O	1:A:773:LYS:HE2	2.21	0.41
1:B:427:THR:HG21	1:B:462:SER:HB3	2.02	0.41
1:B:581:ASN:HB2	1:B:583:ASN:ND2	2.36	0.41
1:B:646:HIS:CE1	1:B:673:ALA:CA	3.04	0.41
1:B:739:HIS:ND1	1:B:750:GLU:OE1	2.47	0.41
1:C:356:ARG:HD2	1:C:379:MET:HE1	2.02	0.41
1:C:663:LEU:HD22	1:C:663:LEU:HA	1.95	0.41
1:C:823:LEU:O	1:D:730:LEU:HD21	2.21	0.41
1:C:968:MET:HE2	1:C:968:MET:HB2	1.98	0.41
1:D:788:PRO:HD2	1:D:968:MET:HG3	2.03	0.41
1:B:340:GLY:O	1:B:561:ARG:HG2	2.21	0.41
1:C:375:ASP:O	1:C:379:MET:HG3	2.21	0.41
1:C:431:ARG:HB3	6:C:9587:HOH:O	2.20	0.41
1:D:16:TRP:CE3	1:D:189:LEU:HD11	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:390:SER:HA	1:D:391:HIS:HA	1.95	0.41
1:D:543:GLY:N	6:D:9750:HOH:O	2.43	0.41
1:B:540[A]:HIS:HA	1:B:568:TRP:O	2.21	0.40
1:B:903:GLN:HB2	6:B:8832:HOH:O	2.20	0.40
1:C:230:ARG:O	1:C:238:ALA:HA	2.21	0.40
1:D:88:SER:HA	1:D:366:VAL:HG21	2.03	0.40
1:D:773:LYS:HG2	1:D:775:GLN:NE2	2.37	0.40
1:C:859:ASP:OD1	1:C:861:SER:OG	2.26	0.40
1:A:360:HIS:HE1	1:A:362:LEU:HD12	1.86	0.40
1:B:499:ILE:HG22	1:B:501:PRO:HD3	2.04	0.40
1:B:634:GLN:CG	1:B:682:LEU:O	2.69	0.40
1:C:157:ARG:HD3	6:C:9706:HOH:O	2.21	0.40
1:D:986:ILE:HG23	1:D:986:ILE:HD13	1.72	0.40
5:A:8408:DMS:H21	6:A:9230:HOH:O	2.21	0.40
1:D:670:LEU:HD23	1:D:670:LEU:HA	1.82	0.40
5:D:8421:DMS:H11	6:D:9369:HOH:O	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)
6:A:9583:HOH:O	6:D:9783:HOH:O[4_545]	2.05	0.15

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	1011/1023 (99%)	972 (96%)	38 (4%)	1 (0%)	51	36
1	B	1011/1023 (99%)	974 (96%)	35 (4%)	2 (0%)	47	33
1	C	1011/1023 (99%)	979 (97%)	31 (3%)	1 (0%)	51	36
1	D	1011/1023 (99%)	973 (96%)	37 (4%)	1 (0%)	51	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
All	All	4044/4092 (99%)	3898 (96%)	141 (4%)	5 (0%)	51 36

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	732	ALA
1	D	164	ASP
1	B	164	ASP
1	C	734	SER
1	A	683	PRO

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	865/875 (99%)	834 (96%)	31 (4%)	35 20
1	B	865/875 (99%)	835 (96%)	30 (4%)	36 21
1	C	865/875 (99%)	832 (96%)	33 (4%)	33 18
1	D	865/875 (99%)	829 (96%)	36 (4%)	30 15
All	All	3460/3500 (99%)	3330 (96%)	130 (4%)	33 18

All (130) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	71	GLU
1	A	76	CYS
1	A	90	TRP
1	A	131	GLU
1	A	237	ARG
1	A	250	LEU
1	A	333	ARG
1	A	392	TYR
1	A	394	ASN
1	A	473	ARG

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Mol	Chain	Res	Type
1	A	519	SER
1	A	546	LEU
1	A	580	GLU
1	A	600	GLN
1	A	632	SER
1	A	634	GLN
1	A	653	HIS
1	A	655	MET
1	A	663	LEU
1	A	665	SER
1	A	667	GLU
1	A	684	GLU
1	A	735	HIS
1	A	737	ILE
1	A	773	LYS
1	A	799	THR
1	A	801	ILE
1	A	817	GLN
1	A	885	ASN
1	A	986	ILE
1	A	1023	LYS
1	B	76	CYS
1	B	80	GLU
1	B	230	ARG
1	B	262	GLN
1	B	264	GLU
1	B	299	LYS
1	B	333	ARG
1	B	362	LEU
1	B	370	GLN
1	B	394	ASN
1	B	535	LEU
1	B	554	GLN
1	B	600	GLN
1	B	651	LEU
1	B	661	LYS
1	B	663	LEU
1	B	667	GLU
1	B	684	GLU
1	B	687	GLN
1	B	690	SER
1	B	730	LEU

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Mol	Chain	Res	Type
1	B	745	MET
1	B	799	THR
1	B	800	ARG
1	B	819	GLU
1	B	845	GLN
1	B	847	LYS
1	B	863	GLN
1	B	956	GLN
1	B	1023	LYS
1	C	49	GLN
1	C	71	GLU
1	C	80	GLU
1	C	135	GLN
1	C	178	ARG
1	C	237	ARG
1	C	262	GLN
1	C	333	ARG
1	C	392	TYR
1	C	394	ASN
1	C	519	SER
1	C	546	LEU
1	C	595	THR
1	C	634	GLN
1	C	651	LEU
1	C	655	MET
1	C	663	LEU
1	C	672	VAL
1	C	681	GLU
1	C	685	LEU
1	C	687	GLN
1	C	730	LEU
1	C	734	SER
1	C	735	HIS
1	C	737	ILE
1	C	750	GLU
1	C	761	GLN
1	C	773	LYS
1	C	800	ARG
1	C	809	ARG
1	C	819	GLU
1	C	986	ILE
1	C	1023	LYS

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Mol	Chain	Res	Type
1	D	13	ARG
1	D	112	PRO
1	D	116	THR
1	D	237	ARG
1	D	277	GLU
1	D	333	ARG
1	D	344	LEU
1	D	370	GLN
1	D	392	TYR
1	D	394	ASN
1	D	519	SER
1	D	546	LEU
1	D	581	ASN
1	D	594	ASP
1	D	632	SER
1	D	653	HIS
1	D	655	MET
1	D	661	LYS
1	D	663	LEU
1	D	685	LEU
1	D	687	GLN
1	D	699	ARG
1	D	703	PRO
1	D	737	ILE
1	D	755	ARG
1	D	772	ASP
1	D	773	LYS
1	D	799	THR
1	D	809	ARG
1	D	845	GLN
1	D	885	ASN
1	D	893	GLU
1	D	986	ILE
1	D	1018	LEU
1	D	1022	GLN
1	D	1023	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	135	GLN
1	A	262	GLN

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Mol	Chain	Res	Type
1	A	600	GLN
1	A	624	GLN
1	A	634	GLN
1	A	817	GLN
1	A	844	HIS
1	A	878	HIS
1	A	977	HIS
1	B	262	GLN
1	B	363	HIS
1	B	583	ASN
1	B	600	GLN
1	B	624	GLN
1	B	628	GLN
1	B	634	GLN
1	B	675	GLN
1	B	687	GLN
1	B	804	ASN
1	B	878	HIS
1	C	266	GLN
1	C	363	HIS
1	C	646	HIS
1	C	653	HIS
1	C	761	GLN
1	C	824	GLN
1	C	878	HIS
1	C	977	HIS
1	D	135	GLN
1	D	294	ASN
1	D	363	HIS
1	D	624	GLN
1	D	628	GLN
1	D	634	GLN
1	D	653	HIS
1	D	804	ASN
1	D	824	GLN
1	D	878	HIS
1	D	977	HIS
1	D	1022	GLN

5.3.3 RNA

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)

8 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	0.62	0	17,17,17	1.63	7 (41%)
2	GAL	E	2	4,2	11,11,12	0.82	0	15,15,17	1.34	3 (20%)
2	BGC	F	1	2	12,12,12	0.75	0	17,17,17	1.88	5 (29%)
2	GAL	F	2	4,2	11,11,12	0.76	0	15,15,17	1.17	2 (13%)
2	BGC	G	1	2	12,12,12	0.98	0	17,17,17	1.50	3 (17%)
2	GAL	G	2	4,2	11,11,12	1.27	1 (9%)	15,15,17	0.77	0
2	BGC	H	1	2	12,12,12	0.89	0	17,17,17	1.24	1 (5%)
2	GAL	H	2	4,2	11,11,12	1.07	1 (9%)	15,15,17	1.11	1 (6%)

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	-	0/2/22/22	0/1/1/1
2	GAL	E	2	4,2	-	1/2/19/22	0/1/1/1
2	BGC	F	1	2	-	0/2/22/22	0/1/1/1
2	GAL	F	2	4,2	-	1/2/19/22	0/1/1/1
2	BGC	G	1	2	-	0/2/22/22	0/1/1/1
2	GAL	G	2	4,2	-	1/2/19/22	0/1/1/1
2	BGC	H	1	2	-	0/2/22/22	0/1/1/1
2	GAL	H	2	4,2	-	1/2/19/22	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	2	GAL	O5-C1	-3.93	1.37	1.43
2	H	2	GAL	O5-C1	-2.81	1.39	1.43

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	1	BGC	O5-C1-C2	-3.87	103.38	110.28
2	F	1	BGC	O1-C1-C2	-3.83	98.24	109.03
2	G	1	BGC	O1-C1-O5	-3.39	100.20	110.38
2	E	1	BGC	O3-C3-C2	-3.10	103.17	110.35
2	E	2	GAL	C1-C2-C3	2.80	113.11	109.67
2	F	2	GAL	O5-C5-C4	-2.61	104.47	110.83
2	F	1	BGC	O4-C4-C5	-2.58	102.90	109.30
2	H	1	BGC	O4-C4-C5	-2.52	103.03	109.30
2	H	2	GAL	C1-O5-C5	-2.44	108.89	112.19
2	E	1	BGC	O2-C2-C3	-2.43	104.74	110.35
2	E	1	BGC	O5-C1-C2	-2.36	106.07	110.28
2	E	1	BGC	O2-C2-C1	2.27	114.42	109.16
2	G	1	BGC	O5-C5-C6	-2.23	100.88	106.44
2	E	1	BGC	O4-C4-C5	-2.21	103.80	109.30
2	E	1	BGC	O1-C1-O5	-2.19	103.81	110.38
2	F	2	GAL	O3-C3-C2	-2.17	105.84	109.99
2	E	2	GAL	O3-C3-C2	-2.17	105.84	109.99
2	F	1	BGC	O3-C3-C2	-2.17	105.34	110.35
2	F	1	BGC	C6-C5-C4	-2.15	107.96	113.00
2	G	1	BGC	O5-C1-C2	-2.09	106.55	110.28
2	E	2	GAL	O2-C2-C3	2.02	114.18	110.14
2	E	1	BGC	C3-C4-C5	-2.01	106.65	110.24

There are no chirality outliers.

All (4) torsion outliers are listed below:

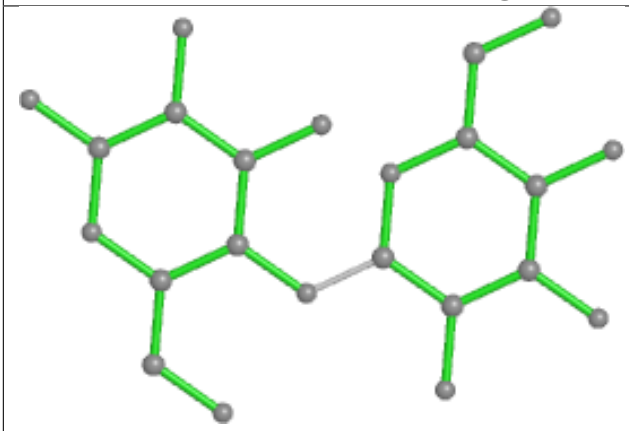
Mol	Chain	Res	Type	Atoms
2	G	2	GAL	O5-C5-C6-O6
2	E	2	GAL	O5-C5-C6-O6
2	H	2	GAL	O5-C5-C6-O6
2	F	2	GAL	O5-C5-C6-O6

There are no ring outliers.

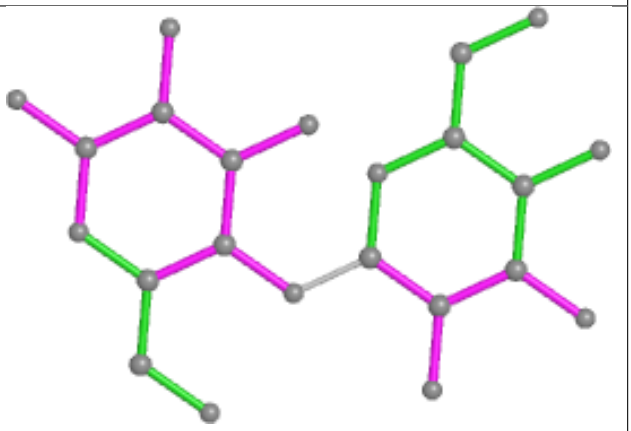
No monomer is involved in short contacts.

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

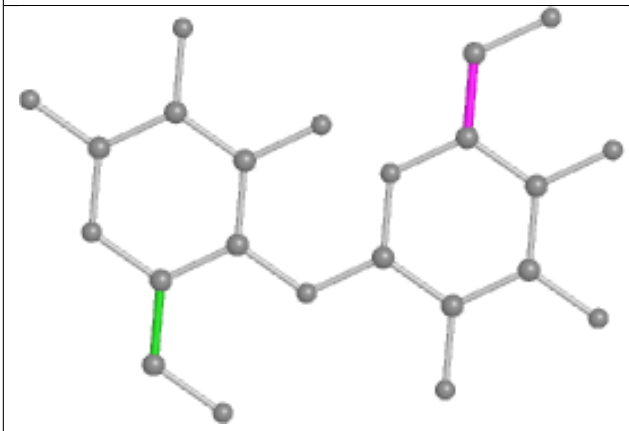
Oligosaccharide Chain E



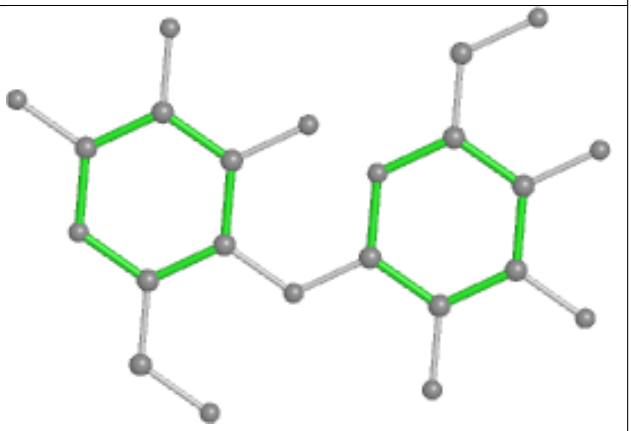
Bond lengths



Bond angles

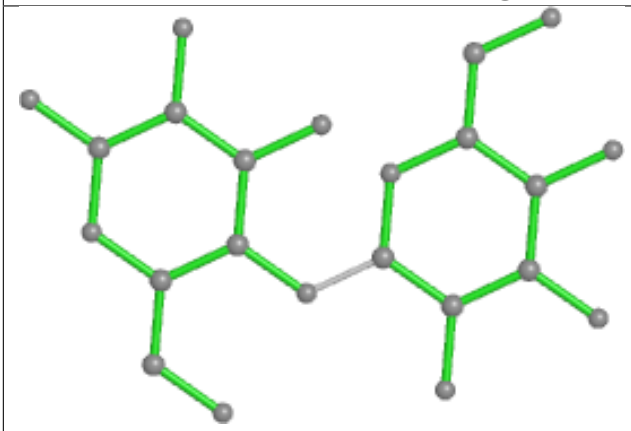


Torsions

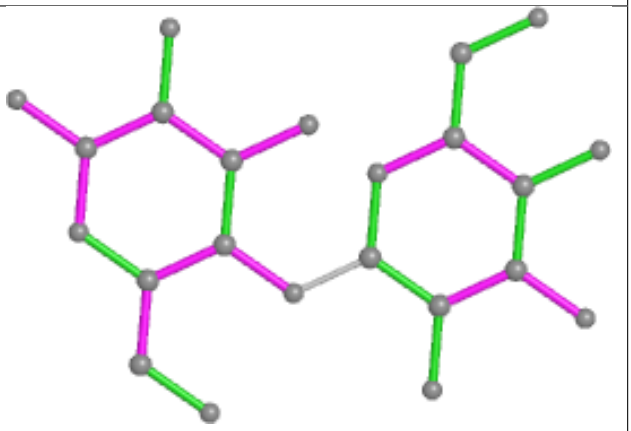


Rings

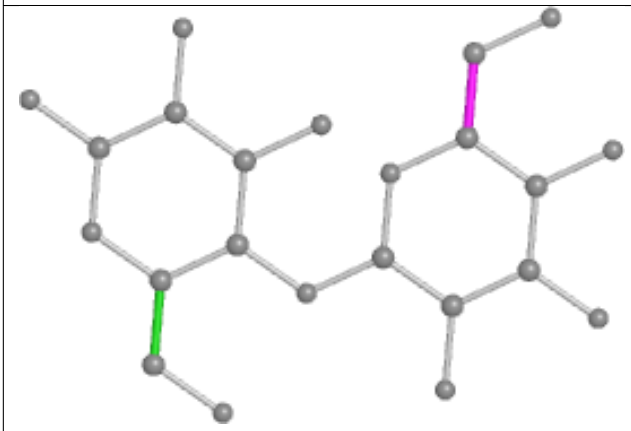
Oligosaccharide Chain F



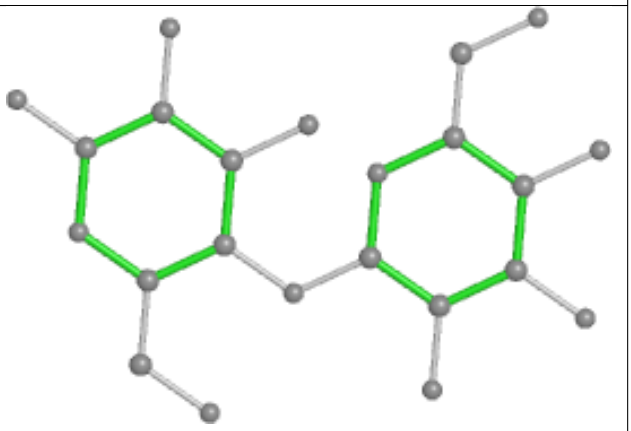
Bond lengths



Bond angles

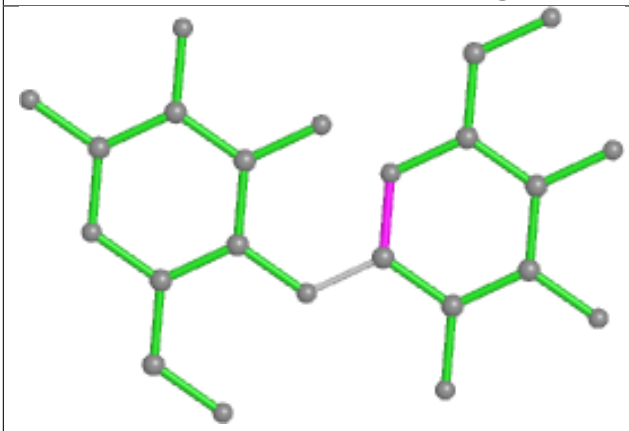


Torsions

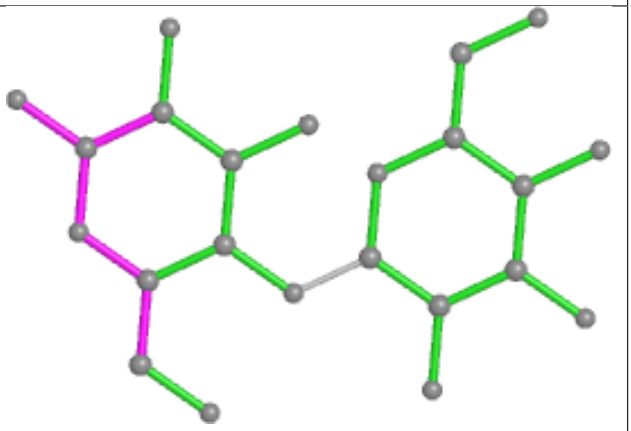


Rings

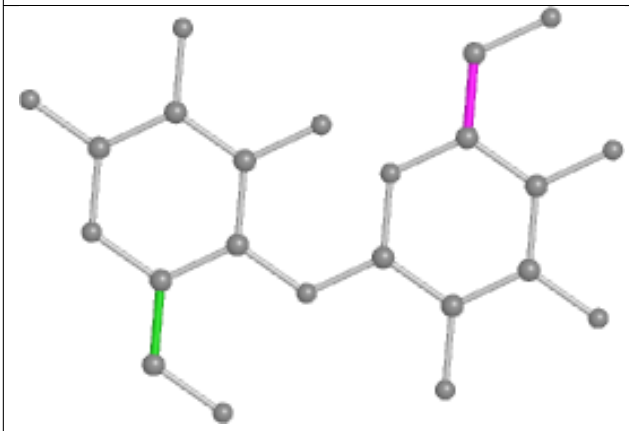
Oligosaccharide Chain G



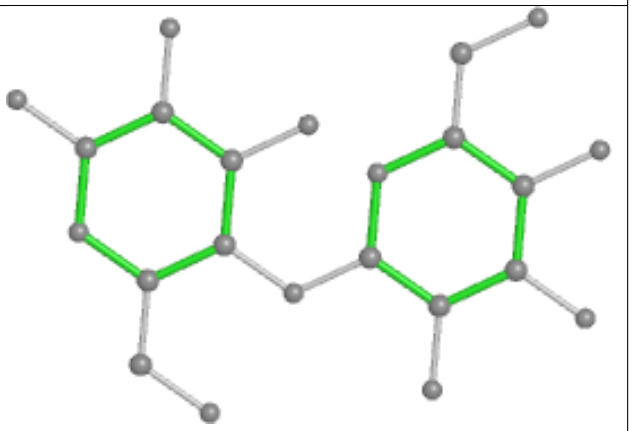
Bond lengths



Bond angles

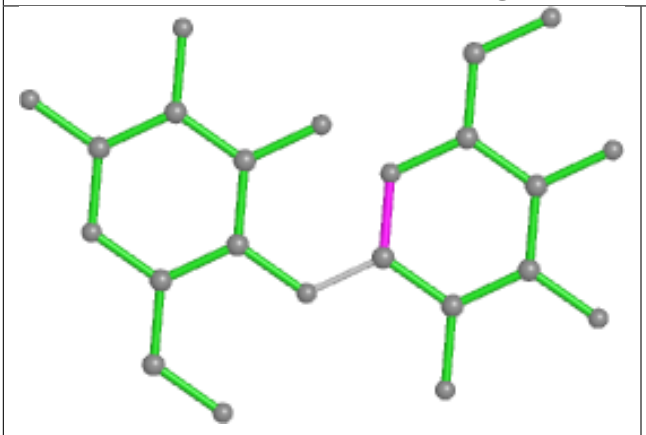


Torsions

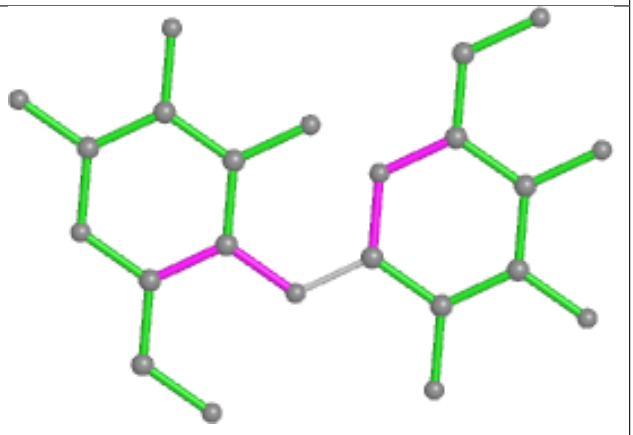


Rings

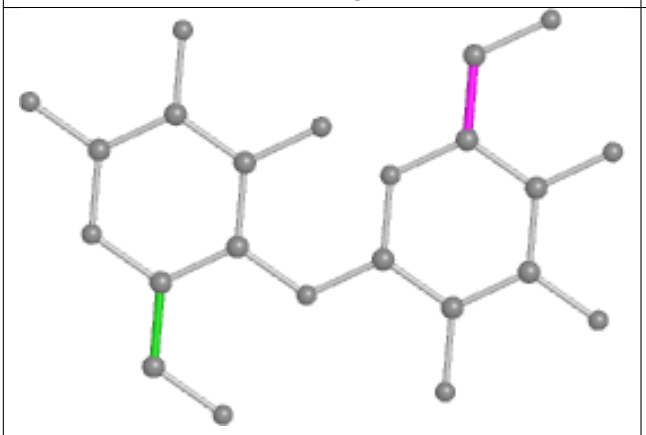
Oligosaccharide Chain H



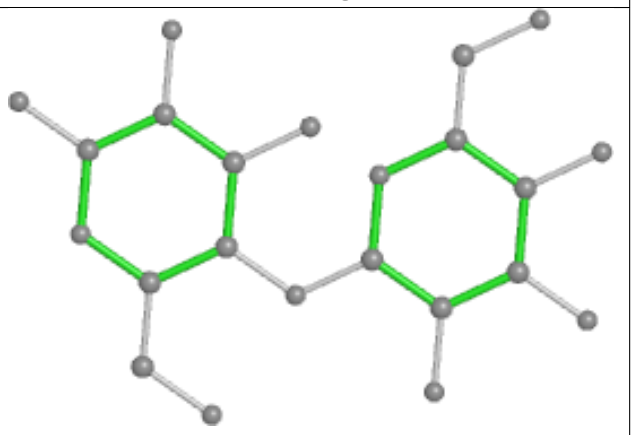
Bond lengths



Bond angles



Torsions



Rings

5.6 Ligand geometry (i)

Of 125 ligands modelled in this entry, 29 are monoatomic - leaving 96 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
5	DMS	A	8404	-	3,3,3	0.77	0	3,3,3	0.10	0
5	DMS	A	8507	-	3,3,3	1.45	0	3,3,3	0.38	0
5	DMS	C	8408	-	3,3,3	1.04	0	3,3,3	0.37	0
5	DMS	C	8415	-	3,3,3	1.25	0	3,3,3	0.40	0
5	DMS	A	8412	-	3,3,3	0.19	0	3,3,3	0.20	0
5	DMS	A	8409	-	3,3,3	1.05	0	3,3,3	0.16	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	DMS	B	8409	-	3,3,3	1.17	0	3,3,3	0.30	0
5	DMS	C	8401	-	3,3,3	0.61	0	3,3,3	0.27	0
5	DMS	D	8416	-	3,3,3	0.41	0	3,3,3	0.20	0
5	DMS	C	8412	-	3,3,3	0.78	0	3,3,3	0.40	0
5	DMS	C	8602	-	3,3,3	0.59	0	3,3,3	0.20	0
5	DMS	C	8413	-	3,3,3	1.30	0	3,3,3	0.25	0
5	DMS	D	8404	-	3,3,3	1.22	0	3,3,3	0.12	0
5	DMS	D	8406	-	3,3,3	0.88	0	3,3,3	0.57	0
5	DMS	A	8503	-	3,3,3	0.45	0	3,3,3	0.15	0
5	DMS	B	8508	-	3,3,3	2.15	1 (33%)	3,3,3	0.59	0
5	DMS	D	8705	-	3,3,3	1.16	0	3,3,3	0.56	0
5	DMS	C	8423	-	3,3,3	0.62	0	3,3,3	0.43	0
5	DMS	A	8419	-	3,3,3	0.49	0	3,3,3	0.36	0
5	DMS	D	8405	-	3,3,3	0.39	0	3,3,3	0.38	0
5	DMS	C	8407	-	3,3,3	0.95	0	3,3,3	0.14	0
5	DMS	C	8405	-	3,3,3	1.18	0	3,3,3	0.36	0
5	DMS	D	8408	-	3,3,3	0.93	0	3,3,3	0.06	0
5	DMS	C	8504	-	3,3,3	0.66	0	3,3,3	0.17	0
5	DMS	D	8412	-	3,3,3	0.25	0	3,3,3	0.25	0
5	DMS	D	8421	-	3,3,3	0.15	0	3,3,3	0.16	0
5	DMS	C	8425	4	3,3,3	0.97	0	3,3,3	0.29	0
5	DMS	D	8413	-	3,3,3	0.98	0	3,3,3	0.26	0
5	DMS	B	8404	-	3,3,3	0.85	0	3,3,3	0.31	0
5	DMS	D	8407	-	3,3,3	1.87	2 (66%)	3,3,3	0.60	0
5	DMS	D	8410	-	3,3,3	0.63	0	3,3,3	0.25	0
5	DMS	B	8417	-	3,3,3	0.48	0	3,3,3	0.08	0
5	DMS	D	8508	-	3,3,3	0.82	0	3,3,3	0.23	0
5	DMS	C	8421	-	3,3,3	0.77	0	3,3,3	0.47	0
5	DMS	D	8402	-	3,3,3	0.76	0	3,3,3	0.25	0
5	DMS	B	8403	-	3,3,3	1.16	0	3,3,3	0.43	0
5	DMS	C	8403	-	3,3,3	0.52	0	3,3,3	0.39	0
5	DMS	B	8416	-	3,3,3	0.76	0	3,3,3	0.17	0
5	DMS	B	8425	4	3,3,3	1.40	1 (33%)	3,3,3	0.65	0
5	DMS	D	8403	-	3,3,3	0.54	0	3,3,3	0.22	0
5	DMS	D	8701	-	3,3,3	1.66	0	3,3,3	0.42	0
5	DMS	B	8411	-	3,3,3	0.84	0	3,3,3	0.23	0
5	DMS	B	8502	-	3,3,3	0.91	0	3,3,3	1.16	1 (33%)
5	DMS	A	8423	-	3,3,3	0.93	0	3,3,3	0.33	0
5	DMS	C	8417	-	3,3,3	0.64	0	3,3,3	0.35	0
5	DMS	C	8402	-	3,3,3	1.42	1 (33%)	3,3,3	0.32	0
5	DMS	C	8409	-	3,3,3	0.96	0	3,3,3	0.23	0
5	DMS	A	8420	-	3,3,3	0.35	0	3,3,3	0.61	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	DMS	B	8407	-	3,3,3	1.33	0	3,3,3	0.25	0
5	DMS	A	8504	-	3,3,3	0.24	0	3,3,3	0.16	0
5	DMS	C	8601	-	3,3,3	0.89	0	3,3,3	0.34	0
5	DMS	C	8420	-	3,3,3	0.51	0	3,3,3	0.25	0
5	DMS	A	8501	-	3,3,3	0.90	0	3,3,3	0.13	0
5	DMS	D	8501	-	3,3,3	0.56	0	3,3,3	0.10	0
5	DMS	B	8408	-	3,3,3	0.78	0	3,3,3	0.84	0
5	DMS	B	8415	-	3,3,3	0.85	0	3,3,3	0.54	0
5	DMS	B	8412	-	3,3,3	0.31	0	3,3,3	0.15	0
5	DMS	A	8421	-	3,3,3	0.51	0	3,3,3	0.56	0
5	DMS	C	8416	-	3,3,3	0.94	0	3,3,3	0.19	0
5	DMS	D	8409	-	3,3,3	1.20	1 (33%)	3,3,3	0.94	0
5	DMS	D	8414	-	3,3,3	0.14	0	3,3,3	0.26	0
5	DMS	B	8401	-	3,3,3	0.81	0	3,3,3	0.40	0
5	DMS	C	8404	-	3,3,3	0.92	0	3,3,3	0.64	0
5	DMS	A	8407	-	3,3,3	1.10	0	3,3,3	0.88	0
5	DMS	B	8413	-	3,3,3	1.65	1 (33%)	3,3,3	0.39	0
5	DMS	B	8410	-	3,3,3	1.03	0	3,3,3	0.77	0
5	DMS	A	8405	-	3,3,3	0.25	0	3,3,3	0.61	0
5	DMS	A	8411	-	3,3,3	0.29	0	3,3,3	0.40	0
5	DMS	B	8601	-	3,3,3	0.91	0	3,3,3	0.44	0
5	DMS	A	8408	-	3,3,3	0.96	0	3,3,3	0.58	0
5	DMS	A	8401	-	3,3,3	0.65	0	3,3,3	0.27	0
5	DMS	A	8413	-	3,3,3	1.66	0	3,3,3	0.43	0
5	DMS	B	8423	-	3,3,3	0.26	0	3,3,3	0.45	0
5	DMS	D	8704	-	3,3,3	0.35	0	3,3,3	0.36	0
5	DMS	A	8403	-	3,3,3	1.15	0	3,3,3	0.37	0
5	DMS	A	8410	-	3,3,3	0.26	0	3,3,3	0.29	0
5	DMS	C	8501	-	3,3,3	0.55	0	3,3,3	0.60	0
5	DMS	A	8425	4	3,3,3	1.42	0	3,3,3	0.28	0
5	DMS	D	8401	-	3,3,3	1.11	0	3,3,3	0.35	0
5	DMS	A	8406	-	3,3,3	0.20	0	3,3,3	0.44	0
5	DMS	B	8402	-	3,3,3	1.22	0	3,3,3	0.30	0
5	DMS	C	8411	-	3,3,3	0.56	0	3,3,3	0.10	0
5	DMS	C	8419	-	3,3,3	0.43	0	3,3,3	0.19	0
5	DMS	A	8414	-	3,3,3	0.83	0	3,3,3	0.16	0
5	DMS	D	8703	-	3,3,3	0.71	0	3,3,3	0.55	0
5	DMS	B	8414	-	3,3,3	0.27	0	3,3,3	0.19	0
5	DMS	A	8402	-	3,3,3	0.89	0	3,3,3	0.51	0
5	DMS	D	8411	-	3,3,3	0.47	0	3,3,3	0.53	0
5	DMS	B	8405	-	3,3,3	0.90	0	3,3,3	0.24	0
5	DMS	D	8419	-	3,3,3	0.33	0	3,3,3	0.22	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
5	DMS	B	8421	-	3,3,3	0.53	0	3,3,3	0.37	0
5	DMS	B	8420	-	3,3,3	0.58	0	3,3,3	0.23	0
5	DMS	C	8410	-	3,3,3	0.93	0	3,3,3	0.16	0
5	DMS	B	8504	-	3,3,3	0.12	0	3,3,3	0.25	0
5	DMS	C	8414	-	3,3,3	1.07	0	3,3,3	0.61	0
5	DMS	D	8423	-	3,3,3	0.75	0	3,3,3	0.18	0

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	B	8508	DMS	C1-S	3.50	2.01	1.75
5	D	8407	DMS	O-S	2.28	1.65	1.50
5	D	8407	DMS	C2-S	2.20	1.92	1.75
5	B	8413	DMS	O-S	2.16	1.64	1.50
5	B	8425	DMS	O-S	2.16	1.64	1.50
5	C	8402	DMS	C2-S	2.15	1.91	1.75
5	D	8409	DMS	O-S	2.01	1.63	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	8502	DMS	C2-S-C1	2.00	108.75	98.44

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

14 monomers are involved in 21 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	C	8408	DMS	2	0
5	A	8412	DMS	3	0
5	C	8602	DMS	1	0
5	B	8508	DMS	1	0
5	D	8412	DMS	2	0
5	D	8421	DMS	1	0
5	B	8417	DMS	2	0
5	D	8508	DMS	1	0
5	A	8420	DMS	1	0
5	C	8420	DMS	2	0
5	B	8410	DMS	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
5	A	8408	DMS	1	0
5	A	8425	DMS	1	0
5	D	8703	DMS	1	0

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	1011/1023 (98%)	-0.80	14 (1%)	75 72	6, 13, 41, 100	0
1	B	1011/1023 (98%)	-0.80	9 (0%)	84 82	6, 12, 40, 94	0
1	C	1011/1023 (98%)	-0.80	10 (0%)	82 80	6, 13, 42, 100	0
1	D	1011/1023 (98%)	-0.77	19 (1%)	66 63	6, 13, 43, 95	0
All	All	4044/4092 (98%)	-0.79	52 (1%)	77 74	6, 13, 42, 100	0

All (52) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	735	HIS	7.9
1	D	735	HIS	7.4
1	D	732	ALA	6.3
1	A	686	PRO	6.0
1	B	689	GLU	6.0
1	A	689	GLU	5.9
1	C	732	ALA	5.8
1	B	731	PRO	5.5
1	A	685	LEU	5.2
1	B	685	LEU	5.1
1	C	731	PRO	4.9
1	A	687	GLN	4.8
1	C	730	LEU	4.4
1	D	730	LEU	4.4
1	B	732	ALA	4.3
1	D	689	GLU	4.3
1	C	689	GLU	4.2
1	C	735	HIS	4.1
1	A	730	LEU	4.0
1	D	731	PRO	4.0
1	B	733	ALA	4.0

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Mol	Chain	Res	Type	RSRZ
1	A	731	PRO	3.7
1	D	686	PRO	3.6
1	B	730	LEU	3.6
1	D	734	SER	3.6
1	D	684	GLU	3.5
1	D	687	GLN	3.5
1	B	684	GLU	3.2
1	B	686	PRO	3.1
1	D	733	ALA	3.1
1	D	685	LEU	3.1
1	A	733	ALA	3.0
1	C	733	ALA	2.8
1	A	1023	LYS	2.8
1	D	580	GLU	2.8
1	A	732	ALA	2.7
1	D	771	GLY	2.6
1	A	684	GLU	2.6
1	B	687	GLN	2.6
1	C	685	LEU	2.6
1	C	686	PRO	2.5
1	D	800	ARG	2.5
1	D	581	ASN	2.4
1	D	683	PRO	2.4
1	C	687	GLN	2.4
1	A	580	GLU	2.2
1	D	1023	LYS	2.2
1	D	688	PRO	2.1
1	D	799	THR	2.1
1	A	799	THR	2.1
1	C	800	ARG	2.0
1	A	634	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)

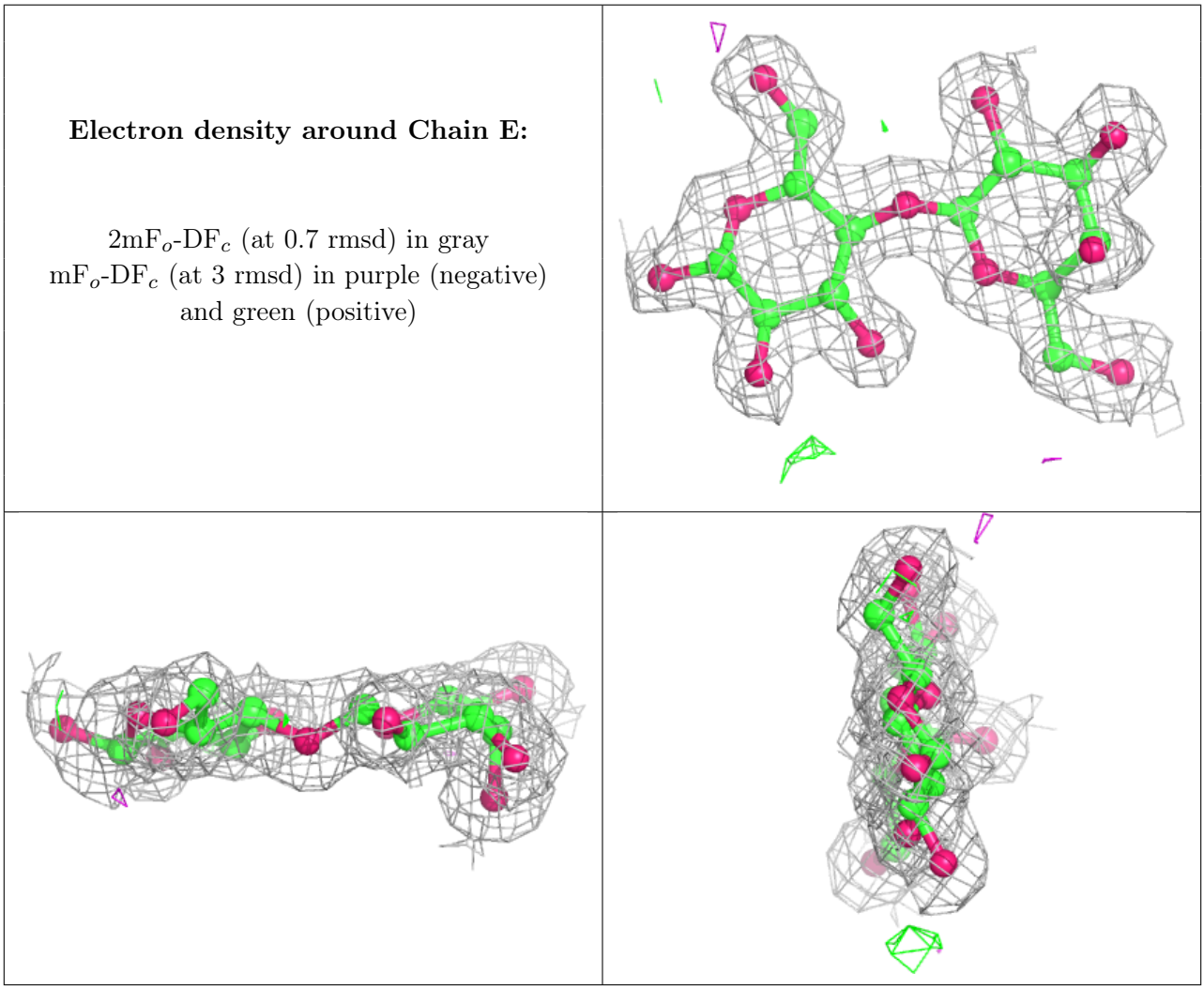
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' 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	BGC	G	1	12/12	0.95	0.09	6,16,32,45	12
2	BGC	H	1	12/12	0.95	0.10	8,23,29,100	0
2	BGC	E	1	12/12	0.96	0.10	9,19,28,42	0
2	BGC	F	1	12/12	0.96	0.09	7,19,30,32	0
2	GAL	E	2	11/12	0.98	0.06	8,9,13,15	0
2	GAL	H	2	11/12	0.98	0.05	7,10,12,13	0
2	GAL	F	2	11/12	0.99	0.06	2,5,10,13	0
2	GAL	G	2	11/12	0.99	0.05	4,5,8,10	11

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.

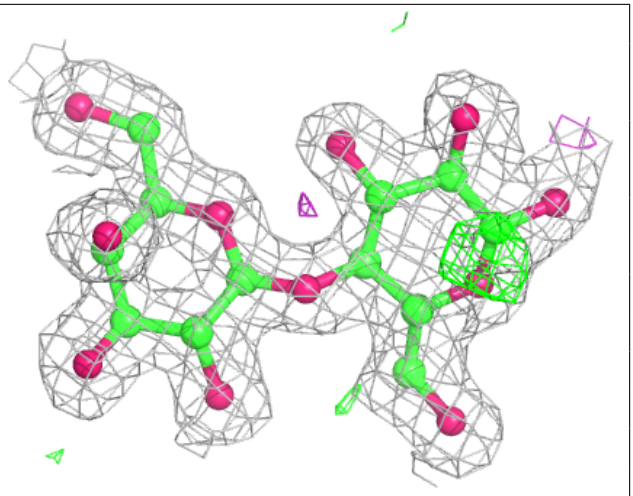
Electron density around Chain E:

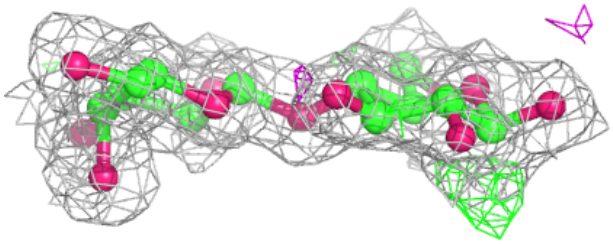
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)



Electron density around Chain F:

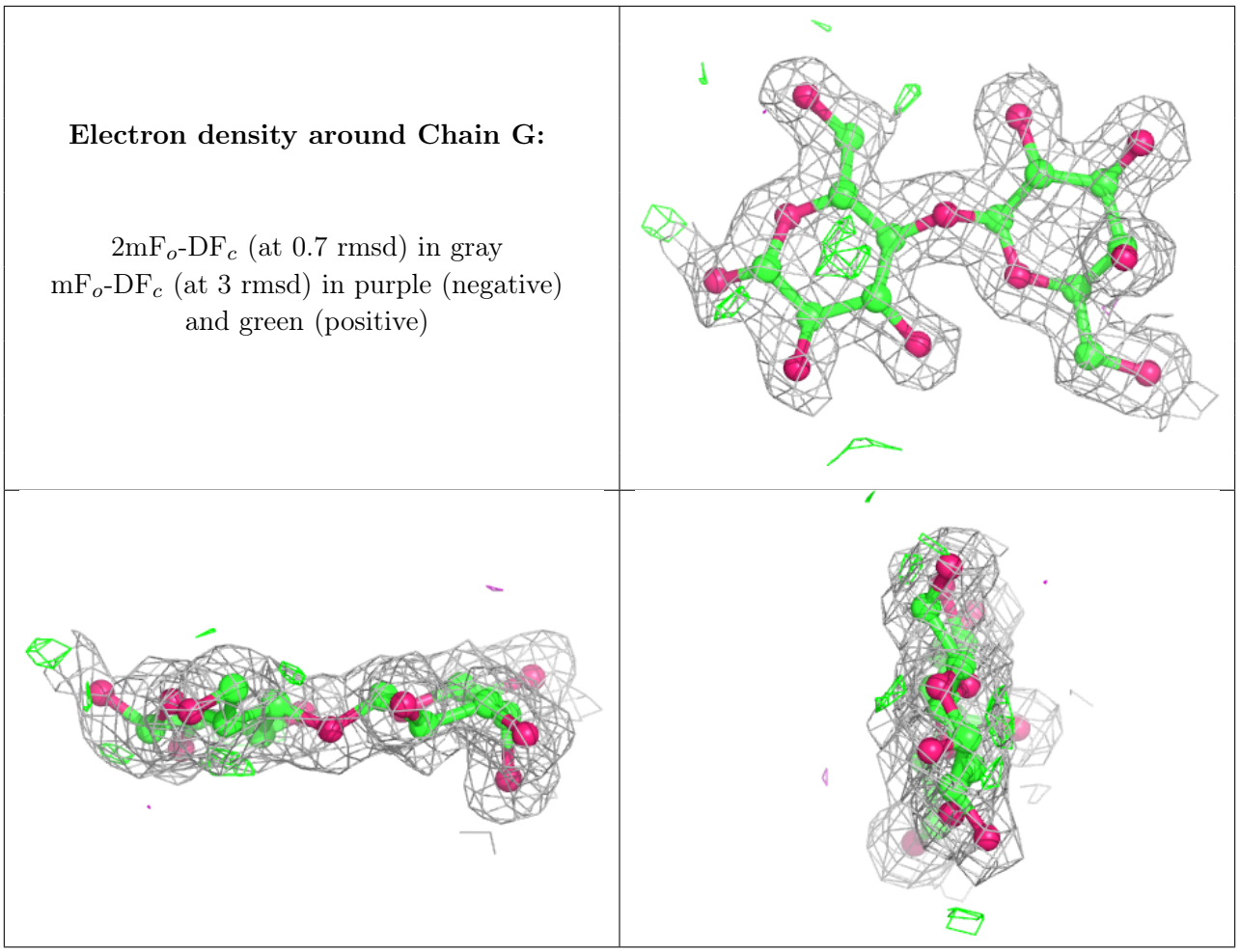
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)





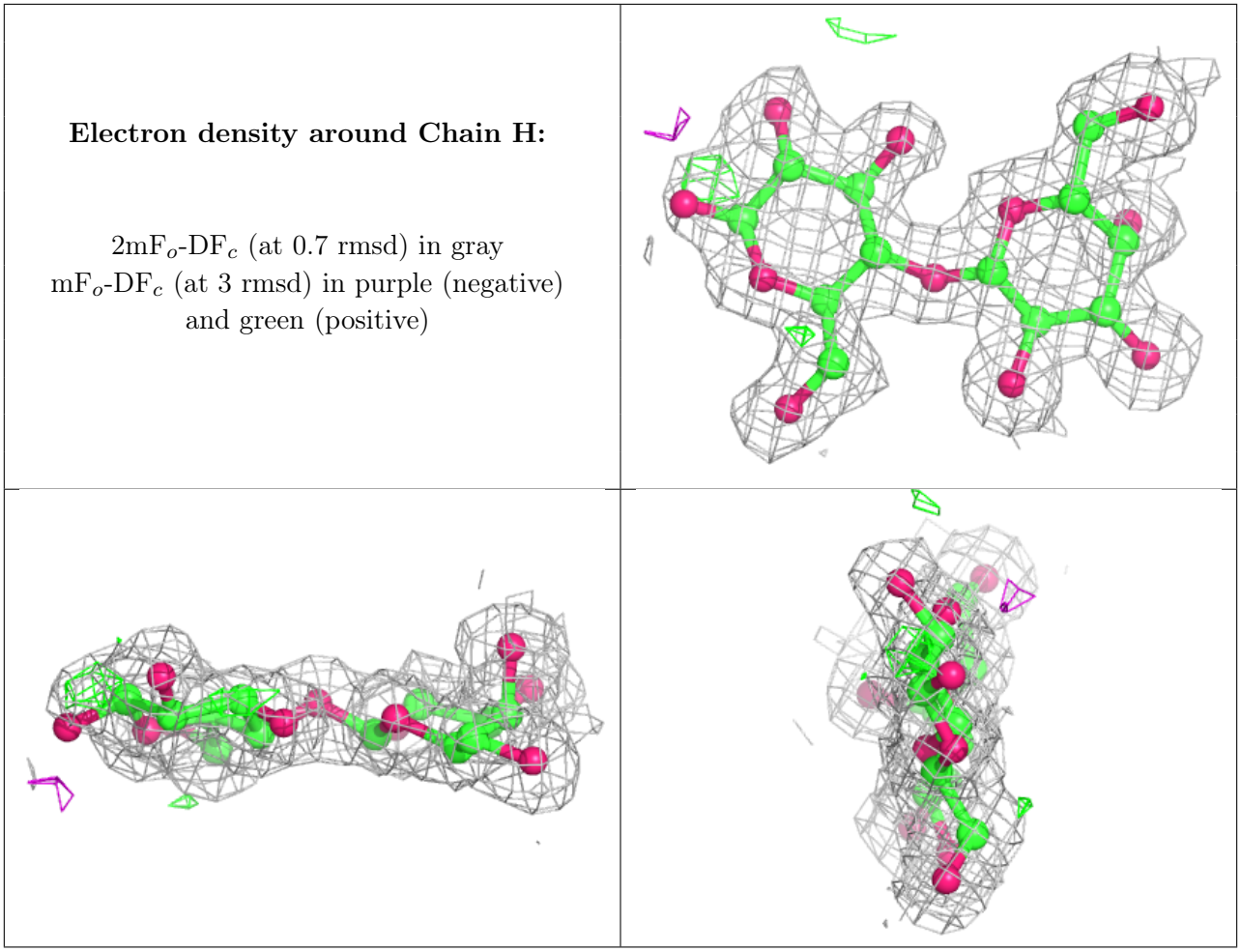
Electron density around Chain G:

$2mF_o$-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 H:

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



6.4 Ligands

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} 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
5	DMS	A	8507	4/4	0.84	0.16	23,26,35,72	0
5	DMS	D	8703	4/4	0.87	0.16	29,55,61,61	0
5	DMS	D	8705	4/4	0.87	0.13	30,37,42,43	0
3	MG	A	3105	1/1	0.89	0.10	77,77,77,77	0
3	MG	D	3003	1/1	0.90	0.24	55,55,55,55	0
5	DMS	C	8417	4/4	0.92	0.14	25,27,63,74	0
5	DMS	C	8423	4/4	0.92	0.13	31,31,46,51	0
5	DMS	D	8423	4/4	0.92	0.17	27,46,56,65	0
5	DMS	B	8415	4/4	0.92	0.14	21,31,32,59	0
5	DMS	B	8417	4/4	0.92	0.12	22,32,68,74	0
5	DMS	B	8420	4/4	0.93	0.15	41,43,64,72	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	DMS	B	8425	4/4	0.93	0.15	21,26,37,42	0
5	DMS	C	8415	4/4	0.93	0.14	15,33,50,60	0
5	DMS	D	8704	4/4	0.93	0.16	32,63,100,100	0
5	DMS	A	8423	4/4	0.93	0.12	27,33,43,56	0
5	DMS	C	8420	4/4	0.94	0.13	26,32,43,64	0
5	DMS	A	8421	4/4	0.94	0.20	36,42,50,59	0
5	DMS	C	8504	4/4	0.94	0.10	29,32,45,52	0
5	DMS	B	8413	4/4	0.94	0.15	27,36,38,39	0
5	DMS	D	8508	4/4	0.94	0.10	29,34,36,53	0
5	DMS	B	8508	4/4	0.94	0.15	15,34,46,47	0
5	DMS	A	8406	4/4	0.94	0.12	23,42,59,61	0
5	DMS	A	8425	4/4	0.94	0.12	26,35,37,40	0
5	DMS	C	8501	4/4	0.95	0.11	18,35,37,38	0
5	DMS	A	8412	4/4	0.95	0.13	34,44,51,54	0
5	DMS	D	8407	4/4	0.95	0.12	27,31,37,44	0
4	NA	B	3104	1/1	0.95	0.08	27,27,27,27	0
5	DMS	D	8501	4/4	0.95	0.08	21,29,32,50	0
5	DMS	B	8407	4/4	0.95	0.16	30,31,36,37	0
5	DMS	C	8419	4/4	0.95	0.12	33,39,43,54	0
5	DMS	B	8423	4/4	0.95	0.13	24,28,46,100	0
3	MG	A	3005	1/1	0.95	0.08	31,31,31,31	0
5	DMS	D	8416	4/4	0.96	0.18	22,36,46,100	0
5	DMS	C	8416	4/4	0.96	0.18	31,34,36,40	0
5	DMS	C	8425	4/4	0.96	0.17	32,40,40,41	0
5	DMS	A	8413	4/4	0.96	0.15	24,26,32,41	0
5	DMS	A	8420	4/4	0.96	0.12	30,33,39,44	0
5	DMS	D	8404	4/4	0.96	0.10	17,17,42,58	0
3	MG	C	3004	1/1	0.96	0.15	37,37,37,37	0
4	NA	C	3104	1/1	0.97	0.11	26,26,26,26	0
5	DMS	A	8414	4/4	0.97	0.12	26,26,43,100	0
5	DMS	B	8409	4/4	0.97	0.11	28,28,31,32	0
5	DMS	B	8410	4/4	0.97	0.09	15,37,37,38	0
5	DMS	A	8419	4/4	0.97	0.10	34,37,38,42	0
5	DMS	C	8421	4/4	0.97	0.12	31,35,46,100	0
4	NA	A	3104	1/1	0.97	0.09	26,26,26,26	0
5	DMS	B	8416	4/4	0.97	0.13	28,35,43,58	0
5	DMS	A	8407	4/4	0.97	0.09	16,24,25,33	0
5	DMS	A	8409	4/4	0.97	0.11	26,26,26,40	0
5	DMS	C	8601	4/4	0.97	0.13	43,43,55,81	0
5	DMS	C	8602	4/4	0.97	0.10	46,51,58,69	0
5	DMS	B	8421	4/4	0.97	0.13	22,46,51,73	0
5	DMS	D	8406	4/4	0.97	0.10	18,19,22,29	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	MG	C	3006	1/1	0.97	0.15	27,27,27,27	0
5	DMS	D	8409	4/4	0.97	0.09	25,28,30,33	0
5	DMS	A	8501	4/4	0.97	0.08	11,24,32,36	0
5	DMS	B	8504	4/4	0.97	0.07	17,25,33,36	0
5	DMS	A	8503	4/4	0.97	0.15	34,37,46,50	0
5	DMS	B	8601	4/4	0.97	0.13	35,35,39,48	0
5	DMS	C	8408	4/4	0.97	0.08	15,20,28,29	0
5	DMS	C	8409	4/4	0.97	0.10	27,32,37,38	0
5	DMS	C	8413	4/4	0.97	0.12	25,31,31,32	0
4	NA	A	3103	1/1	0.98	0.05	21,21,21,21	0
5	DMS	B	8412	4/4	0.98	0.07	22,30,32,32	0
3	MG	D	3005	1/1	0.98	0.08	21,21,21,21	0
5	DMS	C	8405	4/4	0.98	0.10	16,22,25,27	0
5	DMS	C	8407	4/4	0.98	0.12	26,26,31,32	0
5	DMS	B	8414	4/4	0.98	0.10	21,42,100,100	0
5	DMS	A	8408	4/4	0.98	0.09	23,25,29,41	0
5	DMS	C	8410	4/4	0.98	0.07	25,28,31,35	0
5	DMS	C	8412	4/4	0.98	0.08	23,29,32,56	0
5	DMS	A	8504	4/4	0.98	0.10	19,33,55,100	0
5	DMS	D	8413	4/4	0.98	0.12	27,27,27,31	0
5	DMS	D	8414	4/4	0.98	0.11	21,36,100,100	0
5	DMS	C	8414	4/4	0.98	0.09	16,36,37,51	0
5	DMS	D	8419	4/4	0.98	0.10	22,33,39,41	0
5	DMS	D	8421	4/4	0.98	0.12	33,46,52,100	0
4	NA	D	3103	1/1	0.98	0.06	26,26,26,26	0
5	DMS	B	8404	4/4	0.98	0.07	17,25,28,31	0
5	DMS	A	8410	4/4	0.98	0.06	18,28,29,35	0
5	DMS	B	8408	4/4	0.98	0.11	17,26,29,46	0
5	DMS	A	8404	4/4	0.98	0.07	18,21,27,27	0
5	DMS	B	8502	4/4	0.98	0.10	19,24,33,33	0
5	DMS	C	8403	4/4	0.99	0.07	16,17,18,18	0
5	DMS	C	8404	4/4	0.99	0.06	15,18,18,25	0
5	DMS	A	8411	4/4	0.99	0.06	17,17,22,36	0
5	DMS	A	8403	4/4	0.99	0.06	15,15,16,20	0
5	DMS	D	8401	4/4	0.99	0.05	11,11,14,15	0
5	DMS	D	8402	4/4	0.99	0.05	13,15,18,19	0
5	DMS	D	8403	4/4	0.99	0.04	13,20,20,22	0
4	NA	B	3103	1/1	0.99	0.04	19,19,19,19	0
5	DMS	D	8405	4/4	0.99	0.06	21,23,31,36	0
5	DMS	A	8405	4/4	0.99	0.06	16,22,25,57	0
5	DMS	B	8401	4/4	0.99	0.05	11,12,14,16	0
5	DMS	D	8408	4/4	0.99	0.09	16,27,27,31	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
5	DMS	C	8411	4/4	0.99	0.09	16,21,23,28	0
5	DMS	D	8410	4/4	0.99	0.05	15,25,28,34	0
5	DMS	D	8411	4/4	0.99	0.06	15,17,22,48	0
5	DMS	D	8412	4/4	0.99	0.07	21,25,30,46	0
5	DMS	B	8402	4/4	0.99	0.05	9,16,17,20	0
5	DMS	B	8403	4/4	0.99	0.05	14,15,20,20	0
3	MG	D	3001	1/1	0.99	0.04	9,9,9,9	0
5	DMS	B	8405	4/4	0.99	0.11	22,26,31,34	0
4	NA	C	3103	1/1	0.99	0.05	19,19,19,19	0
3	MG	D	3002	1/1	0.99	0.04	12,12,12,12	0
3	MG	B	3002	1/1	0.99	0.04	13,13,13,13	0
5	DMS	A	8402	4/4	0.99	0.06	12,19,20,21	0
5	DMS	D	8701	4/4	0.99	0.07	9,12,16,32	0
5	DMS	B	8411	4/4	0.99	0.06	18,22,22,80	0
5	DMS	C	8401	4/4	0.99	0.04	8,10,16,21	0
5	DMS	C	8402	4/4	0.99	0.06	11,16,21,24	0
4	NA	D	3102	1/1	1.00	0.03	10,10,10,10	0
4	NA	A	3102	1/1	1.00	0.03	12,12,12,12	0
5	DMS	A	8401	4/4	1.00	0.05	11,11,12,12	0
3	MG	B	3001	1/1	1.00	0.03	8,8,8,8	0
3	MG	A	3001	1/1	1.00	0.03	10,10,10,10	0
4	NA	B	3101	1/1	1.00	0.04	11,11,11,11	0
4	NA	B	3102	1/1	1.00	0.05	10,10,10,10	0
3	MG	C	3001	1/1	1.00	0.02	10,10,10,10	0
3	MG	C	3002	1/1	1.00	0.03	9,9,9,9	0
4	NA	C	3101	1/1	1.00	0.04	9,9,9,9	0
4	NA	C	3102	1/1	1.00	0.04	11,11,11,11	0
3	MG	A	3002	1/1	1.00	0.04	12,12,12,12	0
4	NA	A	3101	1/1	1.00	0.04	10,10,10,10	0
4	NA	D	3101	1/1	1.00	0.03	10,10,10,10	0

6.5 Other polymers (i)

There are no such residues in this entry.