



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 10:07 AM UTC

PDB ID : 4BSS / pdb_00004bss
Title : Structure of the ectodomain of LGR5 in complex with R-spondin-1 (Fu1Fu2) in P21 crystal form
Authors : Peng, W.C.; de Lau, W.; Forneris, F.; Granneman, J.C.M.; Huch, M.; Clevers, H.; Gros, P.
Deposited on : 2013-06-11
Resolution : 3.20 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

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

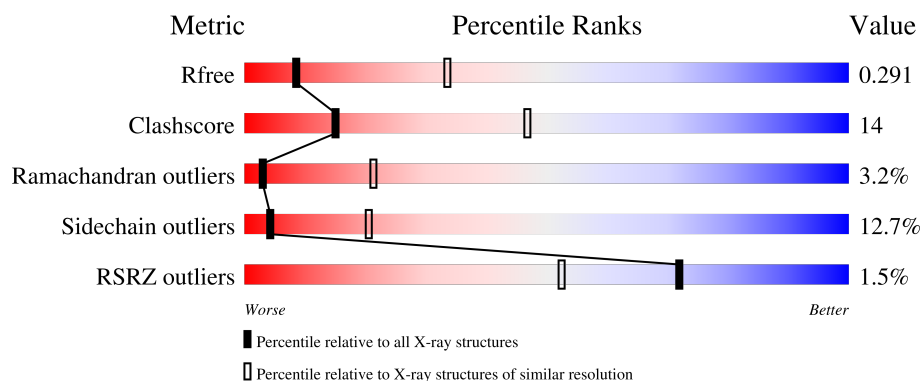
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	1466 (3.20-3.20)
Clashscore	190562	1573 (3.20-3.20)
Ramachandran outliers	187476	1548 (3.20-3.20)
Sidechain outliers	187428	1547 (3.20-3.20)
RSRZ outliers	180081	1466 (3.20-3.20)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	539	% 58% 24% • 14%
1	B	539	% 56% 26% 5% 13%
1	E	539	3% 47% 32% 7% 13%
1	F	539	% 54% 26% 6% 14%
2	C	126	53% 22% 5% • 18%

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
2	D	126	
2	G	126	
2	H	126	
3	I	2	
3	J	2	
3	K	2	
3	L	2	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	J	1	X	-	-	-
4	NAG	F	1077	X	-	-	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 17925 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 LEUCINE-RICH REPEAT-CONTAINING G-PROTEIN COUPLED RECEPTOR 5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	466	Total	C	N	O	S	68	0	0
			3653	2328	627	682	16			
1	B	469	Total	C	N	O	S	42	0	0
			3671	2342	633	679	17			
1	E	468	Total	C	N	O	S	53	0	0
			3672	2339	630	686	17			
1	F	464	Total	C	N	O	S	46	0	0
			3637	2320	626	674	17			

There are 68 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	8	HIS	-	expression tag	UNP O75473
A	9	HIS	-	expression tag	UNP O75473
A	10	HIS	-	expression tag	UNP O75473
A	11	HIS	-	expression tag	UNP O75473
A	12	HIS	-	expression tag	UNP O75473
A	13	HIS	-	expression tag	UNP O75473
A	14	GLU	-	expression tag	UNP O75473
A	15	ASN	-	expression tag	UNP O75473
A	16	LEU	-	expression tag	UNP O75473
A	17	TYR	-	expression tag	UNP O75473
A	18	PHE	-	expression tag	UNP O75473
A	19	GLN	-	expression tag	UNP O75473
A	20	GLY	-	expression tag	UNP O75473
A	21	SER	-	expression tag	UNP O75473
A	544	ALA	-	expression tag	UNP O75473
A	545	ALA	-	expression tag	UNP O75473
A	546	ALA	-	expression tag	UNP O75473
B	8	HIS	-	expression tag	UNP O75473
B	9	HIS	-	expression tag	UNP O75473
B	10	HIS	-	expression tag	UNP O75473

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
B	11	HIS	-	expression tag	UNP O75473
B	12	HIS	-	expression tag	UNP O75473
B	13	HIS	-	expression tag	UNP O75473
B	14	GLU	-	expression tag	UNP O75473
B	15	ASN	-	expression tag	UNP O75473
B	16	LEU	-	expression tag	UNP O75473
B	17	TYR	-	expression tag	UNP O75473
B	18	PHE	-	expression tag	UNP O75473
B	19	GLN	-	expression tag	UNP O75473
B	20	GLY	-	expression tag	UNP O75473
B	21	SER	-	expression tag	UNP O75473
B	544	ALA	-	expression tag	UNP O75473
B	545	ALA	-	expression tag	UNP O75473
B	546	ALA	-	expression tag	UNP O75473
E	8	HIS	-	expression tag	UNP O75473
E	9	HIS	-	expression tag	UNP O75473
E	10	HIS	-	expression tag	UNP O75473
E	11	HIS	-	expression tag	UNP O75473
E	12	HIS	-	expression tag	UNP O75473
E	13	HIS	-	expression tag	UNP O75473
E	14	GLU	-	expression tag	UNP O75473
E	15	ASN	-	expression tag	UNP O75473
E	16	LEU	-	expression tag	UNP O75473
E	17	TYR	-	expression tag	UNP O75473
E	18	PHE	-	expression tag	UNP O75473
E	19	GLN	-	expression tag	UNP O75473
E	20	GLY	-	expression tag	UNP O75473
E	21	SER	-	expression tag	UNP O75473
E	544	ALA	-	expression tag	UNP O75473
E	545	ALA	-	expression tag	UNP O75473
E	546	ALA	-	expression tag	UNP O75473
F	8	HIS	-	expression tag	UNP O75473
F	9	HIS	-	expression tag	UNP O75473
F	10	HIS	-	expression tag	UNP O75473
F	11	HIS	-	expression tag	UNP O75473
F	12	HIS	-	expression tag	UNP O75473
F	13	HIS	-	expression tag	UNP O75473
F	14	GLU	-	expression tag	UNP O75473
F	15	ASN	-	expression tag	UNP O75473
F	16	LEU	-	expression tag	UNP O75473
F	17	TYR	-	expression tag	UNP O75473
F	18	PHE	-	expression tag	UNP O75473

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
F	19	GLN	-	expression tag	UNP O75473
F	20	GLY	-	expression tag	UNP O75473
F	21	SER	-	expression tag	UNP O75473
F	544	ALA	-	expression tag	UNP O75473
F	545	ALA	-	expression tag	UNP O75473
F	546	ALA	-	expression tag	UNP O75473

- Molecule 2 is a protein called R-SPONDIN-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	103	Total	C	N	O	S	0	0	0
			778	480	137	143	18			
2	D	104	Total	C	N	O	S	0	0	0
			784	483	138	145	18			
2	G	103	Total	C	N	O	S	0	0	0
			778	480	137	143	18			
2	H	104	Total	C	N	O	S	0	0	0
			784	483	138	145	18			

There are 40 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	29	GLY	-	expression tag	UNP Q2MKA7
C	30	SER	-	expression tag	UNP Q2MKA7
C	147	ALA	-	expression tag	UNP Q2MKA7
C	148	ALA	-	expression tag	UNP Q2MKA7
C	149	HIS	-	expression tag	UNP Q2MKA7
C	150	HIS	-	expression tag	UNP Q2MKA7
C	151	HIS	-	expression tag	UNP Q2MKA7
C	152	HIS	-	expression tag	UNP Q2MKA7
C	153	HIS	-	expression tag	UNP Q2MKA7
C	154	HIS	-	expression tag	UNP Q2MKA7
D	29	GLY	-	expression tag	UNP Q2MKA7
D	30	SER	-	expression tag	UNP Q2MKA7
D	147	ALA	-	expression tag	UNP Q2MKA7
D	148	ALA	-	expression tag	UNP Q2MKA7
D	149	HIS	-	expression tag	UNP Q2MKA7
D	150	HIS	-	expression tag	UNP Q2MKA7
D	151	HIS	-	expression tag	UNP Q2MKA7
D	152	HIS	-	expression tag	UNP Q2MKA7
D	153	HIS	-	expression tag	UNP Q2MKA7
D	154	HIS	-	expression tag	UNP Q2MKA7

Continued on next page...

Continued from previous page...

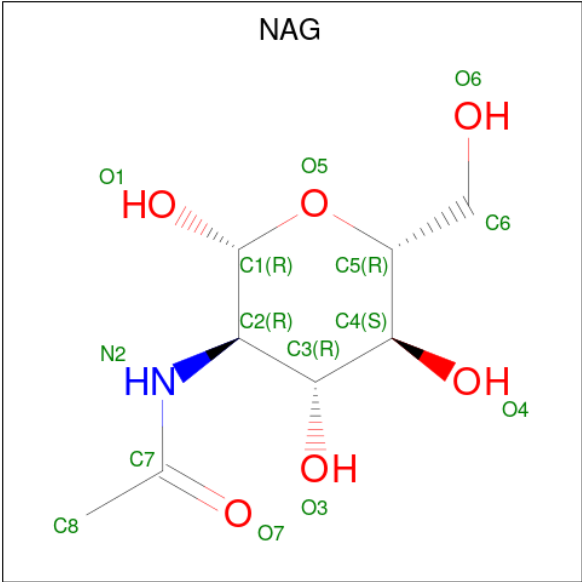
Chain	Residue	Modelled	Actual	Comment	Reference
G	29	GLY	-	expression tag	UNP Q2MKA7
G	30	SER	-	expression tag	UNP Q2MKA7
G	147	ALA	-	expression tag	UNP Q2MKA7
G	148	ALA	-	expression tag	UNP Q2MKA7
G	149	HIS	-	expression tag	UNP Q2MKA7
G	150	HIS	-	expression tag	UNP Q2MKA7
G	151	HIS	-	expression tag	UNP Q2MKA7
G	152	HIS	-	expression tag	UNP Q2MKA7
G	153	HIS	-	expression tag	UNP Q2MKA7
G	154	HIS	-	expression tag	UNP Q2MKA7
H	29	GLY	-	expression tag	UNP Q2MKA7
H	30	SER	-	expression tag	UNP Q2MKA7
H	147	ALA	-	expression tag	UNP Q2MKA7
H	148	ALA	-	expression tag	UNP Q2MKA7
H	149	HIS	-	expression tag	UNP Q2MKA7
H	150	HIS	-	expression tag	UNP Q2MKA7
H	151	HIS	-	expression tag	UNP Q2MKA7
H	152	HIS	-	expression tag	UNP Q2MKA7
H	153	HIS	-	expression tag	UNP Q2MKA7
H	154	HIS	-	expression tag	UNP Q2MKA7

- Molecule 3 is an oligosaccharide called 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose.

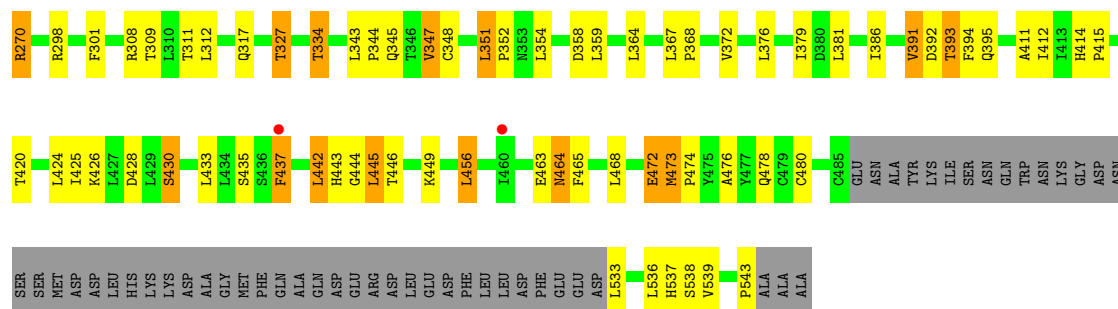


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	I	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	J	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	K	2	Total	C	N	O	0	0	0
			28	16	2	10			
3	L	2	Total	C	N	O	0	0	0
			28	16	2	10			

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: C₈H₁₅NO₆).

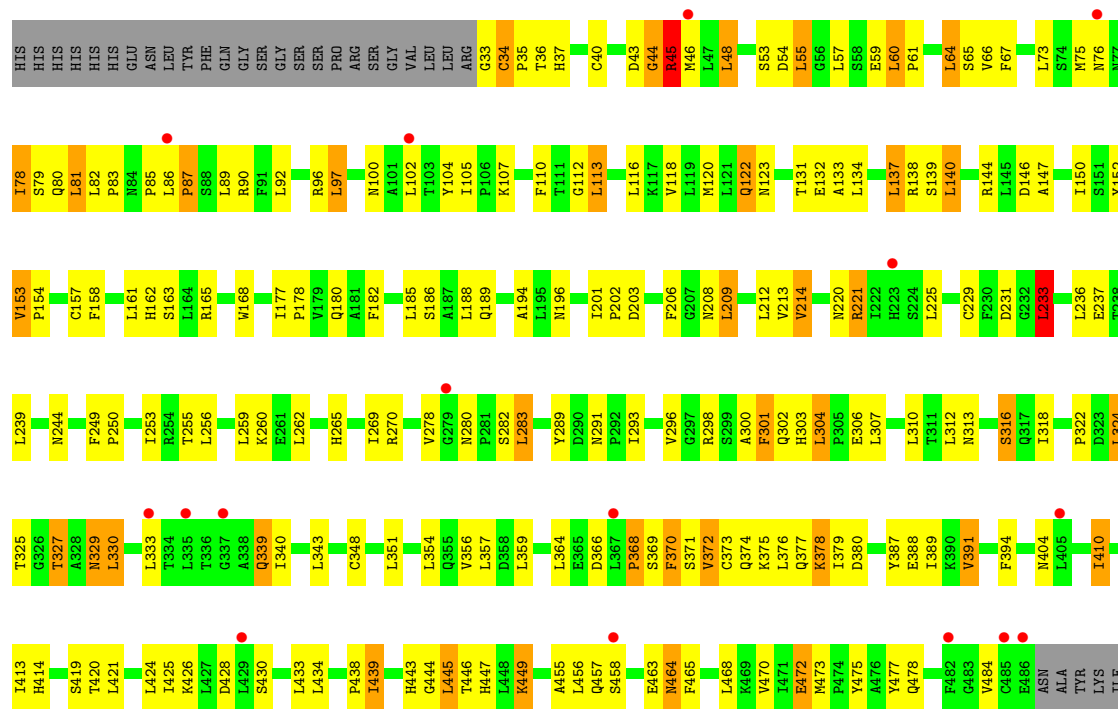


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		
4	E	1	Total	C	N	O	0	0
			14	8	1	5		
4	F	1	Total	C	N	O	0	0
			14	8	1	5		



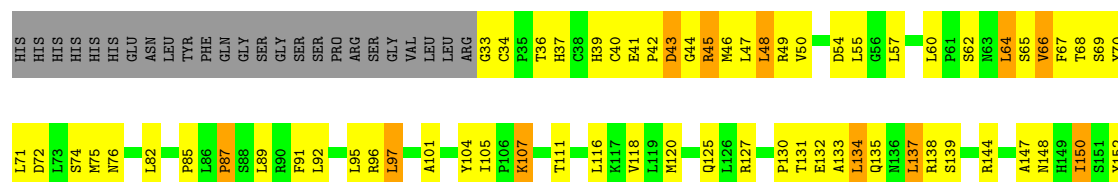
• Molecule 1: LEUCINE-RICH REPEAT-CONTAINING G-PROTEIN COUPLED RECEPTOR

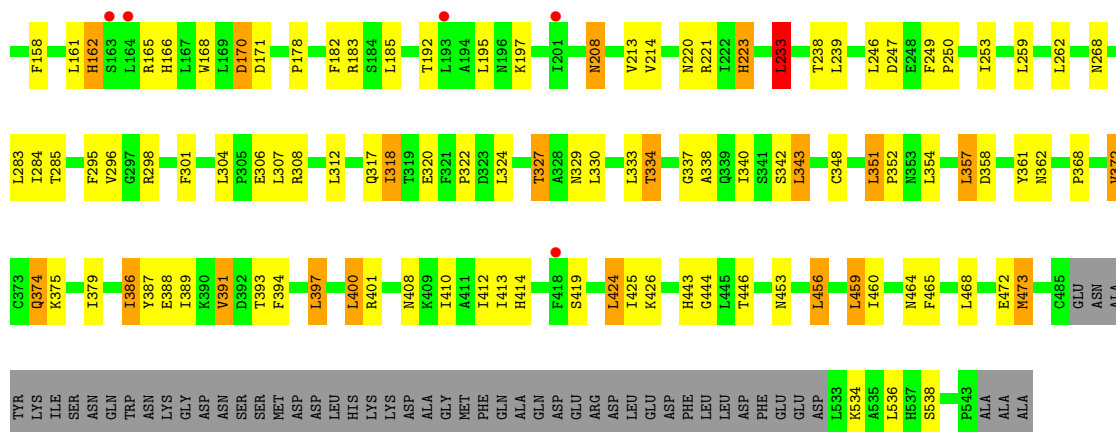
5



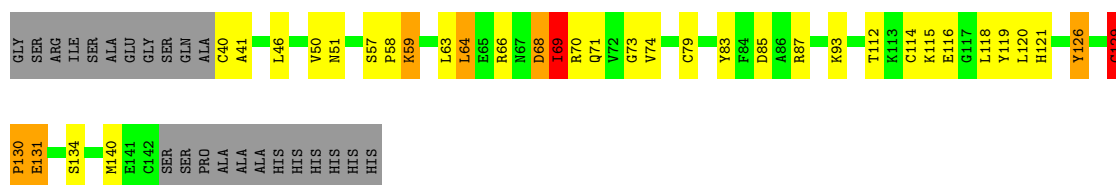
• Molecule 1: LEUCINE-RICH REPEAT-CONTAINING G-PROTEIN COUPLED RECEPTOR

5

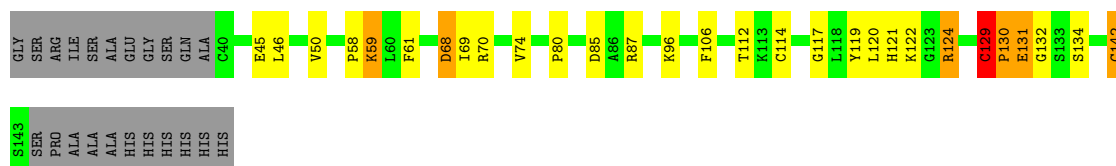




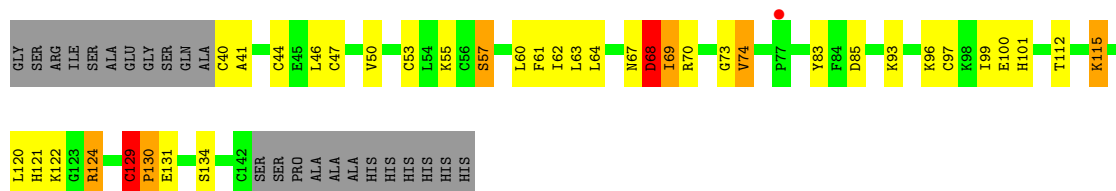
• Molecule 2: R-SPONDIN-1



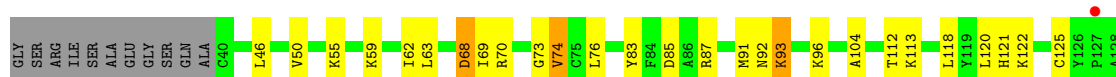
• Molecule 2: R-SPONDIN-1

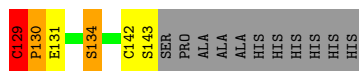


• Molecule 2: R-SPONDIN-1



• Molecule 2: R-SPONDIN-1





- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain I: 100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain J: 100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain K: 100%



- Molecule 3: 2-acetamido-2-deoxy-beta-D-glucopyranose-(1-4)-2-acetamido-2-deoxy-beta-D-glucopyranose

Chain L: 100%



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	120.36Å 111.30Å 130.61Å 90.00° 109.19° 90.00°	Depositor
Resolution (Å)	28.90 – 3.20 28.90 – 3.20	Depositor EDS
% Data completeness (in resolution range)	97.1 (28.90-3.20) 97.0 (28.90-3.20)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.52 (at 3.18Å)	Xtriage
Refinement program	PHENIX (PHENIX.REFINE)	Depositor
R, R_{free}	0.246 , 0.290 0.251 , 0.291	Depositor DCC
R_{free} test set	2664 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	87.3	Xtriage
Anisotropy	0.455	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 87.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	17925	wwPDB-VP
Average B, all atoms (Å ²)	126.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.84% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

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

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# $ Z > 5$	RMSZ	# $ Z > 5$
1	A	0.35	0/3734	0.89	7/5085 (0.1%)
1	B	0.35	0/3752	0.86	5/5109 (0.1%)
1	E	0.37	0/3753	0.89	4/5109 (0.1%)
1	F	0.36	0/3718	0.88	6/5062 (0.1%)
2	C	0.39	0/794	0.91	4/1066 (0.4%)
2	D	0.37	0/800	0.94	6/1074 (0.6%)
2	G	0.37	0/794	0.94	4/1066 (0.4%)
2	H	0.39	0/800	0.93	4/1074 (0.4%)
All	All	0.36	0/18145	0.89	40/24645 (0.2%)

There are no bond length outliers.

All (40) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	207	GLY	N-CA-C	8.21	122.85	112.83
2	C	129	CYS	CA-C-N	7.53	129.25	119.84
2	C	129	CYS	C-N-CA	7.53	129.25	119.84
2	D	129	CYS	CA-C-N	7.26	128.92	119.84
2	D	129	CYS	C-N-CA	7.26	128.92	119.84
2	G	129	CYS	CA-C-N	6.86	128.41	119.84
2	G	129	CYS	C-N-CA	6.86	128.41	119.84
2	H	129	CYS	CA-C-N	6.78	128.31	119.84
2	H	129	CYS	C-N-CA	6.78	128.31	119.84
1	A	351	LEU	CA-C-N	-6.35	114.19	120.98
1	A	351	LEU	C-N-CA	-6.35	114.19	120.98
1	A	105	ILE	CA-C-N	6.31	127.73	119.84
1	A	105	ILE	C-N-CA	6.31	127.73	119.84
1	B	435	SER	N-CA-C	-6.16	106.74	114.56
1	B	105	ILE	CA-C-N	5.86	127.16	119.84
1	B	105	ILE	C-N-CA	5.86	127.16	119.84

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	105	ILE	CA-C-N	5.62	126.86	119.84
1	F	105	ILE	C-N-CA	5.62	126.86	119.84
2	G	130	PRO	CA-C-N	5.48	131.56	121.70
2	G	130	PRO	C-N-CA	5.48	131.56	121.70
1	A	58	SER	N-CA-C	-5.41	106.73	113.55
2	D	80	PRO	O-C-N	5.41	123.80	121.31
1	E	536	LEU	CB-CA-C	-5.31	110.43	116.54
1	E	535	ALA	CB-CA-C	-5.30	110.44	116.54
2	D	130	PRO	CA-C-N	5.29	131.23	121.70
2	D	130	PRO	C-N-CA	5.29	131.23	121.70
2	H	130	PRO	CA-C-N	5.22	131.10	121.70
2	H	130	PRO	C-N-CA	5.22	131.10	121.70
2	C	130	PRO	CA-C-N	5.22	131.10	121.70
2	C	130	PRO	C-N-CA	5.22	131.10	121.70
1	E	419	SER	N-CA-C	5.21	117.04	111.36
2	D	117	GLY	N-CA-C	-5.13	107.92	114.85
1	E	157	CYS	N-CA-C	-5.13	106.80	113.16
1	F	351	LEU	CA-C-N	-5.12	115.50	120.98
1	F	351	LEU	C-N-CA	-5.12	115.50	120.98
1	F	419	SER	N-CA-C	5.08	116.89	111.36
1	F	223	HIS	N-CA-C	-5.07	107.48	113.97
1	B	351	LEU	CA-C-N	-5.06	115.57	120.98
1	B	351	LEU	C-N-CA	-5.06	115.57	120.98
1	A	157	CYS	N-CA-C	-5.02	106.93	113.16

There are no chirality outliers.

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	3653	0	3652	76	9
1	B	3671	0	3685	98	0
1	E	3672	0	3674	143	1
1	F	3637	0	3652	100	8
2	C	778	0	744	23	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	D	784	0	749	17	0
2	G	778	0	744	22	0
2	H	784	0	749	21	0
3	I	28	0	25	0	0
3	J	28	0	25	0	0
3	K	28	0	25	0	0
3	L	28	0	25	0	0
4	B	28	0	26	2	0
4	E	14	0	13	1	0
4	F	14	0	13	0	0
All	All	17925	0	17801	482	9

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 14.

All (482) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:408:ASN:HD21	1:F:410:ILE:HG13	1.23	1.01
1:E:343:LEU:HD11	1:E:368:PRO:HG3	1.53	0.87
1:A:282:SER:HA	1:A:306:GLU:HG3	1.58	0.86
1:E:259:LEU:HD13	1:E:262:LEU:HD11	1.57	0.85
1:B:107:LYS:HD2	1:B:132:GLU:HB2	1.57	0.85
1:E:430:SER:HB3	1:E:449:LYS:HD2	1.60	0.81
1:E:153:VAL:HG21	1:E:178:PRO:HG3	1.61	0.80
1:E:60:LEU:HD12	1:E:61:PRO:HD2	1.64	0.80
1:A:146:ASP:OD2	2:C:87:ARG:NH1	2.16	0.79
1:B:428:ASP:OD1	1:B:430:SER:OG	2.00	0.78
1:E:304:LEU:HD13	1:E:307:LEU:HD21	1.64	0.78
1:B:100:ASN:O	1:B:124:ASN:ND2	2.17	0.78
1:F:298:ARG:HB2	1:F:322:PRO:HA	1.65	0.78
1:A:177:ILE:HD13	1:A:205:ALA:HB1	1.66	0.77
1:E:316:SER:O	1:E:339:GLN:NE2	2.18	0.76
1:B:182:PHE:HB3	1:B:209:LEU:HD11	1.68	0.76
1:E:324:LEU:HD13	1:E:330:LEU:HD21	1.67	0.75
1:E:213:VAL:HG13	1:E:214:VAL:HG13	1.68	0.74
1:E:161:LEU:HD11	1:E:185:LEU:HD23	1.71	0.73
1:E:301:PHE:CE1	1:E:322:PRO:HB3	2.22	0.73
1:E:206:PHE:HB3	1:E:209:LEU:HD11	1.69	0.73
1:A:182:PHE:HB3	1:A:209:LEU:HD11	1.70	0.72
1:E:182:PHE:HA	1:E:185:LEU:HD12	1.71	0.72

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:357:LEU:HD11	1:F:379:ILE:HG12	1.72	0.71
1:E:302:GLN:HE22	1:E:325:THR:HB	1.54	0.71
2:H:130:PRO:HA	2:H:131:GLU:HB2	1.72	0.71
1:F:60:LEU:HG	1:F:82:LEU:HD11	1.72	0.71
1:B:480:CYS:SG	2:C:66:ARG:NH2	2.63	0.71
1:B:480:CYS:HB3	2:C:66:ARG:HH12	1.56	0.70
1:E:57:LEU:HB2	1:E:76:ASN:OD1	1.92	0.69
1:E:140:LEU:HD11	1:E:161:LEU:HB2	1.74	0.68
2:G:130:PRO:HA	2:G:131:GLU:HB2	1.76	0.68
1:F:82:LEU:HD13	1:F:85:PRO:HA	1.75	0.68
1:A:92:LEU:HD21	1:A:95:LEU:HB3	1.76	0.68
1:A:428:ASP:OD1	1:A:430:SER:OG	2.11	0.67
2:C:70:ARG:NH2	2:C:71:GLN:O	2.27	0.67
1:E:439:ILE:HD11	1:E:464:ASN:HB3	1.77	0.67
1:F:295:PHE:HB2	1:F:317:GLN:HB2	1.76	0.67
1:B:66:VAL:HG22	1:B:67:PHE:H	1.61	0.66
1:B:153:VAL:O	1:F:298:ARG:NH2	2.28	0.66
1:E:413:ILE:HG21	1:E:438:PRO:HG3	1.76	0.66
2:G:83:TYR:CD1	2:G:96:LYS:HA	2.30	0.66
1:F:343:LEU:HD12	1:F:343:LEU:H	1.60	0.66
1:E:233:LEU:HD23	1:E:256:LEU:HD21	1.77	0.66
1:E:137:LEU:O	1:E:139:SER:N	2.29	0.66
1:A:258:ASN:N	1:A:258:ASN:OD1	2.30	0.65
1:B:102:LEU:HG	1:B:124:ASN:HD22	1.62	0.65
1:F:170:ASP:OD1	1:F:170:ASP:N	2.26	0.65
1:E:237:GLU:HA	1:E:259:LEU:HA	1.78	0.64
1:B:334:THR:HB	1:B:358:ASP:HB3	1.79	0.64
1:E:376:LEU:HD23	1:E:379:ILE:HD11	1.80	0.64
2:C:114:CYS:H	2:C:120:LEU:HD12	1.62	0.64
2:D:130:PRO:HA	2:D:131:GLU:CG	2.28	0.64
1:F:379:ILE:HD12	1:F:400:LEU:HD21	1.80	0.64
2:H:91:MET:SD	2:H:93:LYS:NZ	2.71	0.64
1:E:177:ILE:HD11	1:E:201:ILE:HG12	1.80	0.64
1:B:104:TYR:OH	1:B:107:LYS:NZ	2.31	0.63
1:B:107:LYS:NZ	1:B:131:THR:OG1	2.28	0.63
1:B:155:PRO:HA	1:B:180:GLN:HE21	1.64	0.63
1:E:260:LYS:NZ	1:E:282:SER:O	2.31	0.63
2:C:51:ASN:HA	2:C:70:ARG:NH2	2.14	0.62
1:F:104:TYR:OH	1:F:131:THR:OG1	2.16	0.62
1:A:132:GLU:O	1:A:134:LEU:N	2.33	0.62
1:F:107:LYS:H	1:F:107:LYS:HD2	1.62	0.62

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:233:LEU:HD13	1:E:233:LEU:H	1.65	0.62
1:F:386:ILE:O	1:F:408:ASN:ND2	2.33	0.62
1:F:144:ARG:NH1	2:H:85:ASP:OD2	2.33	0.62
1:F:306:GLU:O	1:F:308:ARG:NH1	2.34	0.61
1:E:158:PHE:O	1:E:161:LEU:HG	2.01	0.61
1:B:201:ILE:HG22	1:B:229:CYS:HB2	1.82	0.61
1:A:425:ILE:HB	1:A:446:THR:HG22	1.81	0.60
1:E:380:ASP:HA	1:E:404:ASN:HB3	1.83	0.60
1:F:223:HIS:NE2	1:F:247:ASP:OD2	2.34	0.60
1:E:318:ILE:HG22	1:E:340:ILE:HD11	1.83	0.60
1:B:180:GLN:HE22	1:F:298:ARG:HH21	1.49	0.60
1:F:101:ALA:HB1	1:F:125:GLN:HE22	1.66	0.60
1:F:137:LEU:O	1:F:139:SER:N	2.35	0.60
1:E:327:THR:O	1:E:327:THR:OG1	2.15	0.60
1:A:137:LEU:O	1:A:139:SER:N	2.35	0.60
1:F:148:ASN:HB2	1:F:150:ILE:HG22	1.83	0.60
1:F:171:ASP:OD2	2:H:59:LYS:NZ	2.34	0.60
1:B:425:ILE:HG13	1:B:426:LYS:HG3	1.84	0.60
1:E:446:THR:HG23	1:E:447:HIS:ND1	2.17	0.60
1:F:66:VAL:HG22	1:F:67:PHE:H	1.66	0.60
2:D:130:PRO:HA	2:D:131:GLU:HG2	1.84	0.59
1:E:236:LEU:HD22	1:E:256:LEU:HD13	1.82	0.59
1:E:356:VAL:HG13	1:E:378:LYS:HG2	1.83	0.59
1:E:225:LEU:HD21	1:E:250:PRO:HB3	1.84	0.59
1:E:449:LYS:HG2	1:E:472:GLU:HG3	1.85	0.59
1:B:147:ALA:HB2	2:D:87:ARG:HH12	1.67	0.58
1:A:66:VAL:HG22	1:A:67:PHE:H	1.69	0.58
1:F:43:ASP:OD1	1:F:49:ARG:HG3	2.02	0.58
1:E:137:LEU:O	1:E:140:LEU:HD12	2.03	0.58
1:E:351:LEU:HD23	1:E:354:LEU:HD11	1.85	0.58
1:B:473:MET:HG3	1:B:474:PRO:HD2	1.85	0.58
1:E:66:VAL:HG22	1:E:67:PHE:H	1.69	0.58
2:G:122:LYS:NZ	2:G:124:ARG:HH12	2.03	0.57
1:A:144:ARG:NH1	2:C:85:ASP:OD2	2.37	0.57
1:E:209:LEU:HD13	1:E:212:LEU:HD22	1.87	0.57
1:A:473:MET:HG3	1:A:474:PRO:HD2	1.86	0.57
1:B:449:LYS:HG2	1:B:472:GLU:HG3	1.86	0.57
1:F:446:THR:HA	1:F:468:LEU:HA	1.87	0.57
1:B:465:PHE:HB3	1:B:468:LEU:HD12	1.86	0.57
1:F:107:LYS:HD2	1:F:107:LYS:N	2.20	0.57
1:A:465:PHE:HB3	1:A:468:LEU:HD12	1.87	0.57

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:43:ASP:OD2	1:F:69:SER:OG	2.23	0.57
1:F:465:PHE:HB3	1:F:468:LEU:HD12	1.87	0.56
1:A:201:ILE:HG22	1:A:229:CYS:HB2	1.88	0.56
1:E:302:GLN:NE2	1:E:325:THR:O	2.39	0.56
1:F:131:THR:O	1:F:135:GLN:NE2	2.39	0.56
1:F:397:LEU:HD13	1:F:400:LEU:HD22	1.87	0.56
1:F:351:LEU:HB3	1:F:354:LEU:HD12	1.88	0.56
2:D:121:HIS:NE2	2:D:130:PRO:HG2	2.21	0.56
1:F:49:ARG:HG2	1:F:70:TYR:HB3	1.87	0.56
1:E:43:ASP:O	1:E:45:ARG:N	2.38	0.56
1:A:234:HIS:O	1:A:258:ASN:ND2	2.38	0.56
1:E:140:LEU:HD11	1:E:161:LEU:CB	2.36	0.56
1:F:74:SER:O	1:F:76:ASN:ND2	2.39	0.56
2:G:130:PRO:HA	2:G:131:GLU:CB	2.36	0.56
1:E:458:SER:O	1:E:478:GLN:NE2	2.37	0.56
1:E:348:CYS:HB2	1:E:372:VAL:HG23	1.88	0.56
1:B:183:ARG:O	1:B:208:ASN:ND2	2.39	0.55
2:G:64:LEU:HG	2:G:93:LYS:HE3	1.87	0.55
2:D:59:LYS:HE2	2:D:87:ARG:HH22	1.71	0.55
1:F:178:PRO:HD2	1:F:182:PHE:HE2	1.71	0.55
1:A:334:THR:HB	1:A:358:ASP:HB3	1.87	0.55
1:A:420:THR:O	1:A:420:THR:OG1	2.23	0.55
1:A:343:LEU:HD13	1:A:364:LEU:HD21	1.88	0.55
1:E:237:GLU:OE2	2:G:124:ARG:NH2	2.40	0.55
1:B:442:LEU:HD13	1:B:445:LEU:HD21	1.89	0.55
1:B:327:THR:O	1:B:327:THR:OG1	2.19	0.55
1:E:282:SER:HA	1:E:306:GLU:HG3	1.89	0.55
2:G:40:CYS:SG	2:G:41:ALA:N	2.80	0.55
1:F:104:TYR:HE1	1:F:130:PRO:HA	1.72	0.55
1:F:460:ILE:HD13	1:F:473:MET:HE3	1.90	0.54
1:E:161:LEU:O	1:E:163:SER:N	2.39	0.54
1:F:386:ILE:HG23	1:F:408:ASN:ND2	2.22	0.54
1:A:391:VAL:HG22	1:A:414:HIS:CG	2.42	0.54
1:E:457:GLN:O	1:E:477:TYR:OH	2.25	0.54
1:B:425:ILE:HB	1:B:446:THR:HG22	1.90	0.54
2:C:51:ASN:HA	2:C:70:ARG:HH22	1.71	0.54
2:G:47:CYS:HA	2:G:53:CYS:HA	1.89	0.54
2:H:63:LEU:HD11	2:H:83:TYR:CE2	2.43	0.54
1:B:82:LEU:HD13	1:B:85:PRO:HA	1.89	0.54
1:A:144:ARG:HG2	1:A:168:TRP:CE3	2.43	0.53
1:A:351:LEU:HG	1:A:354:LEU:HD22	1.91	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:391:VAL:HG22	1:B:414:HIS:CD2	2.43	0.53
1:E:280:ASN:O	1:E:283:LEU:HD12	2.08	0.53
1:A:231:ASP:HA	1:A:255:THR:HG21	1.90	0.53
1:B:137:LEU:O	1:B:139:SER:N	2.42	0.53
1:B:197:LYS:HD3	1:B:221:ARG:HH12	1.74	0.53
1:E:253:ILE:HD12	1:E:256:LEU:HD12	1.88	0.53
1:F:213:VAL:HG21	2:H:122:LYS:HB2	1.89	0.53
1:B:180:GLN:NE2	1:F:298:ARG:HH21	2.06	0.53
1:F:327:THR:O	1:F:327:THR:OG1	2.14	0.53
1:B:180:GLN:OE1	1:B:180:GLN:N	2.41	0.53
1:B:233:LEU:HD13	1:B:233:LEU:H	1.74	0.53
1:E:82:LEU:HD13	1:E:85:PRO:HA	1.91	0.53
1:E:457:GLN:HG2	1:E:475:TYR:HE2	1.74	0.53
1:B:237:GLU:OE2	2:D:124:ARG:NH2	2.42	0.52
2:H:130:PRO:HA	2:H:131:GLU:CB	2.37	0.52
1:A:389:ILE:HG23	1:A:393:THR:HG21	1.90	0.52
1:E:144:ARG:HG2	1:E:168:TRP:CE3	2.45	0.52
2:C:126:TYR:N	2:C:126:TYR:CD1	2.77	0.52
1:E:144:ARG:NH2	1:E:146:ASP:OD2	2.43	0.52
1:A:327:THR:O	1:A:327:THR:OG1	2.26	0.52
2:C:130:PRO:HA	2:C:131:GLU:CB	2.40	0.52
1:A:100:ASN:O	1:A:124:ASN:ND2	2.43	0.52
1:B:476:ALA:HB2	1:B:543:PRO:HB3	1.92	0.52
1:B:57:LEU:HB3	1:B:76:ASN:HB3	1.92	0.51
1:E:404:ASN:HA	1:E:428:ASP:OD1	2.09	0.51
1:A:177:ILE:HD12	1:A:206:PHE:CZ	2.46	0.51
1:F:425:ILE:HG13	1:F:426:LYS:HG3	1.93	0.51
1:E:60:LEU:HD12	1:E:61:PRO:CD	2.38	0.51
1:F:144:ARG:HG2	1:F:168:TRP:CE3	2.44	0.51
2:H:134:SER:HA	2:H:143:SER:HB3	1.92	0.51
1:B:376:LEU:HD23	1:B:379:ILE:HD11	1.91	0.51
1:E:329:ASN:O	1:E:329:ASN:ND2	2.38	0.51
2:H:121:HIS:CE1	2:H:130:PRO:HG2	2.45	0.51
1:F:214:VAL:HG22	1:F:238:THR:HG22	1.92	0.51
1:F:340:ILE:HG22	1:F:362:ASN:OD1	2.11	0.51
1:A:353:ASN:HA	1:A:375:LYS:HD2	1.92	0.51
1:E:425:ILE:HB	1:E:446:THR:HG22	1.93	0.51
1:E:302:GLN:HG3	1:E:303:HIS:ND1	2.25	0.50
1:B:480:CYS:CB	2:C:66:ARG:HH12	2.24	0.50
1:A:33:GLY:O	1:A:65:SER:HB3	2.11	0.50
1:A:41:GLU:OE1	1:A:42:PRO:HD2	2.11	0.50

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:64:LEU:HD23	1:E:89:LEU:HD21	1.93	0.50
1:E:104:TYR:OH	1:E:131:THR:OG1	2.25	0.50
1:F:348:CYS:HB2	1:F:372:VAL:HB	1.94	0.50
1:A:96:ARG:HA	1:A:120:MET:HB2	1.93	0.50
1:B:311:THR:HG22	1:B:334:THR:HG23	1.94	0.50
1:B:442:LEU:HD12	1:B:442:LEU:O	2.12	0.50
1:F:340:ILE:HD11	1:F:342:SER:O	2.12	0.50
1:F:386:ILE:HG13	1:F:387:TYR:N	2.26	0.50
1:F:96:ARG:HA	1:F:120:MET:HB2	1.92	0.50
1:F:318:ILE:HG13	1:F:338:ALA:HB1	1.93	0.50
1:B:147:ALA:HB2	2:D:87:ARG:NH1	2.27	0.50
1:B:437:PHE:HE2	1:B:456:LEU:HD11	1.75	0.50
2:G:121:HIS:NE2	2:G:122:LYS:HE3	2.26	0.50
2:D:45:GLU:OE2	2:D:58:PRO:HD3	2.12	0.50
2:C:64:LEU:HD22	2:C:93:LYS:HE3	1.94	0.49
1:E:158:PHE:HB3	1:E:161:LEU:HD21	1.93	0.49
1:E:389:ILE:HB	1:E:413:ILE:HD13	1.94	0.49
1:B:343:LEU:HD13	1:B:364:LEU:HD21	1.94	0.49
1:E:231:ASP:HA	1:E:255:THR:HG21	1.95	0.49
1:E:369:SER:C	1:E:371:SER:H	2.21	0.49
1:A:82:LEU:HD12	1:A:83:PRO:HD2	1.93	0.49
1:F:95:LEU:HD21	1:F:97:LEU:HD22	1.93	0.49
1:A:296:VAL:HG11	1:A:301:PHE:HE1	1.77	0.49
1:B:169:LEU:HB2	1:B:193:LEU:HD23	1.94	0.49
2:G:121:HIS:NE2	2:G:130:PRO:HG2	2.28	0.49
1:B:194:ALA:O	1:B:196:ASN:ND2	2.46	0.49
1:E:132:GLU:O	1:E:134:LEU:N	2.45	0.49
1:A:192:THR:HG23	1:A:216:HIS:HB2	1.95	0.49
2:C:116:GLU:HA	2:C:140:MET:SD	2.52	0.49
1:E:387:TYR:HA	1:E:410:ILE:HA	1.93	0.49
2:C:40:CYS:SG	2:C:41:ALA:N	2.86	0.49
1:E:213:VAL:HG23	1:E:237:GLU:HG3	1.94	0.49
1:F:132:GLU:O	1:F:134:LEU:N	2.46	0.49
1:A:92:LEU:HD23	1:A:94:GLU:H	1.77	0.49
1:E:351:LEU:HB3	1:E:354:LEU:HD11	1.95	0.49
1:F:233:LEU:HD13	1:F:233:LEU:H	1.78	0.49
1:F:320:GLU:HA	1:F:340:ILE:HD13	1.95	0.49
2:G:67:ASN:HB3	2:G:70:ARG:HE	1.78	0.49
1:B:170:ASP:N	1:B:170:ASP:OD1	2.45	0.49
1:F:389:ILE:HG23	1:F:393:THR:HG21	1.94	0.49
1:F:334:THR:HB	1:F:358:ASP:HB3	1.94	0.48

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:102:LEU:HD13	1:B:105:ILE:HD11	1.95	0.48
2:C:58:PRO:C	2:C:59:LYS:HD2	2.38	0.48
1:F:87:PRO:C	1:F:89:LEU:H	2.21	0.48
2:H:63:LEU:O	2:H:73:GLY:HA2	2.14	0.48
1:E:81:LEU:HD21	1:E:102:LEU:HD13	1.94	0.48
1:E:380:ASP:OD1	1:E:404:ASN:ND2	2.47	0.48
1:B:414:HIS:CG	1:B:415:PRO:HD2	2.49	0.48
2:C:126:TYR:N	2:C:126:TYR:HD1	2.11	0.48
1:E:283:LEU:HD11	1:E:304:LEU:HB3	1.95	0.48
1:A:352:PRO:C	1:A:354:LEU:H	2.22	0.48
1:E:180:GLN:OE1	1:E:180:GLN:N	2.42	0.48
2:G:97:CYS:SG	2:G:99:ILE:HD12	2.54	0.48
2:C:121:HIS:CE1	2:C:130:PRO:HG2	2.49	0.48
1:A:165:ARG:HA	1:A:188:LEU:HA	1.96	0.47
1:F:386:ILE:HD11	1:F:388:GLU:O	2.14	0.47
1:A:74:SER:O	1:A:76:ASN:ND2	2.46	0.47
1:B:104:TYR:HE1	1:B:130:PRO:HA	1.79	0.47
1:E:140:LEU:HD13	1:E:140:LEU:O	2.13	0.47
2:G:62:ILE:HA	2:G:74:VAL:O	2.14	0.47
1:F:41:GLU:CD	1:F:42:PRO:HD2	2.40	0.47
1:E:465:PHE:HB3	1:E:468:LEU:HD13	1.95	0.47
1:A:45:ARG:HD3	1:A:46:MET:H	1.79	0.47
1:A:425:ILE:HG13	1:A:426:LYS:HG3	1.96	0.47
1:B:104:TYR:OH	1:B:131:THR:OG1	2.20	0.47
1:B:165:ARG:HA	1:B:188:LEU:HA	1.97	0.47
1:B:208:ASN:OD1	4:B:1208:NAG:N2	2.48	0.47
1:E:33:GLY:O	1:E:65:SER:HB3	2.15	0.47
1:E:425:ILE:HG13	1:E:426:LYS:HG3	1.97	0.47
1:F:147:ALA:HA	1:F:171:ASP:HB3	1.96	0.47
1:F:150:ILE:HD12	1:F:152:TYR:H	1.80	0.47
2:H:83:TYR:CD1	2:H:96:LYS:HA	2.49	0.47
1:B:75:MET:SD	1:B:75:MET:N	2.87	0.47
1:B:344:PRO:O	1:B:347:VAL:HG22	2.15	0.47
1:E:388:GLU:N	1:E:388:GLU:OE1	2.48	0.47
1:A:129:VAL:HG21	1:A:153:VAL:HG13	1.96	0.47
4:B:1077:NAG:O7	4:B:1077:NAG:O3	2.30	0.47
1:F:197:LYS:HD3	1:F:221:ARG:HH12	1.79	0.47
1:F:333:LEU:O	1:F:357:LEU:HA	2.15	0.47
1:E:75:MET:SD	1:E:75:MET:N	2.87	0.47
1:B:392:ASP:HA	1:B:395:GLN:HG2	1.97	0.46
1:E:60:LEU:HD13	1:E:73:LEU:HD11	1.96	0.46

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:189:GLN:O	1:E:213:VAL:HG12	2.15	0.46
1:E:203:ASP:HA	1:E:229:CYS:HA	1.96	0.46
1:A:306:GLU:O	1:A:308:ARG:NH1	2.48	0.46
2:D:119:TYR:HB3	2:D:142:CYS:SG	2.55	0.46
1:E:97:LEU:HD12	1:E:100:ASN:ND2	2.30	0.46
1:E:368:PRO:HD2	1:E:370:PHE:CE2	2.50	0.46
1:E:391:VAL:HG22	1:E:414:HIS:CD2	2.50	0.46
1:E:463:GLU:O	1:E:464:ASN:HB2	2.14	0.46
1:F:72:ASP:HA	1:F:96:ARG:HB2	1.97	0.46
2:G:124:ARG:H	2:G:124:ARG:HG2	1.52	0.46
1:B:105:ILE:HA	1:B:106:PRO:HD2	1.76	0.46
1:B:262:LEU:HD22	1:B:264:PHE:HD1	1.81	0.46
1:E:153:VAL:HG21	1:E:178:PRO:CG	2.39	0.46
1:E:373:CYS:O	1:E:376:LEU:HD13	2.16	0.46
1:F:40:CYS:HB3	1:F:48:LEU:HD21	1.97	0.46
1:E:194:ALA:O	1:E:196:ASN:ND2	2.48	0.46
1:B:127:ARG:C	1:B:150:ILE:HA	2.41	0.46
1:B:411:ALA:HA	1:B:433:LEU:O	2.16	0.46
1:E:43:ASP:C	1:E:45:ARG:N	2.74	0.46
1:E:201:ILE:HG22	1:E:229:CYS:HB2	1.97	0.46
1:E:374:GLN:HG3	1:E:375:LYS:HG2	1.98	0.46
1:A:87:PRO:C	1:A:89:LEU:H	2.24	0.46
1:B:164:LEU:HD23	1:B:185:LEU:HD22	1.98	0.46
1:E:434:LEU:O	1:E:455:ALA:HB3	2.16	0.46
1:A:75:MET:SD	1:A:75:MET:N	2.89	0.46
1:B:367:LEU:HD11	1:B:386:ILE:HD13	1.97	0.45
1:E:80:GLN:HG2	1:E:83:PRO:HD3	1.98	0.45
2:G:122:LYS:HZ2	2:G:124:ARG:HH12	1.64	0.45
2:H:63:LEU:HD11	2:H:83:TYR:HE2	1.80	0.45
1:E:40:CYS:HB3	1:E:48:LEU:HD21	1.97	0.45
1:E:189:GLN:C	1:E:212:LEU:HD12	2.41	0.45
1:E:220:ASN:N	1:E:244:ASN:OD1	2.45	0.45
1:B:43:ASP:CG	1:B:44:GLY:H	2.22	0.45
1:E:457:GLN:HG2	1:E:475:TYR:CE2	2.52	0.45
1:F:62:SER:C	1:F:64:LEU:H	2.23	0.45
1:A:82:LEU:CD1	1:A:84:ASN:H	2.29	0.45
1:B:53:SER:HA	1:B:76:ASN:HD21	1.81	0.45
1:B:393:THR:HG22	1:B:394:PHE:CD2	2.51	0.45
1:F:134:LEU:O	1:F:161:LEU:HD11	2.17	0.45
1:F:171:ASP:HB2	2:H:87:ARG:HD3	1.97	0.45
1:B:359:LEU:HB2	1:B:381:LEU:HD23	1.98	0.45

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:393:THR:HG23	1:F:394:PHE:CD2	2.52	0.45
1:F:165:ARG:O	1:F:166:HIS:ND1	2.49	0.45
1:F:459:LEU:HD23	1:F:459:LEU:HA	1.72	0.45
1:A:324:LEU:HD22	1:A:330:LEU:HD11	1.98	0.45
1:B:78:ILE:O	1:B:78:ILE:HG13	2.16	0.45
1:B:120:MET:HA	1:B:144:ARG:HB2	1.98	0.45
1:E:259:LEU:HD22	1:E:262:LEU:HD21	1.98	0.45
1:A:43:ASP:CG	1:A:44:GLY:H	2.21	0.45
1:B:203:ASP:HA	1:B:229:CYS:HA	1.98	0.45
2:D:68:ASP:C	2:D:70:ARG:H	2.24	0.45
1:E:165:ARG:HA	1:E:188:LEU:HA	1.99	0.45
1:F:75:MET:SD	1:F:75:MET:N	2.90	0.45
2:H:87:ARG:HG3	2:H:92:ASN:OD1	2.17	0.45
1:B:437:PHE:CD2	1:B:456:LEU:HD21	2.52	0.45
1:F:43:ASP:OD1	1:F:43:ASP:N	2.49	0.45
2:H:68:ASP:C	2:H:70:ARG:H	2.24	0.45
1:A:367:LEU:HD11	1:A:386:ILE:HD13	1.99	0.44
1:E:220:ASN:HB2	1:E:244:ASN:HD21	1.83	0.44
2:H:104:ALA:HB3	2:H:113:LYS:HG2	1.99	0.44
1:A:192:THR:HG22	1:A:194:ALA:H	1.83	0.44
1:A:223:HIS:NE2	1:A:247:ASP:OD2	2.51	0.44
2:C:130:PRO:HA	2:C:131:GLU:CG	2.47	0.44
1:E:43:ASP:CG	1:E:44:GLY:H	2.25	0.44
1:F:223:HIS:O	1:F:223:HIS:CD2	2.71	0.44
1:F:324:LEU:HD22	1:F:330:LEU:HD11	1.99	0.44
1:E:110:PHE:HA	1:E:113:LEU:HD23	1.99	0.44
1:A:144:ARG:NH2	1:A:146:ASP:OD2	2.51	0.44
1:A:295:PHE:HB2	1:A:317:GLN:HB2	1.99	0.44
1:A:194:ALA:O	1:A:196:ASN:ND2	2.50	0.44
1:E:265:HIS:HB2	1:E:289:TYR:O	2.18	0.44
1:F:107:LYS:HG3	1:F:132:GLU:HB2	1.99	0.44
1:A:220:ASN:HB3	1:A:221:ARG:H	1.59	0.44
1:E:59:GLU:HB3	1:E:82:LEU:HD21	1.99	0.44
1:E:177:ILE:HD11	1:E:201:ILE:HA	1.98	0.44
1:A:78:ILE:HB	1:A:100:ASN:HB3	1.99	0.44
1:A:82:LEU:HG	1:A:84:ASN:H	1.82	0.44
1:A:153:VAL:HA	1:A:154:PRO:HD2	1.86	0.44
1:E:249:PHE:HA	1:E:250:PRO:HD3	1.81	0.44
1:B:62:SER:C	1:B:64:LEU:H	2.26	0.44
1:E:122:GLN:HG2	1:E:144:ARG:CZ	2.47	0.44
1:E:356:VAL:HG22	1:E:378:LYS:HE3	2.00	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:LEU:HB2	1:A:76:ASN:HB3	1.99	0.43
1:B:87:PRO:HB3	1:B:112:GLY:HA3	2.00	0.43
1:B:376:LEU:HD12	1:B:376:LEU:HA	1.83	0.43
1:E:394:PHE:CD2	1:E:421:LEU:HD11	2.53	0.43
1:F:352:PRO:C	1:F:354:LEU:H	2.26	0.43
1:B:43:ASP:O	1:B:45:ARG:N	2.51	0.43
1:B:72:ASP:CG	1:B:96:ARG:HD2	2.43	0.43
1:B:237:GLU:CD	2:D:124:ARG:HH21	2.25	0.43
1:E:36:THR:O	1:E:37:HIS:HB2	2.18	0.43
1:F:246:LEU:HD23	1:F:250:PRO:HG3	2.00	0.43
1:B:131:THR:O	1:B:135:GLN:NE2	2.51	0.43
1:B:192:THR:HG22	2:D:106:PHE:HZ	1.83	0.43
1:E:233:LEU:CD2	1:E:256:LEU:HD21	2.46	0.43
1:F:389:ILE:HB	1:F:413:ILE:HD13	1.99	0.43
1:E:152:TYR:CD2	1:E:154:PRO:HD3	2.54	0.43
1:B:182:PHE:HA	1:B:185:LEU:HD12	2.00	0.43
1:B:216:HIS:HA	1:B:240:ASP:HB3	2.01	0.43
1:F:60:LEU:H	1:F:82:LEU:HD21	1.84	0.43
1:F:178:PRO:HD2	1:F:182:PHE:CE2	2.53	0.43
1:B:201:ILE:HG13	1:B:222:ILE:HD12	2.01	0.43
1:F:89:LEU:C	1:F:91:PHE:H	2.26	0.43
1:F:301:PHE:O	1:F:327:THR:HG21	2.18	0.43
2:G:115:LYS:HA	2:G:115:LYS:HD3	1.82	0.43
1:B:348:CYS:HB2	1:B:372:VAL:HB	2.00	0.43
2:C:68:ASP:C	2:C:70:ARG:H	2.27	0.43
1:F:361:TYR:HD1	1:F:361:TYR:O	2.02	0.43
2:G:121:HIS:HB2	2:G:129:CYS:HB2	2.00	0.43
1:A:301:PHE:O	1:A:327:THR:HG21	2.19	0.43
1:B:270:ARG:HE	1:B:270:ARG:HB3	1.56	0.43
2:C:68:ASP:O	2:C:69:ILE:HG22	2.19	0.43
2:G:68:ASP:O	2:G:69:ILE:HG22	2.18	0.43
1:A:82:LEU:HG	1:A:84:ASN:C	2.43	0.43
1:E:540:GLN:NE2	1:E:541:CYS:O	2.52	0.43
1:A:390:LYS:O	1:A:393:THR:HG22	2.18	0.43
1:B:213:VAL:HG12	1:B:214:VAL:HG23	2.00	0.43
1:E:73:LEU:HD22	1:E:76:ASN:ND2	2.33	0.43
1:F:374:GLN:C	1:F:375:LYS:HG2	2.44	0.43
1:F:391:VAL:HG22	1:F:414:HIS:CD2	2.54	0.43
1:E:260:LYS:HA	1:E:283:LEU:HA	2.00	0.42
1:E:304:LEU:HD13	1:E:307:LEU:CD2	2.42	0.42
1:B:248:GLU:OE1	1:E:270:ARG:NE	2.52	0.42

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:308:ARG:HG3	1:B:309:THR:N	2.33	0.42
2:D:61:PHE:CZ	2:D:85:ASP:HB3	2.54	0.42
1:E:59:GLU:HA	1:E:78:ILE:HG23	2.01	0.42
1:E:333:LEU:HD23	1:E:351:LEU:HD21	2.00	0.42
1:F:284:ILE:O	1:F:307:LEU:HD12	2.19	0.42
2:H:121:HIS:ND1	2:H:130:PRO:HG2	2.34	0.42
2:D:121:HIS:NE2	2:D:122:LYS:HE2	2.34	0.42
1:E:96:ARG:HA	1:E:120:MET:HB2	2.00	0.42
1:A:416:ASN:HA	1:A:440:THR:HG21	2.02	0.42
1:B:231:ASP:HA	1:B:255:THR:HG21	2.02	0.42
1:E:87:PRO:HB3	1:E:112:GLY:HA3	2.02	0.42
1:A:324:LEU:HD13	1:A:351:LEU:HD11	2.01	0.42
2:D:59:LYS:HE2	2:D:87:ARG:NH2	2.34	0.42
1:E:177:ILE:HD13	1:E:202:PRO:HD2	2.01	0.42
1:E:351:LEU:CD2	1:E:354:LEU:HD11	2.48	0.42
1:E:426:LYS:HA	1:E:447:HIS:HB2	2.02	0.42
2:D:130:PRO:HB3	2:D:132:GLY:N	2.35	0.42
1:E:97:LEU:HD12	1:E:97:LEU:HA	1.93	0.42
1:F:183:ARG:HA	1:F:208:ASN:HB2	2.02	0.42
1:A:105:ILE:HA	1:A:106:PRO:HD2	1.71	0.42
1:F:33:GLY:O	1:F:65:SER:HB3	2.18	0.42
2:G:61:PHE:CZ	2:G:85:ASP:HB3	2.54	0.42
1:A:321:PHE:HA	1:A:322:PRO:HD3	1.94	0.42
1:A:414:HIS:CG	1:A:415:PRO:HD2	2.55	0.42
1:B:352:PRO:C	1:B:354:LEU:H	2.28	0.42
1:A:154:PRO:HA	1:A:155:PRO:HD3	1.92	0.42
1:A:180:GLN:OE1	1:A:180:GLN:N	2.43	0.42
1:A:262:LEU:HD22	1:A:264:PHE:HD1	1.85	0.42
1:E:81:LEU:HD11	1:E:105:ILE:HD13	2.02	0.42
1:E:293:ILE:HD11	1:E:296:VAL:HG22	2.02	0.42
1:A:97:LEU:HB3	1:A:121:LEU:HD23	2.02	0.42
1:B:153:VAL:HA	1:B:154:PRO:HD2	1.83	0.42
2:C:63:LEU:O	2:C:73:GLY:HA2	2.20	0.42
1:E:343:LEU:CD1	1:E:368:PRO:HG3	2.38	0.42
1:B:75:MET:SD	1:B:99:GLY:HA3	2.60	0.41
1:B:463:GLU:O	1:B:464:ASN:HB2	2.20	0.41
1:E:53:SER:O	1:E:55:LEU:HD22	2.20	0.41
2:H:91:MET:HE2	2:H:91:MET:HB3	1.72	0.41
1:A:267:ASN:HB3	1:A:268:ASN:H	1.64	0.41
1:B:301:PHE:O	1:B:327:THR:HG21	2.20	0.41
1:E:100:ASN:O	1:E:102:LEU:HG	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:413:ILE:CG2	1:E:438:PRO:HG3	2.48	0.41
1:F:249:PHE:HA	1:F:250:PRO:HD3	1.89	0.41
1:F:259:LEU:HD21	1:F:262:LEU:HG	2.02	0.41
1:A:59:GLU:HG2	1:A:82:LEU:HD13	2.02	0.41
1:E:269:ILE:HG22	1:E:291:ASN:CG	2.45	0.41
1:E:123:ASN:H	1:E:147:ALA:HB3	1.86	0.41
1:E:447:HIS:HA	1:E:470:VAL:HG13	2.03	0.41
2:H:83:TYR:HD1	2:H:96:LYS:HA	1.86	0.41
1:F:130:PRO:HB2	1:F:134:LEU:HD13	2.02	0.41
2:G:63:LEU:O	2:G:73:GLY:HA2	2.20	0.41
2:G:68:ASP:C	2:G:70:ARG:H	2.27	0.41
1:B:473:MET:HG2	1:B:478:GLN:CB	2.51	0.41
1:F:36:THR:O	1:F:37:HIS:HB2	2.21	0.41
1:F:71:LEU:HB2	1:F:92:LEU:HD21	2.03	0.41
2:H:62:ILE:HA	2:H:74:VAL:O	2.21	0.41
1:B:226:GLY:O	1:B:252:ALA:HB2	2.21	0.41
1:E:369:SER:O	1:E:371:SER:N	2.54	0.41
1:E:428:ASP:OD1	1:E:428:ASP:N	2.54	0.41
1:B:94:GLU:OE2	1:B:96:ARG:NH2	2.54	0.41
1:B:391:VAL:HG22	1:B:414:HIS:CG	2.56	0.41
2:C:130:PRO:HA	2:C:131:GLU:HB3	2.03	0.41
2:D:114:CYS:HB2	2:D:120:LEU:HD13	2.03	0.41
1:E:34:CYS:HA	1:E:35:PRO:HD3	1.94	0.41
1:E:79:SER:HB3	4:E:1077:NAG:O7	2.19	0.41
1:E:304:LEU:HD12	1:E:327:THR:HB	2.03	0.41
1:E:425:ILE:C	1:E:445:LEU:HG	2.46	0.41
1:F:220:ASN:HB3	1:F:221:ARG:H	1.64	0.41
1:F:318:ILE:HG13	1:F:318:ILE:O	2.20	0.41
1:B:445:LEU:HB2	1:B:446:THR:H	1.63	0.41
2:C:79:CYS:HB3	2:C:83:TYR:HB2	2.02	0.41
1:E:259:LEU:O	1:E:259:LEU:HD12	2.20	0.41
1:B:97:LEU:HD12	1:B:100:ASN:ND2	2.36	0.40
1:F:158:PHE:CD2	1:F:185:LEU:HD11	2.56	0.40
1:A:148:ASN:HB2	1:A:150:ILE:HG22	2.04	0.40
1:A:233:LEU:HD13	1:A:233:LEU:H	1.84	0.40
1:B:102:LEU:HG	1:B:124:ASN:ND2	2.34	0.40
2:G:57:SER:HB3	2:G:60:LEU:HD12	2.04	0.40
1:A:45:ARG:HD3	1:A:45:ARG:HA	1.86	0.40
1:B:132:GLU:O	1:B:134:LEU:N	2.55	0.40
1:E:220:ASN:HB3	1:E:221:ARG:H	1.66	0.40
1:E:322:PRO:O	1:E:324:LEU:HD23	2.21	0.40

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:F:43:ASP:O	1:F:45:ARG:N	2.50	0.40
1:F:453:ASN:HB3	1:F:456:LEU:HB2	2.04	0.40
1:F:337:GLY:HA2	1:F:361:TYR:CD1	2.56	0.40
2:H:113:LYS:HG3	2:H:113:LYS:O	2.20	0.40
1:A:443:HIS:NE2	1:A:464:ASN:HA	2.36	0.40
1:B:348:CYS:HA	1:B:351:LEU:HB2	2.03	0.40
1:F:246:LEU:CD2	1:F:250:PRO:HG3	2.51	0.40
1:F:401:ARG:O	1:F:424:LEU:HD23	2.22	0.40

All (9) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:531:GLU:OE2	1:F:67:PHE:CE2[1_454]	0.65	1.55
1:A:531:GLU:OE2	1:F:67:PHE:CZ[1_454]	0.80	1.40
1:A:531:GLU:CD	1:F:67:PHE:CE2[1_454]	1.47	0.73
1:A:531:GLU:CD	1:F:67:PHE:CZ[1_454]	1.67	0.53
1:A:531:GLU:OE2	1:F:67:PHE:CD2[1_454]	1.91	0.29
1:A:531:GLU:OE1	1:E:45:ARG:NH1[1_455]	1.95	0.25
1:A:531:GLU:OE2	1:F:67:PHE:CE1[1_454]	2.02	0.18
1:A:531:GLU:OE1	1:F:67:PHE:CZ[1_454]	2.19	0.01
1:A:531:GLU:CG	1:F:67:PHE:CE2[1_454]	2.19	0.01

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	462/539 (86%)	383 (83%)	69 (15%)	10 (2%)	5	29
1	B	465/539 (86%)	385 (83%)	67 (14%)	13 (3%)	4	25
1	E	464/539 (86%)	386 (83%)	61 (13%)	17 (4%)	2	18
1	F	460/539 (85%)	377 (82%)	69 (15%)	14 (3%)	3	23

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	C	101/126 (80%)	81 (80%)	16 (16%)	4 (4%)	2	17
2	D	102/126 (81%)	81 (79%)	16 (16%)	5 (5%)	1	13
2	G	101/126 (80%)	79 (78%)	18 (18%)	4 (4%)	2	17
2	H	102/126 (81%)	82 (80%)	15 (15%)	5 (5%)	1	13
All	All	2257/2660 (85%)	1854 (82%)	331 (15%)	72 (3%)	3	21

All (72) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	54	ASP
1	A	133	ALA
1	A	138	ARG
1	B	45	ARG
1	B	54	ASP
1	B	133	ALA
1	B	138	ARG
1	B	537	HIS
2	C	69	ILE
2	D	68	ASP
2	D	69	ILE
2	D	142	CYS
1	E	45	ARG
1	E	54	ASP
1	E	87	PRO
1	E	133	ALA
1	E	138	ARG
1	F	54	ASP
1	F	133	ALA
1	F	138	ARG
2	G	69	ILE
2	H	69	ILE
1	A	87	PRO
1	A	464	ASN
1	B	44	GLY
1	B	87	PRO
1	E	44	GLY
1	E	46	MET
1	E	162	HIS
1	E	233	LEU
1	F	44	GLY
1	F	87	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	464	ASN
1	F	534	LYS
2	G	68	ASP
2	H	142	CYS
1	A	45	ARG
1	A	46	MET
1	A	444	GLY
1	B	46	MET
1	B	233	LEU
2	C	68	ASP
2	C	134	SER
2	D	134	SER
1	E	64	LEU
1	E	300	ALA
1	E	433	LEU
1	E	532	ASP
2	G	134	SER
2	H	68	ASP
1	A	233	LEU
1	B	464	ASN
1	F	45	ARG
1	F	233	LEU
1	F	444	GLY
1	B	444	GLY
2	C	129	CYS
2	D	129	CYS
1	E	370	PHE
1	E	464	ASN
1	F	162	HIS
2	G	129	CYS
2	H	129	CYS
2	H	134	SER
1	A	44	GLY
1	B	162	HIS
1	F	46	MET
1	E	444	GLY
1	F	66	VAL
1	F	368	PRO
1	B	368	PRO
1	E	368	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	421/484 (87%)	375 (89%)	46 (11%)	6	26
1	B	423/484 (87%)	375 (89%)	48 (11%)	5	24
1	E	424/484 (88%)	361 (85%)	63 (15%)	3	15
1	F	420/484 (87%)	366 (87%)	54 (13%)	4	20
2	C	89/105 (85%)	75 (84%)	14 (16%)	2	13
2	D	90/105 (86%)	81 (90%)	9 (10%)	7	30
2	G	89/105 (85%)	75 (84%)	14 (16%)	2	13
2	H	90/105 (86%)	79 (88%)	11 (12%)	5	22
All	All	2046/2356 (87%)	1787 (87%)	259 (13%)	4	20

All (259) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	34	CYS
1	A	36	THR
1	A	46	MET
1	A	48	LEU
1	A	55	LEU
1	A	60	LEU
1	A	71	LEU
1	A	82	LEU
1	A	90	ARG
1	A	95	LEU
1	A	97	LEU
1	A	113	LEU
1	A	116	LEU
1	A	118	VAL
1	A	122	GLN
1	A	135	GLN
1	A	145	LEU
1	A	150	ILE
1	A	165	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	A	179	VAL
1	A	233	LEU
1	A	239	LEU
1	A	253	ILE
1	A	258	ASN
1	A	270	ARG
1	A	287	HIS
1	A	298	ARG
1	A	312	LEU
1	A	327	THR
1	A	334	THR
1	A	351	LEU
1	A	356	VAL
1	A	357	LEU
1	A	372	VAL
1	A	374	GLN
1	A	391	VAL
1	A	420	THR
1	A	424	LEU
1	A	430	SER
1	A	440	THR
1	A	443	HIS
1	A	456	LEU
1	A	472	GLU
1	A	473	MET
1	A	533	LEU
1	A	538	SER
1	B	32	ARG
1	B	34	CYS
1	B	48	LEU
1	B	55	LEU
1	B	57	LEU
1	B	64	LEU
1	B	71	LEU
1	B	78	ILE
1	B	92	LEU
1	B	97	LEU
1	B	116	LEU
1	B	118	VAL
1	B	150	ILE
1	B	170	ASP
1	B	175	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	176	GLU
1	B	186	SER
1	B	192	THR
1	B	227	LYS
1	B	233	LEU
1	B	238	THR
1	B	239	LEU
1	B	253	ILE
1	B	270	ARG
1	B	298	ARG
1	B	312	LEU
1	B	317	GLN
1	B	327	THR
1	B	334	THR
1	B	345	GLN
1	B	347	VAL
1	B	391	VAL
1	B	393	THR
1	B	412	ILE
1	B	420	THR
1	B	424	LEU
1	B	430	SER
1	B	437	PHE
1	B	442	LEU
1	B	443	HIS
1	B	445	LEU
1	B	456	LEU
1	B	472	GLU
1	B	473	MET
1	B	533	LEU
1	B	536	LEU
1	B	538	SER
1	B	539	VAL
2	C	46	LEU
2	C	50	VAL
2	C	57	SER
2	C	59	LYS
2	C	64	LEU
2	C	69	ILE
2	C	74	VAL
2	C	112	THR
2	C	115	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	C	118	LEU
2	C	119	TYR
2	C	126	TYR
2	C	129	CYS
2	C	131	GLU
2	D	46	LEU
2	D	50	VAL
2	D	59	LYS
2	D	74	VAL
2	D	96	LYS
2	D	112	THR
2	D	124	ARG
2	D	129	CYS
2	D	131	GLU
1	E	34	CYS
1	E	45	ARG
1	E	48	LEU
1	E	55	LEU
1	E	60	LEU
1	E	78	ILE
1	E	81	LEU
1	E	86	LEU
1	E	90	ARG
1	E	92	LEU
1	E	97	LEU
1	E	107	LYS
1	E	113	LEU
1	E	116	LEU
1	E	118	VAL
1	E	122	GLN
1	E	137	LEU
1	E	140	LEU
1	E	150	ILE
1	E	153	VAL
1	E	186	SER
1	E	208	ASN
1	E	209	LEU
1	E	214	VAL
1	E	221	ARG
1	E	233	LEU
1	E	239	LEU
1	E	278	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	283	LEU
1	E	298	ARG
1	E	301	PHE
1	E	304	LEU
1	E	310	LEU
1	E	312	LEU
1	E	313	ASN
1	E	316	SER
1	E	324	LEU
1	E	327	THR
1	E	329	ASN
1	E	330	LEU
1	E	339	GLN
1	E	357	LEU
1	E	359	LEU
1	E	364	LEU
1	E	366	ASP
1	E	372	VAL
1	E	377	GLN
1	E	378	LYS
1	E	391	VAL
1	E	410	ILE
1	E	420	THR
1	E	424	LEU
1	E	439	ILE
1	E	443	HIS
1	E	445	LEU
1	E	449	LYS
1	E	456	LEU
1	E	472	GLU
1	E	473	MET
1	E	484	VAL
1	E	530	GLU
1	E	533	LEU
1	E	540	GLN
1	F	34	CYS
1	F	39	HIS
1	F	43	ASP
1	F	47	LEU
1	F	48	LEU
1	F	50	VAL
1	F	55	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	57	LEU
1	F	64	LEU
1	F	68	THR
1	F	97	LEU
1	F	107	LYS
1	F	111	THR
1	F	116	LEU
1	F	118	VAL
1	F	127	ARG
1	F	134	LEU
1	F	137	LEU
1	F	150	ILE
1	F	162	HIS
1	F	170	ASP
1	F	192	THR
1	F	195	LEU
1	F	208	ASN
1	F	233	LEU
1	F	239	LEU
1	F	253	ILE
1	F	268	ASN
1	F	283	LEU
1	F	285	THR
1	F	296	VAL
1	F	304	LEU
1	F	312	LEU
1	F	318	ILE
1	F	327	THR
1	F	329	ASN
1	F	334	THR
1	F	343	LEU
1	F	357	LEU
1	F	372	VAL
1	F	374	GLN
1	F	386	ILE
1	F	391	VAL
1	F	397	LEU
1	F	400	LEU
1	F	412	ILE
1	F	424	LEU
1	F	443	HIS
1	F	456	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	F	459	LEU
1	F	472	GLU
1	F	473	MET
1	F	536	LEU
1	F	538	SER
2	G	44	CYS
2	G	46	LEU
2	G	50	VAL
2	G	55	LYS
2	G	57	SER
2	G	68	ASP
2	G	74	VAL
2	G	100	GLU
2	G	101	HIS
2	G	112	THR
2	G	115	LYS
2	G	120	LEU
2	G	124	ARG
2	G	129	CYS
2	H	46	LEU
2	H	50	VAL
2	H	55	LYS
2	H	74	VAL
2	H	76	LEU
2	H	93	LYS
2	H	112	THR
2	H	118	LEU
2	H	120	LEU
2	H	125	CYS
2	H	129	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (29) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	HIS
1	A	162	HIS
1	A	166	HIS
1	A	219	ASN
1	A	374	GLN
1	A	377	GLN
1	B	76	ASN
1	B	80	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	B	135	GLN
1	B	200	HIS
1	B	395	GLN
1	B	457	GLN
2	D	51	ASN
1	E	84	ASN
1	E	200	HIS
1	E	219	ASN
1	E	302	GLN
1	E	443	HIS
1	E	457	GLN
1	E	540	GLN
1	F	135	GLN
1	F	180	GLN
1	F	219	ASN
1	F	258	ASN
1	F	329	ASN
1	F	374	GLN
1	F	396	GLN
2	H	51	ASN
2	H	121	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

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
3	NAG	I	1	3,1	14,14,15	0.83	1 (7%)	17,19,21	0.64	0
3	NAG	I	2	3	14,14,15	0.60	0	17,19,21	0.73	1 (5%)
3	NAG	J	1	3,1	14,14,15	0.44	0	17,19,21	0.67	0
3	NAG	J	2	3	14,14,15	0.64	0	17,19,21	0.60	0
3	NAG	K	1	3,1	14,14,15	0.36	0	17,19,21	0.92	0
3	NAG	K	2	3	14,14,15	0.61	0	17,19,21	0.46	0
3	NAG	L	1	3,1	14,14,15	0.52	0	17,19,21	0.54	0
3	NAG	L	2	3	14,14,15	0.34	0	17,19,21	0.65	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NAG	I	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	I	2	3	-	0/6/23/26	0/1/1/1
3	NAG	J	1	3,1	1/1/5/7	1/6/23/26	0/1/1/1
3	NAG	J	2	3	-	2/6/23/26	0/1/1/1
3	NAG	K	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	K	2	3	-	0/6/23/26	0/1/1/1
3	NAG	L	1	3,1	-	2/6/23/26	0/1/1/1
3	NAG	L	2	3	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	1	NAG	C1-C2	2.90	1.56	1.52

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	2	NAG	C1-O5-C5	2.15	115.06	112.19

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	J	1	NAG	C1

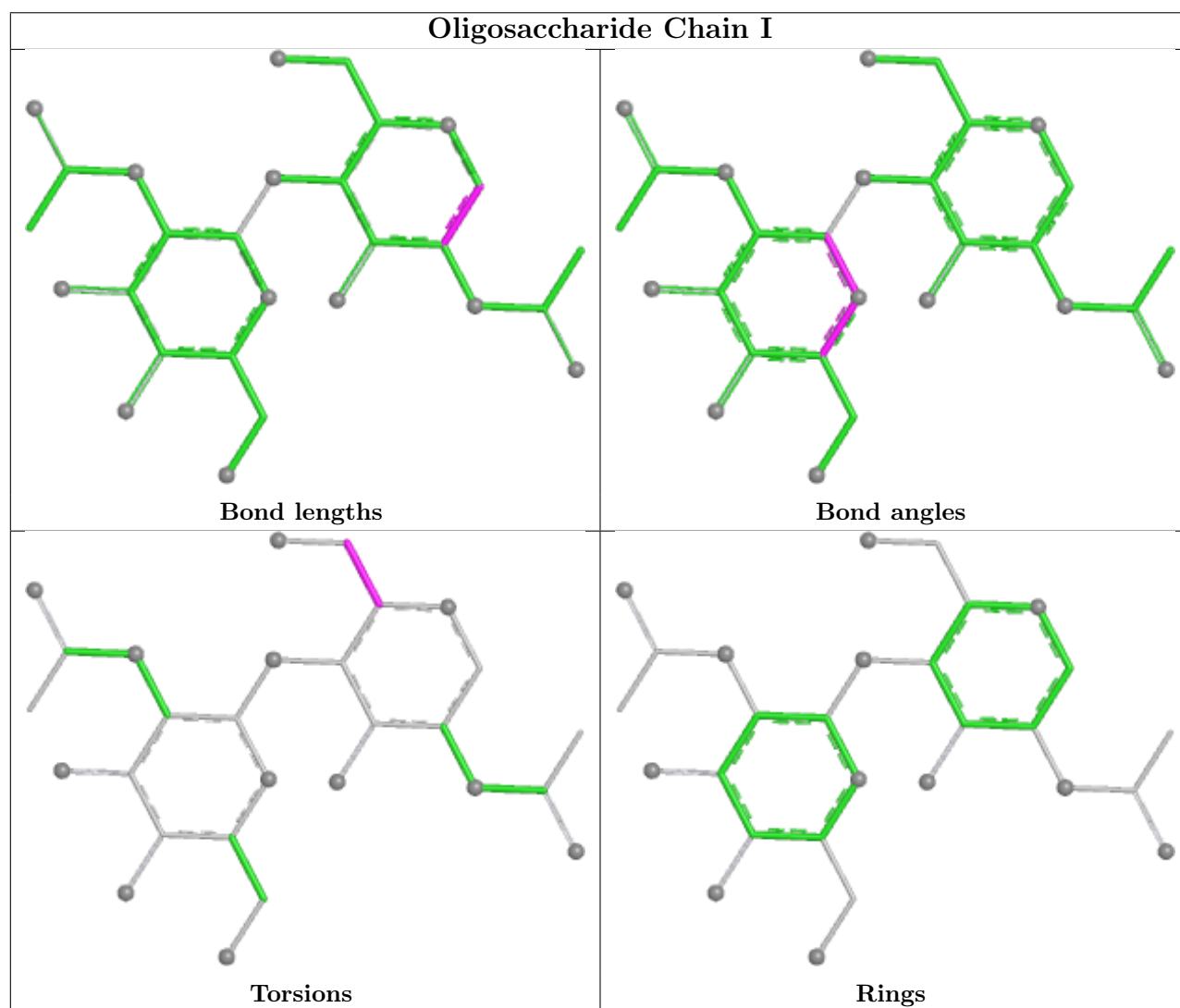
All (10) torsion outliers are listed below:

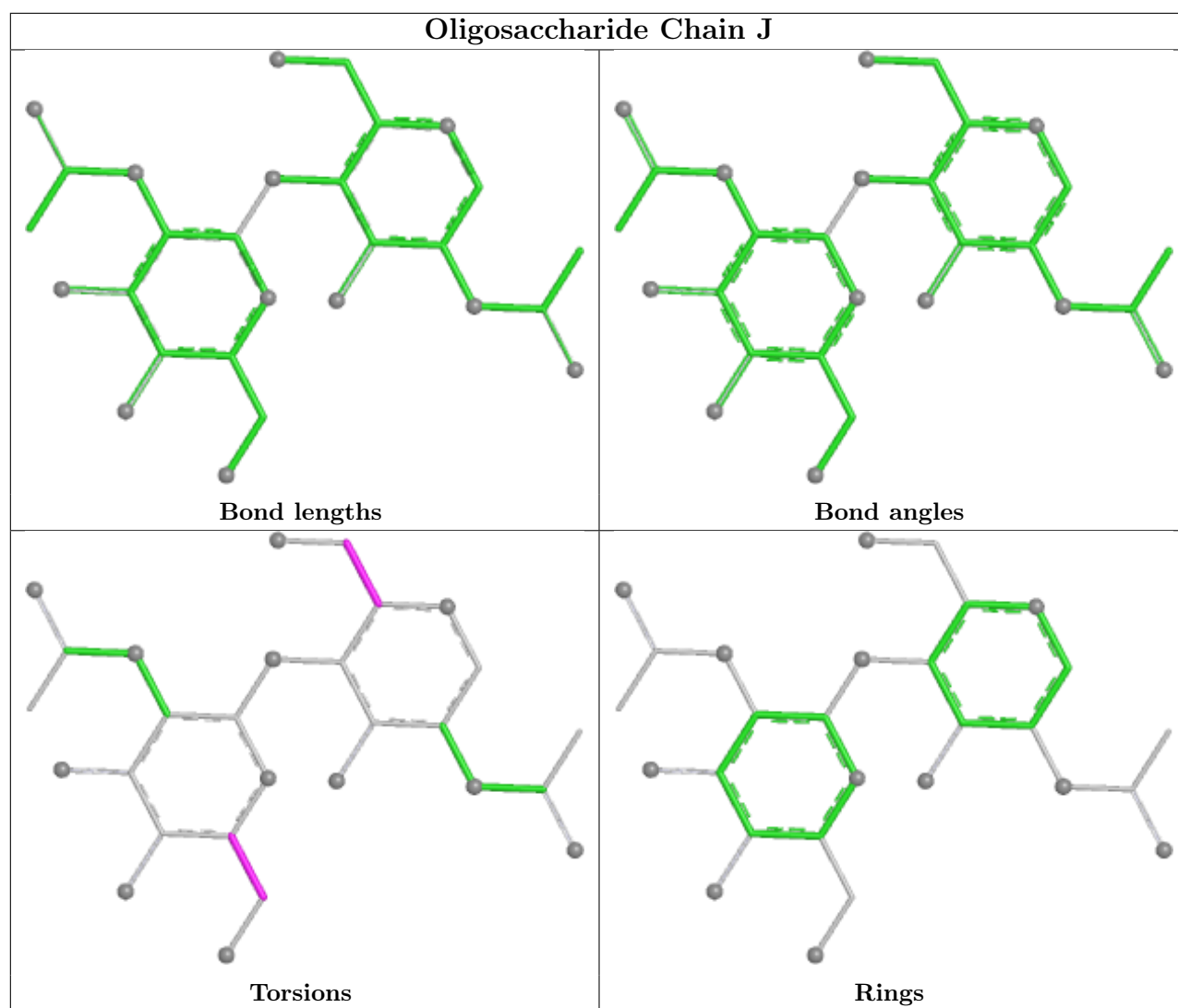
Mol	Chain	Res	Type	Atoms
3	L	1	NAG	O5-C5-C6-O6
3	L	1	NAG	C4-C5-C6-O6
3	K	1	NAG	O5-C5-C6-O6
3	J	2	NAG	O5-C5-C6-O6
3	I	1	NAG	C4-C5-C6-O6
3	K	1	NAG	C4-C5-C6-O6
3	I	1	NAG	O5-C5-C6-O6
3	J	2	NAG	C4-C5-C6-O6
3	J	1	NAG	C4-C5-C6-O6
3	L	2	NAG	C1-C2-N2-C7

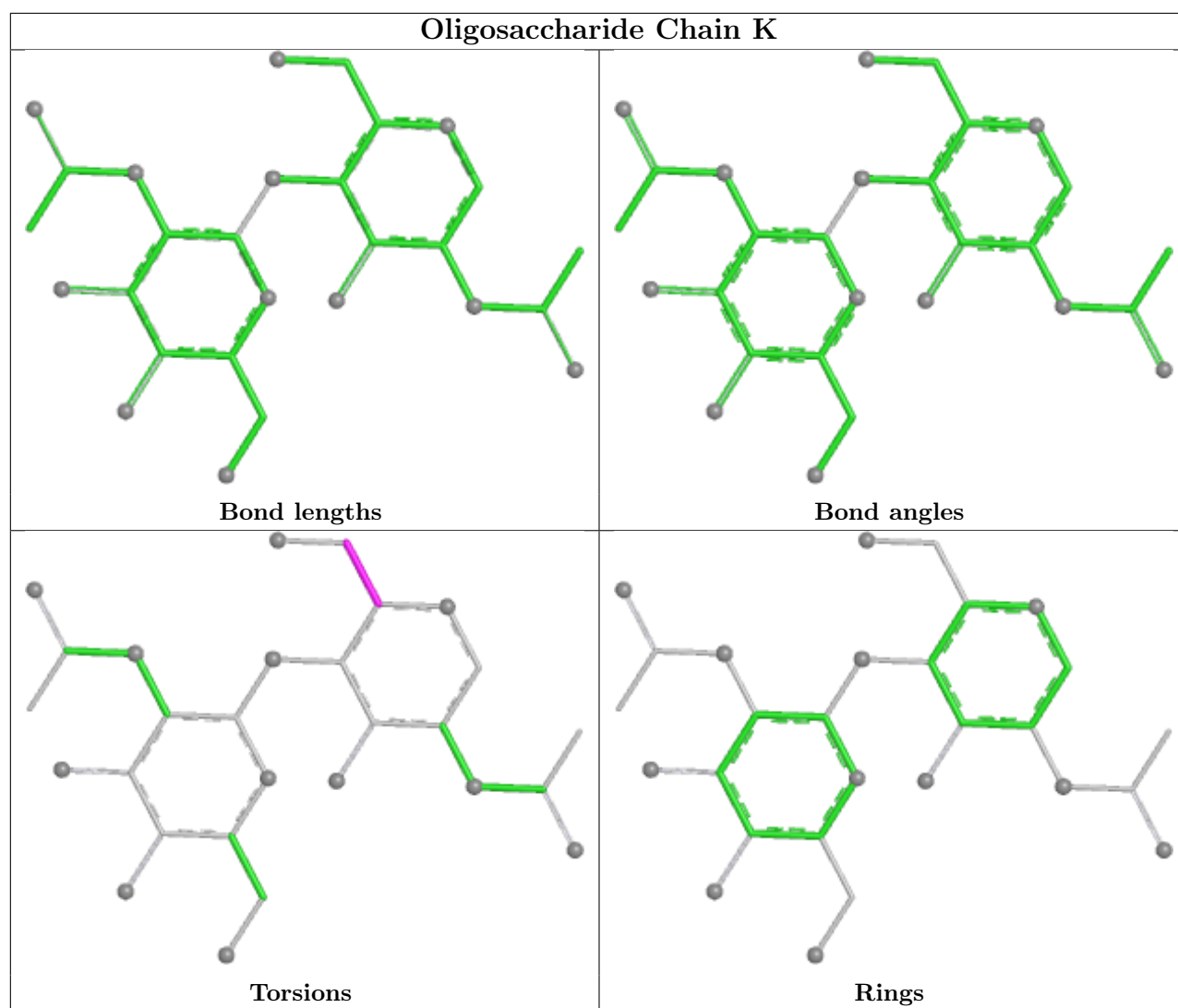
There are no ring outliers.

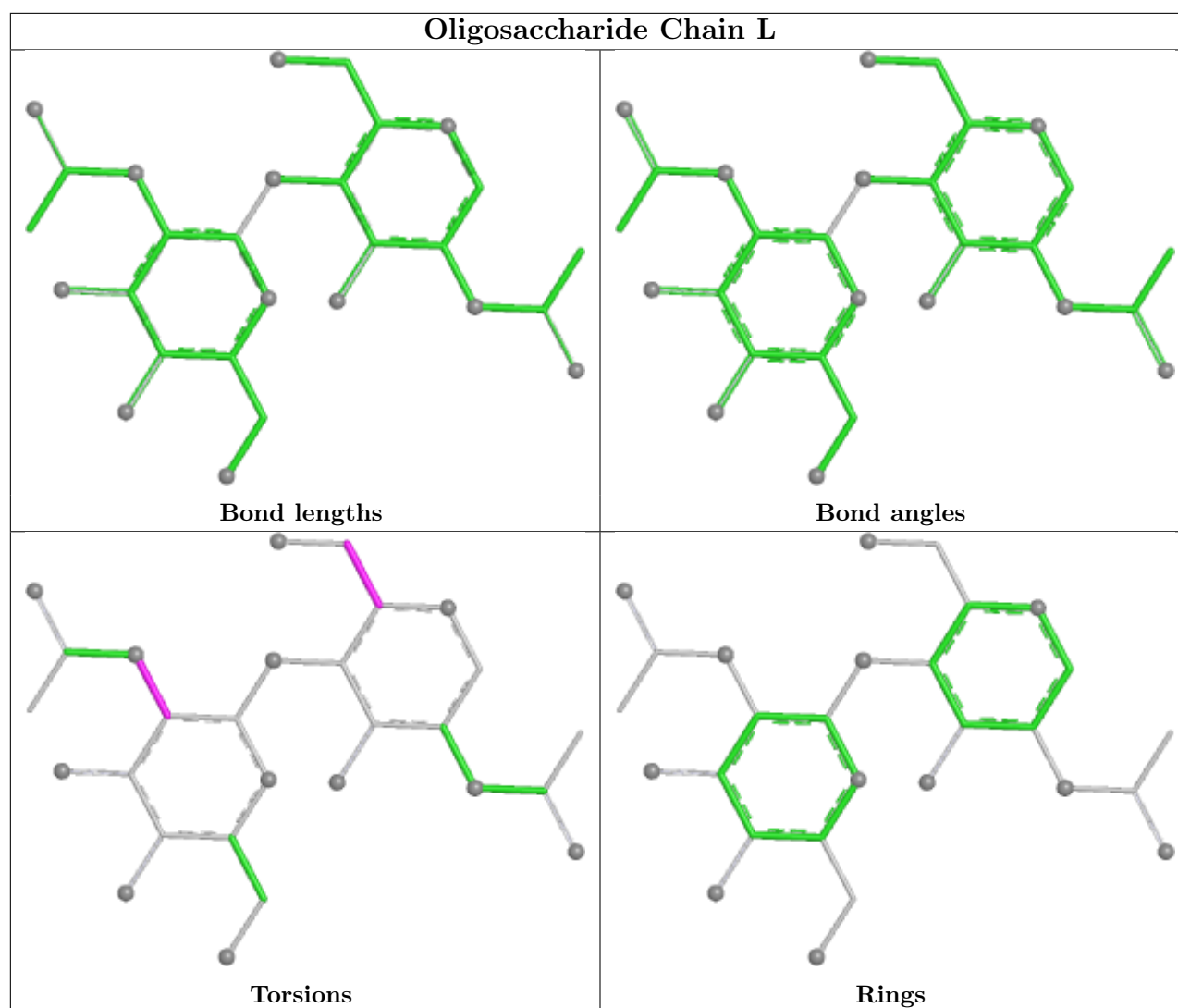
No monomer is involved in short contacts.

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









5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
4	NAG	B	1077	1	14,14,15	0.45	0	17,19,21	0.99	1 (5%)
4	NAG	F	1077	1	14,14,15	0.74	1 (7%)	17,19,21	1.24	1 (5%)
4	NAG	B	1208	1	14,14,15	0.55	0	17,19,21	0.46	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	NAG	E	1077	1	14,14,15	0.71	0	17,19,21	0.51	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	NAG	B	1077	1	-	1/6/23/26	0/1/1/1
4	NAG	B	1208	1	-	2/6/23/26	0/1/1/1
4	NAG	F	1077	1	1/1/5/7	2/6/23/26	0/1/1/1
4	NAG	E	1077	1	-	1/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	F	1077	NAG	O5-C1	-2.41	1.39	1.43

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	1077	NAG	C3-C4-C5	3.51	116.59	110.23
4	B	1077	NAG	C2-N2-C7	-2.70	119.28	122.90

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
4	F	1077	NAG	C1

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	B	1208	NAG	O5-C5-C6-O6
4	F	1077	NAG	C4-C5-C6-O6
4	B	1208	NAG	C4-C5-C6-O6
4	F	1077	NAG	O5-C5-C6-O6
4	B	1077	NAG	O5-C5-C6-O6
4	E	1077	NAG	C4-C5-C6-O6

There are no ring outliers.

3 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1077	NAG	1	0
4	B	1208	NAG	1	0
4	E	1077	NAG	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, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2	OWAB(Å ²)	Q < 0.9
1	A	457/539 (84%)	-0.07	3 (0%) 84 69	36, 85, 149, 296	0
1	B	463/539 (85%)	-0.14	6 (1%) 75 55	42, 86, 161, 250	0
1	E	462/539 (85%)	0.35	17 (3%) 45 28	12, 152, 223, 276	1 (0%)
1	F	458/539 (84%)	0.19	5 (1%) 78 61	89, 143, 196, 310	0
2	C	103/126 (81%)	0.08	0 100 100	64, 120, 210, 233	0
2	D	104/126 (82%)	0.10	0 100 100	64, 113, 205, 350	0
2	G	103/126 (81%)	0.38	1 (0%) 79 63	112, 173, 257, 293	0
2	H	104/126 (82%)	0.28	1 (0%) 79 63	97, 160, 240, 267	0
All	All	2254/2660 (84%)	0.10	33 (1%) 72 52	12, 125, 210, 350	1 (0%)

All (33) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	279	GLY	4.7
1	A	439	ILE	3.9
1	E	485	CYS	3.6
1	E	46	MET	3.2
1	E	486	GLU	3.2
1	E	335	LEU	2.9
1	B	230	PHE	2.9
1	F	193	LEU	2.8
1	A	46	MET	2.6
1	B	46	MET	2.6
1	E	405	LEU	2.6
1	E	429	LEU	2.5
1	E	86	LEU	2.5
1	E	367	LEU	2.4
1	E	102	LEU	2.3
1	B	204	TYR	2.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	F	164	LEU	2.3
1	B	460	ILE	2.2
1	B	437	PHE	2.2
1	E	531	GLU	2.2
1	E	333	LEU	2.2
1	F	163	SER	2.1
1	B	61	PRO	2.1
2	G	77	PRO	2.1
1	F	201	ILE	2.1
2	H	127	PRO	2.1
1	A	436	SER	2.1
1	E	76	ASN	2.1
1	E	482	PHE	2.1
1	F	418	PHE	2.1
1	E	337	GLY	2.0
1	E	458	SER	2.0
1	E	223	HIS	2.0

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

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

6.3 Carbohydrates [i](#)

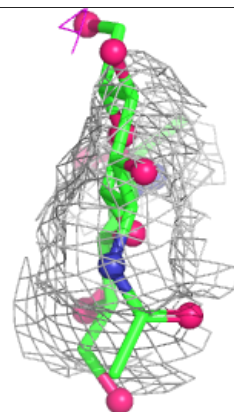
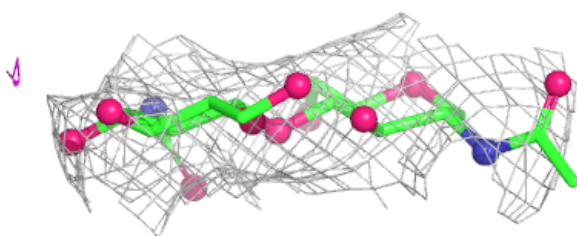
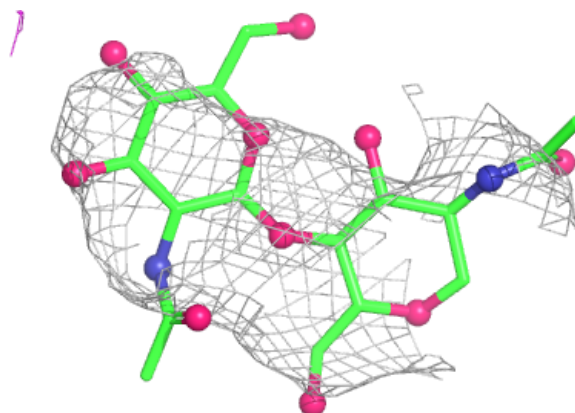
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	NAG	J	1	14/15	-0.15	0.16	167,181,192,200	0
3	NAG	J	2	14/15	0.27	0.11	173,191,200,201	0
3	NAG	K	2	14/15	0.44	0.11	219,230,233,235	0
3	NAG	L	1	14/15	0.44	0.14	191,204,213,213	0
3	NAG	L	2	14/15	0.49	0.12	202,216,225,228	0
3	NAG	I	2	14/15	0.53	0.10	188,200,224,227	0
3	NAG	I	1	14/15	0.54	0.10	141,178,197,205	0
3	NAG	K	1	14/15	0.71	0.10	174,189,216,220	0

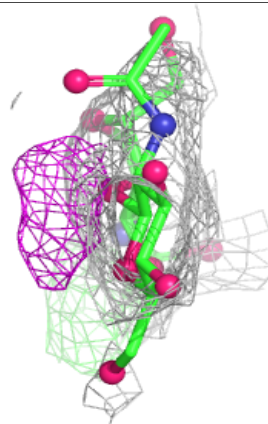
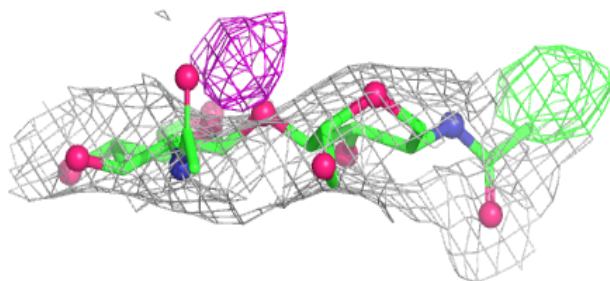
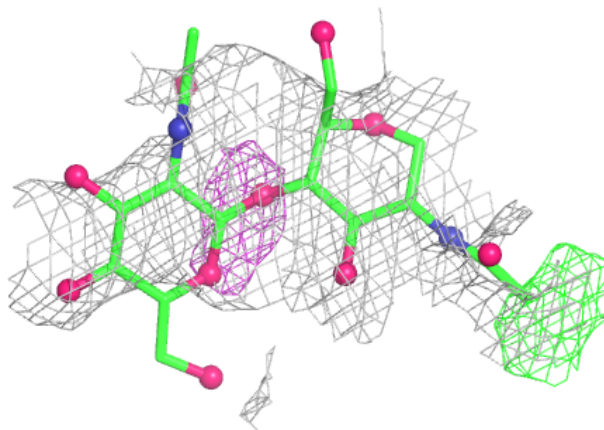
The following is a graphical depiction of the model fit to experimental electron density for oligosaccharide. Each fit is shown from different orientation to approximate a three-dimensional view.

Electron density around Chain I:

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

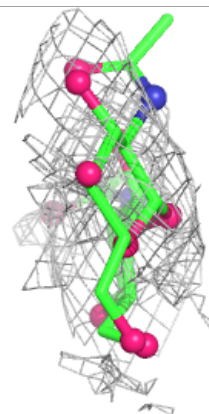
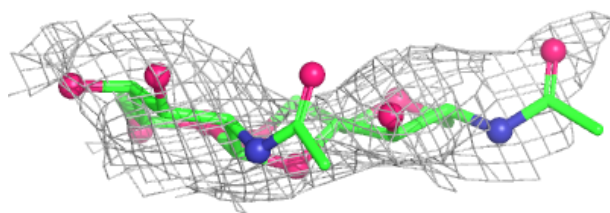
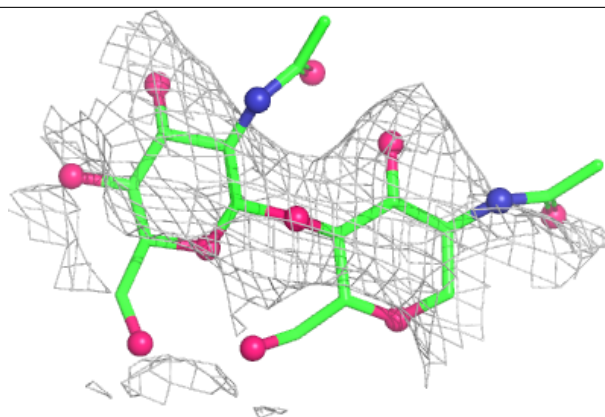
**Electron density around Chain J:**

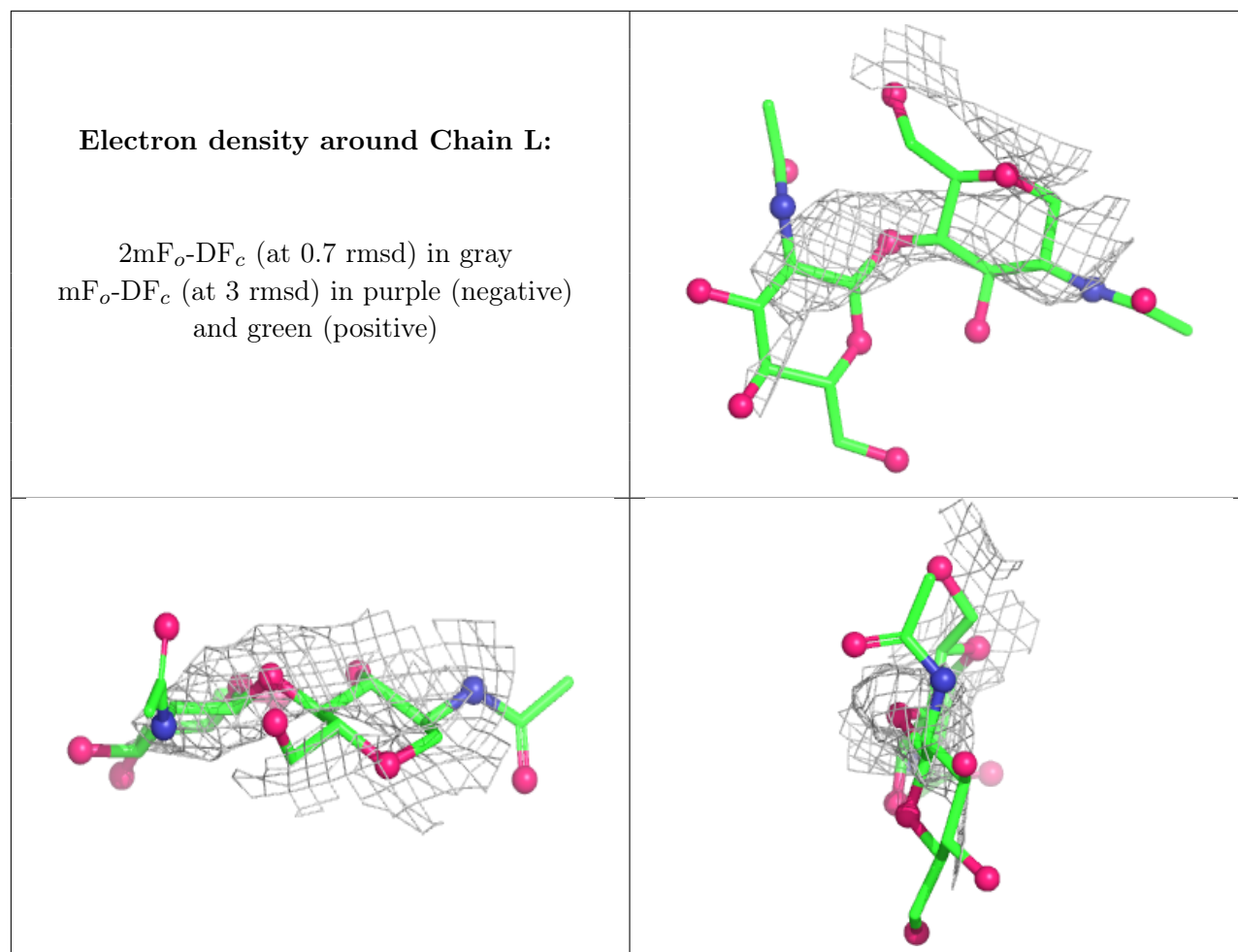
$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around Chain K:

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





6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
4	NAG	E	1077	14/15	0.20	0.10	169,181,184,186	0
4	NAG	B	1208	14/15	0.34	0.12	144,191,199,206	0
4	NAG	B	1077	14/15	0.48	0.13	109,149,161,170	0
4	NAG	F	1077	14/15	0.49	0.11	148,163,167,172	0

6.5 Other polymers [i](#)

There are no such residues in this entry.