



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 5, 2026 – 04:05 AM UTC

PDB ID : 9R9L / pdb_00009r9l
Title : sucrose hydrolase SuxB from Xanthomonas oryzae pv. oryzae in complex with glucose
Authors : Zoellner, N.; Applegate, V.; Smits, S.H.J.; Hoepfner, A.
Deposited on : 2025-05-20
Resolution : 2.95 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

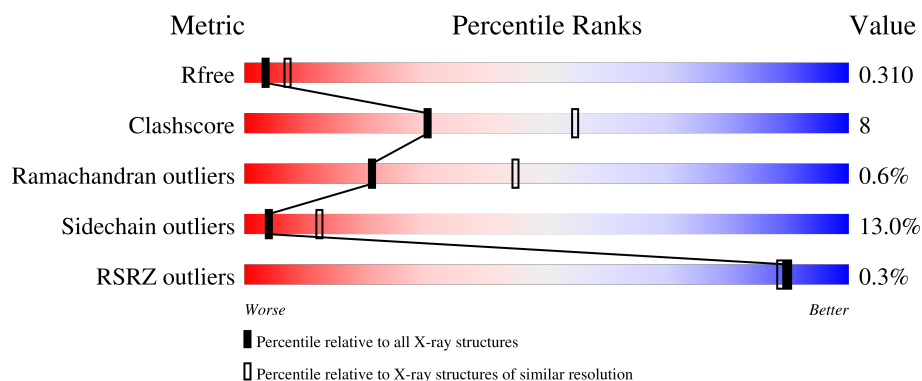
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION




The reported resolution of this entry is 2.95 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	1130 (2.98-2.94)
Clashscore	190562	1157 (2.98-2.94)
Ramachandran outliers	187476	1101 (2.98-2.94)
Sidechain outliers	187428	1101 (2.98-2.94)
RSRZ outliers	180081	1130 (2.98-2.94)

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	638	
1	B	638	
1	C	638	

2 Entry composition [i](#)

There are 4 unique types of molecules in this entry. The entry contains 14524 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.

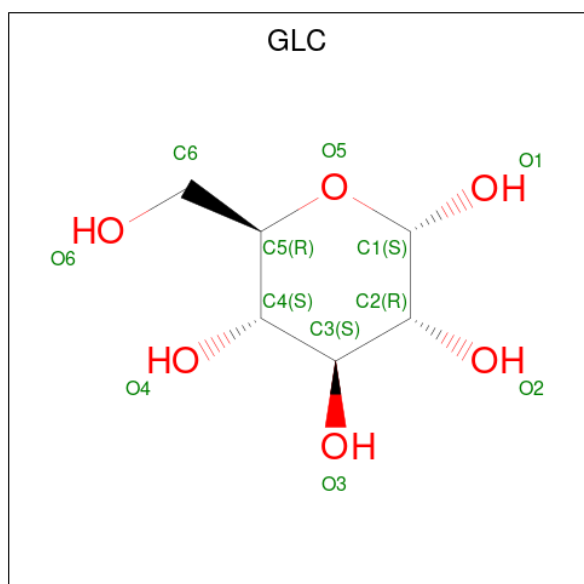
- Molecule 1 is a protein called Amylosucrase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	623	Total	C	N	O	S	0	0	0
			4837	3059	872	886	20			
1	B	624	Total	C	N	O	S	0	0	0
			4844	3064	873	887	20			
1	C	617	Total	C	N	O	S	0	0	0
			4800	3042	865	873	20			

- Molecule 2 is POTASSIUM ION (CCD ID: K) (formula: K).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	K	0	0
			1	1		
2	B	1	Total	K	0	0
			1	1		

- Molecule 3 is alpha-D-glucopyranose (CCD ID: GLC) (formula: C₆H₁₂O₆) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			12	6	6		
3	B	1	Total	C	O	0	0
			12	6	6		
3	C	1	Total	C	O	0	0
			12	6	6		

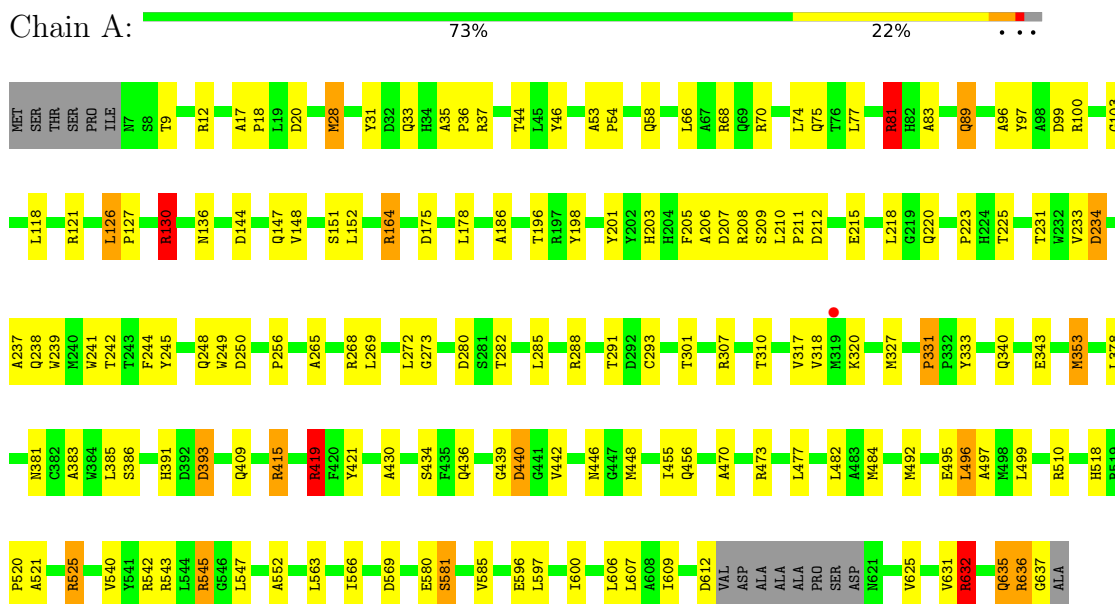
- Molecule 4 is water.

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

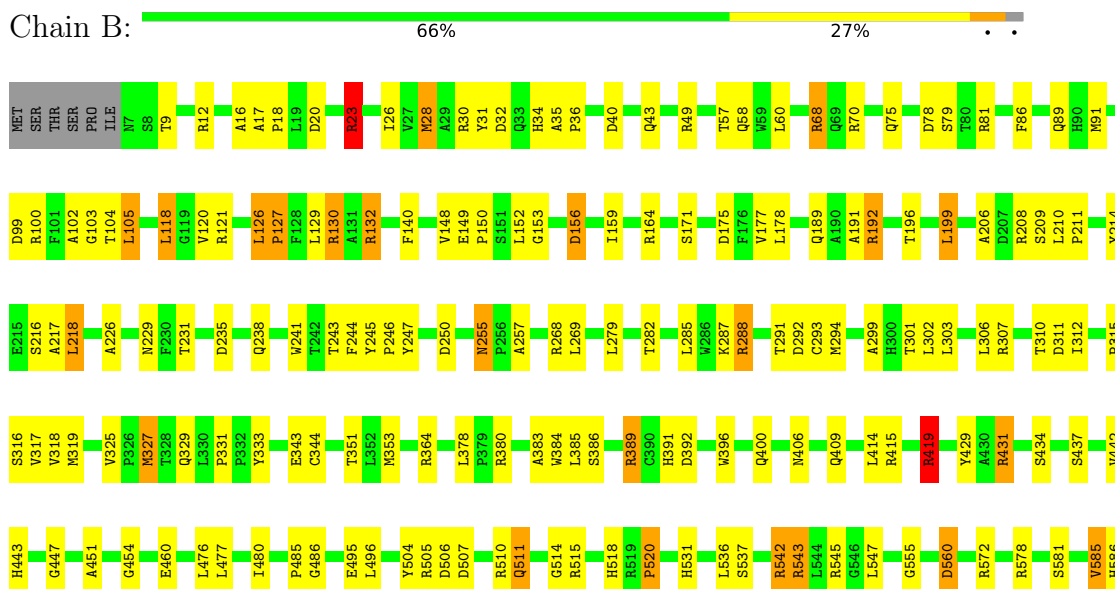
3 Residue-property plots [i](#)

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: Amylosucrase

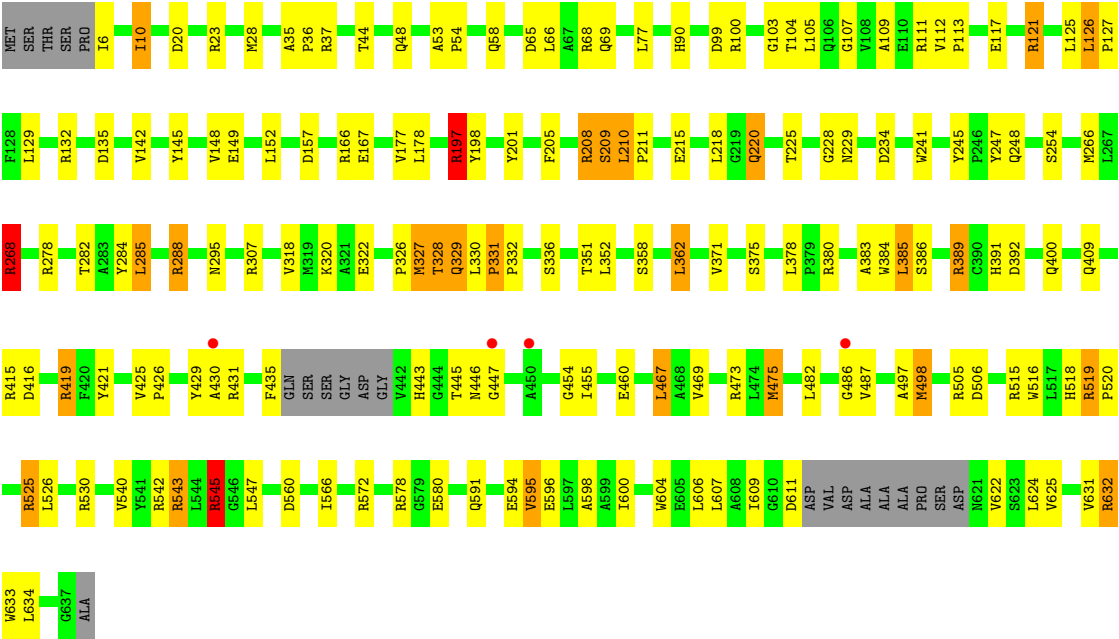


• Molecule 1: Amylosucrase





● Molecule 1: Amylosucrase



4 Data and refinement statistics

Property	Value	Source
Space group	I 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	100.53Å 172.73Å 259.78Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.75 – 2.95 49.75 – 2.95	Depositor EDS
% Data completeness (in resolution range)	99.8 (49.75-2.95) 99.8 (49.75-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.11 (at 2.96Å)	Xtriage
Refinement program	REFMAC 5.8.0403	Depositor
R, R_{free}	0.229 , 0.302 0.241 , 0.310	Depositor DCC
R_{free} test set	2468 reflections (5.14%)	wwPDB-VP
Wilson B-factor (Å ²)	91.5	Xtriage
Anisotropy	0.357	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 108.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	14524	wwPDB-VP
Average B, all atoms (Å ²)	118.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.50% 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: K, GLC

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	0.54	0/4969	0.93	3/6781 (0.0%)
1	B	0.51	0/4976	0.93	1/6791 (0.0%)
1	C	0.50	0/4931	0.91	1/6729 (0.0%)
All	All	0.52	0/14876	0.92	5/20301 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	15
1	B	0	24
1	C	0	19
All	All	0	58

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	331	PRO	N-CA-C	7.80	120.22	110.70
1	B	331	PRO	N-CA-C	6.97	119.21	110.70
1	A	244	PHE	O-C-N	6.31	126.20	121.47
1	A	331	PRO	N-CA-C	5.83	117.81	110.70
1	A	569	ASP	CA-CB-CG	5.27	117.87	112.60

There are no chirality outliers.

All (58) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	12	ARG	Sidechain
1	A	121	ARG	Sidechain
1	A	130	ARG	Sidechain
1	A	164	ARG	Sidechain
1	A	288	ARG	Sidechain
1	A	37	ARG	Sidechain
1	A	415	ARG	Sidechain
1	A	419	ARG	Sidechain
1	A	510	ARG	Sidechain
1	A	542	ARG	Sidechain
1	A	543	ARG	Sidechain
1	A	545	ARG	Sidechain
1	A	632	ARG	Sidechain
1	A	636	ARG	Sidechain
1	A	81	ARG	Sidechain
1	B	12	ARG	Sidechain
1	B	121	ARG	Sidechain
1	B	130	ARG	Sidechain
1	B	132	ARG	Sidechain
1	B	164	ARG	Sidechain
1	B	192	ARG	Sidechain
1	B	208	ARG	Sidechain
1	B	23	ARG	Sidechain
1	B	268	ARG	Sidechain
1	B	288	ARG	Sidechain
1	B	307	ARG	Sidechain
1	B	364	ARG	Sidechain
1	B	389	ARG	Sidechain
1	B	419	ARG	Sidechain
1	B	431	ARG	Sidechain
1	B	49	ARG	Sidechain
1	B	515	ARG	Sidechain
1	B	542	ARG	Sidechain
1	B	543	ARG	Sidechain
1	B	545	ARG	Sidechain
1	B	632	ARG	Sidechain
1	B	636	ARG	Sidechain
1	B	68	ARG	Sidechain
1	B	81	ARG	Sidechain
1	C	121	ARG	Sidechain
1	C	166	ARG	Sidechain
1	C	197	ARG	Sidechain
1	C	23	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	268	ARG	Sidechain
1	C	288	ARG	Sidechain
1	C	37	ARG	Sidechain
1	C	389	ARG	Sidechain
1	C	419	ARG	Sidechain
1	C	431	ARG	Sidechain
1	C	473	ARG	Sidechain
1	C	519	ARG	Sidechain
1	C	525	ARG	Sidechain
1	C	530	ARG	Sidechain
1	C	543	ARG	Sidechain
1	C	545	ARG	Sidechain
1	C	572	ARG	Sidechain
1	C	578	ARG	Sidechain
1	C	632	ARG	Sidechain

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4837	0	4633	79	0
1	B	4844	0	4642	89	0
1	C	4800	0	4611	74	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	12	0	12	1	0
3	B	12	0	12	1	0
3	C	12	0	12	0	0
4	A	3	0	0	0	0
4	B	2	0	0	0	0
All	All	14524	0	13922	239	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (239) 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:B:99:ASP:HA	1:B:103:GLY:HA2	1.53	0.89
1:C:105:LEU:HD11	1:C:148:VAL:HG11	1.65	0.79
1:C:149:GLU:HB3	1:C:152:LEU:HD12	1.69	0.74
1:B:476:LEU:HD11	1:B:586:HIS:HB3	1.73	0.70
1:A:448:MET:HE2	1:A:520:PRO:HG3	1.73	0.70
1:B:126:LEU:HD21	1:B:391:HIS:CG	2.28	0.68
1:A:495:GLU:HG2	1:A:496:LEU:HG	1.77	0.66
1:C:129:LEU:HD13	1:C:145:TYR:HA	1.78	0.66
1:A:100:ARG:HB3	1:A:521:ALA:HA	1.79	0.66
1:B:518:HIS:O	1:B:520:PRO:HD3	1.96	0.65
1:C:518:HIS:O	1:C:520:PRO:HD3	1.97	0.65
1:A:497:ALA:HB2	1:A:540:VAL:HG21	1.79	0.65
1:B:100:ARG:HH11	1:B:520:PRO:HA	1.62	0.65
1:B:17:ALA:HB3	1:B:18:PRO:HD3	1.78	0.65
1:A:241:TRP:HB3	1:A:250:ASP:HB2	1.79	0.64
1:C:278:ARG:CZ	1:C:322:GLU:HG3	2.28	0.63
1:B:178:LEU:HG	1:B:285:LEU:HD21	1.80	0.63
1:B:607:LEU:HD11	1:B:635:GLN:HB2	1.81	0.62
1:C:53:ALA:HB3	1:C:54:PRO:HD3	1.82	0.61
1:B:78:ASP:HB3	1:B:315:PRO:HG2	1.81	0.61
1:B:17:ALA:HB3	1:B:18:PRO:CD	2.30	0.61
1:C:126:LEU:HD21	1:C:391:HIS:CG	2.35	0.61
1:C:497:ALA:HB2	1:C:540:VAL:HG21	1.83	0.60
1:A:518:HIS:O	1:A:520:PRO:HD3	2.02	0.59
1:C:429:TYR:HB2	1:C:454:GLY:HA3	1.82	0.59
1:B:132:ARG:HD2	1:B:247:TYR:HB2	1.85	0.59
1:C:378:LEU:HD13	1:C:383:ALA:HA	1.85	0.59
1:B:189:GLN:HA	1:B:192:ARG:HD2	1.85	0.59
1:B:99:ASP:HA	1:B:103:GLY:CA	2.30	0.58
1:B:431:ARG:HB2	1:B:451:ALA:HB1	1.85	0.57
1:C:595:VAL:HG13	1:C:624:LEU:HB3	1.85	0.57
1:C:327:MET:HA	1:C:330:LEU:HD12	1.87	0.57
1:A:17:ALA:HB3	1:A:18:PRO:HD3	1.86	0.57
1:B:437:SER:HB2	1:B:443:HIS:HB3	1.86	0.57
1:A:96:ALA:HB2	1:A:492:MET:HB2	1.86	0.56
1:A:206:ALA:HA	1:A:238:GLN:HG2	1.86	0.56
1:B:602:ASP:O	1:B:636:ARG:NH2	2.38	0.56
1:A:203:HIS:HB2	1:A:241:TRP:HB2	1.88	0.56
1:B:429:TYR:HB2	1:B:454:GLY:HA3	1.87	0.56
1:A:291:THR:C	1:A:293:CYS:H	2.14	0.55
1:B:196:THR:HA	1:B:199:LEU:HB2	1.87	0.55
1:C:100:ARG:HH11	1:C:520:PRO:HA	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:229:ASN:HA	1:B:243:THR:HA	1.88	0.55
1:A:210:LEU:HB2	1:A:211:PRO:HD3	1.88	0.55
1:C:284:TYR:O	1:C:285:LEU:C	2.50	0.55
1:C:126:LEU:HD21	1:C:391:HIS:CD2	2.42	0.54
1:A:70:ARG:HG2	1:A:75:GLN:HG3	1.89	0.54
1:A:525:ARG:NH2	1:B:217:ALA:HB2	2.23	0.54
1:C:542:ARG:HH22	1:C:543:ARG:HG2	1.72	0.53
1:C:105:LEU:HD12	1:C:157:ASP:HB2	1.91	0.53
1:C:604:TRP:HB3	1:C:634:LEU:HB3	1.91	0.53
1:A:126:LEU:HD21	1:A:391:HIS:CG	2.44	0.53
1:B:140:PHE:CZ	3:B:702:GLC:H2	2.44	0.53
1:A:126:LEU:HD21	1:A:391:HIS:CE1	2.45	0.52
1:B:30:ARG:NH1	1:B:312:ILE:O	2.41	0.52
1:A:482:LEU:HD13	1:A:547:LEU:HB3	1.90	0.52
1:A:53:ALA:HB3	1:A:54:PRO:HD3	1.92	0.51
1:C:383:ALA:HB1	1:C:486:GLY:HA2	1.92	0.51
1:B:636:ARG:O	1:B:637:GLY:C	2.53	0.51
1:B:78:ASP:HA	1:B:316:SER:HB3	1.92	0.51
1:C:329:GLN:O	1:C:332:PRO:HD2	2.10	0.51
1:B:495:GLU:HG2	1:B:496:LEU:HG	1.93	0.51
1:A:223:PRO:HG2	1:A:436:GLN:HB3	1.92	0.51
1:B:378:LEU:HD13	1:B:383:ALA:HA	1.93	0.51
1:C:475:MET:HE1	1:C:540:VAL:HG13	1.92	0.51
1:B:477:LEU:HA	1:B:480:ILE:HD12	1.93	0.50
1:B:149:GLU:HB3	1:B:152:LEU:HD12	1.92	0.50
1:B:504:TYR:HB2	1:B:510:ARG:HB3	1.93	0.50
1:A:74:LEU:HD21	1:A:273:GLY:HA2	1.93	0.50
1:A:606:LEU:HD23	1:A:632:ARG:HG2	1.92	0.50
1:A:378:LEU:HD13	1:A:383:ALA:HA	1.93	0.50
1:A:607:LEU:HD11	1:A:635:GLN:HG3	1.94	0.49
1:B:507:ASP:HB3	1:B:510:ARG:HB2	1.93	0.49
1:C:278:ARG:NH2	1:C:322:GLU:HG3	2.26	0.49
1:A:46:TYR:HB3	1:A:256:PRO:HG3	1.93	0.49
1:C:208:ARG:NE	1:C:211:PRO:HB2	2.28	0.49
1:C:178:LEU:H	1:C:178:LEU:HD23	1.77	0.49
1:A:208:ARG:HH21	1:A:212:ASP:HA	1.78	0.49
1:B:572:ARG:HD2	1:B:589:SER:HB3	1.95	0.49
1:C:358:SER:O	1:C:362:LEU:HB2	2.13	0.49
1:A:205:PHE:HB2	1:A:239:TRP:HB2	1.94	0.49
1:B:597:LEU:HD13	1:B:600:ILE:HD11	1.95	0.49
1:A:215:GLU:HA	1:A:218:LEU:HB2	1.94	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:485:PRO:HD3	1:B:578:ARG:HD3	1.94	0.48
1:C:99:ASP:HA	1:C:103:GLY:HA2	1.95	0.48
1:C:383:ALA:HB1	1:C:486:GLY:CA	2.43	0.48
1:C:198:TYR:O	1:C:201:TYR:HB2	2.12	0.48
1:C:109:ALA:HA	1:C:112:VAL:HG23	1.95	0.48
1:B:126:LEU:O	1:B:127:PRO:C	2.55	0.48
1:B:226:ALA:HB2	1:B:245:TYR:CD1	2.48	0.48
1:A:97:TYR:HB2	1:A:100:ARG:HG2	1.96	0.48
1:A:415:ARG:CZ	1:A:440:ASP:HB2	2.44	0.48
1:A:234:ASP:HA	1:A:237:ALA:HA	1.96	0.48
1:C:210:LEU:HB2	1:C:211:PRO:HD3	1.95	0.48
1:B:150:PRO:HA	1:B:153:GLY:O	2.13	0.47
1:C:421:TYR:HA	1:C:430:ALA:CB	2.45	0.47
1:A:291:THR:C	1:A:293:CYS:N	2.71	0.47
1:A:415:ARG:NH2	1:A:439:GLY:O	2.47	0.47
1:B:129:LEU:HD11	1:B:269:LEU:HD21	1.96	0.47
1:C:607:LEU:HD12	1:C:633:TRP:HB3	1.97	0.47
1:B:279:LEU:HD11	1:B:319:MET:HE3	1.96	0.47
1:B:595:VAL:HG13	1:B:624:LEU:HB3	1.97	0.47
1:C:596:GLU:C	1:C:598:ALA:H	2.22	0.47
1:C:378:LEU:HD11	1:C:384:TRP:CD1	2.49	0.46
1:C:545:ARG:HD2	1:C:545:ARG:HA	1.75	0.46
1:A:70:ARG:CZ	1:A:74:LEU:HB3	2.46	0.46
1:A:89:GLN:HG3	1:A:552:ALA:O	2.16	0.46
1:B:279:LEU:HD13	1:B:303:LEU:HD22	1.97	0.46
1:A:233:VAL:O	1:A:237:ALA:N	2.48	0.46
1:B:585:VAL:HB	1:B:626:LEU:HD11	1.96	0.46
1:C:498:MET:HG2	1:C:526:LEU:HD23	1.97	0.46
1:A:320:LYS:HD2	1:A:385:LEU:HD13	1.98	0.46
1:B:210:LEU:HB2	1:B:211:PRO:HD3	1.97	0.46
1:C:205:PHE:HB3	1:C:210:LEU:HD13	1.98	0.46
1:B:89:GLN:OE1	1:B:555:GLY:HA2	2.16	0.45
1:A:421:TYR:HA	1:A:430:ALA:CB	2.45	0.45
1:B:129:LEU:HA	1:B:148:VAL:HA	1.98	0.45
1:C:421:TYR:HB3	1:C:445:THR:HG21	1.97	0.45
1:A:126:LEU:HD21	1:A:391:HIS:ND1	2.31	0.45
1:A:269:LEU:HA	1:A:272:LEU:HD12	1.98	0.45
1:A:607:LEU:HD21	1:A:635:GLN:HB2	1.98	0.45
1:B:118:LEU:HB3	1:B:120:VAL:HG23	1.98	0.45
1:B:306:LEU:O	1:B:310:THR:HG23	2.17	0.45
1:C:90:HIS:HD2	1:C:121:ARG:HG3	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:ARG:HD2	1:A:81:ARG:HA	1.61	0.45
1:B:333:TYR:O	1:B:343:GLU:HB3	2.17	0.45
1:C:208:ARG:HH22	1:C:215:GLU:HG3	1.81	0.45
1:A:456:GLN:HB2	1:A:499:LEU:HD22	1.98	0.45
1:B:353:MET:HE3	1:B:353:MET:HB3	1.84	0.45
1:B:126:LEU:HD21	1:B:391:HIS:CD2	2.52	0.44
1:A:234:ASP:C	1:A:237:ALA:H	2.26	0.44
1:B:231:THR:HG21	1:B:246:PRO:HB3	2.00	0.44
1:B:299:ALA:HA	1:B:302:LEU:HD12	1.99	0.44
1:A:636:ARG:O	1:A:637:GLY:C	2.61	0.44
1:C:218:LEU:HD11	1:C:241:TRP:CZ2	2.52	0.44
1:C:362:LEU:HD22	1:C:362:LEU:HA	1.82	0.44
1:A:208:ARG:NE	1:A:211:PRO:HB2	2.32	0.44
1:B:23:ARG:HH11	1:B:23:ARG:HG2	1.83	0.44
1:B:70:ARG:HG2	1:B:75:GLN:HG3	1.98	0.44
1:B:126:LEU:HD11	1:B:391:HIS:CD2	2.52	0.44
1:B:156:ASP:HA	1:B:159:ILE:HD12	1.99	0.44
1:B:16:ALA:HB2	1:B:28:MET:HE2	1.99	0.44
1:B:196:THR:HA	1:B:199:LEU:CB	2.48	0.44
1:B:35:ALA:HB3	1:B:36:PRO:HD3	1.99	0.44
1:B:389:ARG:HA	1:B:389:ARG:HD2	1.82	0.44
1:A:581:SER:O	1:A:635:GLN:HA	2.17	0.44
1:C:103:GLY:O	1:C:104:THR:C	2.60	0.44
1:B:396:TRP:HB3	1:B:414:LEU:HD22	1.99	0.44
1:C:326:PRO:HB2	1:C:328:THR:HG23	2.00	0.43
1:B:178:LEU:HD23	1:B:178:LEU:H	1.83	0.43
1:B:255:ASN:ND2	1:B:257:ALA:H	2.16	0.43
1:C:320:LYS:HD3	1:C:385:LEU:HD13	1.98	0.43
1:C:516:TRP:HA	1:C:519:ARG:HB2	2.00	0.43
1:B:241:TRP:HB3	1:B:250:ASP:HB2	1.99	0.43
1:A:566:ILE:O	1:A:566:ILE:HG13	2.18	0.43
1:B:105:LEU:HD11	1:B:148:VAL:HG11	1.99	0.43
1:B:118:LEU:HD21	1:B:495:GLU:HG3	2.00	0.43
1:B:587:ASN:O	1:B:629:TYR:HA	2.19	0.43
1:B:35:ALA:N	1:B:36:PRO:CD	2.81	0.43
1:A:28:MET:O	1:A:31:TYR:HB3	2.19	0.43
1:A:77:LEU:HD12	1:A:77:LEU:HA	1.91	0.43
1:B:214:TYR:O	1:B:218:LEU:HB2	2.19	0.43
1:B:299:ALA:O	1:B:302:LEU:HB2	2.18	0.43
1:A:178:LEU:HD11	1:A:285:LEU:HD11	2.00	0.43
1:B:511:GLN:H	1:B:511:GLN:HG3	1.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ALA:HB1	1:A:381:ASN:HD21	1.84	0.43
1:A:178:LEU:HG	1:A:285:LEU:HD21	2.00	0.43
1:B:192:ARG:HB3	1:B:235:ASP:HB3	2.00	0.43
1:C:371:VAL:O	1:C:375:SER:N	2.51	0.42
1:C:392:ASP:HA	1:C:515:ARG:HD2	2.01	0.42
1:A:77:LEU:HG	1:A:81:ARG:HD3	2.00	0.42
1:C:178:LEU:HG	1:C:285:LEU:HD21	2.00	0.42
1:A:333:TYR:O	1:A:343:GLU:HB3	2.20	0.42
1:A:470:ALA:O	1:A:473:ARG:HB2	2.19	0.42
1:C:112:VAL:N	1:C:113:PRO:CD	2.81	0.42
1:A:147:GLN:HG3	1:A:148:VAL:O	2.19	0.42
1:C:107:GLY:O	1:C:111:ARG:HG2	2.19	0.42
1:C:218:LEU:HD13	1:C:229:ASN:HB2	2.01	0.42
1:C:245:TYR:HB2	1:C:248:GLN:OE1	2.19	0.42
1:B:560:ASP:OD1	1:B:560:ASP:N	2.53	0.42
1:C:178:LEU:HD11	1:C:285:LEU:HD11	2.02	0.42
1:C:425:VAL:HB	1:C:426:PRO:HD2	2.00	0.42
1:A:118:LEU:HD12	1:A:545:ARG:HD3	2.02	0.42
1:B:17:ALA:CB	1:B:18:PRO:CD	2.98	0.42
1:B:60:LEU:HD23	1:B:60:LEU:HA	1.91	0.42
1:C:482:LEU:HD13	1:C:547:LEU:HB3	2.01	0.42
1:A:391:HIS:NE2	3:A:702:GLC:H62	2.35	0.42
1:A:597:LEU:HA	1:A:600:ILE:HG12	2.02	0.42
1:B:23:ARG:HA	1:B:23:ARG:HD3	1.98	0.42
1:B:31:TYR:O	1:B:32:ASP:C	2.63	0.42
1:B:191:ALA:HB1	1:B:199:LEU:HD13	2.01	0.42
1:B:327:MET:HB2	1:B:351:THR:HG21	2.02	0.42
1:C:215:GLU:HA	1:C:218:LEU:HB2	2.02	0.41
1:C:389:ARG:HA	1:C:389:ARG:HD2	1.76	0.41
1:C:220:GLN:CD	1:C:228:GLY:H	2.28	0.41
1:B:504:TYR:CE2	1:B:514:GLY:HA2	2.55	0.41
1:C:132:ARG:HD3	1:C:247:TYR:HB2	2.03	0.41
1:C:389:ARG:HH21	1:C:447:GLY:H	1.68	0.41
1:C:596:GLU:C	1:C:598:ALA:N	2.78	0.41
1:B:34:HIS:CD2	1:B:311:ASP:HB3	2.55	0.41
1:A:245:TYR:HB2	1:A:248:GLN:OE1	2.20	0.41
1:A:307:ARG:O	1:A:310:THR:OG1	2.35	0.41
1:A:186:ALA:HB1	1:C:10:ILE:HG13	2.03	0.41
1:B:389:ARG:HH21	1:B:447:GLY:H	1.68	0.41
1:C:100:ARG:NH1	1:C:519:ARG:O	2.54	0.41
1:C:385:LEU:HD12	1:C:487:VAL:HB	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:545:ARG:HD2	1:A:545:ARG:HA	1.88	0.41
1:C:429:TYR:O	1:C:454:GLY:HA2	2.21	0.41
1:A:231:THR:HB	1:A:242:THR:HG21	2.02	0.41
1:A:353:MET:HE3	1:A:353:MET:HB3	1.85	0.41
1:B:86:PHE:O	1:B:91:MET:HG3	2.20	0.41
1:B:384:TRP:O	1:B:486:GLY:HA3	2.21	0.41
1:C:77:LEU:HD12	1:C:77:LEU:HA	1.85	0.41
1:A:178:LEU:HD23	1:A:178:LEU:H	1.85	0.41
1:A:233:VAL:HG21	1:A:249:TRP:CZ2	2.55	0.41
1:A:265:ALA:HA	1:A:268:ARG:HD2	2.01	0.41
1:B:178:LEU:HD11	1:B:285:LEU:HD11	2.03	0.41
1:B:291:THR:C	1:B:293:CYS:H	2.27	0.41
1:C:330:LEU:N	1:C:331:PRO:CD	2.84	0.41
1:C:416:ASP:O	1:C:419:ARG:HB2	2.21	0.41
1:C:467:LEU:HD13	1:C:467:LEU:HA	1.90	0.41
1:A:35:ALA:HB3	1:A:36:PRO:HD3	2.02	0.41
1:A:175:ASP:HB3	1:A:280:ASP:OD2	2.21	0.41
1:A:198:TYR:O	1:A:201:TYR:HB2	2.20	0.41
1:A:327:MET:O	1:A:331:PRO:HD3	2.20	0.41
1:A:70:ARG:NH2	1:A:74:LEU:HB3	2.36	0.40
1:A:415:ARG:HH11	1:A:419:ARG:HE	1.69	0.40
1:B:279:LEU:HD11	1:B:319:MET:HB3	2.03	0.40
1:B:325:VAL:CG2	1:B:329:GLN:HB2	2.51	0.40
1:C:125:LEU:HD23	1:C:125:LEU:HA	1.92	0.40
1:B:206:ALA:N	1:B:238:GLN:HE21	2.20	0.40
1:A:68:ARG:HD2	1:C:197:ARG:HH21	1.86	0.40
1:A:484:MET:HB3	1:A:484:MET:HE3	1.84	0.40
1:B:415:ARG:CZ	1:B:419:ARG:HE	2.35	0.40
1:A:130:ARG:HB2	1:A:144:ASP:HB3	2.02	0.40
1:A:164:ARG:O	1:A:164:ARG:NH1	2.55	0.40
1:A:393:ASP:HB3	1:A:446:ASN:OD1	2.22	0.40
1:C:35:ALA:O	1:C:36:PRO:C	2.65	0.40
1:C:66:LEU:HD21	1:C:268:ARG:HG3	2.03	0.40

There are no symmetry-related clashes.

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	619/638 (97%)	587 (95%)	29 (5%)	3 (0%)	24	49
1	B	620/638 (97%)	581 (94%)	33 (5%)	6 (1%)	12	32
1	C	611/638 (96%)	576 (94%)	32 (5%)	3 (0%)	24	49
All	All	1850/1914 (97%)	1744 (94%)	94 (5%)	12 (1%)	21	45

All (12) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	285	LEU
1	B	102	ALA
1	B	244	PHE
1	C	209	SER
1	A	209	SER
1	B	127	PRO
1	B	216	SER
1	A	393	ASP
1	B	209	SER
1	C	127	PRO
1	A	103	GLY
1	B	520	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.

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	479/490 (98%)	431 (90%)	48 (10%)	7 20
1	B	480/490 (98%)	412 (86%)	68 (14%)	3 9
1	C	475/490 (97%)	404 (85%)	71 (15%)	3 8
All	All	1434/1470 (98%)	1247 (87%)	187 (13%)	4 12

All (187) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	THR
1	A	20	ASP
1	A	28	MET
1	A	33	GLN
1	A	44	THR
1	A	58	GLN
1	A	66	LEU
1	A	81	ARG
1	A	89	GLN
1	A	99	ASP
1	A	126	LEU
1	A	127	PRO
1	A	130	ARG
1	A	136	ASN
1	A	151	SER
1	A	152	LEU
1	A	196	THR
1	A	207	ASP
1	A	220	GLN
1	A	225	THR
1	A	234	ASP
1	A	282	THR
1	A	301	THR
1	A	317	VAL
1	A	318	VAL
1	A	340	GLN
1	A	353	MET
1	A	386	SER
1	A	409	GLN
1	A	419	ARG
1	A	434	SER

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Mol	Chain	Res	Type
1	A	440	ASP
1	A	442	VAL
1	A	455	ILE
1	A	477	LEU
1	A	496	LEU
1	A	525	ARG
1	A	563	LEU
1	A	580	GLU
1	A	581	SER
1	A	585	VAL
1	A	596	GLU
1	A	609	ILE
1	A	612	ASP
1	A	625	VAL
1	A	631	VAL
1	A	632	ARG
1	A	635	GLN
1	B	9	THR
1	B	20	ASP
1	B	23	ARG
1	B	26	ILE
1	B	28	MET
1	B	40	ASP
1	B	43	GLN
1	B	57	THR
1	B	58	GLN
1	B	68	ARG
1	B	79	SER
1	B	104	THR
1	B	105	LEU
1	B	118	LEU
1	B	126	LEU
1	B	130	ARG
1	B	156	ASP
1	B	171	SER
1	B	175	ASP
1	B	177	VAL
1	B	199	LEU
1	B	218	LEU
1	B	255	ASN
1	B	282	THR
1	B	287	LYS

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Mol	Chain	Res	Type
1	B	288	ARG
1	B	292	ASP
1	B	294	MET
1	B	301	THR
1	B	317	VAL
1	B	318	VAL
1	B	327	MET
1	B	344	CYS
1	B	380	ARG
1	B	385	LEU
1	B	386	SER
1	B	392	ASP
1	B	400	GLN
1	B	406	ASN
1	B	409	GLN
1	B	419	ARG
1	B	434	SER
1	B	442	VAL
1	B	460	GLU
1	B	505	ARG
1	B	506	ASP
1	B	511	GLN
1	B	531	HIS
1	B	536	LEU
1	B	537	SER
1	B	542	ARG
1	B	543	ARG
1	B	547	LEU
1	B	560	ASP
1	B	581	SER
1	B	585	VAL
1	B	591	GLN
1	B	593	LEU
1	B	595	VAL
1	B	605	GLU
1	B	606	LEU
1	B	609	ILE
1	B	612	ASP
1	B	622	VAL
1	B	625	VAL
1	B	631	VAL
1	B	632	ARG

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Mol	Chain	Res	Type
1	B	634	LEU
1	C	6	ILE
1	C	10	ILE
1	C	20	ASP
1	C	28	MET
1	C	44	THR
1	C	48	GLN
1	C	58	GLN
1	C	65	ASP
1	C	68	ARG
1	C	69	GLN
1	C	117	GLU
1	C	126	LEU
1	C	135	ASP
1	C	142	VAL
1	C	167	GLU
1	C	177	VAL
1	C	197	ARG
1	C	208	ARG
1	C	209	SER
1	C	210	LEU
1	C	220	GLN
1	C	225	THR
1	C	234	ASP
1	C	254	SER
1	C	266	MET
1	C	268	ARG
1	C	282	THR
1	C	288	ARG
1	C	295	ASN
1	C	307	ARG
1	C	318	VAL
1	C	327	MET
1	C	328	THR
1	C	329	GLN
1	C	336	SER
1	C	351	THR
1	C	352	LEU
1	C	362	LEU
1	C	380	ARG
1	C	385	LEU
1	C	386	SER

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Mol	Chain	Res	Type
1	C	400	GLN
1	C	409	GLN
1	C	415	ARG
1	C	435	PHE
1	C	443	HIS
1	C	446	ASN
1	C	455	ILE
1	C	460	GLU
1	C	467	LEU
1	C	469	VAL
1	C	475	MET
1	C	498	MET
1	C	505	ARG
1	C	506	ASP
1	C	525	ARG
1	C	545	ARG
1	C	560	ASP
1	C	566	ILE
1	C	580	GLU
1	C	591	GLN
1	C	594	GLU
1	C	595	VAL
1	C	600	ILE
1	C	606	LEU
1	C	609	ILE
1	C	611	ASP
1	C	622	VAL
1	C	625	VAL
1	C	631	VAL
1	C	632	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (5) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	GLN
1	A	456	GLN
1	B	75	GLN
1	B	363	GLN
1	B	550	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 5 ligands modelled in this entry, 2 are monoatomic - leaving 3 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	$\# Z > 2$
3	GLC	B	702	2	12,12,12	0.43	0	17,17,17	1.22	1 (5%)
3	GLC	A	702	-	12,12,12	0.81	0	17,17,17	1.61	4 (23%)
3	GLC	C	701	-	12,12,12	0.53	0	17,17,17	0.67	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	GLC	B	702	2	-	0/2/22/22	0/1/1/1
3	GLC	A	702	-	-	2/2/22/22	0/1/1/1
3	GLC	C	701	-	-	1/2/22/22	0/1/1/1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	702	GLC	O5-C5-C4	-3.41	103.56	109.70
3	A	702	GLC	C1-C2-C3	3.16	116.79	110.36
3	B	702	GLC	C3-C4-C5	-3.00	104.80	110.23
3	A	702	GLC	C1-O5-C5	-2.52	108.77	113.65
3	A	702	GLC	C4-C3-C2	2.44	115.11	110.83

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	A	702	GLC	O5-C5-C6-O6
3	A	702	GLC	C4-C5-C6-O6
3	C	701	GLC	O5-C5-C6-O6

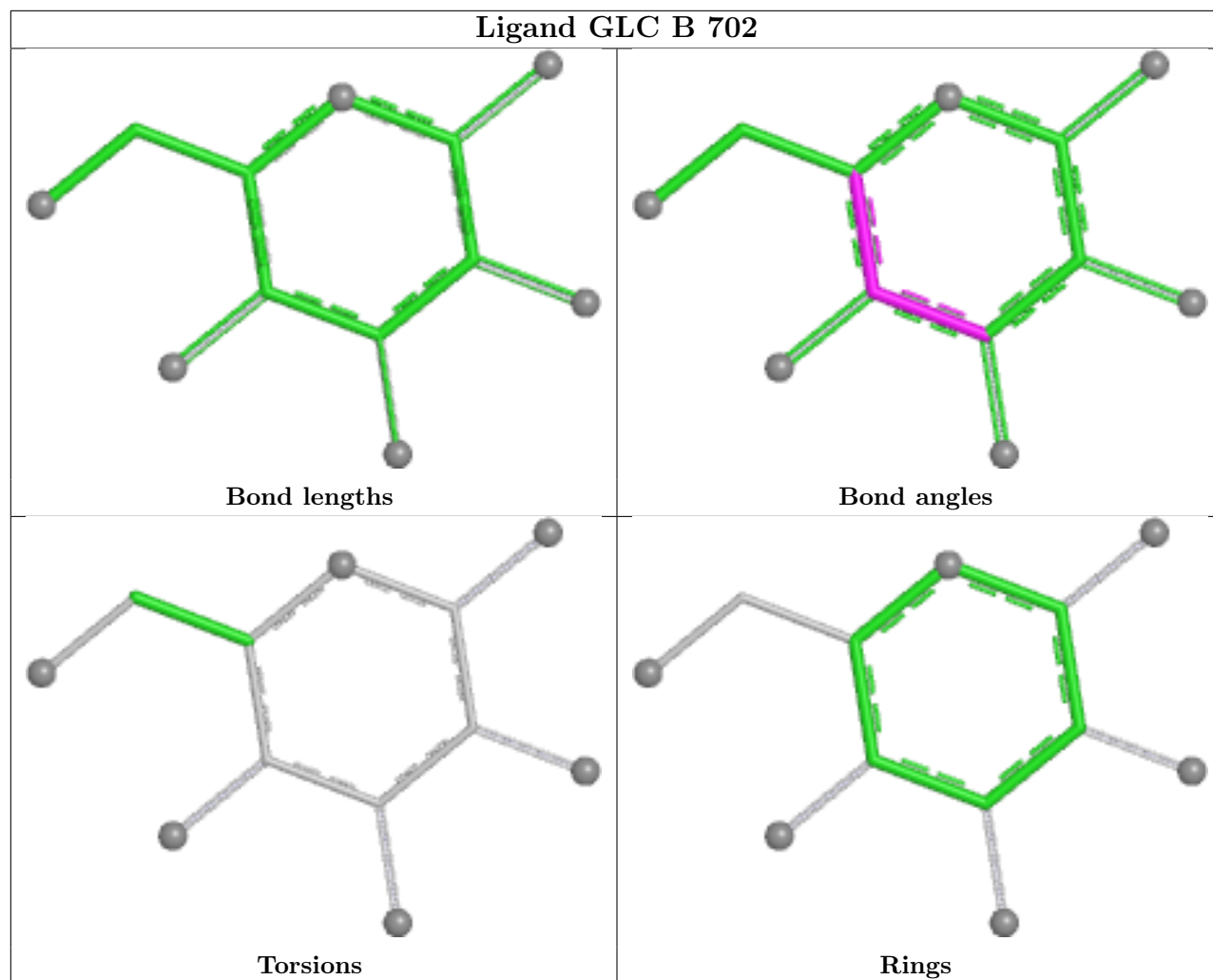
There are no ring outliers.

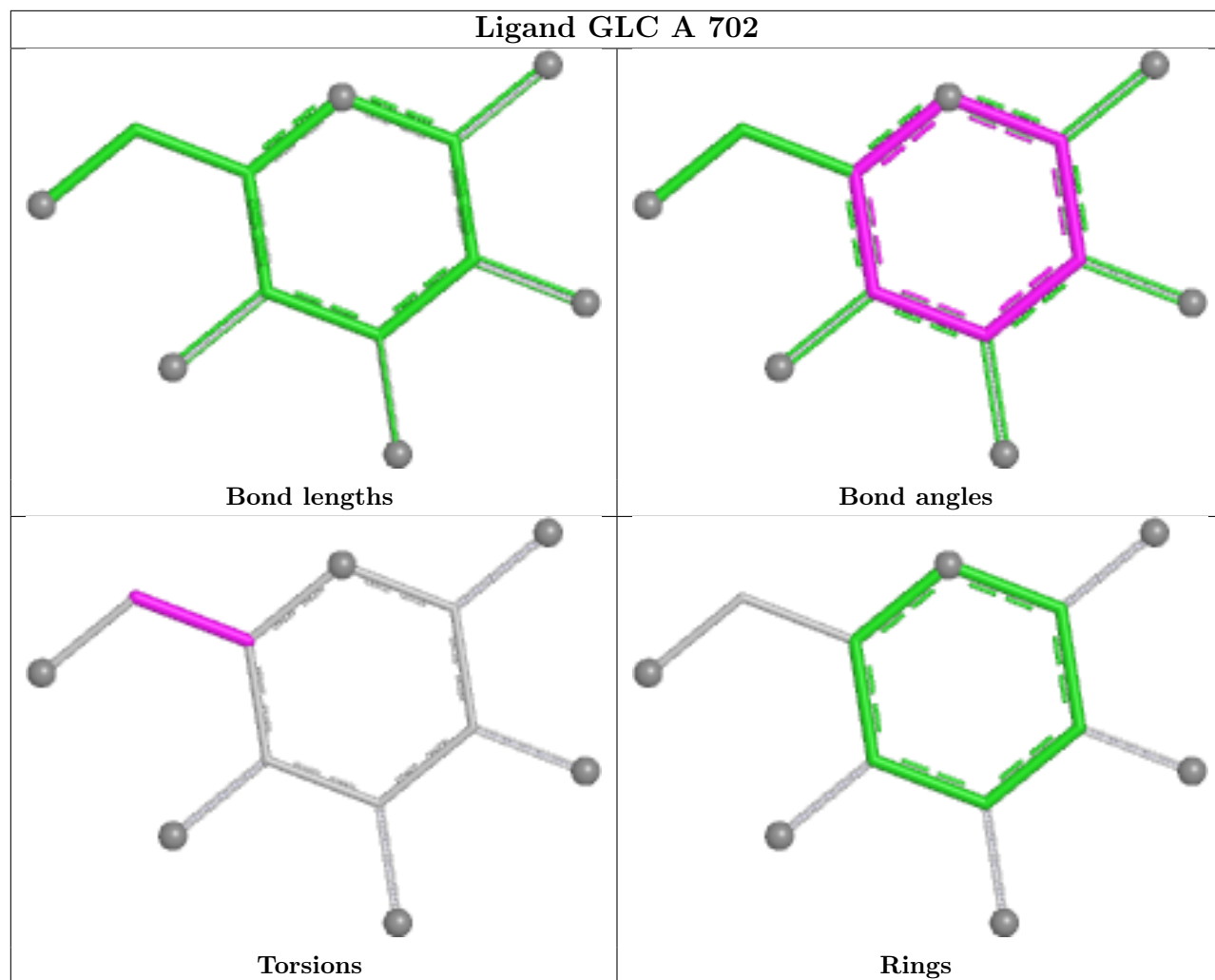
2 monomers are involved in 2 short contacts:

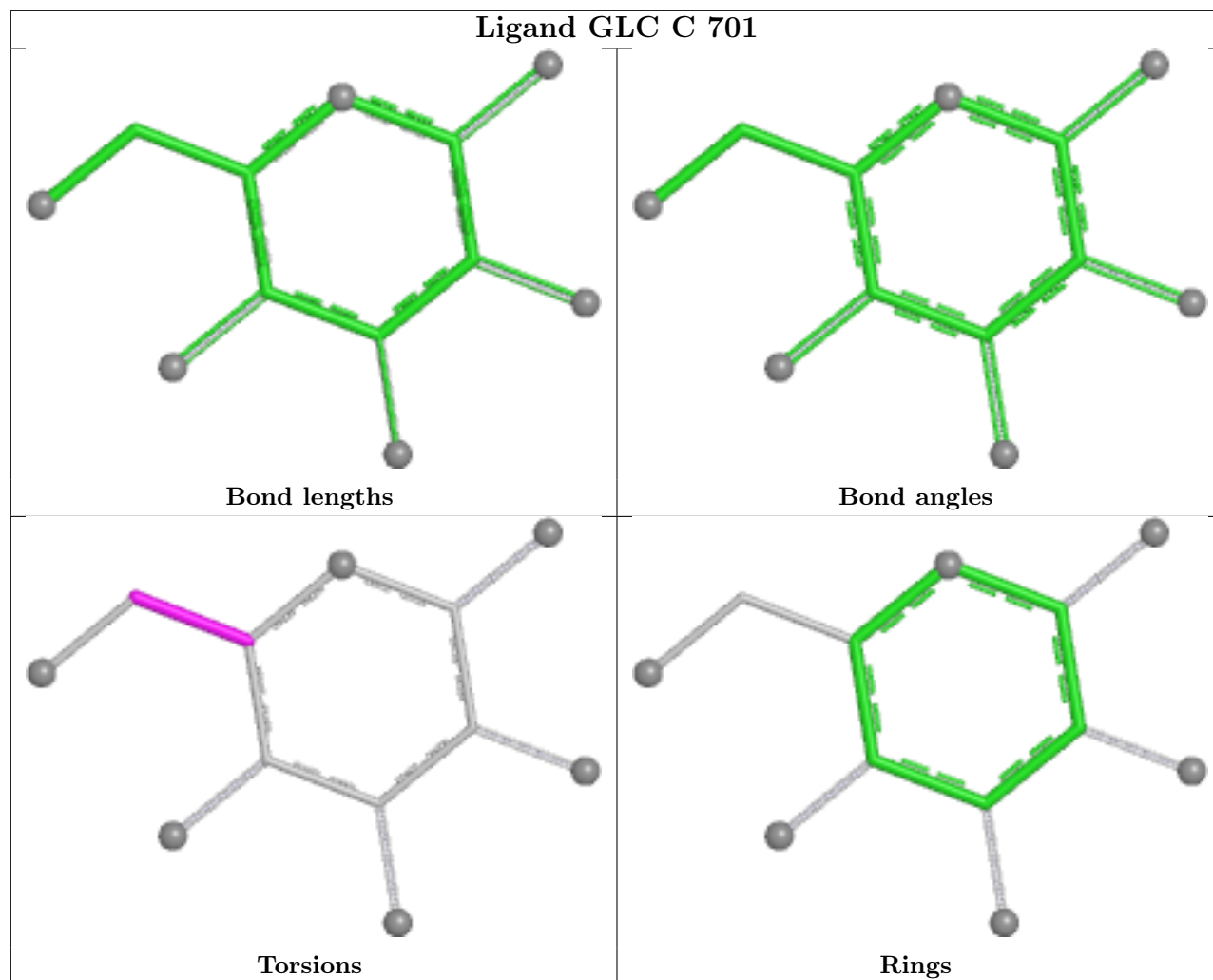
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	702	GLC	1	0
3	A	702	GLC	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand GLC B 702







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	623/638 (97%)	-0.19	1 (0%) 91 90	61, 102, 141, 181	0
1	B	624/638 (97%)	-0.10	0 100 100	75, 121, 174, 220	0
1	C	617/638 (96%)	-0.01	4 (0%) 85 82	78, 124, 164, 209	0
All	All	1864/1914 (97%)	-0.10	5 (0%) 90 88	61, 116, 164, 220	0

All (5) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	447	GLY	3.6
1	C	450	ALA	2.5
1	C	486	GLY	2.3
1	C	430	ALA	2.1
1	A	319	MET	2.1

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](#)

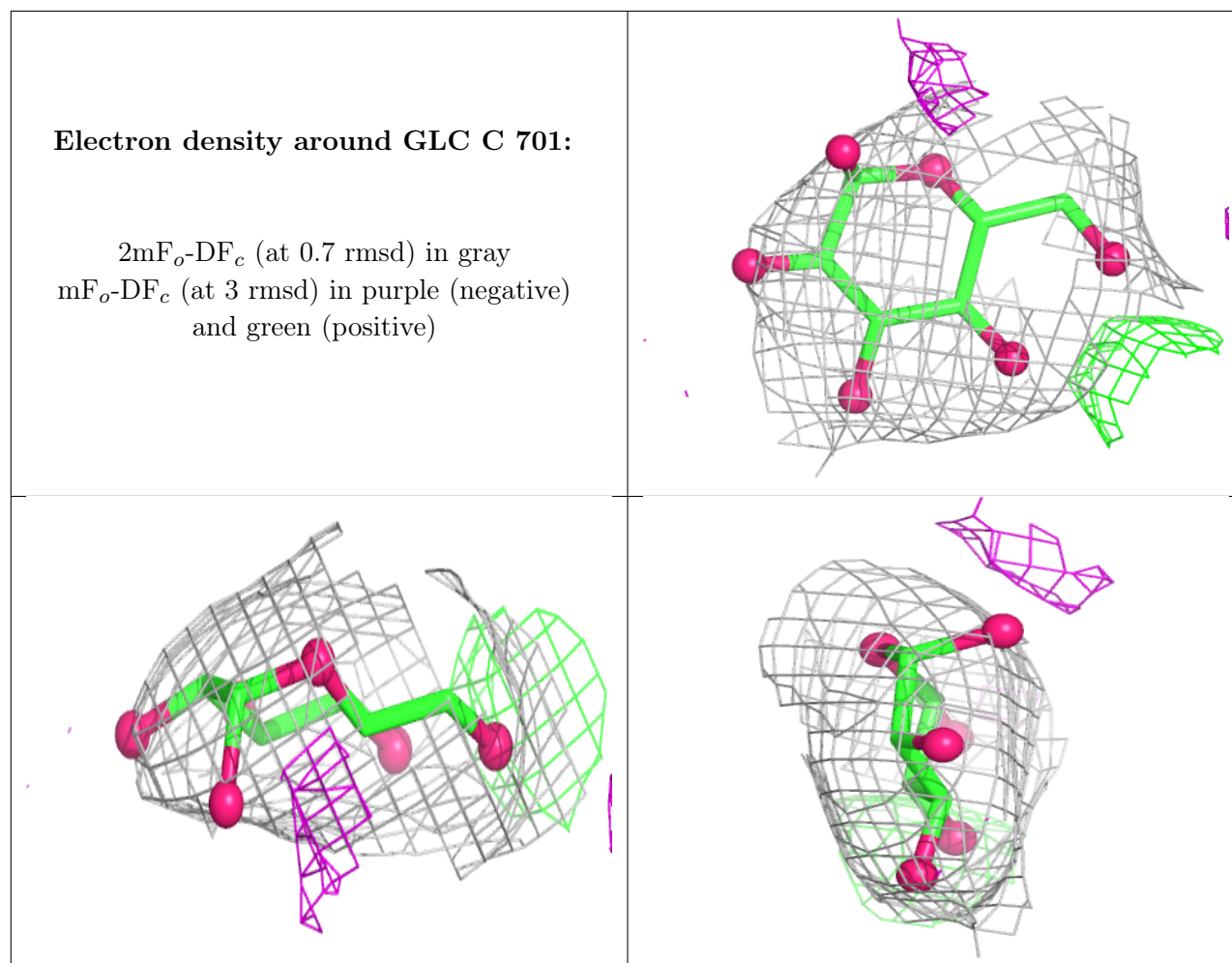
There are no oligosaccharides in this entry.

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.

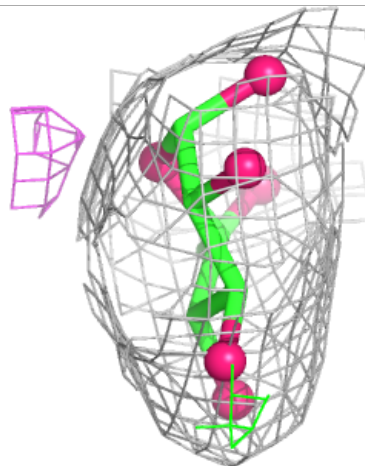
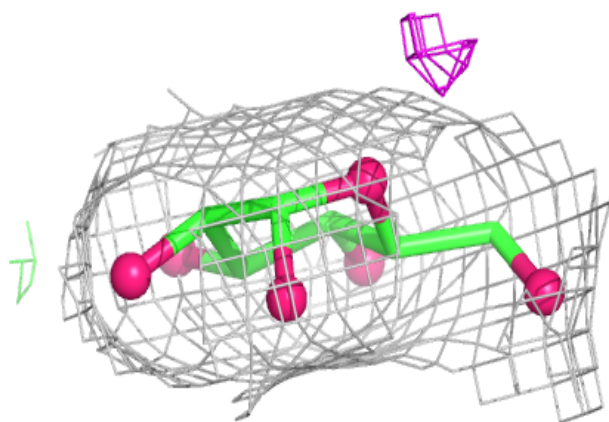
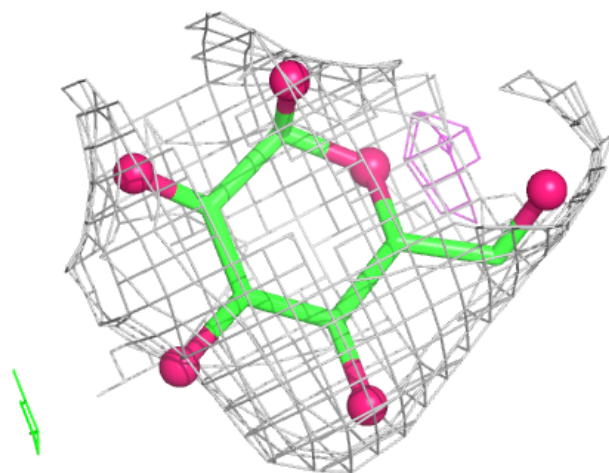
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	GLC	C	701	12/12	0.85	0.10	91,107,128,128	0
3	GLC	B	702	12/12	0.88	0.06	104,128,137,148	0
3	GLC	A	702	12/12	0.89	0.09	63,81,87,92	0
2	K	B	701	1/1	0.92	0.07	118,118,118,118	0
2	K	A	701	1/1	0.92	0.09	94,94,94,94	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



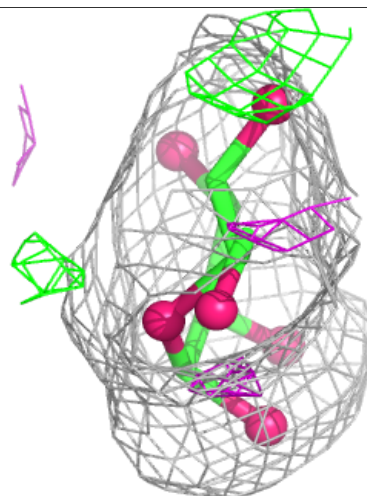
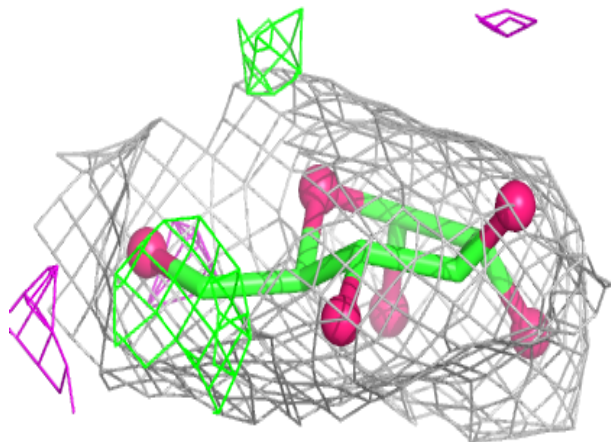
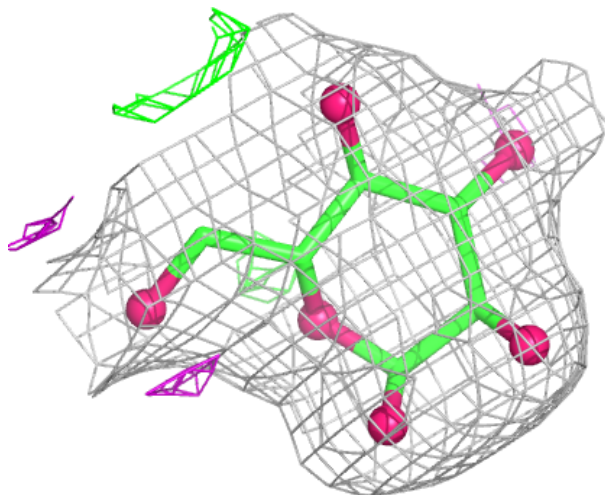
Electron density around GLC B 702:

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



Electron density around GLC A 702:

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



6.5 Other polymers [i](#)

There are no such residues in this entry.