



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 05:53 PM UTC

PDB ID : 7VQM / pdb_00007vqm
Title : GH2 beta-galacturonate AqGalA in complex with galacturonide
Authors : Yang, J.
Deposited on : 2021-10-20
Resolution : 2.40 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

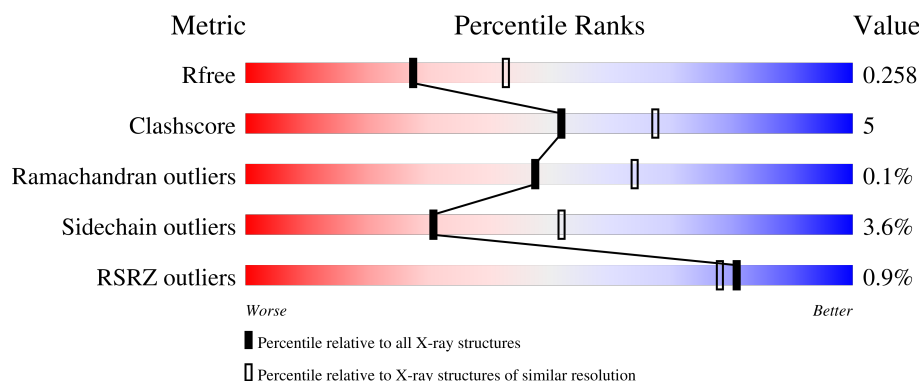
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.40 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	4912 (2.40-2.40)
Clashscore	190562	5391 (2.40-2.40)
Ramachandran outliers	187476	5320 (2.40-2.40)
Sidechain outliers	187428	5321 (2.40-2.40)
RSRZ outliers	180081	4916 (2.40-2.40)

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

Mol	Chain	Length	Quality of chain
1	A	605	
1	B	605	
1	C	605	
1	D	605	

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	GTR	A	702	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 20710 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.

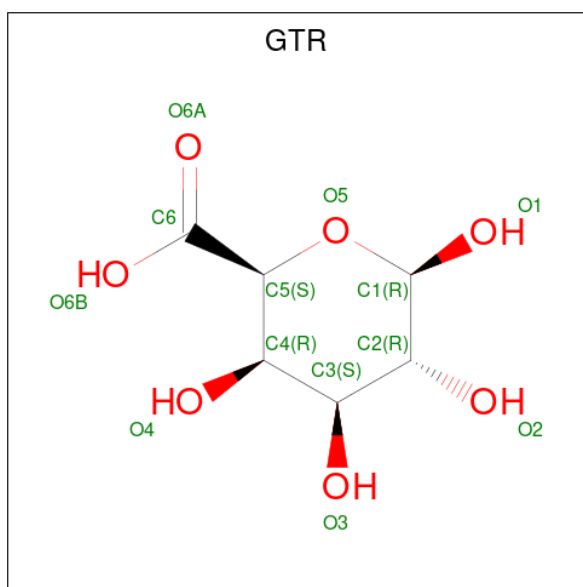
- Molecule 1 is a protein called GH2 beta-galacturonate AqGalA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	584	Total	C	N	O	S	0	0	0
			4847	3103	835	895	14			
1	B	584	Total	C	N	O	S	0	0	0
			4847	3103	835	895	14			
1	C	584	Total	C	N	O	S	0	0	0
			4847	3103	835	895	14			
1	D	584	Total	C	N	O	S	0	0	0
			4847	3103	835	895	14			

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Cl	0	0
			1	1		
2	B	1	Total	Cl	0	0
			1	1		
2	C	1	Total	Cl	0	0
			1	1		
2	D	1	Total	Cl	0	0
			1	1		

- Molecule 3 is beta-D-galactopyranuronic acid (CCD ID: GTR) (formula: C₆H₁₀O₇) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			13	6	7		
3	B	1	Total	C	O	0	0
			13	6	7		
3	C	1	Total	C	O	0	0
			13	6	7		
3	D	1	Total	C	O	0	0
			13	6	7		

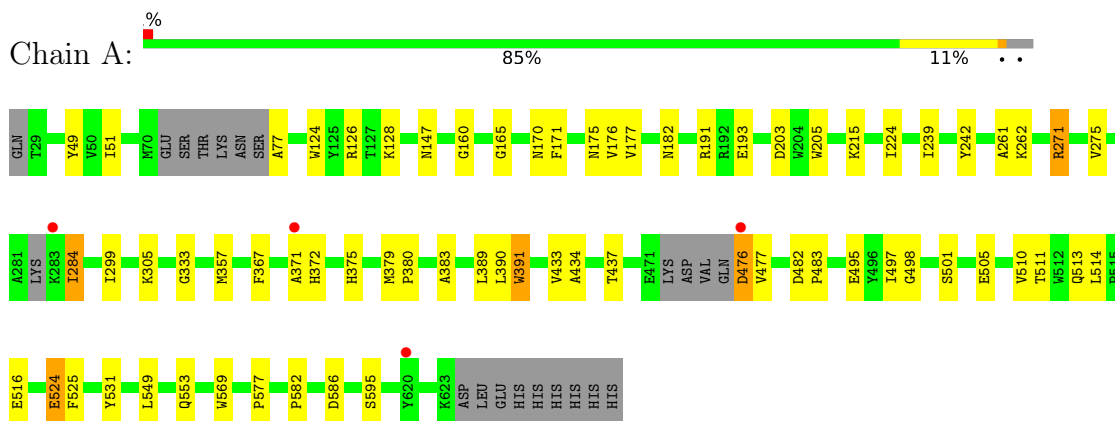
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	338	Total	O	0	0
			338	338		
4	B	299	Total	O	0	0
			299	299		
4	C	349	Total	O	0	0
			349	349		
4	D	280	Total	O	0	0
			280	280		

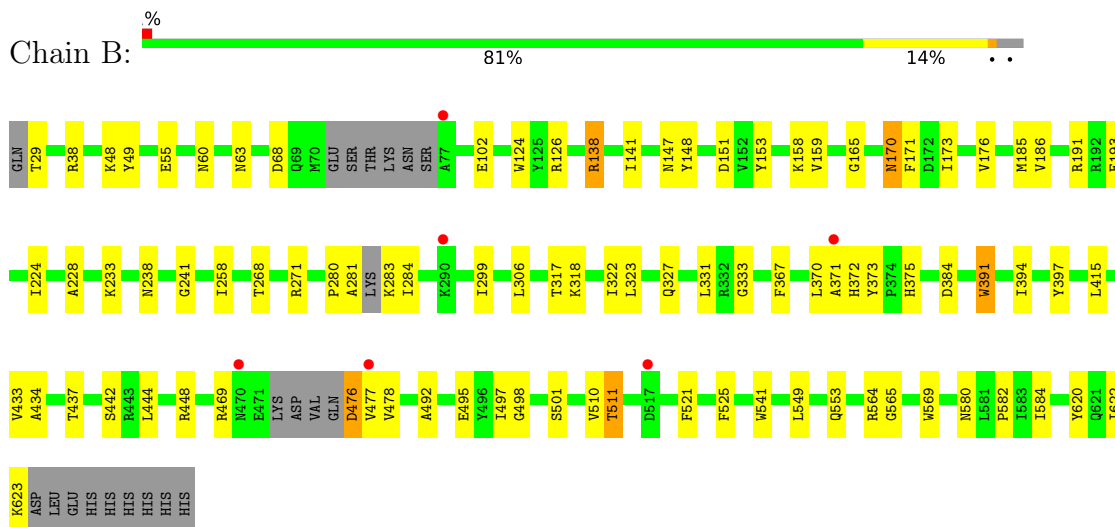
3 Residue-property plots

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.

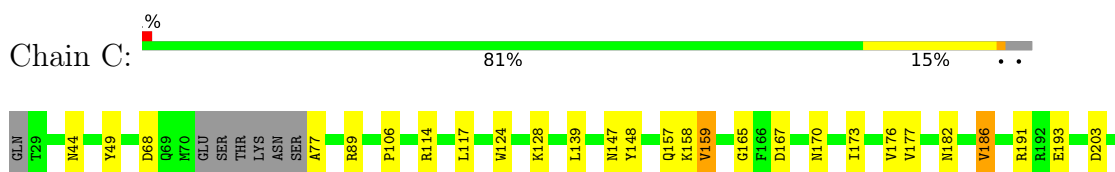
• Molecule 1: GH2 beta-galacturonate AqGalA

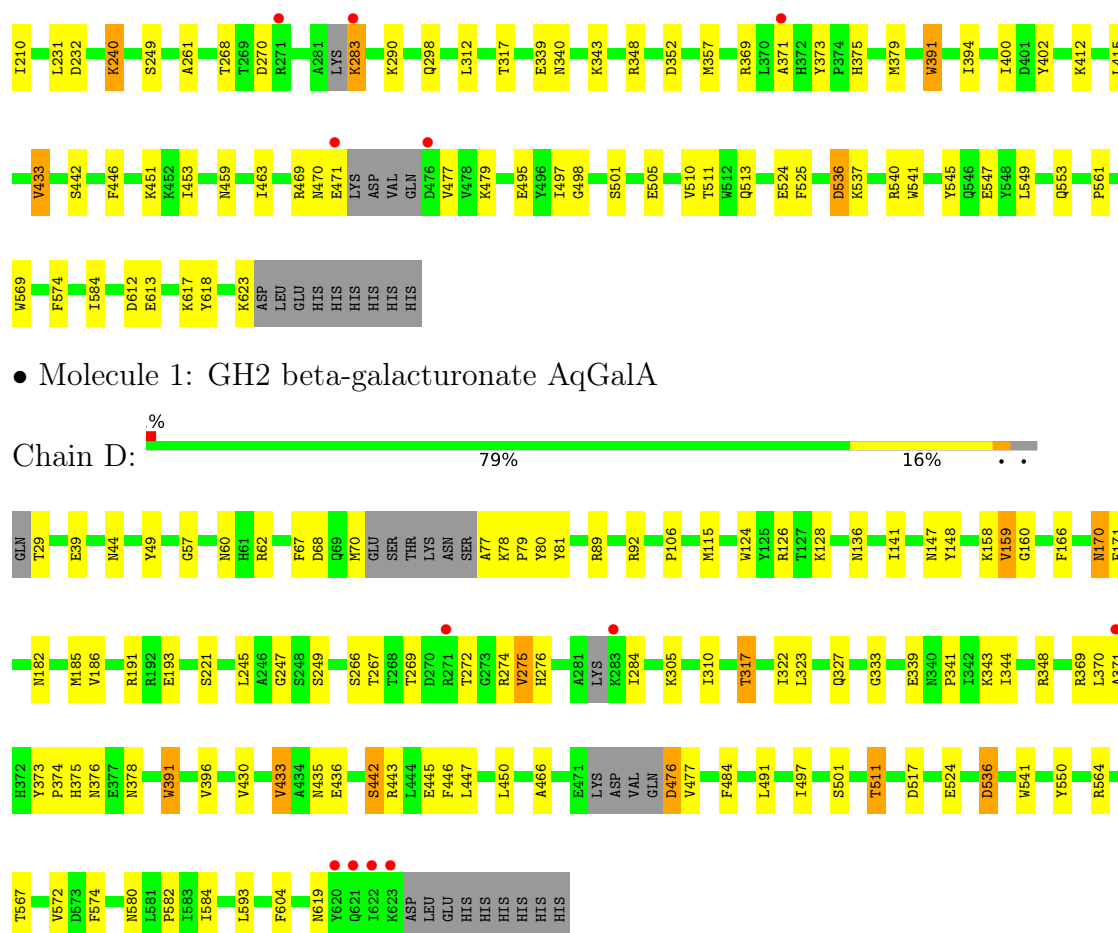


• Molecule 1: GH2 beta-galacturonate AqGalA

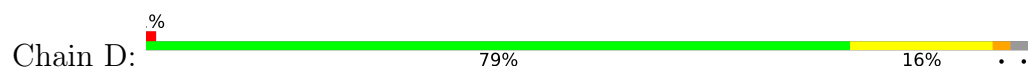


• Molecule 1: GH2 beta-galacturonate AqGalA





● Molecule 1: GH2 beta-galacturonate AqGalA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	83.41Å 154.01Å 115.92Å 90.00° 109.78° 90.00°	Depositor
Resolution (Å)	19.95 – 2.40 19.95 – 2.40	Depositor EDS
% Data completeness (in resolution range)	98.7 (19.95-2.40) 98.7 (19.95-2.40)	Depositor EDS
R_{merge}	0.14	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.25 (at 2.41Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.200 , 0.257 0.205 , 0.258	Depositor DCC
R_{free} test set	5373 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	17.7	Xtriage
Anisotropy	0.618	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 42.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	20710	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.75% 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: GTR, CL

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	1.00	1/4973 (0.0%)	1.30	3/6738 (0.0%)
1	B	1.00	0/4973	1.31	6/6738 (0.1%)
1	C	0.99	0/4973	1.31	13/6738 (0.2%)
1	D	0.99	0/4973	1.31	2/6738 (0.0%)
All	All	1.00	1/19892 (0.0%)	1.31	24/26952 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	C	0	1
1	D	0	3
All	All	0	5

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	514	LEU	N-CA	6.24	1.50	1.46

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	271	ARG	CG-CD-NE	6.74	126.82	112.00
1	B	511	THR	CB-CA-C	6.35	120.70	110.16
1	B	370	LEU	CA-C-N	6.26	133.51	121.54
1	B	370	LEU	C-N-CA	6.26	133.51	121.54
1	C	433	VAL	N-CA-CB	-5.97	105.64	112.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	384	ASP	CA-CB-CG	5.82	118.42	112.60
1	C	613	GLU	CB-CA-C	5.64	121.03	110.70
1	C	167	ASP	CB-CA-C	5.52	115.99	109.47
1	D	476	ASP	CA-CB-CG	5.43	118.03	112.60
1	C	352	ASP	CA-C-N	5.40	127.83	120.54
1	C	352	ASP	C-N-CA	5.40	127.83	120.54
1	C	114	ARG	CA-C-N	5.36	128.00	120.28
1	C	114	ARG	C-N-CA	5.36	128.00	120.28
1	C	547	GLU	CA-C-N	5.25	127.63	120.54
1	C	547	GLU	C-N-CA	5.25	127.63	120.54
1	B	55	GLU	CA-C-N	5.23	127.29	120.28
1	B	55	GLU	C-N-CA	5.23	127.29	120.28
1	D	317	THR	CB-CA-C	5.21	118.89	109.37
1	A	516	GLU	CA-C-N	5.16	130.57	122.11
1	A	516	GLU	C-N-CA	5.16	130.57	122.11
1	C	270	ASP	CA-C-N	5.12	127.39	120.38
1	C	270	ASP	C-N-CA	5.12	127.39	120.38
1	C	317	THR	CB-CA-C	5.07	119.06	109.37
1	C	446	PHE	CA-CB-CG	5.07	118.87	113.80

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	524	GLU	Peptide
1	C	524	GLU	Peptide
1	D	370	LEU	Peptide
1	D	396	VAL	Peptide
1	D	524	GLU	Peptide

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	4847	0	4734	39	0
1	B	4847	0	4734	50	0
1	C	4847	0	4734	58	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	D	4847	0	4734	55	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	13	0	9	6	0
3	B	13	0	9	4	0
3	C	13	0	9	2	0
3	D	13	0	9	1	0
4	A	338	0	0	5	0
4	B	299	0	0	2	0
4	C	349	0	0	5	0
4	D	280	0	0	6	0
All	All	20710	0	18972	197	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 5.

All (197) 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:498:GLY:HA3	1:B:549:LEU:HD13	1.47	0.95
1:C:371:ALA:HB2	1:C:375:HIS:NE2	1.94	0.82
1:B:569:TRP:CZ2	3:B:702:GTR:H3	2.15	0.82
1:D:77:ALA:N	4:D:801:HOH:O	2.13	0.82
1:B:623:LYS:NZ	4:B:801:HOH:O	2.13	0.81
1:C:536:ASP:OD1	1:D:89:ARG:NH1	2.14	0.80
1:D:497:ILE:O	1:D:501:SER:O	2.00	0.80
1:B:525:PHE:CD1	1:B:553:GLN:HG2	2.18	0.79
1:C:159:VAL:HG21	1:C:173:ILE:HG22	1.65	0.77
1:B:48:LYS:HE2	1:B:102:GLU:OE2	1.86	0.76
1:D:68:ASP:OD2	1:D:158:LYS:NZ	2.20	0.75
1:B:498:GLY:HA3	1:B:549:LEU:CD1	2.17	0.74
1:A:569:TRP:CZ2	3:A:702:GTR:H3	2.23	0.74
1:A:497:ILE:O	1:A:501:SER:O	2.05	0.74
1:B:371:ALA:HB2	1:B:375:HIS:NE2	2.03	0.73
1:C:525:PHE:CD1	1:C:553:GLN:HG2	2.22	0.73
1:A:203:ASP:OD2	3:A:702:GTR:O4	2.04	0.73
1:A:203:ASP:CG	3:A:702:GTR:HO4	1.96	0.72
1:A:495:GLU:OE2	1:A:553:GLN:OE1	2.08	0.71
1:C:617:LYS:NZ	4:C:1002:HOH:O	2.22	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:451:LYS:HG3	1:C:463:ILE:HG21	1.73	0.70
1:D:371:ALA:HB2	1:D:375:HIS:NE2	2.08	0.69
1:C:203:ASP:OD2	3:C:702:GTR:O4	2.12	0.68
1:D:49:TYR:HA	1:D:124:TRP:O	1.93	0.68
1:A:372:HIS:NE2	3:A:702:GTR:O2	2.27	0.67
1:B:29:THR:N	4:B:802:HOH:O	2.26	0.67
1:A:77:ALA:N	4:A:804:HOH:O	2.28	0.67
1:A:525:PHE:CD1	1:A:553:GLN:HG2	2.29	0.67
1:C:497:ILE:O	1:C:501:SER:O	2.13	0.66
1:C:191:ARG:HD3	1:C:193:GLU:OE2	1.96	0.66
1:A:191:ARG:HD3	1:A:193:GLU:OE2	1.97	0.65
1:A:498:GLY:HA3	1:A:549:LEU:HD13	1.80	0.64
1:B:159:VAL:HG11	1:B:173:ILE:HG22	1.77	0.64
1:B:497:ILE:O	1:B:501:SER:O	2.15	0.64
1:C:469:ARG:NH2	4:C:1006:HOH:O	2.29	0.64
1:D:267:THR:HG21	1:D:275:VAL:HG21	1.80	0.64
1:C:77:ALA:N	4:C:1009:HOH:O	2.32	0.63
1:A:49:TYR:HA	1:A:124:TRP:O	1.99	0.63
1:B:525:PHE:CE1	1:B:553:GLN:HG2	2.34	0.62
1:B:371:ALA:CB	1:B:375:HIS:NE2	2.63	0.61
1:B:224:ILE:HD13	1:B:299:ILE:HG22	1.83	0.61
1:D:77:ALA:N	4:D:805:HOH:O	2.34	0.61
1:B:569:TRP:CE2	3:B:702:GTR:H3	2.36	0.60
1:A:371:ALA:HB2	1:A:375:HIS:NE2	2.17	0.59
1:B:281:ALA:O	1:B:283:LYS:N	2.35	0.59
1:B:333:GLY:HA2	1:B:367:PHE:O	2.02	0.59
1:B:372:HIS:NE2	3:B:702:GTR:O2	2.36	0.58
1:C:371:ALA:CB	1:C:375:HIS:NE2	2.64	0.58
1:B:495:GLU:OE2	1:B:553:GLN:OE1	2.21	0.58
1:B:228:ALA:O	1:B:241:GLY:HA3	2.04	0.57
1:D:445:GLU:OE1	4:D:802:HOH:O	2.17	0.57
1:B:138:ARG:HG2	1:B:138:ARG:HH11	1.71	0.56
1:B:49:TYR:HA	1:B:124:TRP:O	2.06	0.56
1:D:191:ARG:HD3	1:D:193:GLU:OE2	2.05	0.56
1:D:371:ALA:CB	1:D:375:HIS:NE2	2.69	0.56
1:C:49:TYR:HA	1:C:124:TRP:O	2.06	0.55
1:C:495:GLU:OE2	1:C:553:GLN:NE2	2.40	0.55
1:D:160:GLY:HA3	1:D:171:PHE:CE1	2.42	0.55
1:A:383:ALA:CB	1:A:390:LEU:HD11	2.37	0.55
1:A:261:ALA:O	1:A:262:LYS:HB2	2.06	0.55
1:D:443:ARG:O	1:D:446:PHE:HB3	2.07	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:89:ARG:NH1	1:D:536:ASP:OD1	2.41	0.54
1:B:371:ALA:HB1	1:B:373:TYR:CZ	2.43	0.54
1:D:447:LEU:HB3	1:D:484:PHE:CE2	2.41	0.54
1:B:191:ARG:HD3	1:B:193:GLU:OE2	2.07	0.54
1:C:186:VAL:HG21	1:C:210:ILE:HD11	1.91	0.53
1:A:371:ALA:CB	1:A:375:HIS:NE2	2.73	0.52
1:A:525:PHE:CE1	1:A:553:GLN:HG2	2.44	0.52
1:C:525:PHE:CE1	1:C:553:GLN:HG2	2.44	0.52
1:D:274:ARG:HD3	1:D:276:HIS:NE2	2.25	0.52
1:C:128:LYS:HA	1:C:182:ASN:O	2.09	0.52
1:D:322:ILE:HD12	1:D:564:ARG:HB3	1.92	0.51
1:D:29:THR:N	4:D:815:HOH:O	2.43	0.51
1:C:117:LEU:CD2	1:D:115:MET:HE2	2.41	0.51
1:C:186:VAL:CG2	1:C:210:ILE:HD11	2.40	0.51
1:C:117:LEU:HD23	1:D:115:MET:HE2	1.92	0.50
1:C:343:LYS:HG2	1:C:343:LYS:O	2.11	0.50
1:D:67:PHE:HA	1:D:70:MET:HE2	1.91	0.50
1:C:525:PHE:CG	1:C:553:GLN:HG2	2.47	0.50
1:B:397:TYR:OH	3:B:702:GTR:H2	2.13	0.49
1:D:44:ASN:CG	1:D:106:PRO:HD3	2.38	0.49
1:B:331:LEU:HB2	1:B:565:GLY:HA3	1.95	0.49
1:C:261:ALA:O	1:C:283:LYS:HD2	2.12	0.49
1:C:498:GLY:HA3	1:C:549:LEU:CD1	2.43	0.49
1:D:221:SER:O	1:D:247:GLY:HA3	2.13	0.49
1:B:394:ILE:HD13	1:B:415:LEU:HB2	1.95	0.48
1:D:341:PRO:HG3	1:D:572:VAL:HG21	1.96	0.48
1:C:173:ILE:HD12	1:C:177:VAL:CG1	2.42	0.48
1:A:531:TYR:HB2	1:A:595:SER:HB3	1.94	0.48
1:C:498:GLY:HA3	1:C:549:LEU:HD13	1.94	0.48
1:D:128:LYS:HA	1:D:182:ASN:O	2.13	0.48
1:A:513:GLN:NE2	4:A:823:HOH:O	2.47	0.48
1:A:524:GLU:OE1	3:A:702:GTR:H1	2.14	0.47
1:C:159:VAL:CG2	1:C:173:ILE:HG22	2.41	0.47
1:A:160:GLY:HA3	1:A:171:PHE:CE1	2.49	0.47
1:C:479:LYS:HE3	1:C:513:GLN:NE2	2.29	0.47
1:B:147:ASN:HA	1:B:165:GLY:HA2	1.96	0.47
1:C:617:LYS:HG2	1:C:618:TYR:CD1	2.49	0.47
1:A:582:PRO:HA	1:A:586:ASP:OD1	2.14	0.47
1:B:580:ASN:O	1:B:582:PRO:HD3	2.15	0.47
1:D:147:ASN:HA	1:D:148:TYR:HA	1.76	0.47
1:B:147:ASN:HA	1:B:148:TYR:HA	1.71	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:495:GLU:CD	1:C:553:GLN:HE22	2.24	0.46
1:C:540:ARG:NE	1:D:92:ARG:HB2	2.30	0.46
1:C:612:ASP:O	4:C:1001:HOH:O	2.21	0.46
1:B:141:ILE:O	1:B:170:ASN:HA	2.16	0.46
1:A:357:MET:HE1	1:A:379:MET:O	2.16	0.46
1:A:333:GLY:HA2	1:A:367:PHE:O	2.16	0.45
1:D:267:THR:CG2	1:D:275:VAL:HG21	2.46	0.45
1:D:391:TRP:CE3	1:D:430:VAL:HG11	2.51	0.45
1:B:476:ASP:OD1	1:B:476:ASP:N	2.49	0.45
1:C:44:ASN:CG	1:C:106:PRO:HD3	2.42	0.45
1:D:339:GLU:OE2	1:D:574:PHE:HA	2.17	0.45
1:C:477:VAL:HG12	1:C:511:THR:OG1	2.16	0.45
1:D:191:ARG:NH1	4:D:835:HOH:O	2.49	0.45
1:D:477:VAL:HG12	1:D:511:THR:OG1	2.16	0.45
1:B:38:ARG:NH2	1:B:306:LEU:HD12	2.32	0.45
1:D:136:ASN:O	1:D:221:SER:HB3	2.17	0.45
1:D:436:GLU:OE2	3:D:702:GTR:H1	2.17	0.45
1:B:323:LEU:HA	1:B:327:GLN:O	2.17	0.45
1:D:376:ASN:OD1	1:D:378:ASN:HB2	2.17	0.45
1:D:435:ASN:HA	1:D:466:ALA:HB3	1.99	0.45
1:D:166:PHE:O	1:D:374:PRO:HG2	2.17	0.45
1:D:57:GLY:HA3	1:D:80:TYR:CD2	2.52	0.44
1:B:68:ASP:OD2	1:B:158:LYS:NZ	2.48	0.44
1:B:327:GLN:HG2	1:B:620:TYR:CD1	2.52	0.44
1:C:147:ASN:HA	1:C:148:TYR:HA	1.59	0.44
1:D:141:ILE:O	1:D:170:ASN:HA	2.17	0.44
1:A:205:TRP:CE3	1:A:577:PRO:HD3	2.52	0.44
1:A:379:MET:HB2	1:A:380:PRO:CD	2.47	0.44
1:C:469:ARG:HD2	1:C:471:GLU:OE2	2.17	0.44
1:D:391:TRP:C	1:D:391:TRP:CD1	2.95	0.44
1:D:60:ASN:OD1	1:D:62:ARG:N	2.46	0.44
1:A:147:ASN:HA	1:A:165:GLY:HA2	2.00	0.44
1:A:391:TRP:C	1:A:391:TRP:CD1	2.96	0.44
1:C:357:MET:HE1	1:C:379:MET:O	2.18	0.44
1:C:525:PHE:CD1	1:C:525:PHE:C	2.96	0.44
1:D:333:GLY:HA3	1:D:567:THR:HG22	2.00	0.44
1:A:128:LYS:HA	1:A:182:ASN:O	2.18	0.43
1:D:442:SER:HB2	4:D:999:HOH:O	2.18	0.43
1:A:77:ALA:HB2	4:A:1103:HOH:O	2.18	0.43
1:A:476:ASP:N	4:A:830:HOH:O	2.50	0.43
1:C:623:LYS:O	1:C:623:LYS:HG3	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:322:ILE:HD12	1:B:564:ARG:HB3	2.00	0.43
1:D:81:TYR:HA	1:D:185:MET:HG2	2.00	0.43
1:B:434:ALA:HB1	1:B:437:THR:HG21	2.01	0.43
1:B:444:LEU:HD21	1:B:448:ARG:NH1	2.34	0.43
1:C:541:TRP:CD2	1:C:584:ILE:HG21	2.54	0.43
1:C:545:TYR:C	1:C:545:TYR:CD1	2.97	0.43
1:D:369:ARG:HG3	1:D:391:TRP:CD1	2.53	0.43
1:D:371:ALA:HB1	1:D:373:TYR:CZ	2.54	0.42
1:A:383:ALA:HB2	1:A:390:LEU:HD11	2.00	0.42
1:B:541:TRP:CD2	1:B:584:ILE:HG21	2.55	0.42
1:C:68:ASP:OD2	1:C:158:LYS:NZ	2.44	0.42
1:A:569:TRP:CE2	3:A:702:GTR:H3	2.55	0.42
1:A:239:ILE:HD11	1:A:284:ILE:HD13	2.00	0.42
1:B:391:TRP:CD1	1:B:391:TRP:C	2.96	0.42
1:B:622:ILE:O	1:B:623:LYS:C	2.62	0.42
1:B:151:ASP:OD2	1:B:158:LYS:NZ	2.47	0.42
1:C:569:TRP:CE2	3:C:702:GTR:H4	2.54	0.42
1:A:224:ILE:HD13	1:A:299:ILE:HG22	2.00	0.42
1:C:369:ARG:HG3	1:C:391:TRP:CD1	2.54	0.42
1:D:323:LEU:HA	1:D:327:GLN:O	2.20	0.42
1:D:550:TYR:CZ	1:D:593:LEU:HD21	2.54	0.42
1:C:139:LEU:HD23	1:C:177:VAL:HG11	2.02	0.42
1:A:482:ASP:HA	1:A:483:PRO:HD2	1.84	0.41
1:B:153:TYR:HB2	1:B:185:MET:HB3	2.01	0.41
1:A:175:ASN:HB2	4:A:907:HOH:O	2.19	0.41
1:C:412:LYS:HG3	1:C:453:ILE:HD13	2.01	0.41
1:D:433:VAL:HG22	1:D:450:LEU:HB3	2.02	0.41
1:B:327:GLN:HG2	1:B:620:TYR:CG	2.55	0.41
1:B:492:ALA:HA	1:B:521:PHE:O	2.21	0.41
1:C:394:ILE:HD13	1:C:415:LEU:HB2	2.03	0.41
1:C:561:PRO:HD2	4:C:1048:HOH:O	2.21	0.41
1:D:541:TRP:CD2	1:D:584:ILE:HG21	2.55	0.41
1:A:242:TYR:HA	1:A:275:VAL:O	2.20	0.41
1:D:78:LYS:N	1:D:79:PRO:CD	2.84	0.41
1:B:469:ARG:HB2	1:B:478:VAL:HG13	2.02	0.41
1:C:157:GLN:OE1	1:C:176:VAL:HG23	2.21	0.41
1:C:231:LEU:HG	1:C:312:LEU:HB3	2.01	0.41
1:A:367:PHE:HA	1:A:389:LEU:O	2.21	0.41
1:B:159:VAL:CG1	1:B:171:PHE:HB3	2.51	0.41
1:B:318:LYS:HB2	1:B:323:LEU:HD22	2.03	0.41
1:C:232:ASP:CG	1:C:240:LYS:HE3	2.46	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:434:ALA:HB1	1:A:437:THR:HG21	2.03	0.41
1:B:238:ASN:HA	1:B:280:PRO:HA	2.03	0.40
1:C:339:GLU:OE1	1:C:574:PHE:HA	2.21	0.40
1:D:580:ASN:O	1:D:582:PRO:HD3	2.20	0.40
1:C:400:ILE:HB	1:C:402:TYR:CZ	2.56	0.40
1:C:495:GLU:CD	1:C:553:GLN:NE2	2.79	0.40
1:D:159:VAL:HG13	1:D:171:PHE:HB3	2.03	0.40
1:C:147:ASN:HA	1:C:165:GLY:HA2	2.01	0.40
1:C:340:ASN:OD1	1:C:340:ASN:C	2.64	0.40
1:C:371:ALA:HB1	1:C:373:TYR:CZ	2.57	0.40
1:D:245:LEU:HD12	1:D:269:THR:HG21	2.04	0.40
1:D:604:PHE:CD1	1:D:604:PHE:C	3.00	0.40
1:B:60:ASN:HB3	1:B:63:ASN:OD1	2.21	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	576/605 (95%)	549 (95%)	27 (5%)	0	100	100
1	B	576/605 (95%)	543 (94%)	33 (6%)	0	100	100
1	C	576/605 (95%)	548 (95%)	27 (5%)	1 (0%)	43	58
1	D	576/605 (95%)	546 (95%)	29 (5%)	1 (0%)	43	58
All	All	2304/2420 (95%)	2186 (95%)	116 (5%)	2 (0%)	48	64

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	348	ARG
1	C	348	ARG

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	522/543 (96%)	506 (97%)	16 (3%)	35	57
1	B	522/543 (96%)	504 (97%)	18 (3%)	32	54
1	C	522/543 (96%)	504 (97%)	18 (3%)	32	54
1	D	522/543 (96%)	498 (95%)	24 (5%)	24	41
All	All	2088/2172 (96%)	2012 (96%)	76 (4%)	31	52

All (76) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	51	ILE
1	A	126	ARG
1	A	170	ASN
1	A	176	VAL
1	A	177	VAL
1	A	215	LYS
1	A	271	ARG
1	A	284	ILE
1	A	305	LYS
1	A	391	TRP
1	A	433	VAL
1	A	476	ASP
1	A	477	VAL
1	A	505	GLU
1	A	510	VAL
1	A	511	THR
1	B	126	ARG
1	B	138	ARG
1	B	170	ASN
1	B	176	VAL
1	B	186	VAL
1	B	233	LYS
1	B	258	ILE
1	B	268	THR

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Mol	Chain	Res	Type
1	B	271	ARG
1	B	284	ILE
1	B	317	THR
1	B	391	TRP
1	B	433	VAL
1	B	442	SER
1	B	476	ASP
1	B	477	VAL
1	B	510	VAL
1	B	511	THR
1	C	159	VAL
1	C	170	ASN
1	C	186	VAL
1	C	240	LYS
1	C	249	SER
1	C	268	THR
1	C	283	LYS
1	C	290	LYS
1	C	298	GLN
1	C	391	TRP
1	C	433	VAL
1	C	442	SER
1	C	459	ASN
1	C	470	ASN
1	C	505	GLU
1	C	510	VAL
1	C	536	ASP
1	C	537	LYS
1	D	39	GLU
1	D	126	ARG
1	D	159	VAL
1	D	170	ASN
1	D	186	VAL
1	D	249	SER
1	D	266	SER
1	D	272	THR
1	D	275	VAL
1	D	284	ILE
1	D	305	LYS
1	D	310	ILE
1	D	317	THR
1	D	343	LYS

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Mol	Chain	Res	Type
1	D	344	ILE
1	D	391	TRP
1	D	433	VAL
1	D	442	SER
1	D	476	ASP
1	D	491	LEU
1	D	511	THR
1	D	517	ASP
1	D	536	ASP
1	D	619	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (17) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	37	ASN
1	A	253	ASN
1	A	298	GLN
1	A	309	GLN
1	A	449	GLN
1	A	470	ASN
1	A	553	GLN
1	B	34	ASN
1	B	37	ASN
1	B	46	ASN
1	B	253	ASN
1	B	513	GLN
1	B	605	HIS
1	C	195	HIS
1	C	238	ASN
1	C	410	GLN
1	D	414	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 [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 8 ligands modelled in this entry, 4 are monoatomic - leaving 4 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	GTR	C	702	-	13,13,13	1.77	3 (23%)	18,19,19	2.63	7 (38%)
3	GTR	B	702	-	13,13,13	2.03	3 (23%)	18,19,19	1.75	7 (38%)
3	GTR	A	702	-	13,13,13	2.17	3 (23%)	18,19,19	1.92	5 (27%)
3	GTR	D	702	-	13,13,13	1.69	2 (15%)	18,19,19	1.68	5 (27%)

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	GTR	C	702	-	-	1/4/24/24	0/1/1/1
3	GTR	B	702	-	-	0/4/24/24	0/1/1/1
3	GTR	A	702	-	-	0/4/24/24	0/1/1/1
3	GTR	D	702	-	-	2/4/24/24	0/1/1/1

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	702	GTR	O5-C5	4.56	1.52	1.43
3	B	702	GTR	O5-C1	4.47	1.53	1.42
3	A	702	GTR	O5-C1	4.33	1.53	1.42
3	D	702	GTR	O5-C1	3.74	1.52	1.42
3	B	702	GTR	O3-C3	3.73	1.52	1.43
3	C	702	GTR	O5-C1	3.68	1.51	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	702	GTR	O5-C5	3.52	1.50	1.43
3	B	702	GTR	O5-C5	3.51	1.50	1.43
3	A	702	GTR	O3-C3	3.25	1.51	1.43
3	C	702	GTR	O5-C5	3.13	1.49	1.43
3	C	702	GTR	C4-C5	2.28	1.56	1.53

All (24) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	702	GTR	C1-O5-C5	6.47	121.75	112.22
3	C	702	GTR	O5-C1-C2	4.95	119.00	110.30
3	A	702	GTR	O6B-C6-O6A	-3.95	115.12	124.08
3	D	702	GTR	O6B-C6-O6A	-3.92	115.19	124.08
3	C	702	GTR	C1-C2-C3	3.73	117.96	110.36
3	A	702	GTR	O5-C5-C6	3.39	116.75	106.14
3	B	702	GTR	O5-C5-C6	3.32	116.52	106.14
3	C	702	GTR	C3-C4-C5	3.28	114.93	109.30
3	B	702	GTR	O3-C3-C4	3.20	117.92	110.38
3	C	702	GTR	O5-C5-C4	2.90	115.20	109.48
3	C	702	GTR	C4-C3-C2	2.87	115.87	110.83
3	C	702	GTR	O6B-C6-O6A	-2.81	117.72	124.08
3	A	702	GTR	C3-C4-C5	2.74	114.01	109.30
3	A	702	GTR	O3-C3-C4	2.74	116.83	110.38
3	D	702	GTR	C1-O5-C5	2.68	116.17	112.22
3	D	702	GTR	O6B-C6-C5	2.43	122.41	113.64
3	B	702	GTR	O5-C1-C2	2.42	114.55	110.30
3	A	702	GTR	O4-C4-C5	-2.37	104.35	109.76
3	D	702	GTR	C3-C4-C5	2.28	113.21	109.30
3	D	702	GTR	O5-C1-C2	2.26	114.28	110.30
3	B	702	GTR	O6B-C6-O6A	-2.20	119.08	124.08
3	B	702	GTR	O2-C2-C3	-2.20	105.20	110.38
3	B	702	GTR	C3-C4-C5	2.13	112.96	109.30
3	B	702	GTR	O4-C4-C5	-2.12	104.92	109.76

There are no chirality outliers.

All (3) torsion outliers are listed below:

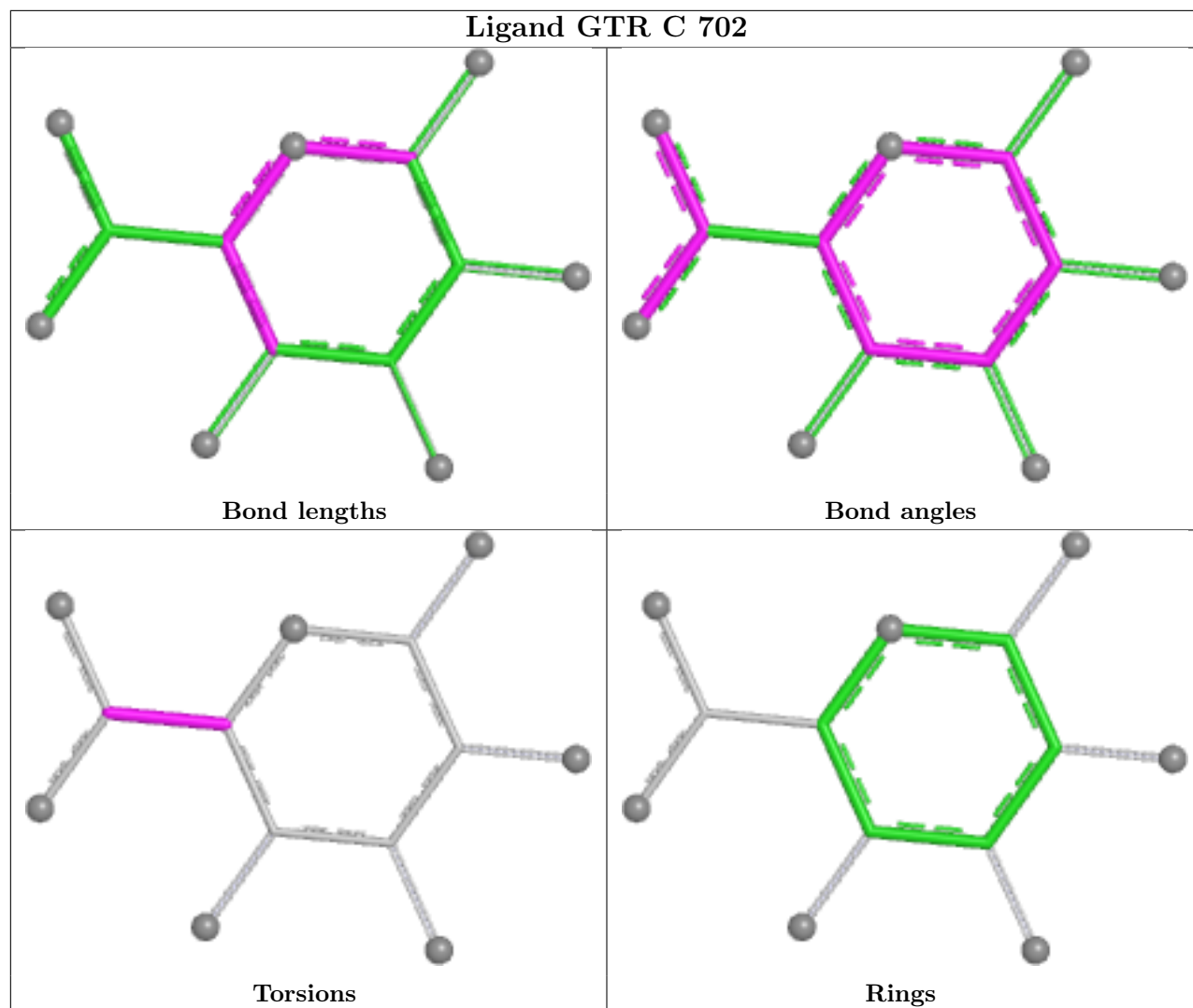
Mol	Chain	Res	Type	Atoms
3	C	702	GTR	O5-C5-C6-O6B
3	D	702	GTR	O5-C5-C6-O6A
3	D	702	GTR	O5-C5-C6-O6B

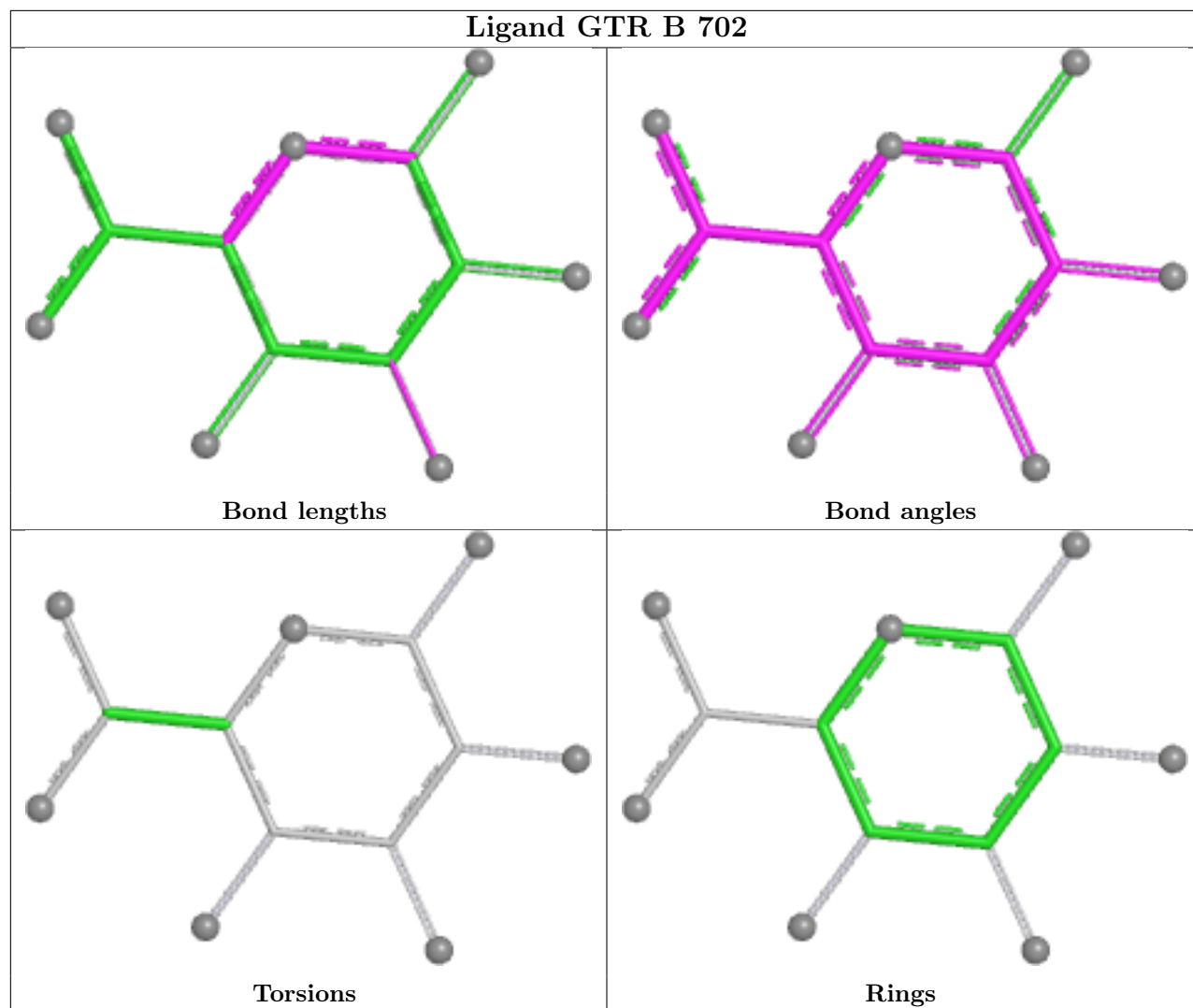
There are no ring outliers.

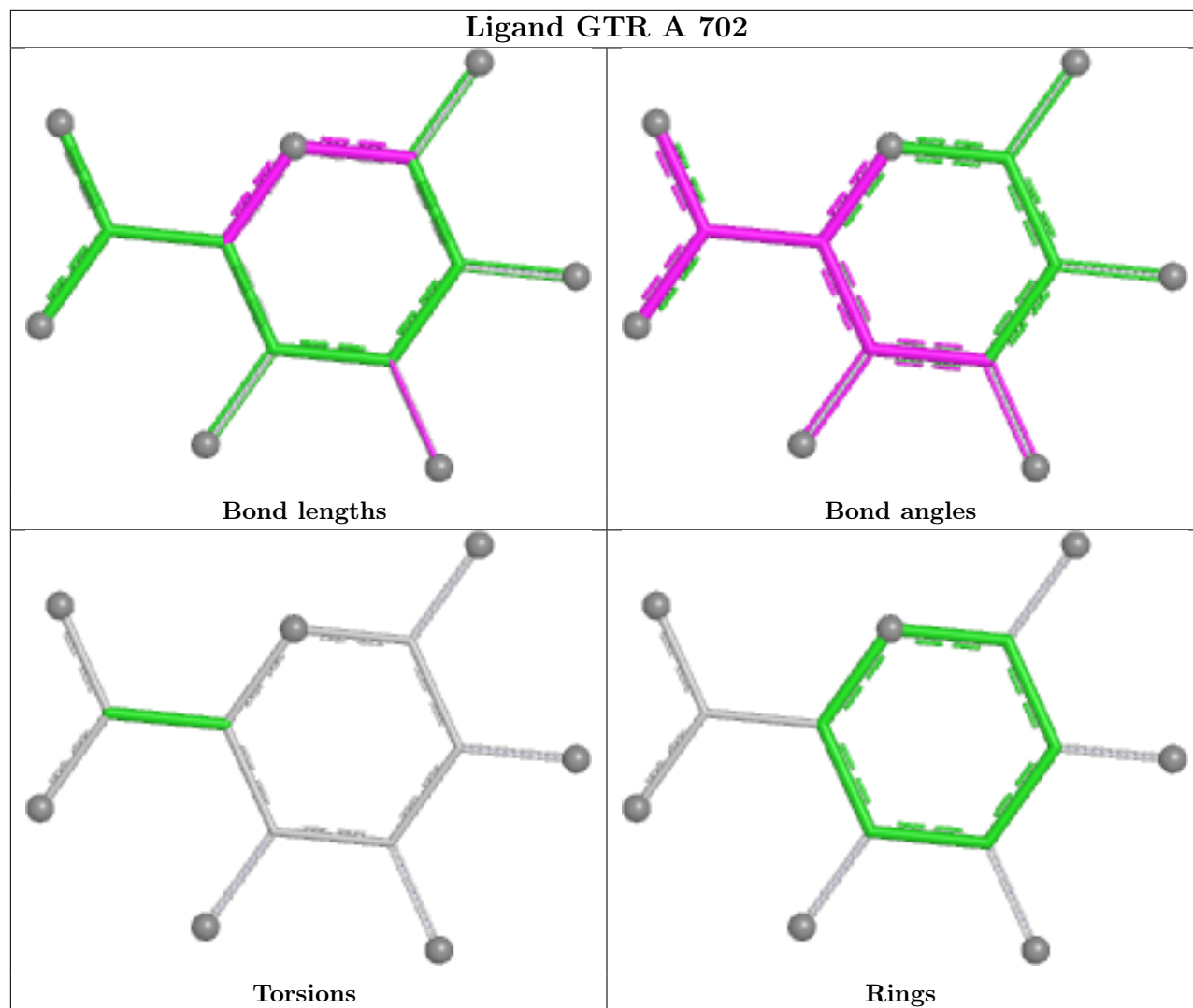
4 monomers are involved in 13 short contacts:

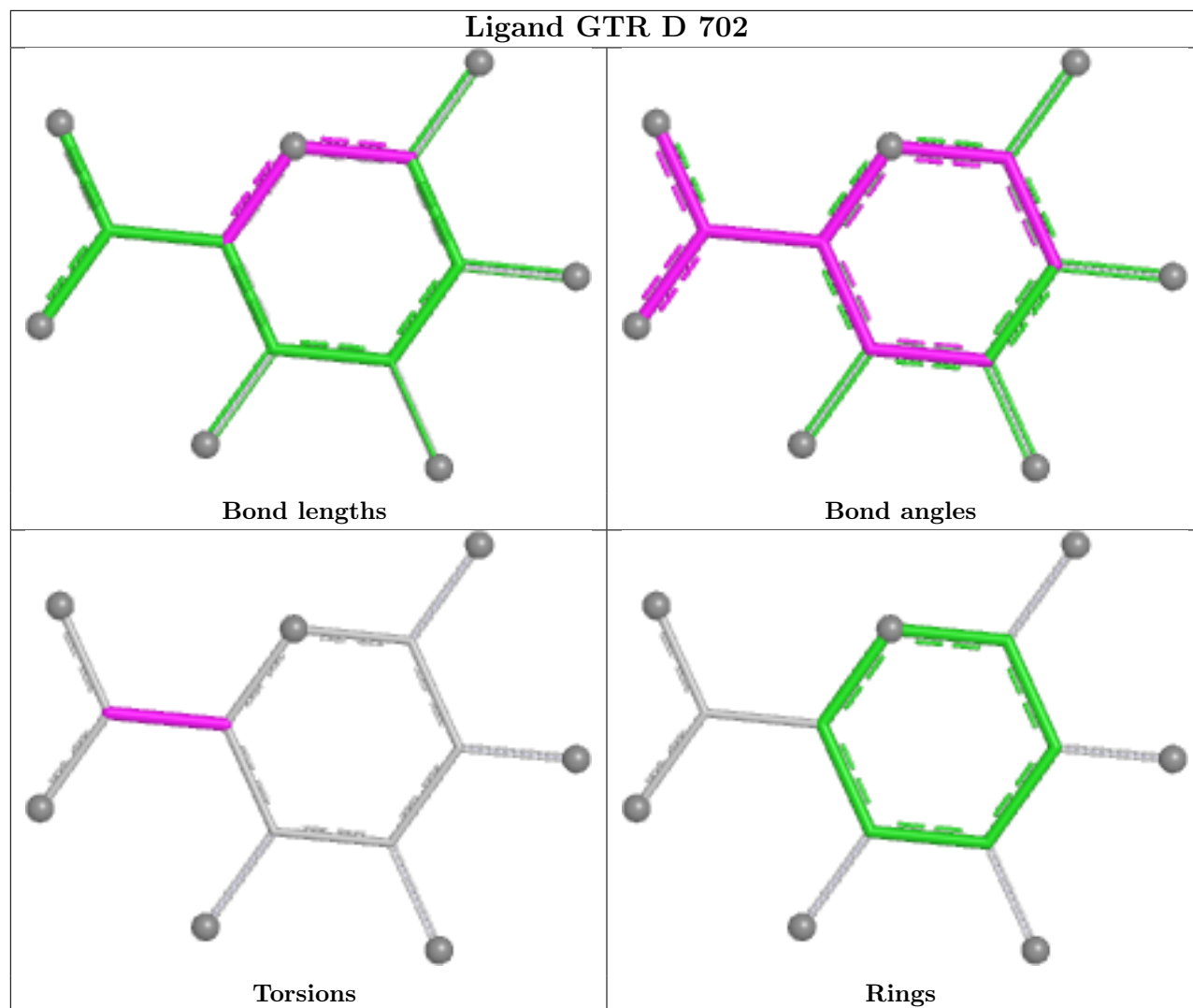
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	702	GTR	2	0
3	B	702	GTR	4	0
3	A	702	GTR	6	0
3	D	702	GTR	1	0

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.









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	584/605 (96%)	-0.33	4 (0%) 84 81	10, 19, 36, 66	0
1	B	584/605 (96%)	-0.22	6 (1%) 79 76	11, 20, 42, 77	0
1	C	584/605 (96%)	-0.31	5 (0%) 81 78	11, 19, 36, 73	0
1	D	584/605 (96%)	-0.11	7 (1%) 76 73	11, 24, 45, 93	0
All	All	2336/2420 (96%)	-0.24	22 (0%) 81 78	10, 20, 42, 93	0

All (22) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	620	TYR	3.4
1	D	623	LYS	3.4
1	A	371	ALA	3.0
1	D	622	ILE	3.0
1	D	371	ALA	2.8
1	A	620	TYR	2.7
1	B	290	LYS	2.7
1	B	517	ASP	2.6
1	C	371	ALA	2.5
1	B	371	ALA	2.5
1	D	621	GLN	2.5
1	B	77	ALA	2.5
1	A	476	ASP	2.4
1	D	283	LYS	2.4
1	B	477	VAL	2.4
1	B	470	ASN	2.3
1	A	283	LYS	2.3
1	C	283	LYS	2.2
1	C	271	ARG	2.2
1	C	471	GLU	2.1
1	D	271	ARG	2.1
1	C	476	ASP	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](#)

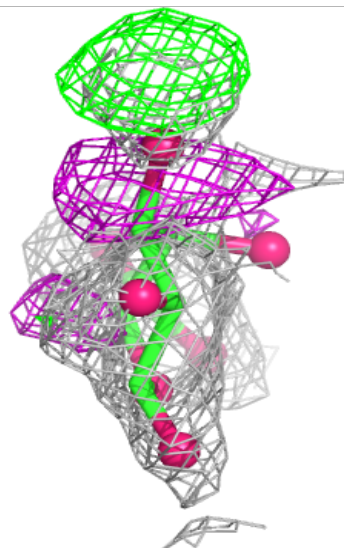
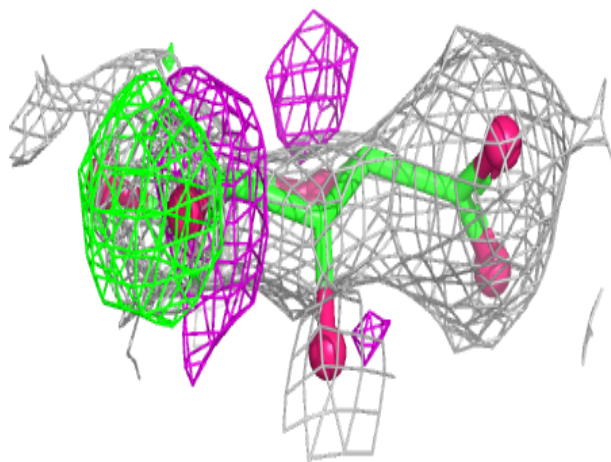
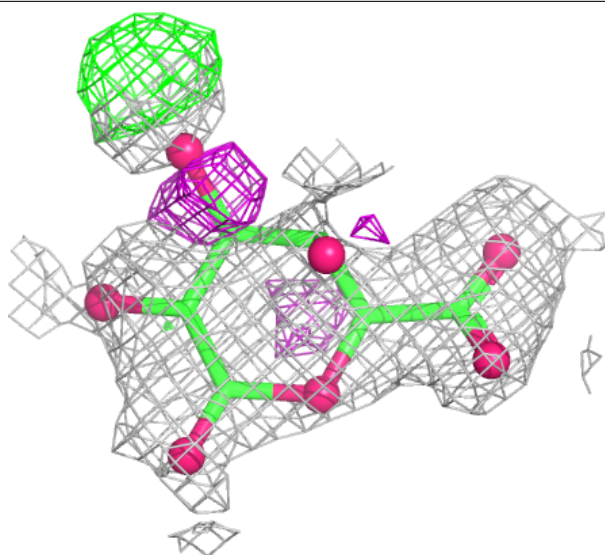
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	GTR	B	702	13/13	0.75	0.17	26,42,45,47	0
3	GTR	A	702	13/13	0.80	0.18	23,42,47,47	0
3	GTR	C	702	13/13	0.82	0.16	28,43,48,55	0
3	GTR	D	702	13/13	0.82	0.20	40,62,73,74	0
2	CL	A	701	1/1	0.98	0.04	17,17,17,17	0
2	CL	C	701	1/1	0.98	0.03	18,18,18,18	0
2	CL	B	701	1/1	0.99	0.02	17,17,17,17	0
2	CL	D	701	1/1	0.99	0.02	20,20,20,20	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.

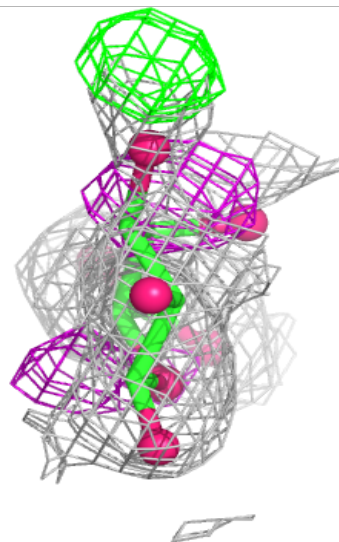
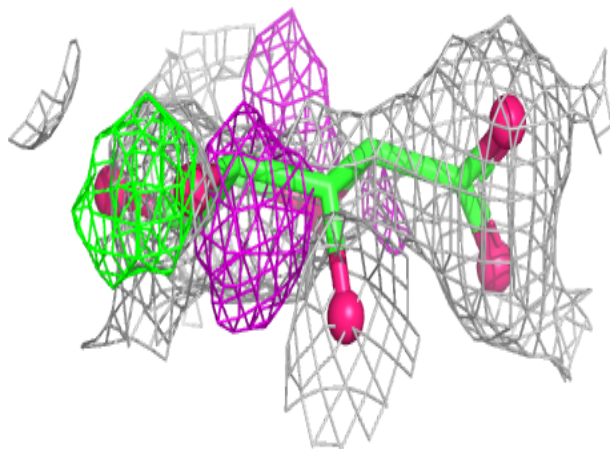
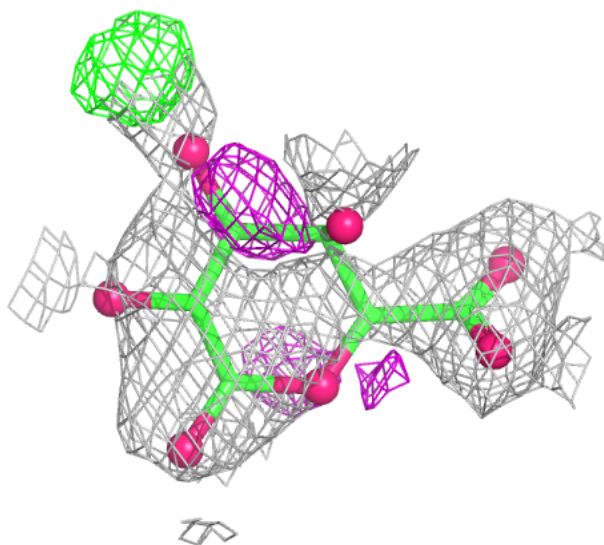
Electron density around GTR B 702:

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



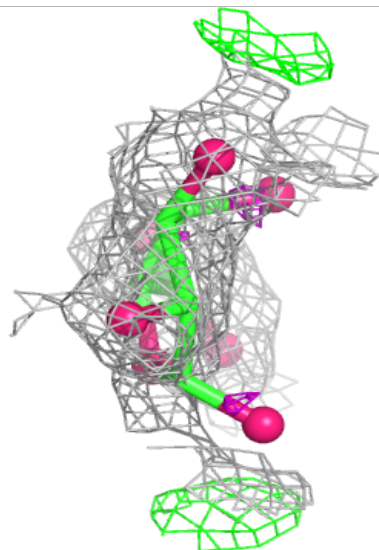
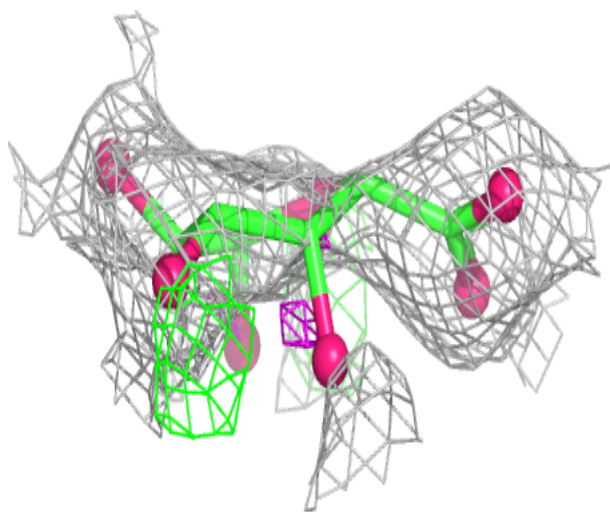
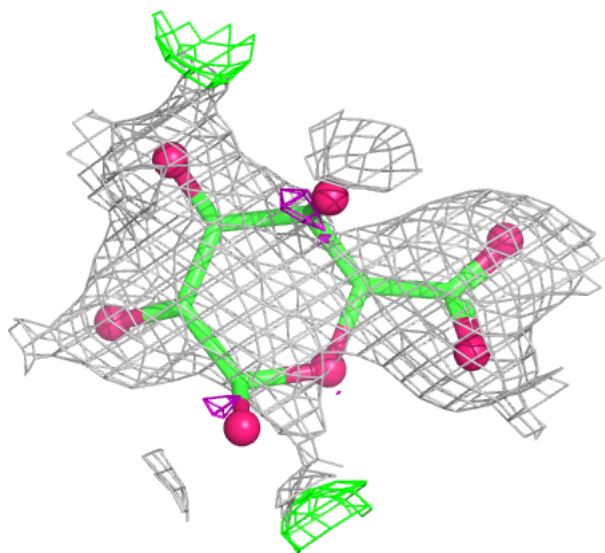
Electron density around GTR A 702:

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



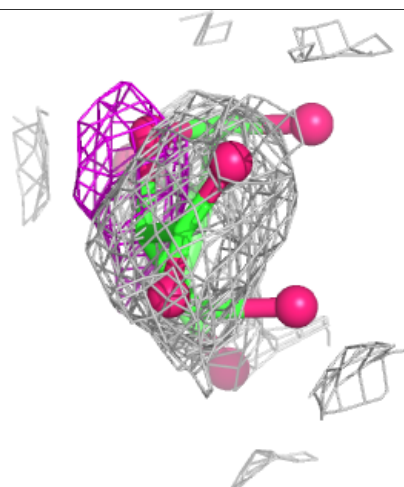
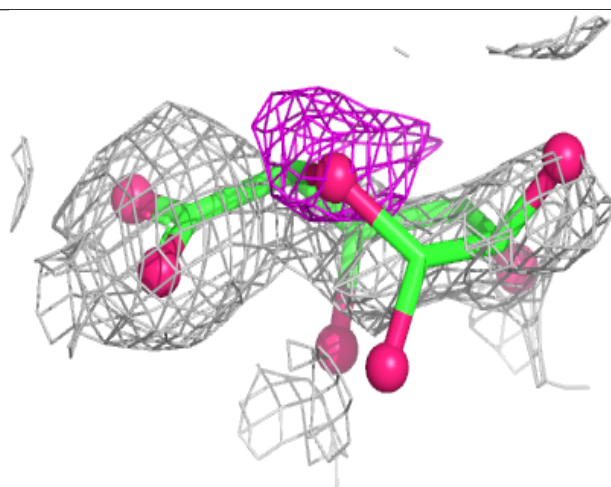
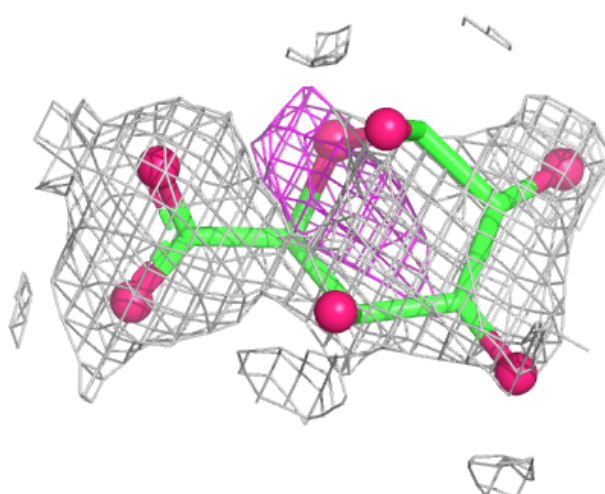
Electron density around GTR C 702:

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



Electron density around GTR D 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.