



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 4, 2025 – 12:16 pm GMT

PDB ID : 9FKC
Title : Crystal structure of human Glucose-6-phosphate isomerase with citraconate ligand
Authors : Jonatansdottir, Y.Y.; Hjorleifsson, G.J.
Deposited on : 2024-06-03
Resolution : 1.60 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	:	4.02b-467
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
CCP4	:	9.0.003 (Gargrove)
Density-Fitness	:	1.0.11
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.41

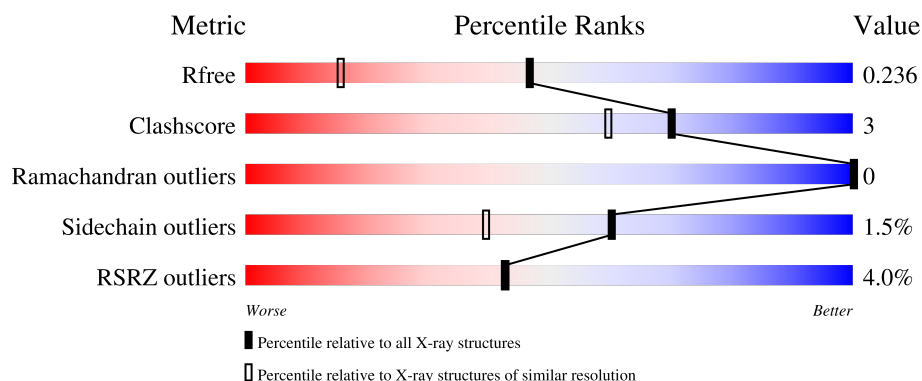
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.60 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}	164625	4274 (1.60-1.60)
Clashscore	180529	4682 (1.60-1.60)
Ramachandran outliers	177936	4583 (1.60-1.60)
Sidechain outliers	177891	4582 (1.60-1.60)
RSRZ outliers	164620	4272 (1.60-1.60)

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	558	<div> <div>0%</div> <div> <div></div> <div>91%</div> <div>8%</div> </div> </div>
1	B	558	<div> <div>6%</div> <div> <div></div> <div>93%</div> <div>6%</div> </div> </div>
1	C	558	<div> <div>7%</div> <div> <div></div> <div>91%</div> <div>8%</div> </div> </div>
1	D	558	<div> <div>2%</div> <div> <div></div> <div>93%</div> <div>6%</div> </div> </div>

2 Entry composition [i](#)

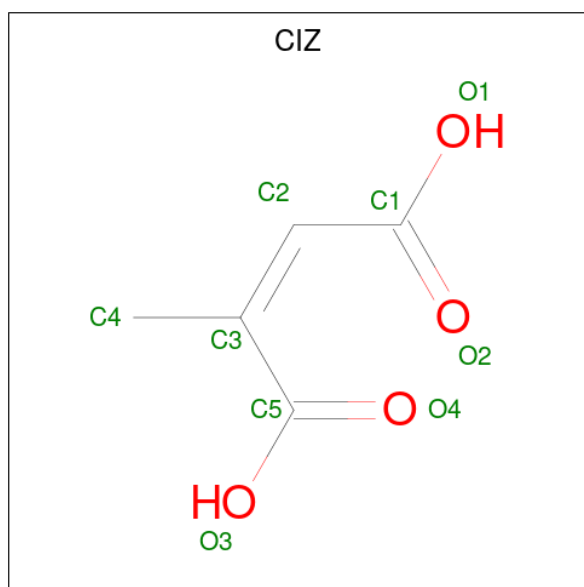
There are 7 unique types of molecules in this entry. The entry contains 37255 atoms, of which 17671 are hydrogens and 0 are deuteriums.

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 Glucose-6-phosphate isomerase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	555	Total	C	H	N	O	S	0	0	0
			8815	2822	4385	781	809	18			
1	B	555	Total	C	H	N	O	S	0	0	0
			8816	2822	4386	781	809	18			
1	C	556	Total	C	H	N	O	S	0	0	0
			8831	2827	4394	782	810	18			
1	D	556	Total	C	H	N	O	S	0	0	0
			8831	2827	4394	782	810	18			

- Molecule 2 is ({Z})-2-methylbut-2-enedioic acid (three-letter code: CIZ) (formula: C₅H₆O₄) (labeled as "Ligand of Interest" by depositor).



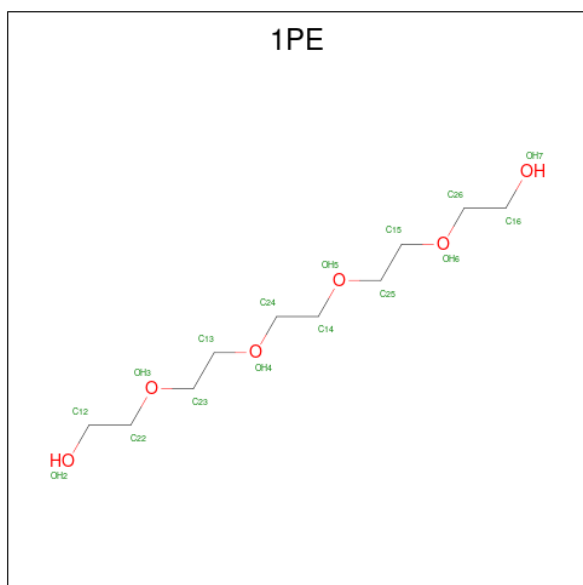
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			13	5	4	4		
2	B	1	Total	C	H	O	0	0
			13	5	4	4		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	H	O	0	0
			13	5	4	4		
2	D	1	Total	C	H	O	0	0
			13	5	4	4		

- Molecule 3 is PENTAETHYLENE GLYCOL (three-letter code: 1PE) (formula: $C_{10}H_{22}O_6$).



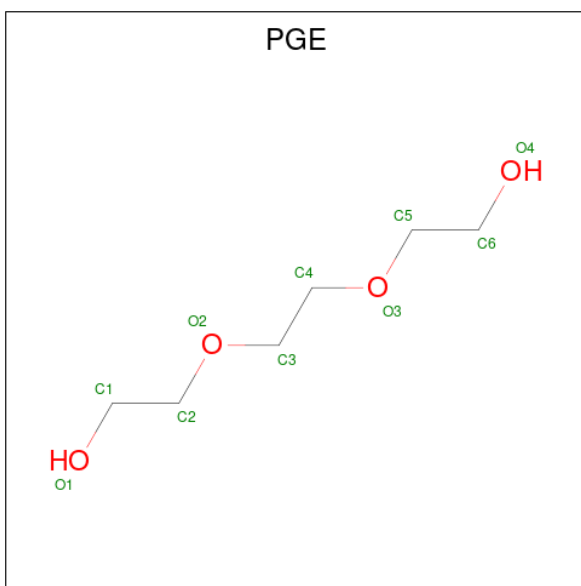
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	H	O	0	0
			38	10	22	6		
3	B	1	Total	C	H	O	0	0
			38	10	22	6		

- Molecule 4 is TETRAETHYLENE GLYCOL (three-letter code: PG4) (formula: $C_8H_{18}O_5$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	H	O	0	0
			31	8	18	5		

- Molecule 5 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	A	1	Total	C	H	O	0	0
			24	6	14	4		
5	C	1	Total	C	H	O	0	0
			24	6	14	4		

- Molecule 6 is BETA-MERCAPTOETHANOL (three-letter code: BME) (formula: C_2H_6OS).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	C	1	Total	C	H	O	S	0	0
			10	2	6	1	1		

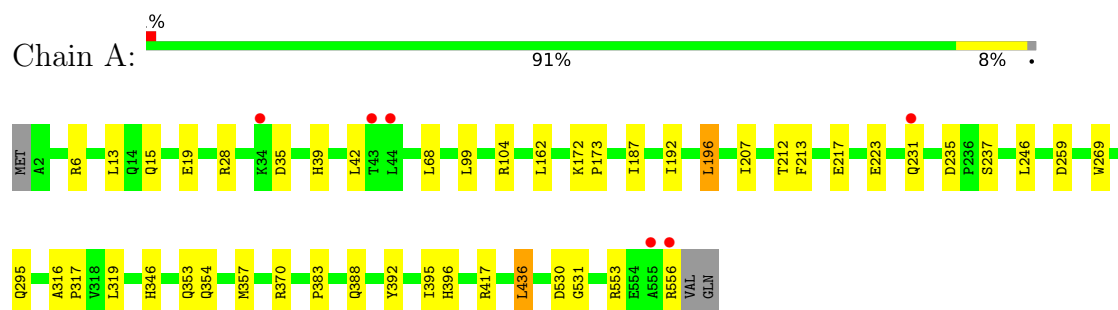
- Molecule 7 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
7	A	459	Total	O	0	0
			459	459		
7	B	449	Total	O	0	0
			449	449		
7	C	398	Total	O	0	0
			398	398		
7	D	439	Total	O	0	0
			439	439		

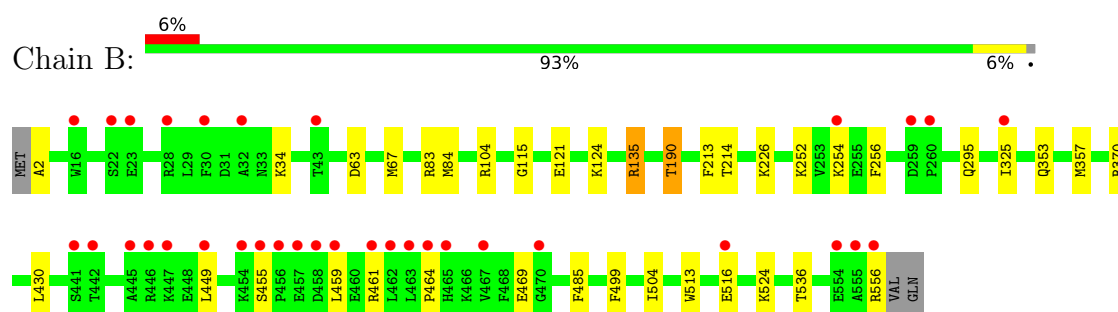
3 Residue-property plots [i](#)

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.

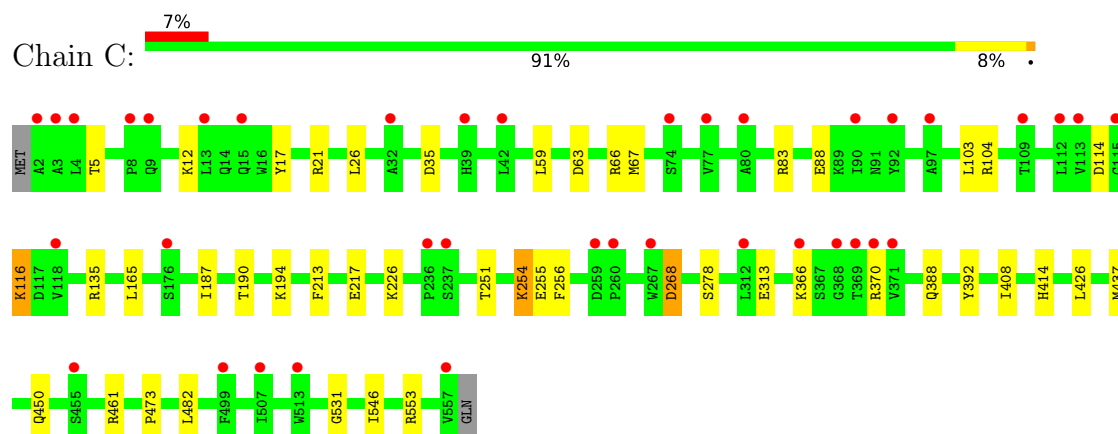
- Molecule 1: Glucose-6-phosphate isomerase



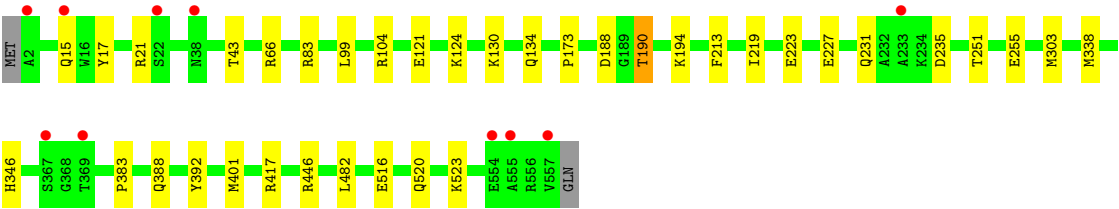
- Molecule 1: Glucose-6-phosphate isomerase



- Molecule 1: Glucose-6-phosphate isomerase



- Molecule 1: Glucose-6-phosphate isomerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	80.72Å 107.84Å 271.48Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.32 – 1.60 46.32 – 1.60	Depositor EDS
% Data completeness (in resolution range)	99.7 (46.32-1.60) 87.5 (46.32-1.60)	Depositor EDS
R_{merge}	0.18	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	0.83 (at 1.60Å)	Xtriage
Refinement program	REFMAC 1.20.1_4487, PHENIX 1.20.1_4487	Depositor
R, R_{free}	0.198 , 0.227 0.209 , 0.236	Depositor DCC
R_{free} test set	16215 reflections (5.02%)	wwPDB-VP
Wilson B-factor (Å ²)	17.5	Xtriage
Anisotropy	0.659	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 36.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.46$, $\langle L^2 \rangle = 0.29$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	37255	wwPDB-VP
Average B, all atoms (Å ²)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 38.45 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 3.6800e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: CIZ, 1PE, PG4, BME, PGE

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	0.37	0/4538	0.57	0/6144
1	B	0.36	0/4538	0.56	0/6144
1	C	0.35	0/4545	0.55	0/6154
1	D	0.36	0/4545	0.56	0/6154
All	All	0.36	0/18166	0.56	0/24596

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	B	0	1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	135	ARG	Sidechain

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	4430	4385	4383	31	0
1	B	4430	4386	4383	30	0
1	C	4437	4394	4392	31	0
1	D	4437	4394	4392	28	0
2	A	9	4	0	1	0
2	B	9	4	0	0	0
2	C	9	4	0	0	0
2	D	9	4	0	0	0
3	A	16	22	22	0	0
3	B	16	22	22	0	0
4	A	13	18	18	2	0
5	A	10	14	14	0	0
5	C	10	14	14	0	0
6	C	4	6	6	0	0
7	A	459	0	0	10	1
7	B	449	0	0	14	0
7	C	398	0	0	10	1
7	D	439	0	0	14	1
All	All	19584	17671	17646	117	3

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 3.

All (117) 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:556:ARG:NH1	7:B:701:HOH:O	1.83	1.10
1:C:135:ARG:NH2	7:C:702:HOH:O	1.85	1.10
1:B:556:ARG:CZ	7:B:701:HOH:O	2.10	1.00
1:A:28:ARG:NE	7:A:701:HOH:O	1.87	0.96
1:B:83:ARG:NH2	7:B:702:HOH:O	2.00	0.93
1:D:235:ASP:OD2	7:D:701:HOH:O	1.88	0.90
1:C:66:ARG:NH2	7:C:701:HOH:O	1.83	0.85
1:C:366:LYS:NZ	7:C:708:HOH:O	2.14	0.80
1:D:173:PRO:O	7:D:702:HOH:O	1.98	0.79
1:D:523:LYS:NZ	7:D:705:HOH:O	2.08	0.78
1:D:523:LYS:HD2	7:D:705:HOH:O	1.84	0.78
1:A:295:GLN:HG3	7:A:1016:HOH:O	1.84	0.77
1:A:223:GLU:OE2	7:A:702:HOH:O	2.02	0.77
1:C:5:THR:O	7:C:703:HOH:O	2.02	0.77
1:C:450:GLN:OE1	7:C:704:HOH:O	2.04	0.74
1:B:455:SER:C	7:B:704:HOH:O	2.26	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:114:ASP:O	7:C:706:HOH:O	2.06	0.73
1:D:231:GLN:OE1	7:D:703:HOH:O	2.06	0.73
1:D:227:GLU:OE2	7:D:704:HOH:O	2.06	0.73
1:C:63:ASP:OD2	7:C:705:HOH:O	2.05	0.72
1:C:66:ARG:NH1	7:C:701:HOH:O	2.20	0.72
1:B:556:ARG:NH2	7:B:701:HOH:O	2.21	0.72
1:D:338:MET:SD	7:D:1073:HOH:O	2.50	0.69
1:A:370:ARG:HG2	1:A:370:ARG:HH11	1.60	0.67
1:C:190:THR:O	1:C:194:LYS:HG2	1.94	0.67
1:B:2:ALA:N	7:B:706:HOH:O	2.28	0.67
1:C:313:GLU:OE2	7:C:707:HOH:O	2.13	0.66
1:D:523:LYS:CD	7:D:705:HOH:O	2.43	0.64
1:A:192:ILE:HG13	1:A:196:LEU:HD22	1.81	0.63
1:B:464:PRO:HA	7:B:782:HOH:O	2.00	0.62
1:A:13:LEU:HD11	1:A:68:LEU:HD23	1.82	0.62
1:B:455:SER:CB	7:B:704:HOH:O	2.48	0.61
1:D:83:ARG:NH2	7:D:708:HOH:O	2.27	0.61
1:D:219:ILE:O	1:D:223:GLU:HG3	1.99	0.61
1:A:6:ARG:NH2	7:A:703:HOH:O	2.12	0.61
1:B:536:THR:HG22	7:B:731:HOH:O	2.00	0.60
1:A:231:GLN:NE2	7:A:708:HOH:O	2.33	0.60
1:C:254:LYS:HA	1:C:254:LYS:HE2	1.85	0.58
1:B:135:ARG:NH2	7:B:711:HOH:O	2.36	0.58
1:A:556:ARG:C	7:A:706:HOH:O	2.42	0.57
1:D:121:GLU:OE1	1:D:124:LYS:NZ	2.36	0.57
1:B:353:GLN:O	1:B:357:MET:HB2	2.04	0.57
1:D:190:THR:HG21	7:D:768:HOH:O	2.05	0.57
1:A:42:LEU:HD11	1:A:319:LEU:HD12	1.88	0.56
1:C:116:LYS:HB2	7:C:706:HOH:O	2.08	0.53
1:A:530:ASP:OD1	7:A:704:HOH:O	2.19	0.53
1:C:59:LEU:HD23	1:C:473:PRO:HB3	1.91	0.52
1:C:268:ASP:N	1:C:268:ASP:OD1	2.42	0.52
1:B:370:ARG:HH11	1:B:370:ARG:HG2	1.76	0.50
1:B:295:GLN:HG2	1:B:485:PHE:HB2	1.94	0.50
1:A:396:HIS:CE1	1:A:436:LEU:HD13	2.47	0.50
1:A:15:GLN:O	1:A:19:GLU:HG3	2.13	0.48
1:B:524:LYS:HD2	7:B:1018:HOH:O	2.13	0.48
1:C:226:LYS:NZ	1:C:256:PHE:O	2.47	0.48
1:D:83:ARG:NH1	7:D:717:HOH:O	2.42	0.48
1:D:446:ARG:NH1	7:D:706:HOH:O	2.19	0.48
1:A:531:GLY:O	1:A:553:ARG:NH2	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:353:GLN:O	1:A:357:MET:HB2	2.13	0.48
1:B:469:GLU:OE1	1:C:370:ARG:NH2	2.47	0.47
1:A:212:THR:HG23	2:A:601:CIZ:O2	2.15	0.47
1:D:251:THR:O	1:D:255:GLU:HG3	2.15	0.47
1:B:115:GLY:N	7:B:703:HOH:O	2.16	0.47
1:D:188:ASP:OD1	1:D:190:THR:HG23	2.15	0.47
1:C:59:LEU:CD2	1:C:473:PRO:HB3	2.46	0.46
1:D:346:HIS:HA	1:D:383:PRO:HG3	1.98	0.46
1:A:395:ILE:HG22	1:A:436:LEU:HD11	1.97	0.46
1:C:83:ARG:HA	1:C:88:GLU:HG3	1.98	0.46
1:A:162:LEU:HD12	1:A:354:GLN:HE21	1.80	0.46
1:B:84:MET:HE1	1:B:499:PHE:CD1	2.51	0.46
1:B:190:THR:HB	1:C:414:HIS:CD2	2.51	0.45
1:C:531:GLY:O	1:C:553:ARG:NH2	2.49	0.45
1:D:130:LYS:NZ	7:D:711:HOH:O	2.36	0.45
1:B:121:GLU:OE2	1:B:124:LYS:HE2	2.16	0.45
1:D:516:GLU:O	1:D:520:GLN:HG3	2.16	0.44
1:A:316:ALA:HB3	1:A:317:PRO:HD3	1.99	0.44
1:B:325:ILE:HD13	1:B:504:ILE:HG21	1.98	0.44
1:B:449:LEU:HD13	1:B:459:LEU:HG	1.98	0.44
1:A:15:GLN:OE1	1:A:15:GLN:HA	2.18	0.44
1:A:388:GLN:HA	1:A:392:TYR:CG	2.53	0.44
1:D:17:TYR:O	1:D:21:ARG:HB2	2.18	0.43
1:A:370:ARG:HH11	1:A:370:ARG:CG	2.30	0.43
1:B:464:PRO:CA	7:B:782:HOH:O	2.64	0.43
1:B:430:LEU:HD13	1:C:546:ILE:HG12	2.00	0.43
1:C:165:LEU:HD23	1:C:165:LEU:C	2.39	0.43
1:A:370:ARG:HH12	4:A:603:PG4:C1	2.32	0.43
1:B:513:TRP:O	1:B:516:GLU:HG2	2.18	0.43
1:D:388:GLN:HA	1:D:392:TYR:CG	2.54	0.43
1:C:26:LEU:HD13	1:C:437:MET:CG	2.49	0.42
1:A:316:ALA:HB3	1:A:317:PRO:CD	2.49	0.42
7:A:702:HOH:O	1:D:417:ARG:NH2	2.25	0.42
1:B:459:LEU:C	1:B:459:LEU:HD23	2.40	0.42
1:C:251:THR:O	1:C:255:GLU:HG3	2.19	0.42
1:A:235:ASP:OD2	1:A:237:SER:OG	2.37	0.42
1:B:226:LYS:NZ	1:B:256:PHE:O	2.52	0.42
1:B:254:LYS:HD3	1:B:254:LYS:C	2.40	0.42
1:D:121:GLU:HG3	7:D:759:HOH:O	2.20	0.42
1:C:26:LEU:HD13	1:C:437:MET:HG3	2.01	0.42
1:A:187:ILE:HB	1:A:217:GLU:CG	2.49	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:190:THR:O	1:D:194:LYS:HG2	2.19	0.42
1:C:12:LYS:HG3	1:C:67:MET:SD	2.59	0.42
1:A:346:HIS:HA	1:A:383:PRO:HG3	2.02	0.41
1:B:63:ASP:O	1:B:67:MET:HG3	2.20	0.41
1:A:172:LYS:N	1:A:173:PRO:CD	2.84	0.41
1:B:214:THR:HG22	1:B:252:LYS:HD3	2.01	0.41
1:C:187:ILE:HB	1:C:217:GLU:HG3	2.03	0.41
7:A:827:HOH:O	1:D:43:THR:HG21	2.20	0.41
1:C:408:ILE:HD13	1:C:426:LEU:HD23	2.02	0.41
1:D:99:LEU:HD23	1:D:99:LEU:HA	1.95	0.41
1:D:303:MET:O	1:D:303:MET:HG3	2.21	0.41
1:A:28:ARG:CZ	7:A:701:HOH:O	2.51	0.41
1:A:99:LEU:HB2	1:A:269:TRP:CE3	2.55	0.41
4:A:603:PG4:H62	1:D:401:MET:HG3	2.03	0.41
1:B:190:THR:HG21	7:B:831:HOH:O	2.20	0.41
1:C:103:LEU:HD13	1:C:278:SER:HB3	2.03	0.41
1:A:207:ILE:HG21	1:A:246:LEU:HD11	2.04	0.40
1:C:17:TYR:O	1:C:21:ARG:HB2	2.21	0.40
1:C:388:GLN:HA	1:C:392:TYR:CG	2.56	0.40

All (3) 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)
7:C:910:HOH:O	7:C:1035:HOH:O[1_455]	1.51	0.69
7:D:706:HOH:O	7:D:994:HOH:O[1_655]	1.82	0.38
7:A:713:HOH:O	7:A:1078:HOH:O[4_445]	2.15	0.05

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	553/558 (99%)	533 (96%)	20 (4%)	0	100	100
1	B	553/558 (99%)	532 (96%)	21 (4%)	0	100	100
1	C	554/558 (99%)	535 (97%)	19 (3%)	0	100	100
1	D	554/558 (99%)	540 (98%)	14 (2%)	0	100	100
All	All	2214/2232 (99%)	2140 (97%)	74 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	474/477 (99%)	466 (98%)	8 (2%)	56	33
1	B	474/477 (99%)	469 (99%)	5 (1%)	70	53
1	C	475/477 (100%)	467 (98%)	8 (2%)	56	33
1	D	475/477 (100%)	468 (98%)	7 (2%)	60	39
All	All	1898/1908 (100%)	1870 (98%)	28 (2%)	60	39

All (28) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	35	ASP
1	A	39	HIS
1	A	104	ARG
1	A	196	LEU
1	A	213	PHE
1	A	259	ASP
1	A	417	ARG
1	A	436	LEU
1	B	34	LYS
1	B	104	ARG
1	B	190	THR
1	B	213	PHE
1	B	461	ARG

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Mol	Chain	Res	Type
1	C	35	ASP
1	C	104	ARG
1	C	116	LYS
1	C	213	PHE
1	C	254	LYS
1	C	268	ASP
1	C	461	ARG
1	C	482	LEU
1	D	15	GLN
1	D	66	ARG
1	D	104	ARG
1	D	134	GLN
1	D	190	THR
1	D	213	PHE
1	D	482	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	39	HIS
1	A	231	GLN
1	A	295	GLN
1	A	354	GLN
1	C	50	HIS
1	D	9	GLN
1	D	15	GLN
1	D	134	GLN
1	D	386	ASN
1	D	450	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](#)

10 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
2	CIZ	D	601	-	8,8,8	1.40	0	10,10,10	1.46	1 (10%)
2	CIZ	C	601	-	8,8,8	1.46	1 (12%)	10,10,10	1.75	3 (30%)
2	CIZ	B	601	-	8,8,8	1.39	0	10,10,10	1.61	2 (20%)
4	PG4	A	603	-	12,12,12	0.25	0	11,11,11	0.38	0
6	BME	C	603	-	3,3,3	0.38	0	1,2,2	0.37	0
5	PGE	C	602	-	9,9,9	0.34	0	8,8,8	0.31	0
2	CIZ	A	601	-	8,8,8	1.41	1 (12%)	10,10,10	1.62	2 (20%)
5	PGE	A	604	-	9,9,9	0.32	0	8,8,8	0.30	0
3	1PE	A	602	-	15,15,15	0.14	0	14,14,14	0.15	0
3	1PE	B	602	-	15,15,15	0.16	0	14,14,14	0.10	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
2	CIZ	D	601	-	-	6/8/8/8	-
2	CIZ	C	601	-	-	4/8/8/8	-
2	CIZ	B	601	-	-	4/8/8/8	-
4	PG4	A	603	-	-	6/10/10/10	-
6	BME	C	603	-	-	1/1/1/1	-
5	PGE	C	602	-	-	3/7/7/7	-
2	CIZ	A	601	-	-	6/8/8/8	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
5	PGE	A	604	-	-	3/7/7/7	-
3	1PE	A	602	-	-	7/13/13/13	-
3	1PE	B	602	-	-	8/13/13/13	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	601	CIZ	C2-C1	2.13	1.53	1.47
2	C	601	CIZ	C2-C1	2.03	1.53	1.47

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	CIZ	O1-C1-C2	2.77	122.11	113.50
2	A	601	CIZ	O1-C1-C2	2.68	121.83	113.50
2	B	601	CIZ	C4-C3-C5	2.68	119.85	115.69
2	C	601	CIZ	C4-C3-C5	2.51	119.59	115.69
2	D	601	CIZ	O1-C1-C2	2.40	120.94	113.50
2	A	601	CIZ	C1-C2-C3	-2.16	121.27	126.81
2	B	601	CIZ	C1-C2-C3	-2.02	121.62	126.81
2	C	601	CIZ	C4-C3-C2	-2.01	118.27	123.87

There are no chirality outliers.

All (48) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	602	1PE	OH4-C13-C23-OH3
5	A	604	PGE	O2-C3-C4-O3
3	A	602	1PE	OH4-C13-C23-OH3
3	B	602	1PE	OH5-C14-C24-OH4
4	A	603	PG4	O3-C5-C6-O4
5	C	602	PGE	O1-C1-C2-O2
4	A	603	PG4	O2-C3-C4-O3
3	A	602	1PE	OH6-C15-C25-OH5
3	B	602	1PE	OH6-C15-C25-OH5
3	B	602	1PE	OH2-C12-C22-OH3
6	C	603	BME	O1-C1-C2-S2
3	A	602	1PE	OH2-C12-C22-OH3
3	B	602	1PE	OH7-C16-C26-OH6
4	A	603	PG4	O1-C1-C2-O2

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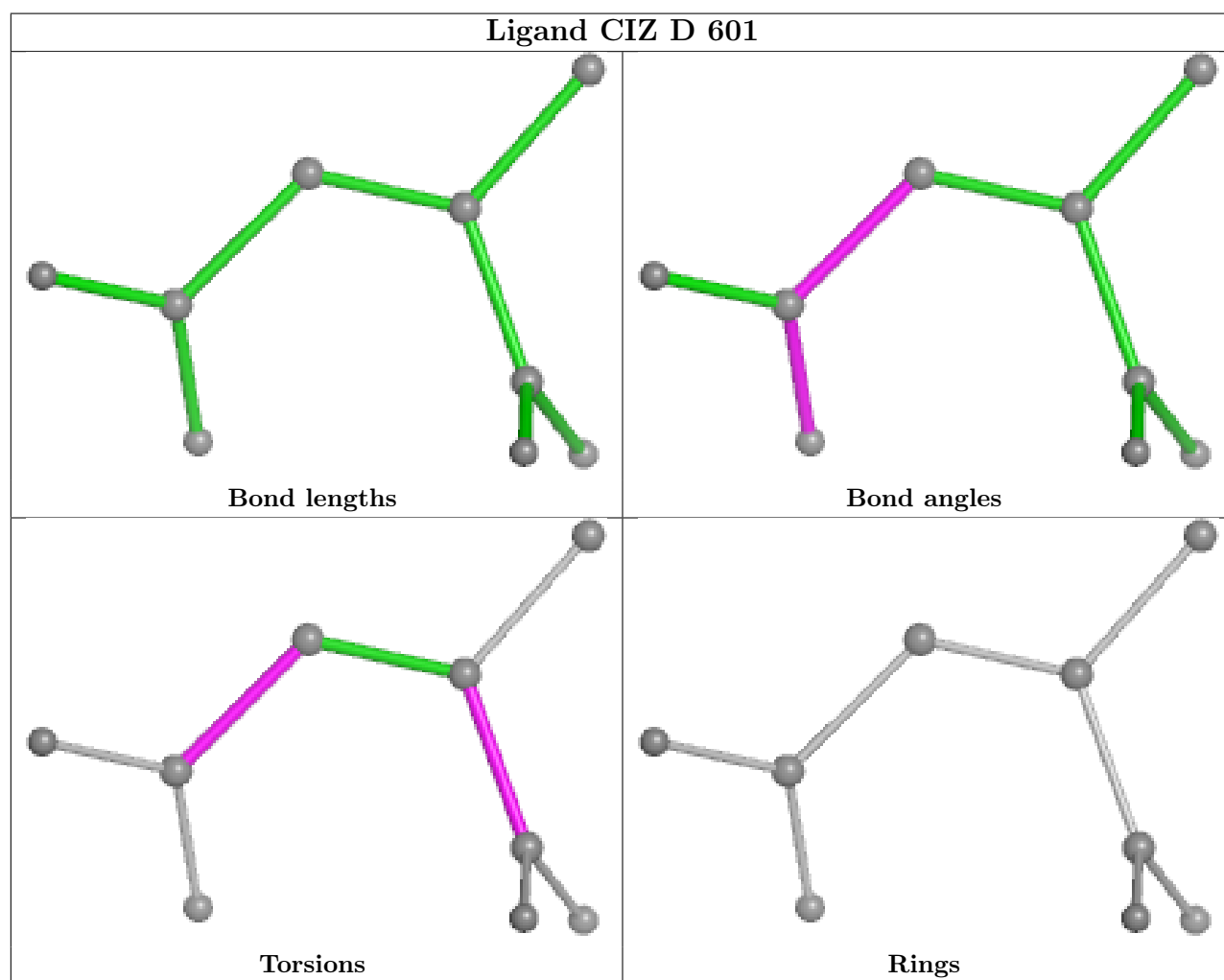
Mol	Chain	Res	Type	Atoms
2	A	601	CIZ	O1-C1-C2-C3
2	A	601	CIZ	O2-C1-C2-C3
2	D	601	CIZ	O1-C1-C2-C3
2	D	601	CIZ	O2-C1-C2-C3
3	A	602	1PE	OH7-C16-C26-OH6
4	A	603	PG4	O4-C7-C8-O5
2	A	601	CIZ	C2-C3-C5-O3
2	B	601	CIZ	C4-C3-C5-O4
2	B	601	CIZ	C2-C3-C5-O4
2	C	601	CIZ	C2-C3-C5-O3
2	D	601	CIZ	C4-C3-C5-O4
2	D	601	CIZ	C2-C3-C5-O4
2	D	601	CIZ	C4-C3-C5-O3
2	D	601	CIZ	C2-C3-C5-O3
5	C	602	PGE	O2-C3-C4-O3
5	A	604	PGE	O3-C5-C6-O4
4	A	603	PG4	C8-C7-O4-C6
3	B	602	1PE	C23-C13-OH4-C24
3	A	602	1PE	C12-C22-OH3-C23
4	A	603	PG4	C1-C2-O2-C3
2	A	601	CIZ	C4-C3-C5-O4
2	A	601	CIZ	C2-C3-C5-O4
2	A	601	CIZ	C4-C3-C5-O3
2	B	601	CIZ	C4-C3-C5-O3
2	B	601	CIZ	C2-C3-C5-O3
2	C	601	CIZ	C4-C3-C5-O4
2	C	601	CIZ	C2-C3-C5-O4
2	C	601	CIZ	C4-C3-C5-O3
3	B	602	1PE	C12-C22-OH3-C23
5	A	604	PGE	C6-C5-O3-C4
3	B	602	1PE	C25-C15-OH6-C26
3	A	602	1PE	C14-C24-OH4-C13
5	C	602	PGE	O3-C5-C6-O4
3	A	602	1PE	OH5-C14-C24-OH4

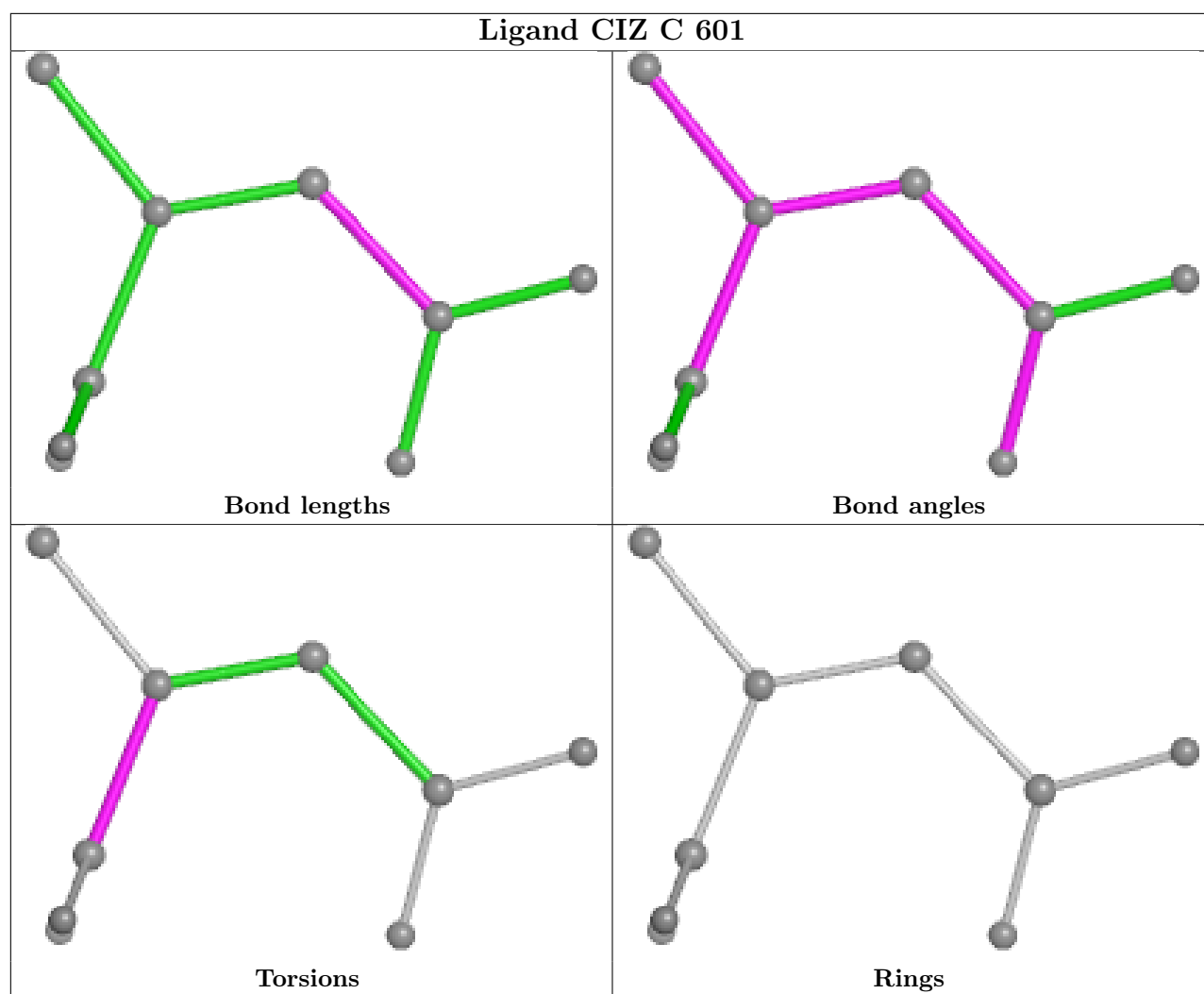
There are no ring outliers.

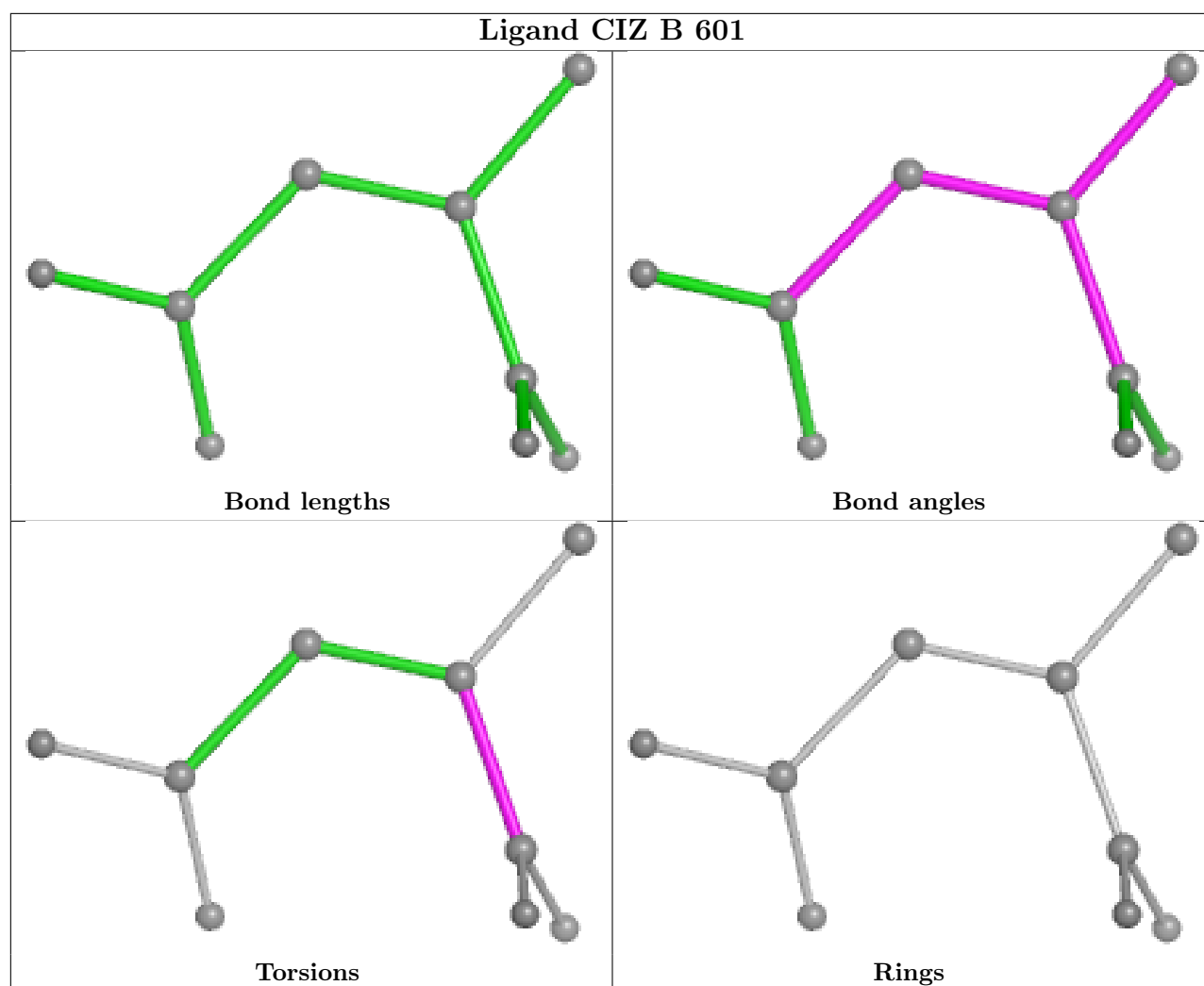
2 monomers are involved in 3 short contacts:

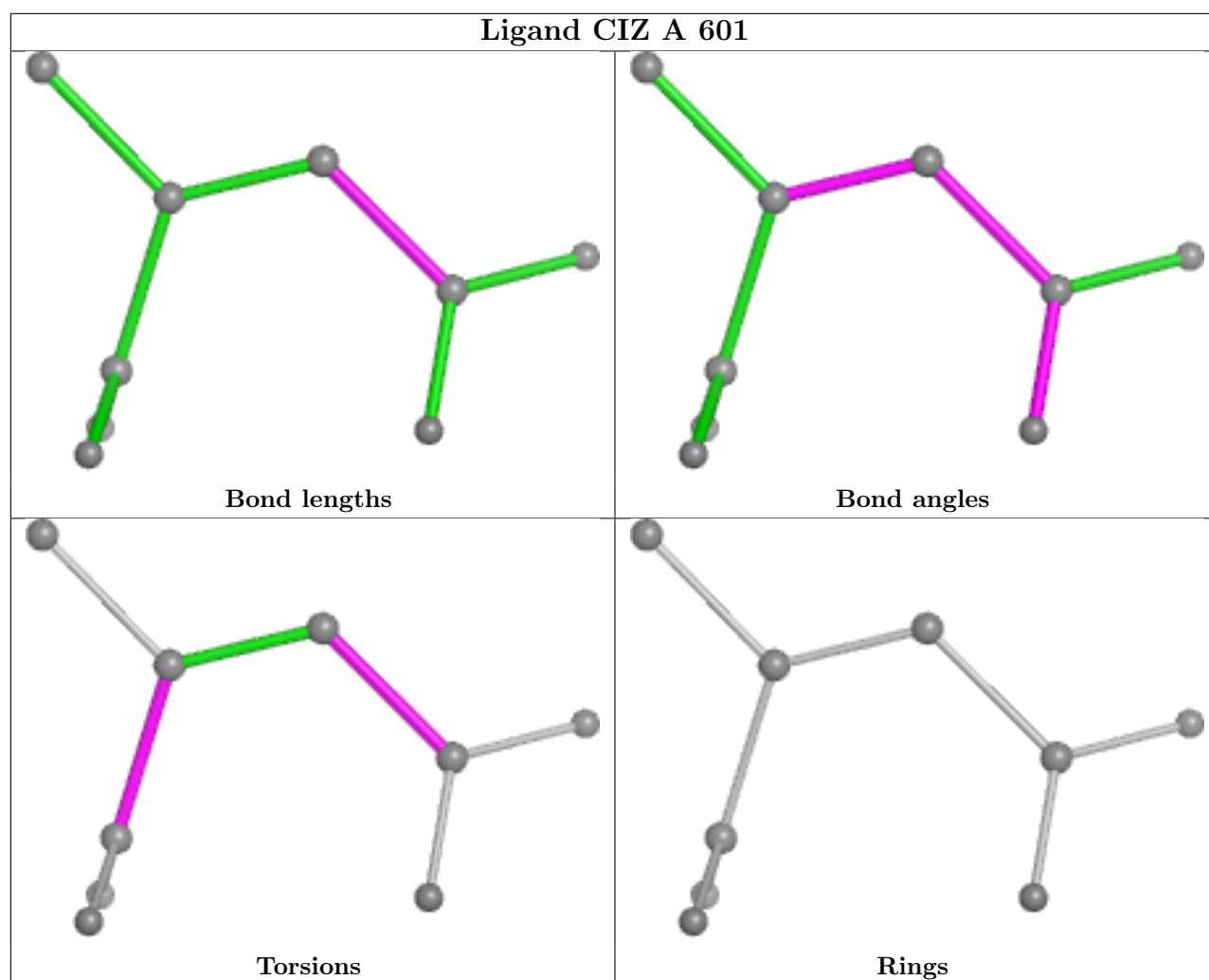
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	603	PG4	2	0
2	A	601	CIZ	1	0

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	555/558 (99%)	0.38	6 (1%) 77 80	19, 28, 49, 76	0
1	B	555/558 (99%)	0.44	34 (6%) 28 28	19, 28, 59, 99	0
1	C	556/558 (99%)	0.69	38 (6%) 25 24	18, 31, 57, 76	0
1	D	556/558 (99%)	0.44	10 (1%) 67 69	18, 29, 49, 80	0
All	All	2222/2232 (99%)	0.49	88 (3%) 43 43	18, 29, 53, 99	0

All (88) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	449	LEU	4.5
1	B	462	LEU	4.4
1	C	115	GLY	4.0
1	C	3	ALA	3.9
1	D	557	VAL	3.8
1	C	371	VAL	3.7
1	B	459	LEU	3.7
1	C	112	LEU	3.4
1	B	554	GLU	3.2
1	B	456	PRO	3.1
1	C	260	PRO	3.1
1	C	368	GLY	3.1
1	C	113	VAL	3.1
1	B	463	LEU	3.0
1	B	556	ARG	3.0
1	C	118	VAL	2.9
1	B	464	PRO	2.8
1	C	2	ALA	2.8
1	D	2	ALA	2.8
1	B	467	VAL	2.7
1	C	369	THR	2.7

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Mol	Chain	Res	Type	RSRZ
1	B	465	HIS	2.6
1	C	109	THR	2.6
1	C	236	PRO	2.6
1	B	260	PRO	2.6
1	B	441	SER	2.6
1	B	23	GLU	2.5
1	C	176	SER	2.5
1	C	4	LEU	2.5
1	C	97	ALA	2.5
1	A	34	LYS	2.5
1	C	455	SER	2.5
1	D	22	SER	2.5
1	B	461	ARG	2.5
1	D	555	ALA	2.5
1	B	458	ASP	2.5
1	C	77	VAL	2.5
1	D	369	THR	2.4
1	B	447	LYS	2.4
1	B	455	SER	2.4
1	A	231	GLN	2.4
1	B	457	GLU	2.4
1	B	516	GLU	2.4
1	C	13	LEU	2.4
1	C	557	VAL	2.3
1	B	470	GLY	2.3
1	D	233	ALA	2.3
1	B	442	THR	2.3
1	C	92	TYR	2.3
1	D	15	GLN	2.2
1	C	32	ALA	2.2
1	C	42	LEU	2.2
1	C	259	ASP	2.2
1	B	446	ARG	2.2
1	C	90	ILE	2.2
1	B	555	ALA	2.2
1	C	237	SER	2.2
1	B	454	LYS	2.2
1	C	9	GLN	2.2
1	A	44	LEU	2.2
1	C	312	LEU	2.2
1	B	325	ILE	2.2
1	B	445	ALA	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	30	PHE	2.2
1	B	22	SER	2.2
1	A	556	ARG	2.1
1	C	74	SER	2.1
1	B	254	LYS	2.1
1	C	507	ILE	2.1
1	B	43	THR	2.1
1	D	38	ASN	2.1
1	B	32	ALA	2.1
1	C	499	PHE	2.1
1	C	513	TRP	2.1
1	B	28	ARG	2.1
1	C	15	GLN	2.1
1	D	554	GLU	2.0
1	B	259	ASP	2.0
1	D	367	SER	2.0
1	C	8	PRO	2.0
1	B	16	TRP	2.0
1	C	267	TRP	2.0
1	C	39	HIS	2.0
1	C	370	ARG	2.0
1	A	43	THR	2.0
1	A	555	ALA	2.0
1	C	80	ALA	2.0
1	C	366	LYS	2.0

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

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

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

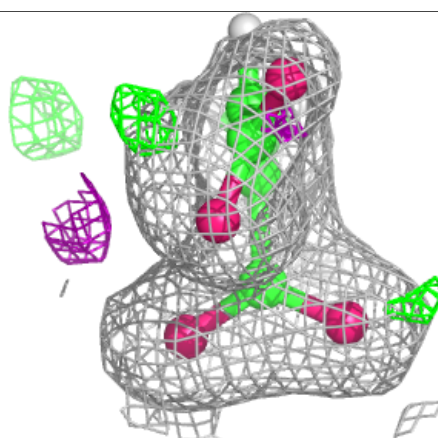
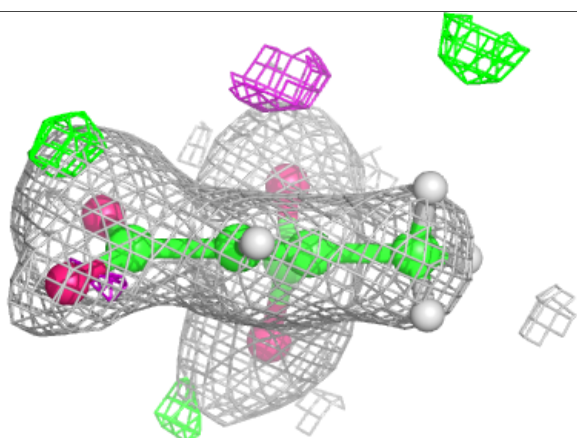
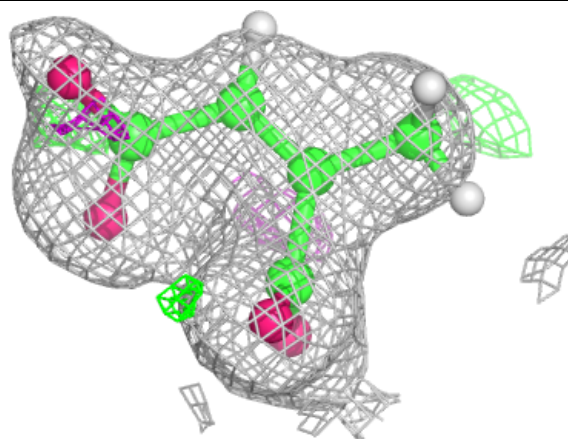
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
5	PGE	A	604	10/10	0.62	0.18	39,50,56,65	0
4	PG4	A	603	13/13	0.77	0.17	28,42,50,57	0
6	BME	C	603	4/4	0.81	0.12	38,46,60,72	0
3	1PE	B	602	16/16	0.82	0.14	36,52,63,65	0
3	1PE	A	602	16/16	0.85	0.13	31,42,54,60	0
5	PGE	C	602	10/10	0.86	0.12	31,45,59,60	0
2	CIZ	B	601	9/9	0.91	0.09	21,25,31,31	0
2	CIZ	C	601	9/9	0.91	0.10	27,32,42,44	0
2	CIZ	D	601	9/9	0.91	0.10	25,33,38,41	0
2	CIZ	A	601	9/9	0.92	0.08	23,26,34,35	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.

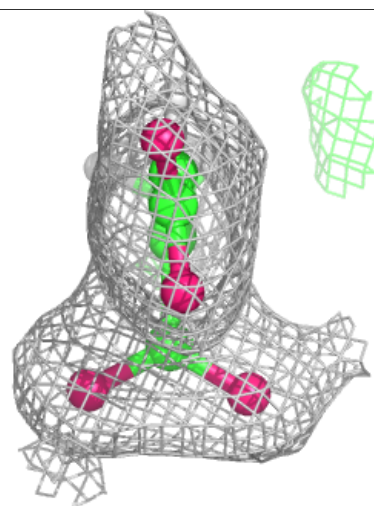
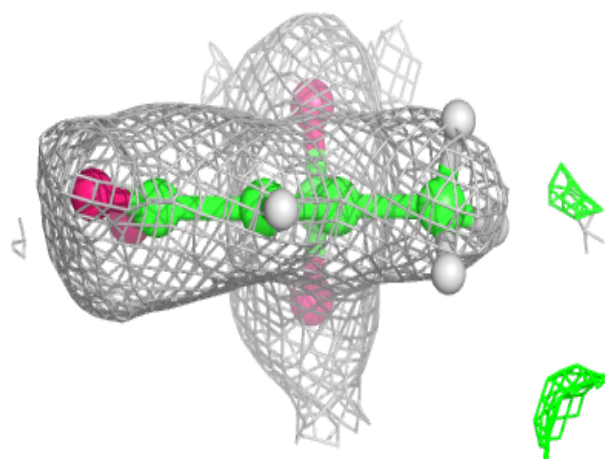
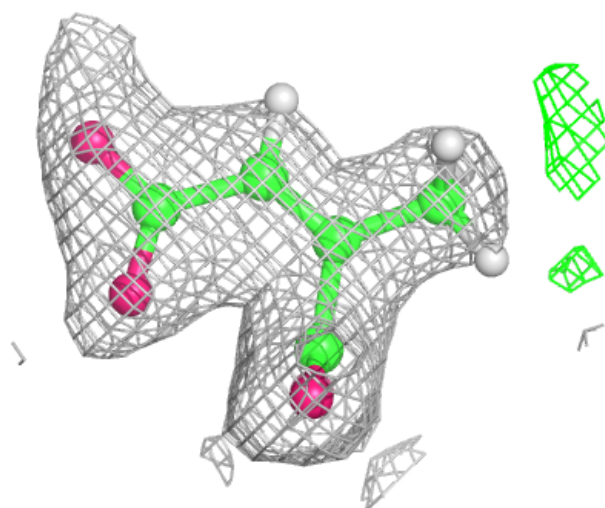
Electron density around CIZ B 601:

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



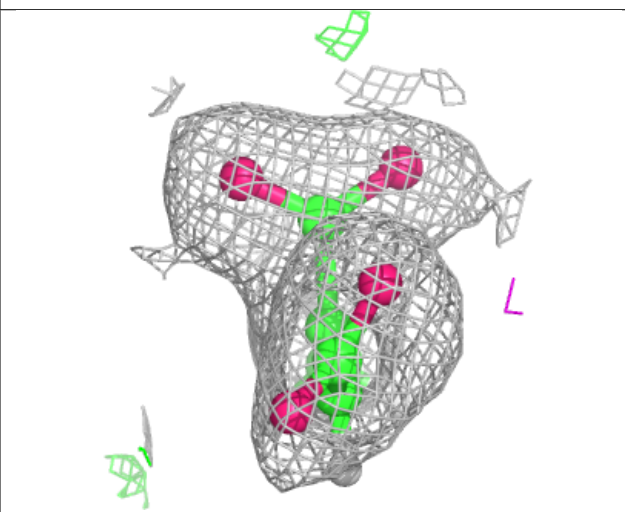
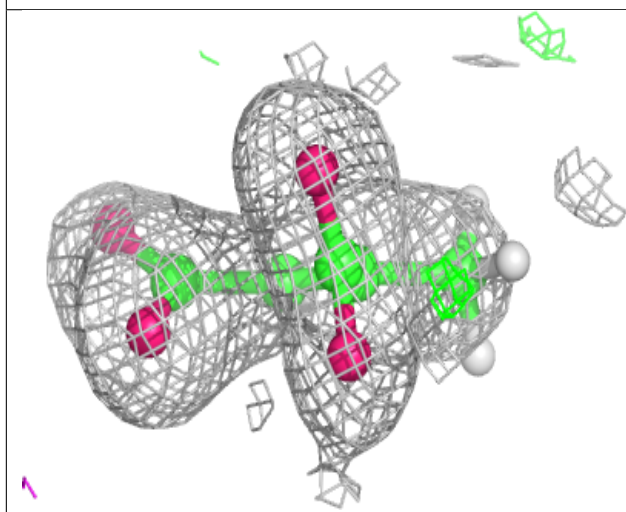
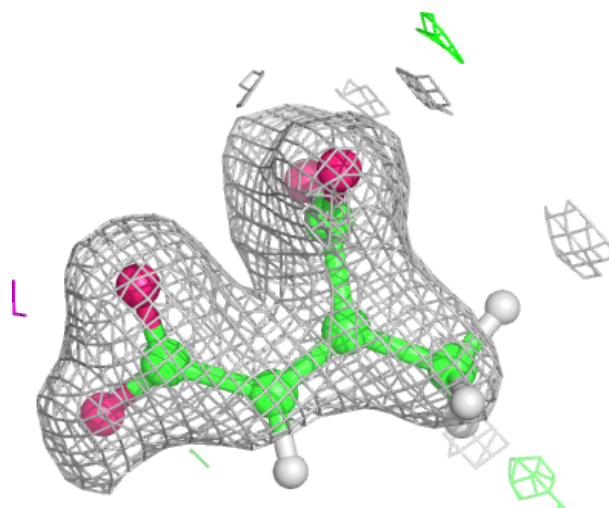
Electron density around CIZ C 601:

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



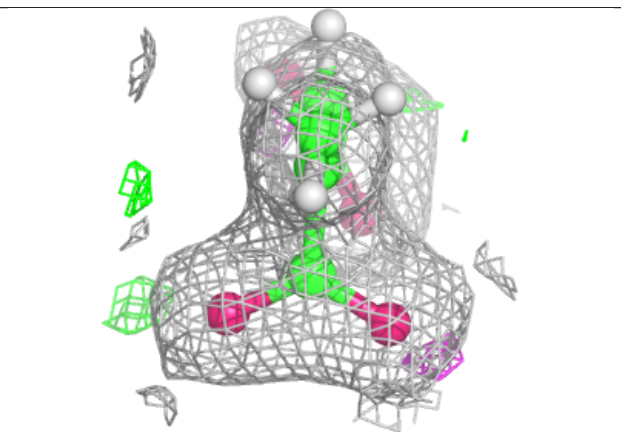
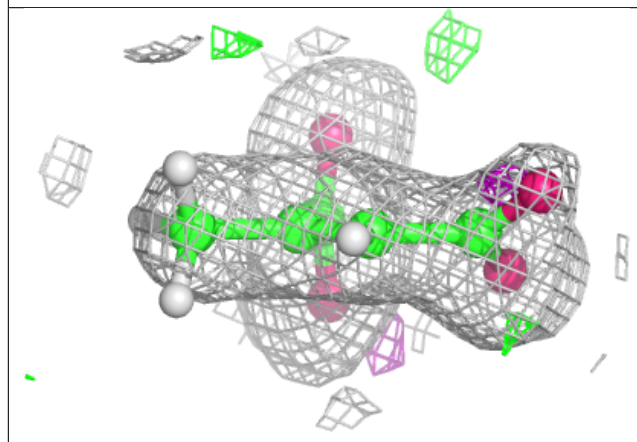
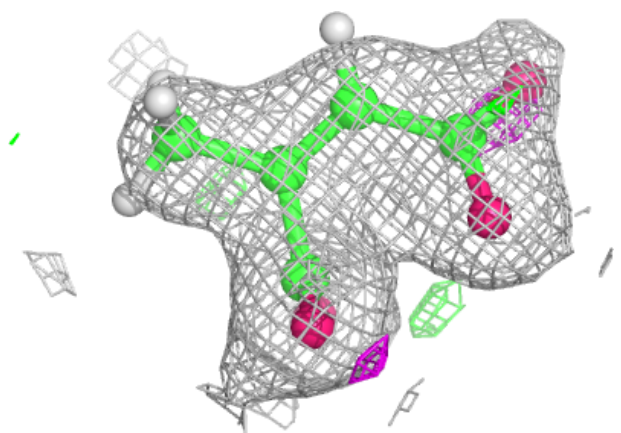
Electron density around CIZ D 601:

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



Electron density around CIZ A 601:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.