



Full wwPDB X-ray Structure Validation Report ⓘ

Jun 24, 2024 – 07:36 AM EDT

PDB ID : 6ZGB
Title : glutamate transporter homologue Glttk in complex with a photo cage compound
Authors : Arkhipova, V.; Slotboom, D.J.; Guskov, A.
Deposited on : 2020-06-18
Resolution : 3.20 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity : 4.02b-467
Mogul : 2022.3.0, CSD as543be (2022)
Xtrriage (Phenix) : 1.20.1
EDS : 2.37.1
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.37.1

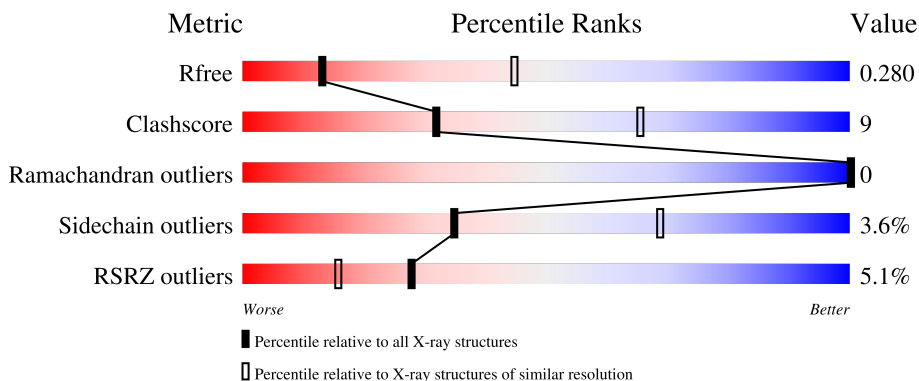
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1133 (3.20-3.20)
Clashscore	141614	1253 (3.20-3.20)
Ramachandran outliers	138981	1234 (3.20-3.20)
Sidechain outliers	138945	1233 (3.20-3.20)
RSRZ outliers	127900	1095 (3.20-3.20)

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

Mol	Chain	Length	Quality of chain
1	A	438	 7% 74% 22% ..
1	B	438	 5% 72% 24% ..
1	C	438	 3% 79% 17% ..

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
2	QJW	A	501	-	-	-	X
2	QJW	B	501	-	-	-	X
3	PEG	A	502	-	-	-	X
3	PEG	B	503	-	-	-	X

2 Entry composition i

There are 4 unique types of molecules in this entry. The entry contains 9583 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 Proton/glutamate symporter, SDF family.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	425	3183	2097	519	551	16	0	1	0
1	B	423	3151	2079	508	548	16	0	0	0
1	C	423	3151	2079	508	548	16	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

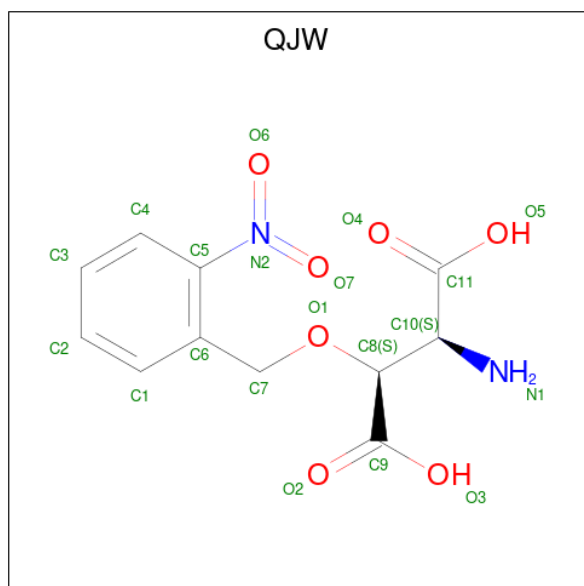
Chain	Residue	Modelled	Actual	Comment	Reference
A	431	HIS	-	expression tag	UNP Q5JID0
A	432	HIS	-	expression tag	UNP Q5JID0
A	433	HIS	-	expression tag	UNP Q5JID0
A	434	HIS	-	expression tag	UNP Q5JID0
A	435	HIS	-	expression tag	UNP Q5JID0
A	436	HIS	-	expression tag	UNP Q5JID0
A	437	HIS	-	expression tag	UNP Q5JID0
A	438	HIS	-	expression tag	UNP Q5JID0
B	431	HIS	-	expression tag	UNP Q5JID0
B	432	HIS	-	expression tag	UNP Q5JID0
B	433	HIS	-	expression tag	UNP Q5JID0
B	434	HIS	-	expression tag	UNP Q5JID0
B	435	HIS	-	expression tag	UNP Q5JID0
B	436	HIS	-	expression tag	UNP Q5JID0
B	437	HIS	-	expression tag	UNP Q5JID0
B	438	HIS	-	expression tag	UNP Q5JID0
C	431	HIS	-	expression tag	UNP Q5JID0
C	432	HIS	-	expression tag	UNP Q5JID0
C	433	HIS	-	expression tag	UNP Q5JID0
C	434	HIS	-	expression tag	UNP Q5JID0
C	435	HIS	-	expression tag	UNP Q5JID0
C	436	HIS	-	expression tag	UNP Q5JID0
C	437	HIS	-	expression tag	UNP Q5JID0

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Chain	Residue	Modelled	Actual	Comment	Reference
C	438	HIS	-	expression tag	UNP Q5JID0

- Molecule 2 is (2 {S},3 {S})-2-azanyl-3-[(2-nitrophenyl)methoxy]butanedioic acid (three-letter code: QJW) (formula: C₁₁H₁₂N₂O₇).



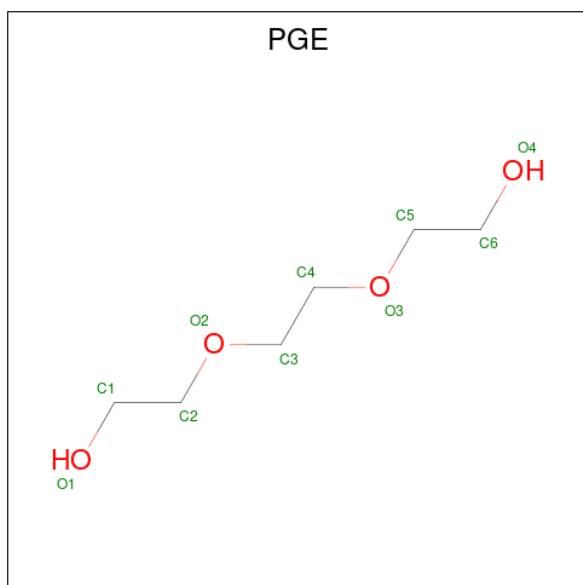
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	Total	C	N	O	0	0
			20	11	2	7		
2	B	1	Total	C	N	O	0	0
			20	11	2	7		
2	C	1	Total	C	N	O	0	0
			20	11	2	7		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (three-letter code: PEG) (formula: C₄H₁₀O₃).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0
3	B	1	Total C O 7 4 3	0	0
3	C	1	Total C O 7 4 3	0	0

- Molecule 4 is TRIETHYLENE GLYCOL (three-letter code: PGE) (formula: $C_6H_{14}O_4$).

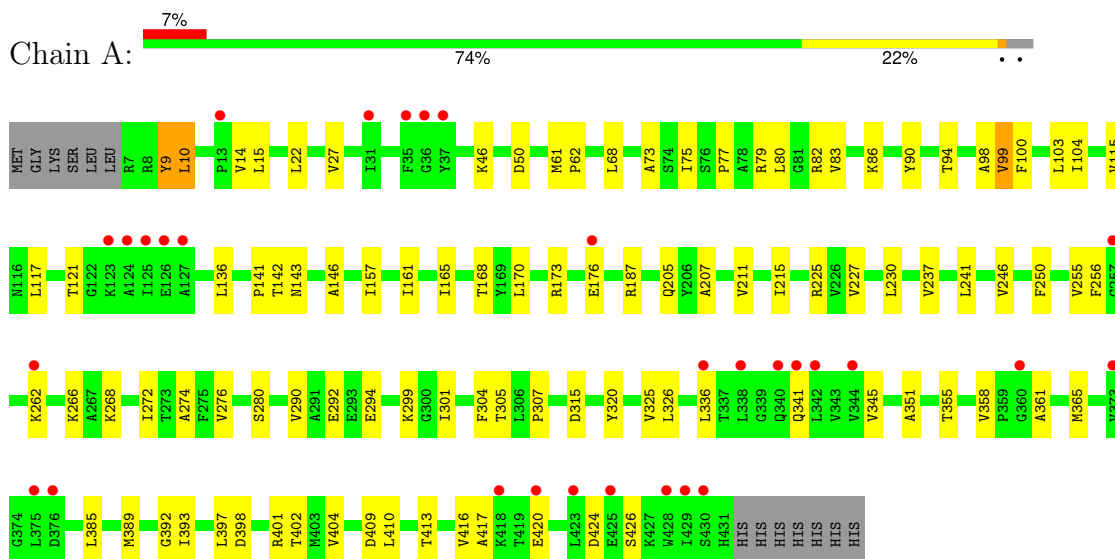


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			10	6	4		

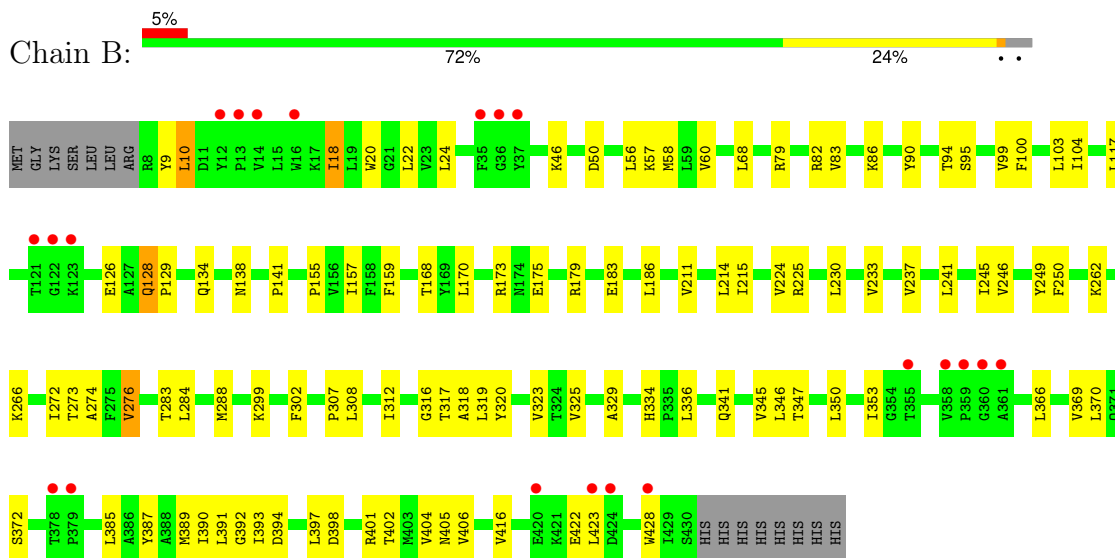
3 Residue-property plots [i](#)

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.

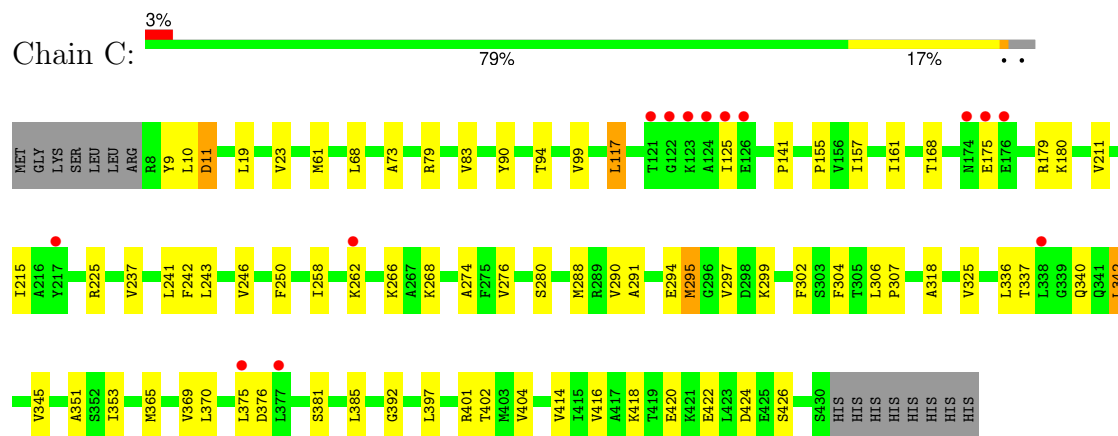
- Molecule 1: Proton/glutamate symporter, SDF family



- Molecule 1: Proton/glutamate symporter, SDF family



- Molecule 1: Proton/glutamate symporter, SDF family



4 Data and refinement statistics

Property	Value	Source
Space group	P 32 2 1	Depositor
Cell constants a, b, c, α , β , γ	115.74Å 115.74Å 308.49Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	45.75 – 3.20 47.66 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.75-3.20) 99.8 (47.66-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 3.19Å)	Xtrriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.232 , 0.275 0.237 , 0.280	Depositor DCC
R_{free} test set	2018 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	137.0	Xtrriage
Anisotropy	0.300	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.25 , 89.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtrriage
Estimated twinning fraction	0.058 for -h,-k,l	Xtrriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	9583	wwPDB-VP
Average B, all atoms (Å ²)	153.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.57% 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: PGE, QJW, PEG

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	0.25	0/3243	0.42	0/4413
1	B	0.26	0/3210	0.43	0/4370
1	C	0.26	0/3210	0.42	0/4370
All	All	0.26	0/9663	0.42	0/13153

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

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	3183	0	3385	57	0
1	B	3151	0	3353	70	0
1	C	3151	0	3353	51	0
2	A	20	0	0	1	0
2	B	20	0	0	1	0
2	C	20	0	0	3	0
3	A	7	0	10	0	0
3	B	14	0	20	2	0
3	C	7	0	10	0	0
4	C	10	0	14	2	0
All	All	9583	0	10145	175	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 9.

All (175) 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:126:GLU:HG2	1:B:128:GLN:HG2	1.60	0.83
1:B:237:VAL:HG12	1:B:323:VAL:HG11	1.59	0.83
1:C:211:VAL:HG13	1:C:276:VAL:HG11	1.61	0.81
1:A:103:LEU:HD13	1:A:341:GLN:HB3	1.64	0.80
1:C:211:VAL:HG22	1:C:276:VAL:HG21	1.69	0.73
1:C:274:ALA:HB1	1:C:402:THR:HG22	1.70	0.73
1:C:157:ILE:HD11	1:C:307:PRO:HB2	1.70	0.73
1:A:211:VAL:HG12	1:A:276:VAL:HG21	1.71	0.73
1:C:237:VAL:HG21	1:C:397:LEU:HD22	1.71	0.73
1:A:99:VAL:HB	1:A:345:VAL:HG22	1.70	0.73
1:B:237:VAL:HG21	1:B:397:LEU:HD22	1.71	0.72
1:B:157:ILE:HD11	1:B:307:PRO:HB2	1.72	0.71
1:B:103:LEU:HD13	1:B:341:GLN:HB3	1.71	0.71
1:A:325:VAL:HG12	1:A:336:LEU:HD11	1.74	0.70
1:C:117:LEU:HD11	1:C:385:LEU:HD23	1.73	0.69
1:C:99:VAL:HG13	1:C:318:ALA:HB1	1.75	0.69
1:B:159:PHE:HE2	3:B:503:PEG:O1	1.76	0.68
1:A:15:LEU:HD13	1:A:268:LYS:HZ1	1.59	0.67
1:A:237:VAL:HG11	1:A:397:LEU:HD22	1.76	0.67
1:A:274:ALA:HB1	1:A:402:THR:HG22	1.78	0.66
1:A:115:VAL:HG12	1:A:117:LEU:HD13	1.77	0.65
1:C:418:LYS:HZ1	4:C:502:PGE:C1	2.10	0.64
1:B:211:VAL:HG22	1:B:276:VAL:HG11	1.79	0.63
1:B:246:VAL:O	1:B:250:PHE:HB2	1.97	0.63
1:A:355:THR:HB	1:A:361:ALA:HB1	1.80	0.63
1:A:241:LEU:HB3	1:A:404:VAL:HG21	1.81	0.62
1:A:77:PRO:HG3	1:A:165:ILE:HD12	1.80	0.62
1:B:141:PRO:HB3	1:B:155:PRO:HB3	1.81	0.61
1:B:159:PHE:CE2	3:B:503:PEG:O1	2.54	0.60
1:B:398:ASP:HA	1:B:401:ARG:HG2	1.84	0.59
1:B:391:LEU:HA	1:B:394:ASP:HB2	1.84	0.59
1:A:157:ILE:HD11	1:A:307:PRO:HB2	1.85	0.59
1:C:141:PRO:HB3	1:C:155:PRO:HB3	1.84	0.58
1:A:246:VAL:O	1:A:250:PHE:HB2	2.04	0.58
1:C:258:ILE:HD13	1:C:414:VAL:HG12	1.84	0.58
1:C:10:LEU:H	1:C:10:LEU:HD23	1.70	0.57
1:B:99:VAL:HG22	1:B:318:ALA:HB1	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:230:LEU:HD21	1:B:389:MET:HG2	1.86	0.57
1:A:398:ASP:HA	1:A:401:ARG:HG2	1.86	0.57
1:C:325:VAL:HG12	1:C:336:LEU:HD11	1.87	0.57
1:B:128:GLN:N	1:B:129:PRO:HD2	2.20	0.57
1:B:46:LYS:NZ	1:B:50:ASP:OD1	2.38	0.56
1:A:117:LEU:HD21	1:A:385:LEU:HD23	1.88	0.56
1:A:22:LEU:HD13	1:A:272:ILE:HD12	1.87	0.56
1:B:10:LEU:H	1:B:10:LEU:HD12	1.71	0.55
1:C:241:LEU:HB3	1:C:404:VAL:HG21	1.89	0.55
1:B:274:ALA:HA	1:B:283:THR:HG21	1.89	0.55
1:B:317:THR:HG23	1:B:405:ASN:HD21	1.72	0.54
1:C:246:VAL:O	1:C:250:PHE:HB2	2.08	0.54
1:A:73:ALA:O	1:A:168:THR:OG1	2.22	0.54
1:A:401:ARG:HE	2:A:501:QJW:C9	2.21	0.54
1:B:134:GLN:O	1:B:138:ASN:ND2	2.41	0.53
1:A:351:ALA:HB1	1:A:365:MET:HG2	1.91	0.53
1:C:83:VAL:HG13	1:C:416:VAL:HG11	1.91	0.53
1:C:125:ILE:H	1:C:376:ASP:HB3	1.74	0.53
1:A:292:GLU:OE2	1:A:299:LYS:NZ	2.35	0.52
1:B:325:VAL:HG22	1:B:336:LEU:HD11	1.92	0.52
1:B:173:ARG:NH2	1:B:175:GLU:OE2	2.39	0.52
1:B:233:VAL:O	1:B:237:VAL:HG13	2.08	0.52
1:C:73:ALA:O	1:C:168:THR:OG1	2.28	0.52
1:C:401:ARG:HH21	2:C:501:QJW:C9	2.23	0.52
1:B:214:LEU:HB2	1:B:276:VAL:HG22	1.92	0.52
1:B:225:ARG:NH1	1:B:392:GLY:O	2.43	0.52
1:B:99:VAL:HG11	1:B:345:VAL:HA	1.92	0.51
1:A:301:ILE:HG21	1:A:417:ALA:HB2	1.92	0.51
1:B:95:SER:O	1:B:99:VAL:HG23	2.09	0.51
1:A:79:ARG:NH2	1:A:420:GLU:O	2.41	0.51
1:B:316:GLY:N	1:B:405:ASN:OD1	2.43	0.51
1:C:241:LEU:HD22	1:C:404:VAL:HG21	1.92	0.51
1:A:230:LEU:HD21	1:A:389:MET:HG2	1.92	0.50
1:C:79:ARG:HH21	1:C:422:GLU:HG2	1.76	0.50
1:B:284:LEU:O	1:B:288:MET:HG3	2.11	0.50
1:C:280:SER:N	2:C:501:QJW:O5	2.45	0.50
1:C:401:ARG:NH2	2:C:501:QJW:O3	2.43	0.49
1:C:11:ASP:OD1	1:C:11:ASP:N	2.45	0.49
1:B:329:ALA:HB1	1:B:334:HIS:O	2.13	0.49
1:A:82:ARG:HG2	1:A:86:LYS:HE3	1.95	0.49
1:C:68:LEU:HD23	1:C:157:ILE:HA	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:VAL:HG22	1:A:420:GLU:HG3	1.94	0.49
1:A:262:LYS:O	1:A:266:LYS:HG3	2.13	0.49
1:B:68:LEU:HD23	1:B:157:ILE:HA	1.94	0.48
1:C:175:GLU:O	1:C:179:ARG:NH1	2.47	0.48
1:C:370:LEU:HB3	1:C:375:LEU:O	2.13	0.48
1:C:291:ALA:HA	1:C:295:MET:HG3	1.94	0.48
1:B:241:LEU:HB3	1:B:404:VAL:HG21	1.95	0.48
1:A:409:ASP:O	1:A:413:THR:HG23	2.14	0.48
1:C:242:PHE:O	1:C:246:VAL:HG22	2.14	0.48
1:B:347:THR:HG21	1:B:372:SER:OG	2.14	0.48
1:C:365:MET:O	1:C:369:VAL:HG23	2.14	0.48
1:A:326:LEU:HD23	1:A:336:LEU:HD12	1.96	0.48
1:B:274:ALA:HB1	1:B:402:THR:HG22	1.94	0.48
1:A:100:PHE:CZ	1:A:104:ILE:HD11	2.49	0.47
1:B:273:THR:HG22	1:B:283:THR:HG22	1.96	0.47
1:B:56:LEU:O	1:B:60:VAL:HG23	2.15	0.47
1:A:98:ALA:HB2	1:A:315:ASP:HB3	1.97	0.46
1:B:175:GLU:O	1:B:179:ARG:NH1	2.48	0.46
1:B:20:TRP:O	1:B:24:LEU:HB2	2.15	0.46
1:B:299:LYS:HA	1:B:302:PHE:CE2	2.51	0.46
1:B:83:VAL:HG13	1:B:416:VAL:HG11	1.98	0.46
1:B:22:LEU:HD13	1:B:272:ILE:HD12	1.98	0.46
1:B:211:VAL:O	1:B:215:ILE:HG22	2.16	0.46
1:A:225:ARG:NH1	1:A:392:GLY:O	2.49	0.45
1:A:68:LEU:HD23	1:A:157:ILE:HA	1.97	0.45
1:B:18:ILE:HG23	1:B:272:ILE:HG21	1.97	0.45
1:C:351:ALA:HB1	1:C:365:MET:HG2	1.98	0.45
1:C:161:ILE:HD11	1:C:304:PHE:CD1	2.52	0.45
1:B:99:VAL:CG2	1:B:318:ALA:HB1	2.46	0.45
1:B:350:LEU:HA	1:B:353:ILE:HG22	1.99	0.45
1:A:83:VAL:HG13	1:A:416:VAL:HG11	1.99	0.45
1:A:161:ILE:HD11	1:A:304:PHE:CD1	2.53	0.44
1:A:237:VAL:O	1:A:241:LEU:HG	2.18	0.44
1:A:211:VAL:O	1:A:215:ILE:HG22	2.17	0.44
1:A:142:THR:O	1:B:57:LYS:HG3	2.17	0.44
1:C:299:LYS:HA	1:C:302:PHE:CE2	2.52	0.44
1:C:19:LEU:O	1:C:23:VAL:HG22	2.18	0.44
1:C:225:ARG:NH1	1:C:392:GLY:O	2.51	0.43
1:A:90:TYR:CZ	1:A:94:THR:HG21	2.53	0.43
1:B:245:ILE:HA	1:B:249:TYR:CD2	2.54	0.43
1:B:262:LYS:O	1:B:266:LYS:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:9:TYR:OH	1:A:205:GLN:O	2.24	0.43
1:A:46:LYS:NZ	1:A:50:ASP:OD1	2.48	0.43
1:B:79:ARG:NH1	1:B:422:GLU:OE2	2.52	0.43
1:B:100:PHE:CZ	1:B:104:ILE:HD11	2.53	0.43
1:B:211:VAL:HA	1:B:276:VAL:HG21	2.01	0.43
1:C:342:LEU:O	1:C:345:VAL:HG22	2.18	0.43
1:A:290:VAL:O	1:A:294:GLU:HB2	2.18	0.43
1:B:320:TYR:HE1	1:B:397:LEU:HD12	1.83	0.43
1:C:290:VAL:O	1:C:294:GLU:HB2	2.19	0.43
1:A:424:ASP:OD2	1:A:426:SER:OG	2.37	0.42
1:B:90:TYR:CZ	1:B:94:THR:HG21	2.54	0.42
1:B:401:ARG:NE	2:B:501:QJW:O3	2.46	0.42
1:A:207:ALA:O	1:A:211:VAL:HG13	2.18	0.42
1:A:211:VAL:HB	1:A:276:VAL:HG11	2.01	0.42
1:C:418:LYS:HZ1	4:C:502:PGE:H1	1.84	0.42
1:B:347:THR:HG23	1:B:369:VAL:HG22	2.02	0.42
1:A:143:ASN:HB3	1:A:146:ALA:HB3	2.02	0.42
1:B:134:GLN:HG3	1:B:138:ASN:HD21	1.84	0.42
1:A:15:LEU:HB3	1:A:268:LYS:CE	2.50	0.42
1:C:180:LYS:HE3	1:C:180:LYS:HB2	1.85	0.42
1:C:291:ALA:O	1:C:297:VAL:HG22	2.19	0.42
1:A:10:LEU:H	1:A:10:LEU:HD12	1.85	0.42
1:B:423:LEU:HD11	1:B:428:TRP:HE1	1.85	0.42
1:C:262:LYS:O	1:C:266:LYS:HG3	2.19	0.42
1:C:306:LEU:HD23	1:C:306:LEU:HA	1.92	0.42
1:A:141:PRO:O	1:B:58:MET:HB2	2.20	0.41
1:A:255:VAL:HG13	1:A:256:PHE:CD2	2.54	0.41
1:B:134:GLN:HG3	1:B:138:ASN:ND2	2.35	0.41
1:B:393:ILE:O	1:B:397:LEU:HG	2.20	0.41
1:B:82:ARG:HG2	1:B:86:LYS:HE3	2.02	0.41
1:B:100:PHE:CE2	1:B:104:ILE:HD11	2.55	0.41
1:B:170:LEU:HD12	1:B:170:LEU:HA	1.90	0.41
1:C:19:LEU:HD23	1:C:19:LEU:HA	1.84	0.41
1:C:288:MET:HE3	1:C:307:PRO:HG3	2.02	0.41
1:C:424:ASP:OD2	1:C:426:SER:OG	2.38	0.41
1:C:90:TYR:CZ	1:C:94:THR:HG21	2.56	0.41
1:A:75:ILE:HG21	1:A:80:LEU:HD12	2.03	0.41
1:B:308:LEU:O	1:B:312:ILE:HG12	2.21	0.41
1:A:320:TYR:HE1	1:A:397:LEU:HD12	1.86	0.41
1:C:337:THR:HG23	1:C:340:GLN:H	1.86	0.41
1:A:410:LEU:HD23	1:A:410:LEU:HA	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:366:LEU:HD23	1:B:387:TYR:CE1	2.56	0.41
1:B:390:ILE:HD13	1:B:390:ILE:HA	1.91	0.41
1:C:79:ARG:NH2	1:C:420:GLU:O	2.54	0.41
1:C:297:VAL:HG23	1:C:302:PHE:CD2	2.55	0.41
1:A:187[A]:ARG:CZ	1:C:180:LYS:HD2	2.51	0.41
1:A:305:THR:OG1	1:A:413:THR:HG22	2.20	0.41
1:A:61:MET:HB2	1:A:62:PRO:HD3	2.04	0.40
1:C:299:LYS:HD2	1:C:302:PHE:CZ	2.56	0.40
1:B:117:LEU:HD23	1:B:117:LEU:HA	1.91	0.40
1:B:319:LEU:O	1:B:323:VAL:HG12	2.20	0.40
1:C:211:VAL:O	1:C:215:ILE:HG22	2.22	0.40
1:A:75:ILE:HD11	1:A:79:ARG:HD3	2.04	0.40
1:A:393:ILE:O	1:A:397:LEU:HG	2.21	0.40
1:B:18:ILE:HD13	1:B:211:VAL:HG21	2.02	0.40
1:B:245:ILE:O	1:B:249:TYR:HB2	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	424/438 (97%)	409 (96%)	15 (4%)	0	100	100
1	B	421/438 (96%)	407 (97%)	14 (3%)	0	100	100
1	C	421/438 (96%)	407 (97%)	14 (3%)	0	100	100
All	All	1266/1314 (96%)	1223 (97%)	43 (3%)	0	100	100

There are no Ramachandran outliers to report.

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	334/345 (97%)	321 (96%)	13 (4%)	32	67
1	B	331/345 (96%)	318 (96%)	13 (4%)	32	67
1	C	331/345 (96%)	321 (97%)	10 (3%)	41	73
All	All	996/1035 (96%)	960 (96%)	36 (4%)	35	69

All (36) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	TYR
1	A	10	LEU
1	A	14	VAL
1	A	27	VAL
1	A	99	VAL
1	A	121	THR
1	A	136	LEU
1	A	170	LEU
1	A	173	ARG
1	A	176	GLU
1	A	227	VAL
1	A	280	SER
1	A	358	VAL
1	B	9	TYR
1	B	10	LEU
1	B	18	ILE
1	B	128	GLN
1	B	168	THR
1	B	183	GLU
1	B	186	LEU
1	B	224	VAL
1	B	276	VAL
1	B	346	LEU
1	B	370	LEU
1	B	385	LEU
1	B	406	VAL

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Mol	Chain	Res	Type
1	C	9	TYR
1	C	11	ASP
1	C	61	MET
1	C	117	LEU
1	C	243	LEU
1	C	268	LYS
1	C	295	MET
1	C	342	LEU
1	C	353	ILE
1	C	381	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	321	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

8 ligands are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
4	PGE	C	502	-	9,9,9	0.14	0	8,8,8	0.11	0
2	QJW	A	501	-	19,20,20	2.61	2 (10%)	24,27,27	1.93	9 (37%)
3	PEG	B	502	-	6,6,6	0.50	0	5,5,5	0.27	0
3	PEG	B	503	-	6,6,6	0.11	0	5,5,5	0.07	0
3	PEG	C	503	-	6,6,6	0.50	0	5,5,5	0.28	0
2	QJW	C	501	-	19,20,20	2.61	2 (10%)	24,27,27	1.79	5 (20%)
3	PEG	A	502	-	6,6,6	0.50	0	5,5,5	0.32	0
2	QJW	B	501	-	19,20,20	2.60	2 (10%)	24,27,27	1.79	4 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	PGE	C	502	-	-	3/7/7/7	-
2	QJW	A	501	-	-	8/21/21/21	0/1/1/1
3	PEG	B	502	-	-	2/4/4/4	-
3	PEG	B	503	-	-	1/4/4/4	-
3	PEG	C	503	-	-	2/4/4/4	-
2	QJW	C	501	-	-	8/21/21/21	0/1/1/1
3	PEG	A	502	-	-	1/4/4/4	-
2	QJW	B	501	-	-	8/21/21/21	0/1/1/1

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	501	QJW	O7-N2	7.68	1.40	1.22
2	A	501	QJW	O6-N2	7.68	1.40	1.22
2	B	501	QJW	O7-N2	7.66	1.40	1.22
2	B	501	QJW	O6-N2	7.65	1.40	1.22
2	C	501	QJW	O6-N2	7.64	1.40	1.22
2	A	501	QJW	O7-N2	7.63	1.40	1.22

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	QJW	C1-C6-C5	4.99	120.21	115.73
2	C	501	QJW	C1-C6-C5	4.77	120.02	115.73
2	B	501	QJW	C1-C6-C5	4.61	119.88	115.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	501	QJW	C4-C5-C6	-4.05	119.77	122.89
2	C	501	QJW	C4-C5-C6	-3.78	119.98	122.89
2	B	501	QJW	C4-C5-C6	-3.71	120.03	122.89
2	C	501	QJW	C7-C6-C5	-3.30	120.30	123.81
2	B	501	QJW	C7-C6-C5	-3.29	120.31	123.81
2	A	501	QJW	C7-C6-C5	-3.21	120.40	123.81
2	B	501	QJW	C4-C5-N2	2.27	119.68	116.68
2	A	501	QJW	C4-C5-N2	2.26	119.66	116.68
2	C	501	QJW	C4-C5-N2	2.25	119.65	116.68
2	A	501	QJW	C8-C10-N1	2.20	113.56	109.20
2	A	501	QJW	O3-C9-C8	2.19	121.56	113.64
2	C	501	QJW	O3-C9-O2	-2.11	119.30	124.08
2	A	501	QJW	O5-C11-O4	-2.10	119.31	124.08
2	A	501	QJW	O3-C9-O2	-2.05	119.44	124.08
2	A	501	QJW	O5-C11-C10	2.00	121.05	114.15

There are no chirality outliers.

All (33) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	QJW	O1-C8-C9-O2
2	A	501	QJW	O1-C8-C9-O3
2	A	501	QJW	C10-C8-O1-C7
2	A	501	QJW	N1-C10-C11-O5
2	B	501	QJW	O1-C8-C9-O2
2	B	501	QJW	O1-C8-C9-O3
2	B	501	QJW	C10-C8-O1-C7
2	B	501	QJW	C8-C10-C11-O4
2	B	501	QJW	C8-C10-C11-O5
2	C	501	QJW	O1-C8-C9-O2
2	C	501	QJW	O1-C8-C9-O3
2	C	501	QJW	C10-C8-O1-C7
2	C	501	QJW	C9-C8-O1-C7
2	C	501	QJW	C8-C10-C11-O4
2	C	501	QJW	C8-C10-C11-O5
2	B	501	QJW	C9-C8-O1-C7
3	B	503	PEG	O2-C3-C4-O4
3	A	502	PEG	O2-C3-C4-O4
3	B	502	PEG	O1-C1-C2-O2
2	B	501	QJW	N1-C10-C11-O5
2	C	501	QJW	N1-C10-C11-O5
4	C	502	PGE	O2-C3-C4-O3

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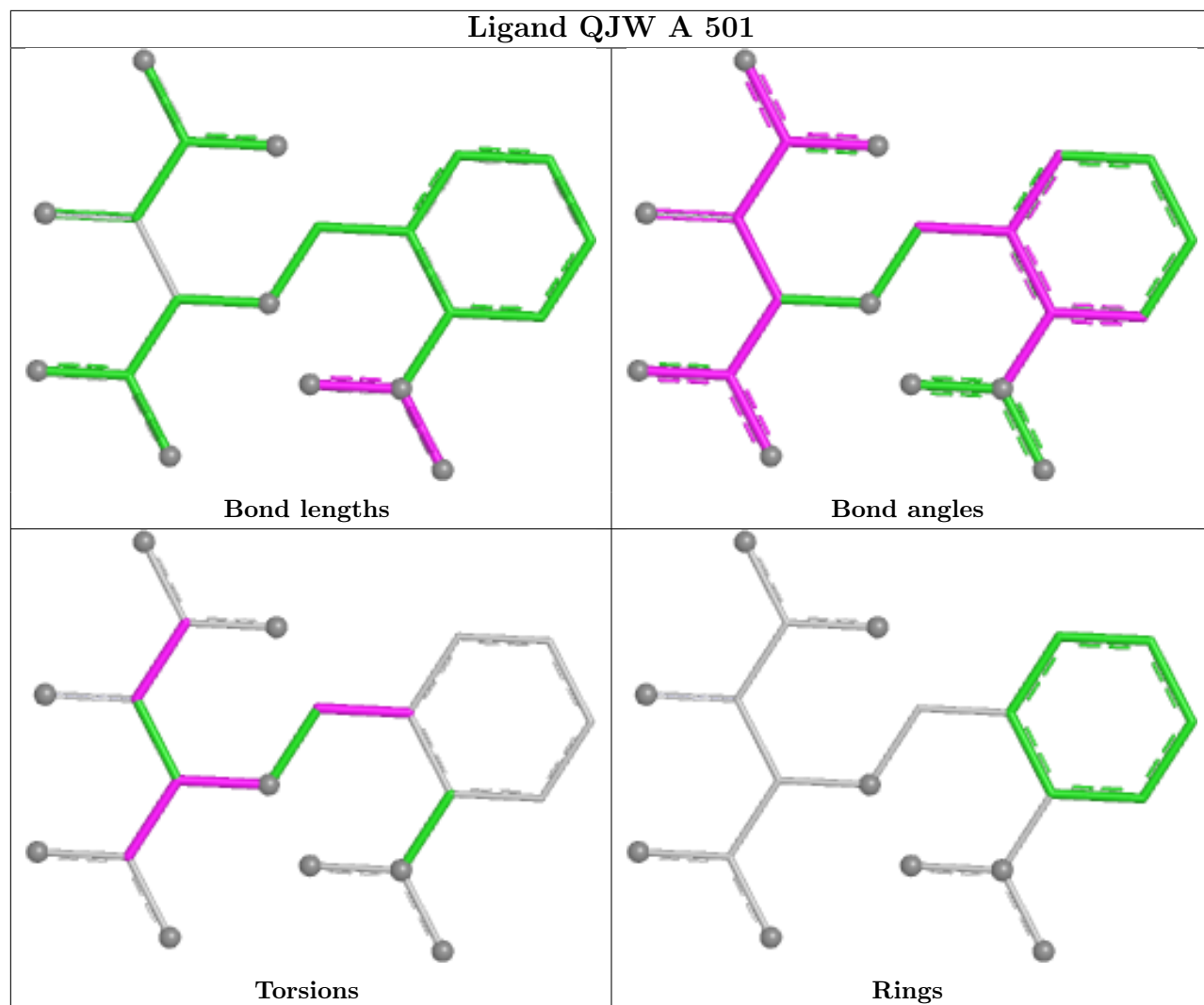
Mol	Chain	Res	Type	Atoms
3	C	503	PEG	C1-C2-O2-C3
4	C	502	PGE	C6-C5-O3-C4
4	C	502	PGE	C3-C4-O3-C5
2	A	501	QJW	N1-C10-C11-O4
3	B	502	PEG	C4-C3-O2-C2
3	C	503	PEG	O1-C1-C2-O2
2	A	501	QJW	C10-C8-C9-O2
2	A	501	QJW	C10-C8-C9-O3
2	A	501	QJW	C5-C6-C7-O1
2	B	501	QJW	C5-C6-C7-O1
2	C	501	QJW	C5-C6-C7-O1

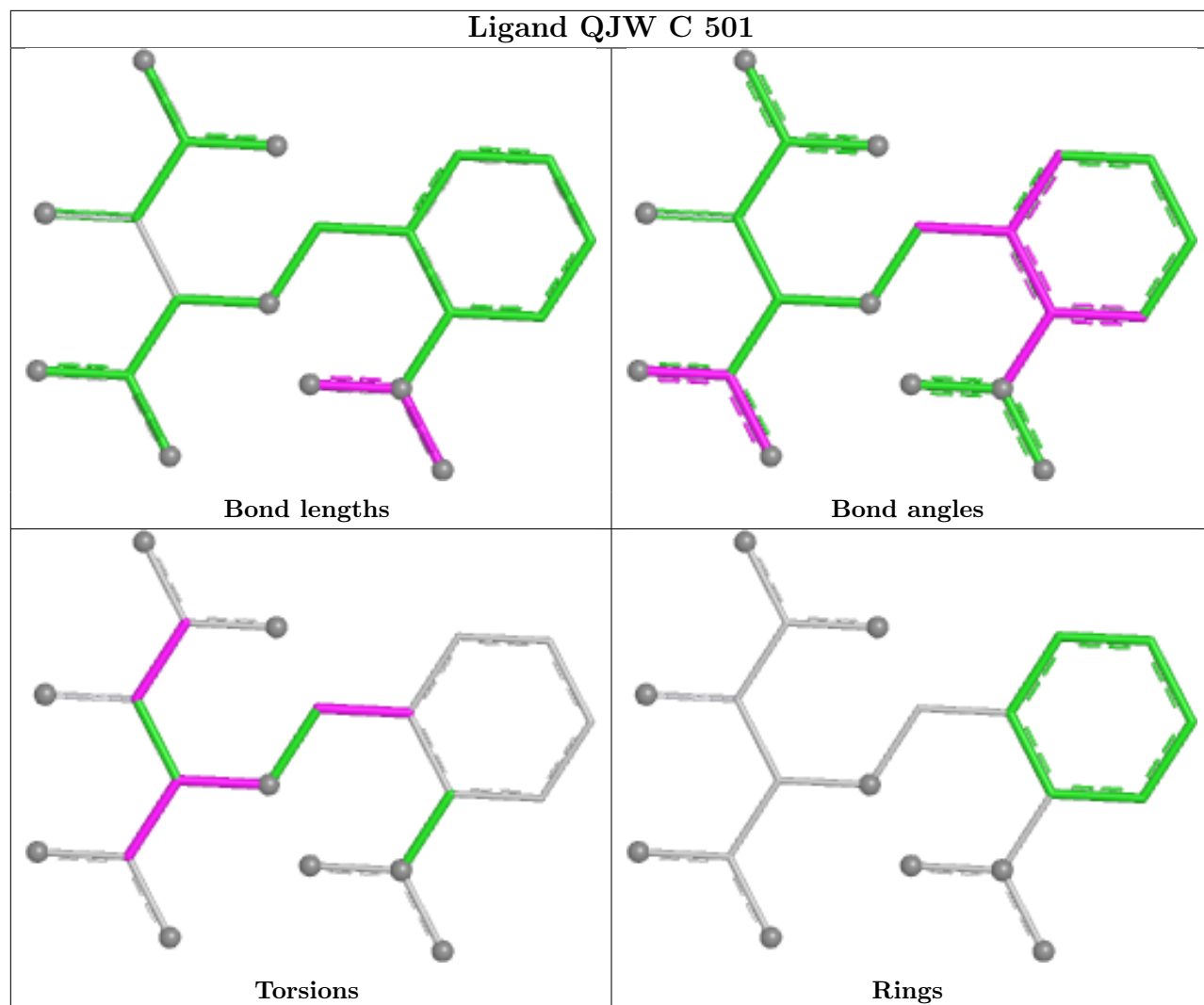
There are no ring outliers.

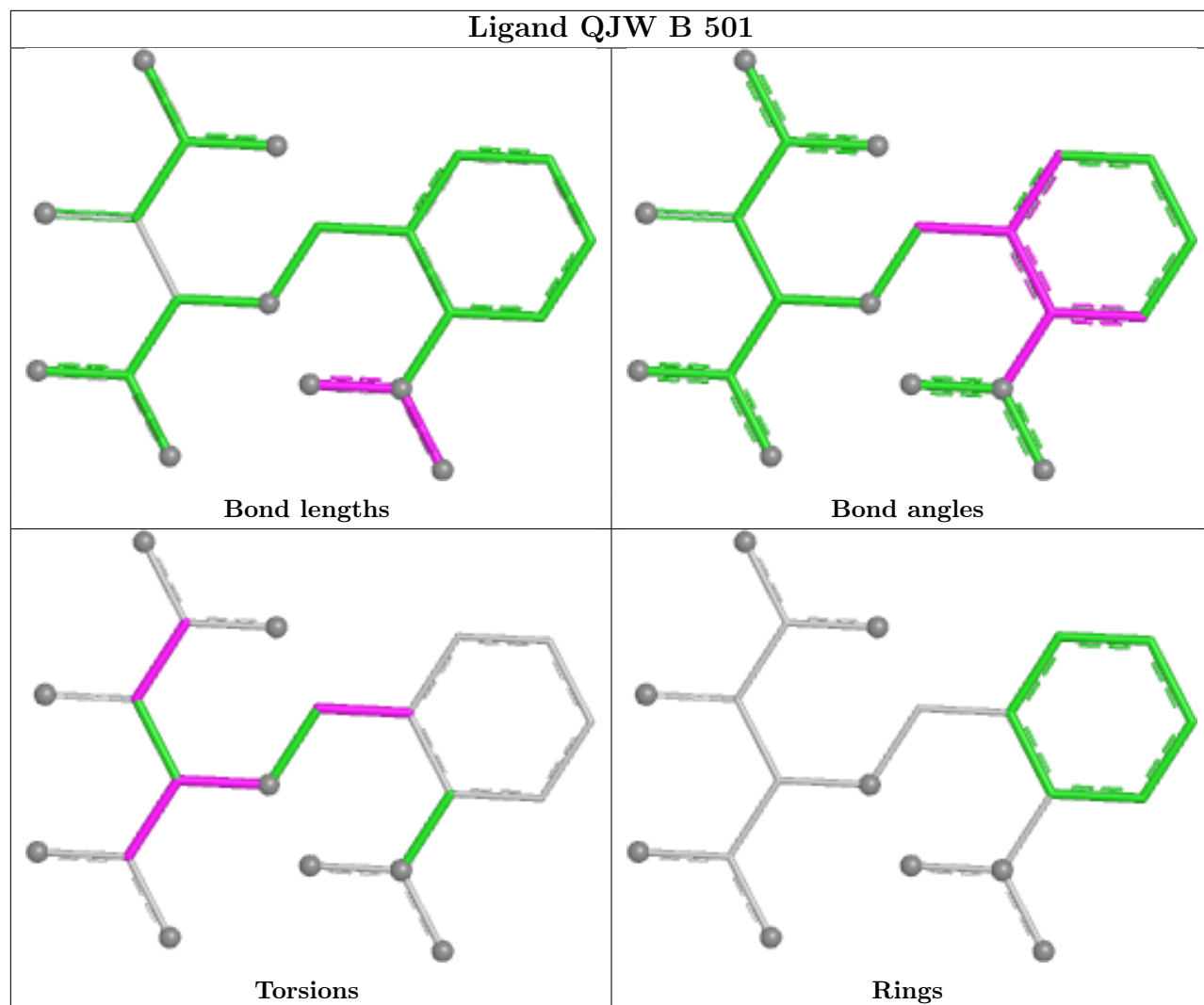
5 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	502	PGE	2	0
2	A	501	QJW	1	0
3	B	503	PEG	2	0
2	C	501	QJW	3	0
2	B	501	QJW	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	425/438 (97%)	0.04	30 (7%) 16 9	100, 143, 214, 308	0
1	B	423/438 (96%)	-0.12	21 (4%) 28 16	91, 148, 214, 267	0
1	C	423/438 (96%)	-0.15	14 (3%) 46 30	109, 145, 206, 354	0
All	All	1271/1314 (96%)	-0.08	65 (5%) 28 16	91, 146, 213, 354	0

All (65) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	359	PRO	8.4
1	C	125	ILE	7.8
1	B	360	GLY	7.7
1	A	125	ILE	6.9
1	B	121	THR	5.5
1	A	429	ILE	5.2
1	C	124	ALA	5.1
1	A	360	GLY	4.8
1	B	424	ASP	4.7
1	A	373	VAL	4.2
1	A	428	TRP	4.1
1	C	121	THR	4.0
1	B	423	LEU	3.9
1	C	174	ASN	3.8
1	A	124	ALA	3.8
1	A	37	TYR	3.7
1	B	35	PHE	3.7
1	A	423	LEU	3.7
1	A	127	ALA	3.6
1	A	342	LEU	3.5
1	B	358	VAL	3.5
1	A	375	LEU	3.4
1	B	123	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	35	PHE	3.2
1	A	430	SER	3.2
1	B	13	PRO	3.1
1	B	12	TYR	3.0
1	C	175	GLU	3.0
1	A	126	GLU	2.9
1	A	418	LYS	2.9
1	C	123	LYS	2.9
1	A	425	GLU	2.8
1	A	338	LEU	2.7
1	A	341	GLN	2.7
1	C	122	GLY	2.7
1	A	123	LYS	2.7
1	B	16	TRP	2.7
1	A	376	ASP	2.6
1	A	176	GLU	2.6
1	C	176	GLU	2.6
1	B	37	TYR	2.6
1	A	336	LEU	2.6
1	B	378	THR	2.6
1	B	361	ALA	2.6
1	A	31	ILE	2.6
1	B	428	TRP	2.5
1	A	36	GLY	2.5
1	A	262	LYS	2.5
1	A	344	VAL	2.5
1	A	340	GLN	2.3
1	B	355	THR	2.3
1	A	420	GLU	2.3
1	B	420	GLU	2.3
1	B	36	GLY	2.2
1	A	13	PRO	2.2
1	C	377	LEU	2.2
1	C	217	TYR	2.2
1	C	262	LYS	2.2
1	C	375	LEU	2.2
1	C	126	GLU	2.1
1	B	122	GLY	2.1
1	A	257	GLY	2.1
1	B	379	PRO	2.1
1	B	14	VAL	2.0
1	C	338	LEU	2.0

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

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

6.3 Carbohydrates [i](#)

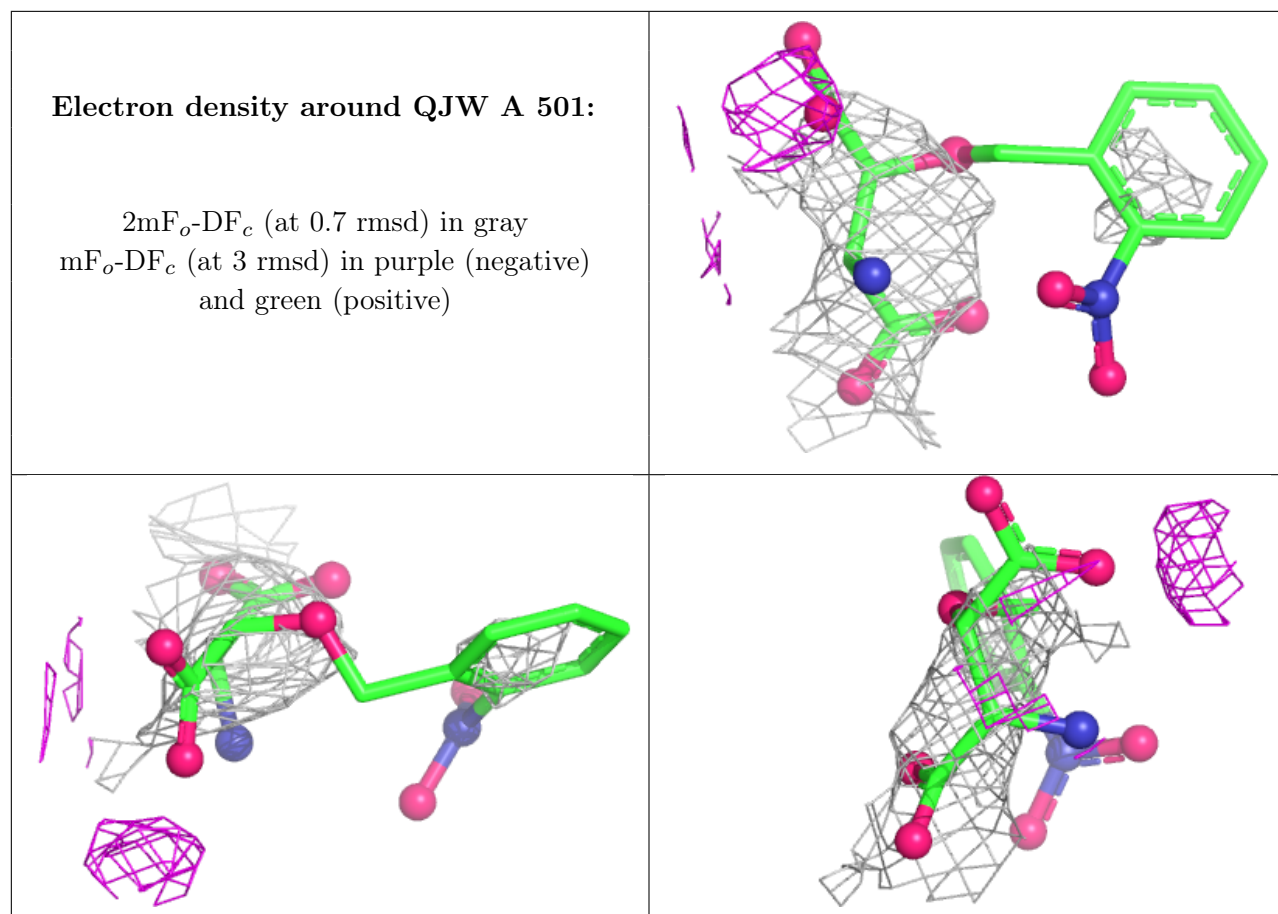
There are no monosaccharides in this entry.

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.

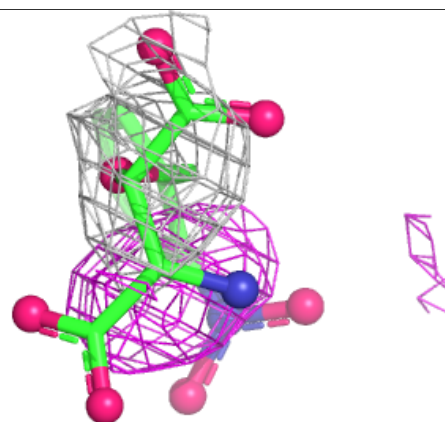
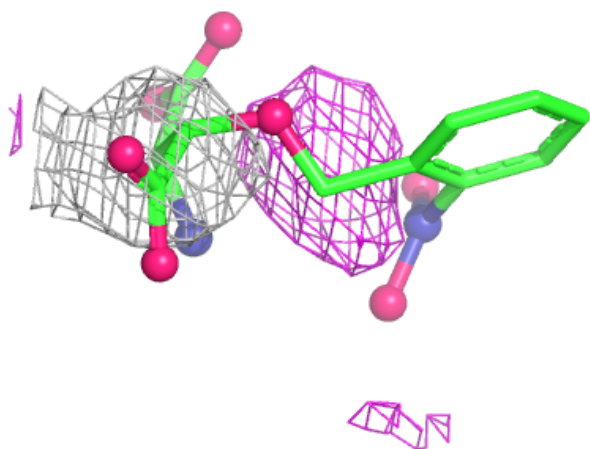
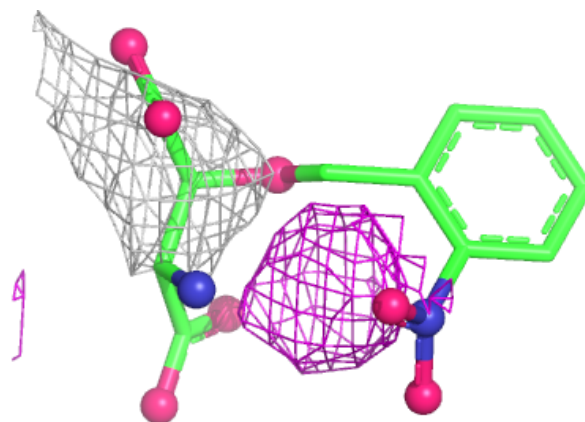
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	PEG	B	503	7/7	0.42	0.47	176,192,229,239	0
4	PGE	C	502	10/10	0.57	0.18	144,171,193,207	0
2	QJW	A	501	20/20	0.74	0.47	204,219,235,238	0
3	PEG	A	502	7/7	0.78	0.55	123,151,189,190	0
2	QJW	B	501	20/20	0.79	0.65	169,188,202,209	0
2	QJW	C	501	20/20	0.80	0.31	160,201,211,212	0
3	PEG	C	503	7/7	0.81	0.34	138,187,205,233	0
3	PEG	B	502	7/7	0.84	0.14	160,165,181,185	0

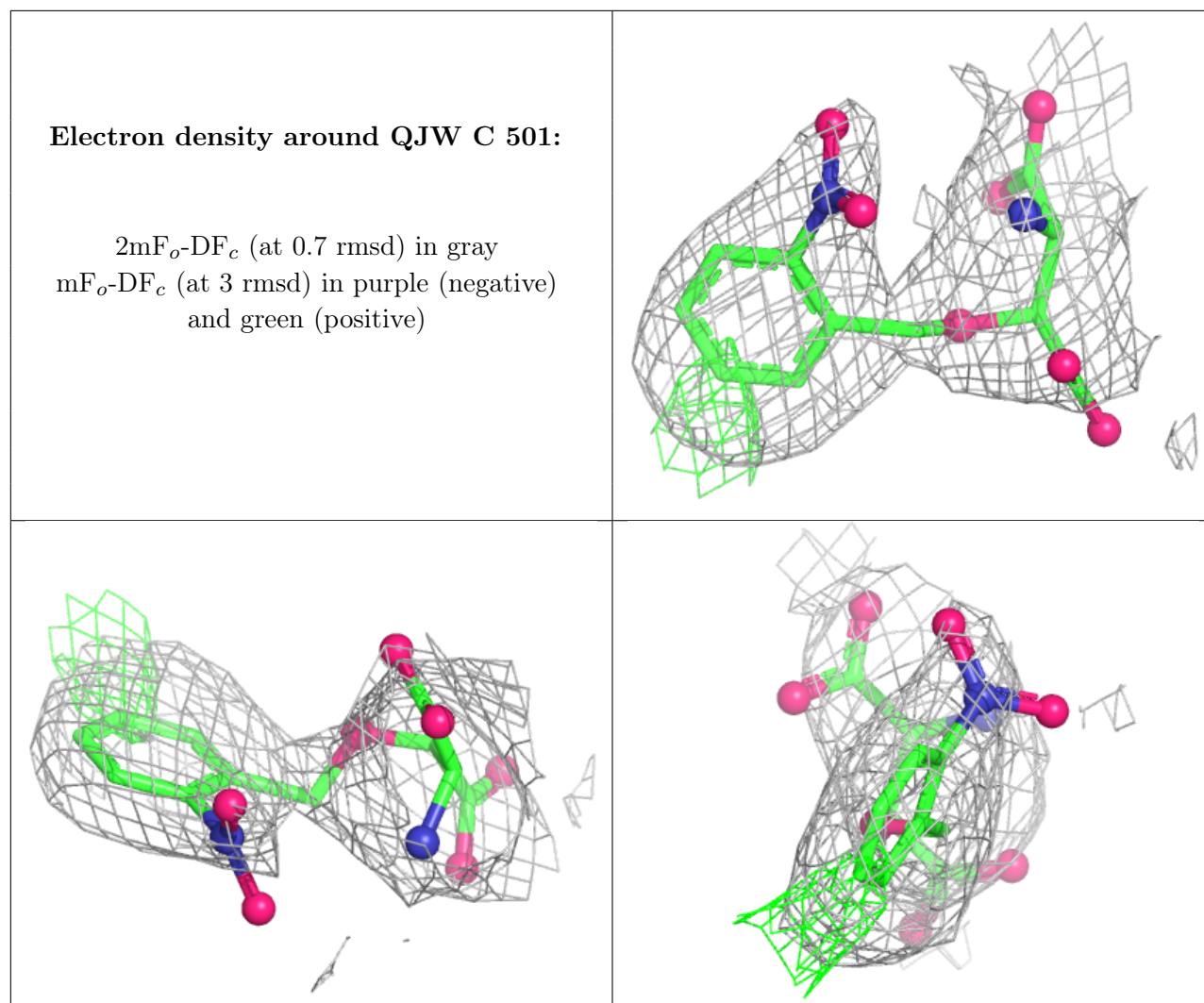
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



Electron density around QJW B 501:

$2mF_o-DF_c$ (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.