



Full wwPDB X-ray Structure Validation Report ⓘ

Apr 15, 2026 – 12:58 AM UTC

PDB ID : 6ZGB / pdb_00006zgb
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	:	4-5-2 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

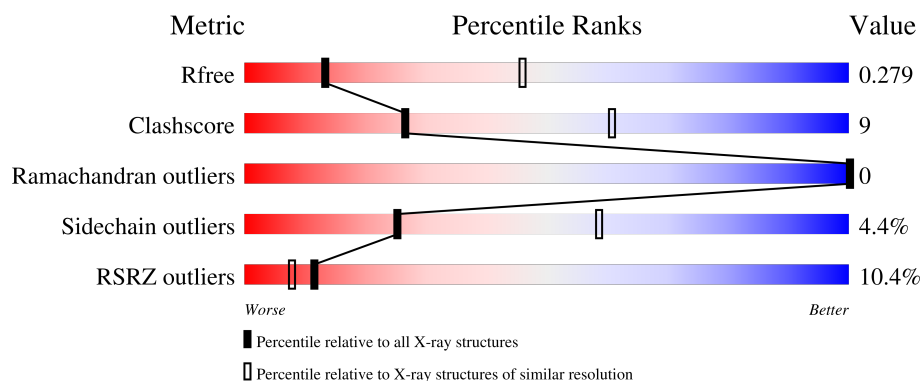
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.20 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	438	8% 74% 23% .
1	B	438	11% 70% 26% ..
1	C	438	11% 77% 19% ..

2 Entry composition

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
1	A	425	Total	C	N	O	S	0	1	0
			3183	2097	519	551	16			
1	B	423	Total	C	N	O	S	0	0	0
			3151	2079	508	548	16			
1	C	423	Total	C	N	O	S	0	0	0
			3151	2079	508	548	16			

There are 24 discrepancies between the modelled and reference sequences:

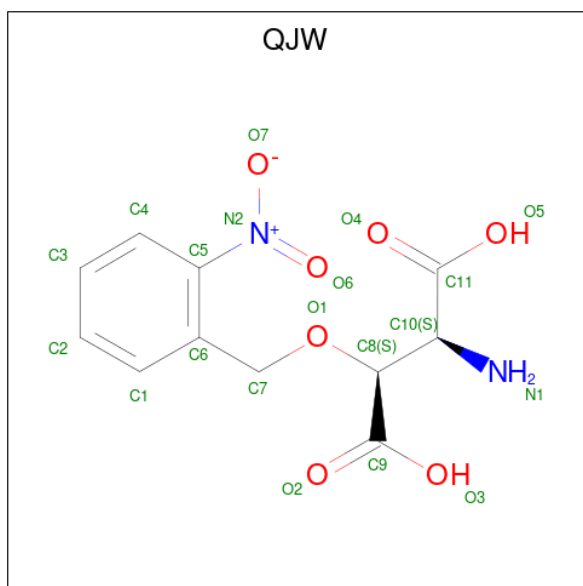
Chain	Residue	Modelled	Actual	Comment	Reference
A	431	HIS	-	expression tag	UNP Q5JID0
A	432	HIS	-	expression tag	UNP Q5JID0
A	433	HIS	-	expression tag	UNP Q5JID0
A	434	HIS	-	expression tag	UNP Q5JID0
A	435	HIS	-	expression tag	UNP Q5JID0
A	436	HIS	-	expression tag	UNP Q5JID0
A	437	HIS	-	expression tag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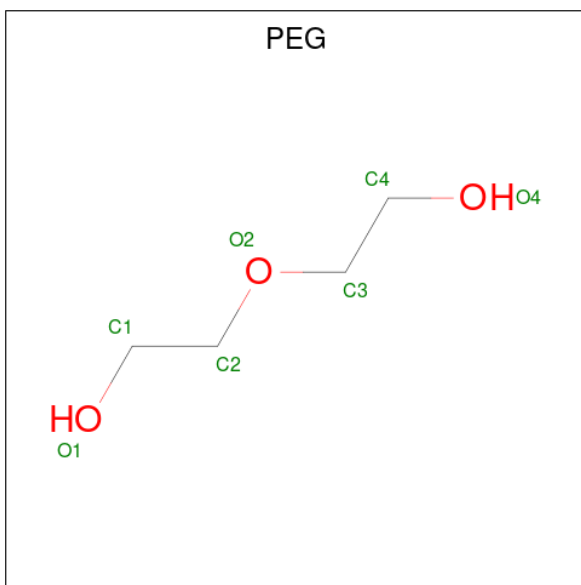
Chain	Residue	Modelled	Actual	Comment	Reference
C	438	HIS	-	expression tag	UNP Q5JID0

- Molecule 2 is (3S)-3-[(2-nitrophenyl)methoxy]-L-aspartic acid (CCD ID: QJW) (formula: $C_{11}H_{12}N_2O_7$).



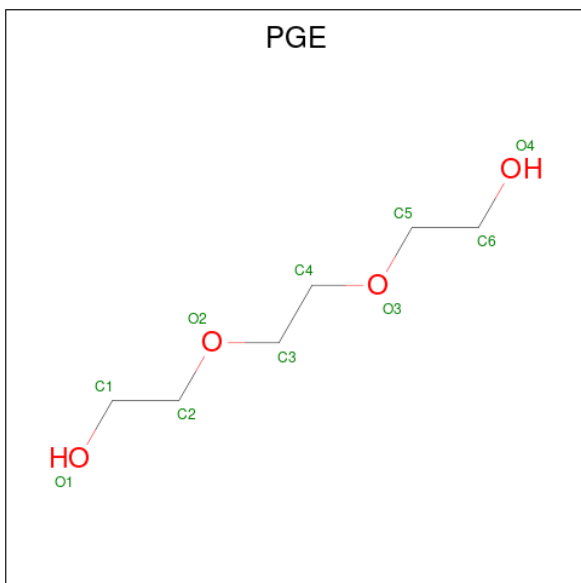
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			20	11	2	7		
2	B	1	Total	C	N	O	0	0
			20	11	2	7		
2	C	1	Total	C	N	O	0	0
			20	11	2	7		

- Molecule 3 is DI(HYDROXYETHYL)ETHER (CCD ID: PEG) (formula: $C_4H_{10}O_3$).



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

- Molecule 4 is TRIETHYLENE GLYCOL (CCD ID: PGE) (formula: $C_6H_{14}O_4$).

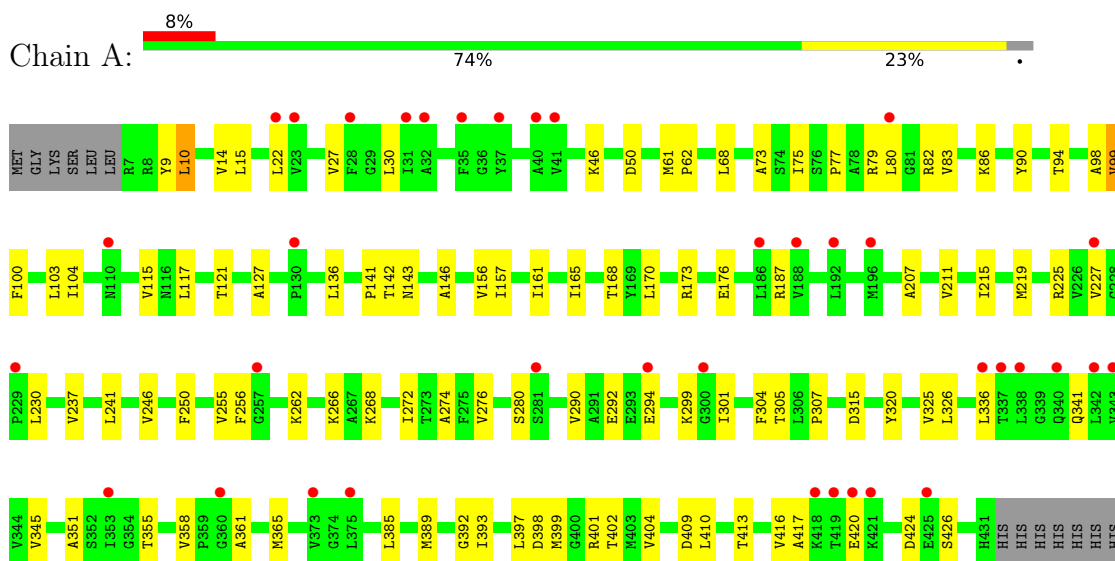


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	C	1	Total	C	O	0	0
			10	6	4		

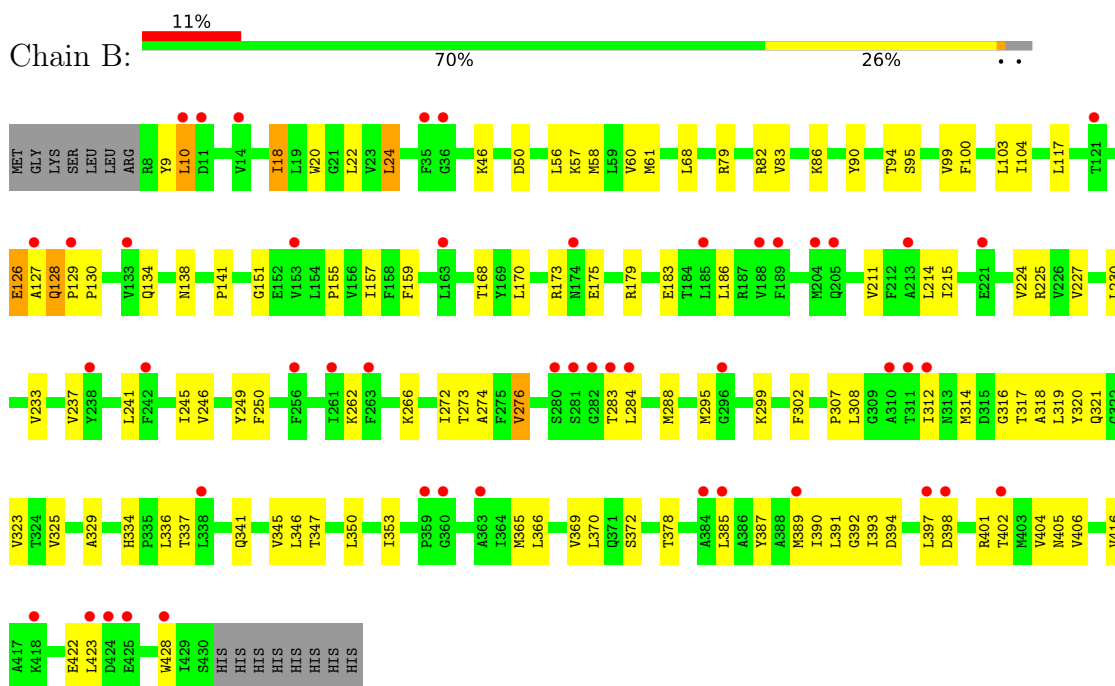
3 Residue-property plots [i](#)

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

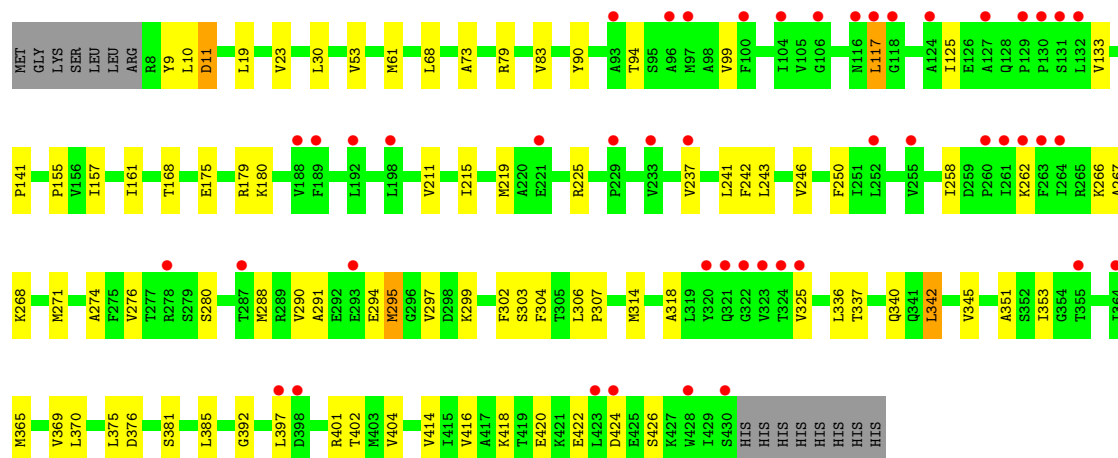


- Molecule 1: Proton/glutamate symporter, SDF family



● Molecule 1: Proton/glutamate symporter, SDF family

Chain C:  11% 77% 19%



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 45.75 – 3.20	Depositor EDS
% Data completeness (in resolution range)	99.6 (45.75-3.20) 99.7 (45.75-3.20)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 3.19Å)	Xtriage
Refinement program	PHENIX 1.16_3549	Depositor
R, R_{free}	0.232 , 0.275 0.237 , 0.279	Depositor DCC
R_{free} test set	2018 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	137.0	Xtriage
Anisotropy	0.300	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.26 , 79.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.44$, $\langle L^2 \rangle = 0.26$	Xtriage
Estimated twinning fraction	0.058 for -h,-k,l	Xtriage
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

Xtriage'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 [i](#)

5.1 Standard geometry [i](#)

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	0.13	0/3243	0.34	1/4413 (0.0%)
1	B	0.18	0/3210	0.41	4/4370 (0.1%)
1	C	0.13	0/3210	0.32	0/4370
All	All	0.15	0/9663	0.36	5/13153 (0.0%)

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	127	ALA	CA-C-N	8.66	130.92	120.09
1	B	127	ALA	C-N-CA	8.66	130.92	120.09
1	A	127	ALA	N-CA-C	5.22	117.01	110.91
1	B	130	PRO	CA-C-N	-5.20	113.67	120.95
1	B	130	PRO	C-N-CA	-5.20	113.67	120.95

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3183	0	3385	59	0
1	B	3151	0	3353	74	0
1	C	3151	0	3353	54	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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	184	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 (184) 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:A:15:LEU:HD13	1:A:268:LYS:HZ1	1.50	0.76
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: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	2.11	0.64
1:B:211:VAL:HG22	1:B:276:VAL:HG11	1.79	0.63
1:B:321:GLN:HE22	1:B:365:MET:HE2	1.62	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:A:61:MET:HE1	1:A:156:VAL:HG21	1.81	0.61
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
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:A:276:VAL:HA	1:A:399:MET:HE2	1.87	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:C:288:MET:HE2	1:C:303:SER:HA	1.95	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:61:MET:HE3	1:B:151:GLY:HA2	1.97	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:30:LEU:HD21	1:A:219:MET:HE3	1.99	0.44
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
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:267:ALA:HB3	1:C:271:MET:HE3	2.01	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:C:30:LEU:HD21	1:C:219:MET:HE3	2.02	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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: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:314:MET:HE3	1:C:314:MET:HB2	1.94	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
1:B:365:MET:HE2	1:B:365:MET:HB3	1.97	0.41
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:C:418:LYS:HZ1	4:C:502:PGE:H1	1.86	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:B:266:LYS:HB2	1:B:295:MET:HE2	2.03	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

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	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

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%)	28	62
1	B	331/345 (96%)	312 (94%)	19 (6%)	18	51
1	C	331/345 (96%)	319 (96%)	12 (4%)	31	63
All	All	996/1035 (96%)	952 (96%)	44 (4%)	25	59

All (44) 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

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Mol	Chain	Res	Type
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	24	LEU
1	B	126	GLU
1	B	128	GLN
1	B	168	THR
1	B	183	GLU
1	B	186	LEU
1	B	224	VAL
1	B	227	VAL
1	B	276	VAL
1	B	314	MET
1	B	337	THR
1	B	346	LEU
1	B	370	LEU
1	B	378	THR
1	B	385	LEU
1	B	406	VAL
1	C	9	TYR
1	C	11	ASP
1	C	53	VAL
1	C	61	MET
1	C	117	LEU
1	C	133	VAL
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 (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	116	ASN
1	A	138	ASN
1	A	313	ASN
1	B	134	GLN
1	B	321	GLN
1	C	334	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

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	$\# Z > 2$
2	QJW	C	501	-	19,20,20	2.53	1 (5%)	21,27,27	1.44	3 (14%)
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
2	QJW	A	501	-	19,20,20	2.55	1 (5%)	21,27,27	1.58	7 (33%)
3	PEG	A	502	-	6,6,6	0.50	0	5,5,5	0.32	0
3	PEG	C	503	-	6,6,6	0.50	0	5,5,5	0.28	0
2	QJW	B	501	-	19,20,20	2.53	1 (5%)	21,27,27	1.46	2 (9%)
4	PGE	C	502	-	9,9,9	0.14	0	8,8,8	0.11	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	QJW	C	501	-	-	10/19/21/21	0/1/1/1
3	PEG	B	502	-	-	2/4/4/4	-
3	PEG	B	503	-	-	1/4/4/4	-
2	QJW	A	501	-	-	8/19/21/21	0/1/1/1
3	PEG	A	502	-	-	1/4/4/4	-
3	PEG	C	503	-	-	2/4/4/4	-
2	QJW	B	501	-	-	10/19/21/21	0/1/1/1
4	PGE	C	502	-	-	3/7/7/7	-

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	QJW	O6-N2	10.52	1.40	1.22
2	B	501	QJW	O6-N2	10.48	1.40	1.22
2	C	501	QJW	O6-N2	10.46	1.40	1.22

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
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	3.00	119.68	116.47
2	A	501	QJW	C4-C5-N2	2.99	119.66	116.47
2	C	501	QJW	C4-C5-N2	2.97	119.65	116.47
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 (37) 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	C4-C5-N2-O6
2	B	501	QJW	C6-C5-N2-O6
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	C4-C5-N2-O6
2	C	501	QJW	C6-C5-N2-O6
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
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:

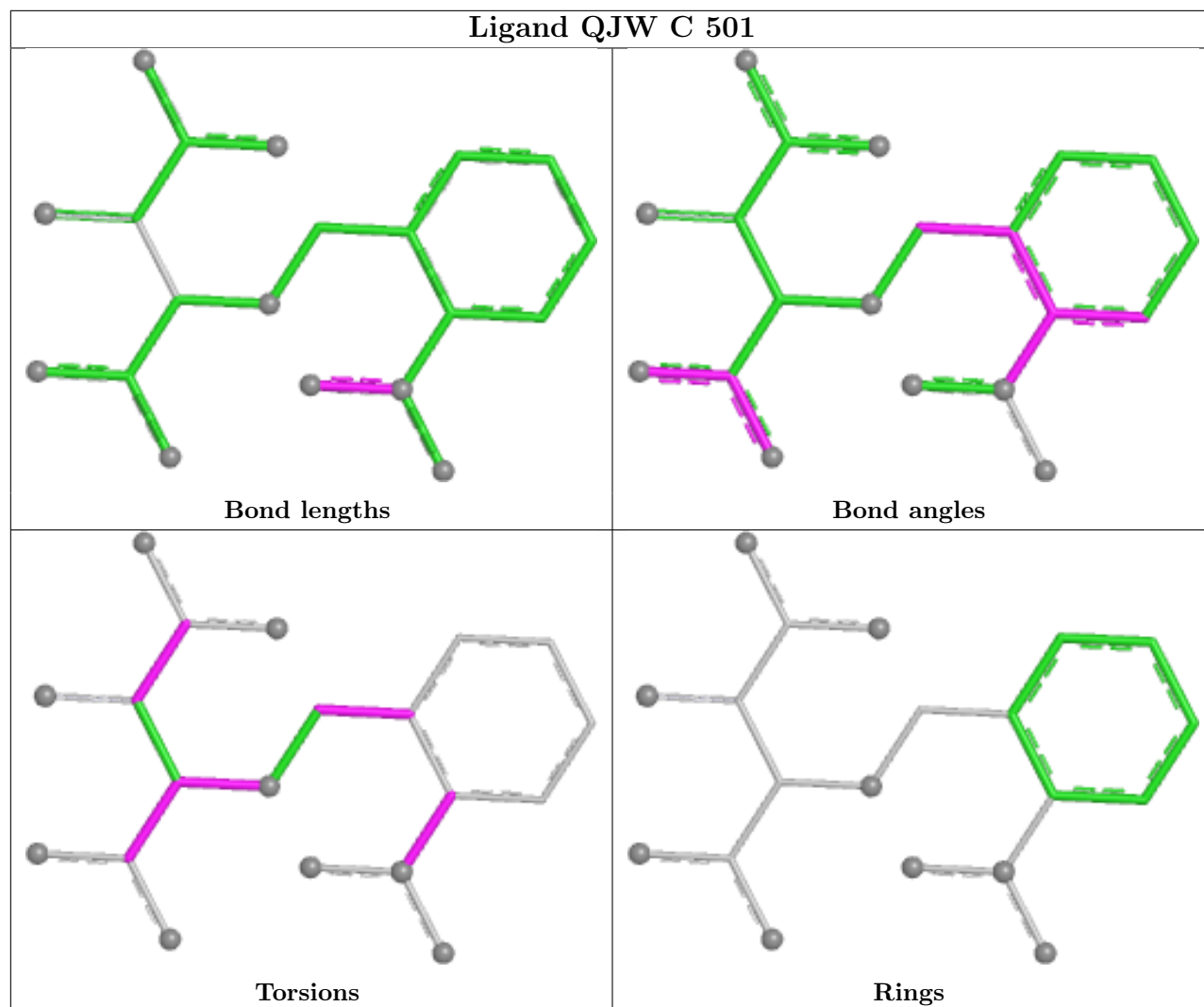
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	C	501	QJW	3	0

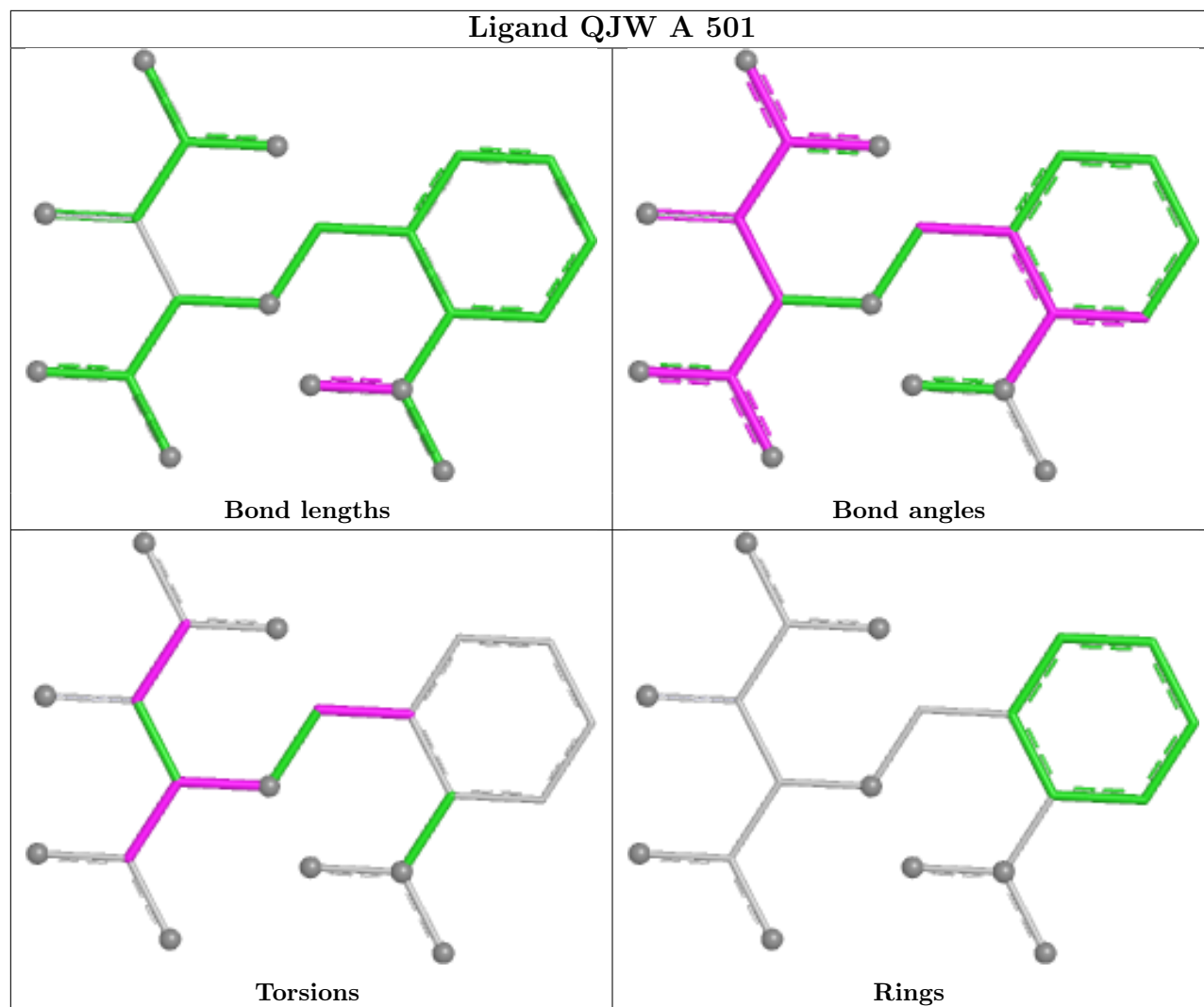
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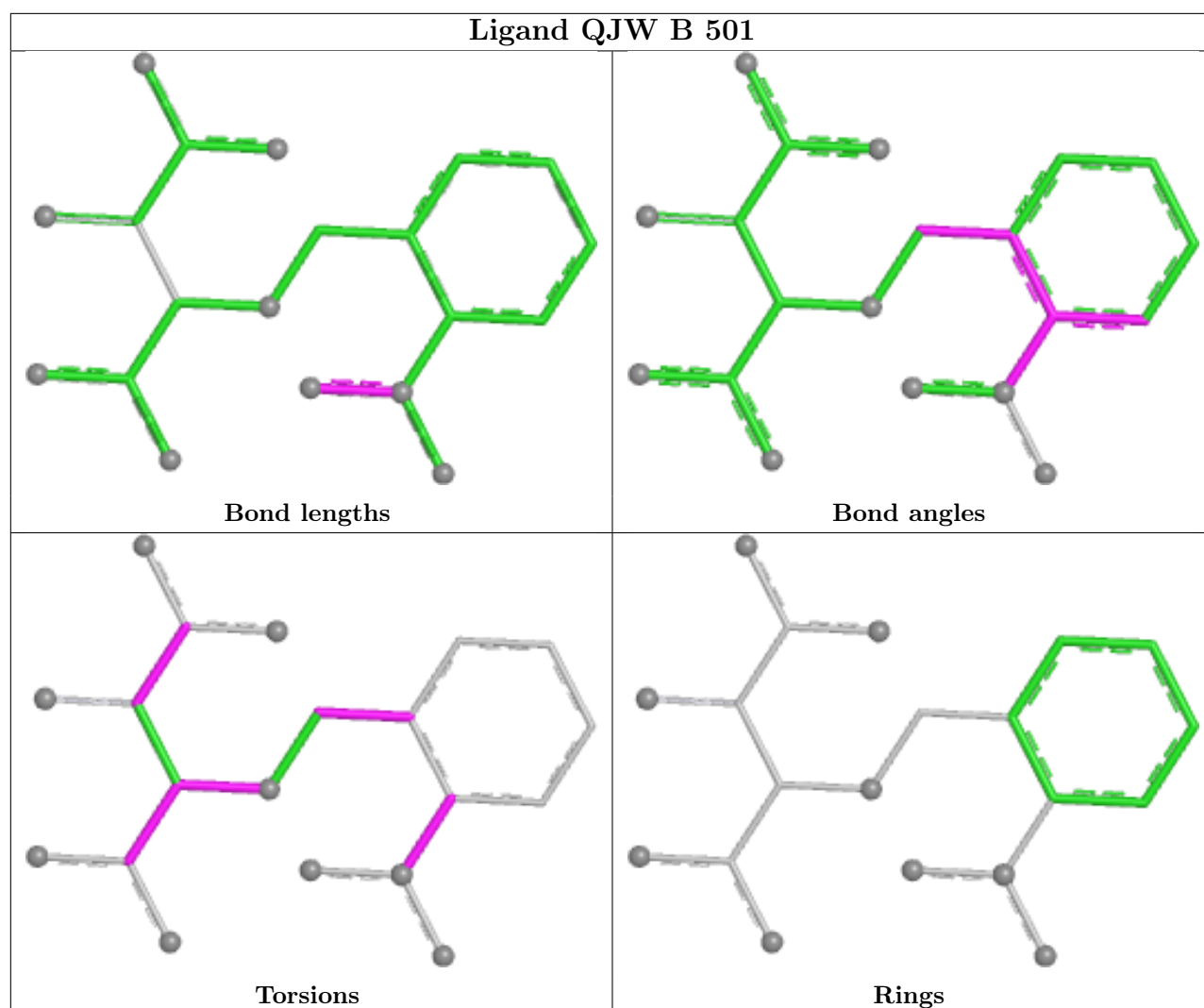
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Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	503	PEG	2	0
2	A	501	QJW	1	0
2	B	501	QJW	1	0
4	C	502	PGE	2	0

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%)	0.24	37 (8%) 16 11	68, 143, 214, 308	1 (0%)
1	B	423/438 (96%)	0.40	48 (11%) 10 7	91, 148, 214, 267	0
1	C	423/438 (96%)	0.33	47 (11%) 10 7	109, 145, 206, 354	0
All	All	1271/1314 (96%)	0.32	132 (10%) 11 8	68, 146, 213, 354	1 (0%)

All (132) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	281	SER	9.3
1	B	359	PRO	7.2
1	B	360	GLY	6.6
1	B	10	LEU	6.4
1	B	423	LEU	5.9
1	C	188	VAL	5.6
1	B	424	ASP	5.6
1	A	31	ILE	5.5
1	B	189	PHE	5.4
1	B	35	PHE	5.3
1	C	130	PRO	5.1
1	A	35	PHE	5.0
1	C	100	PHE	4.9
1	A	28	PHE	4.7
1	C	97	MET	4.7
1	A	80	LEU	4.6
1	A	342	LEU	4.6
1	C	189	PHE	4.6
1	B	398	ASP	4.4
1	B	280	SER	4.4
1	A	421	LYS	4.3
1	C	129	PRO	4.2
1	B	397	LEU	4.2

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Mol	Chain	Res	Type	RSRZ
1	B	121	THR	4.2
1	B	36	GLY	4.1
1	B	185	LEU	4.0
1	C	323	VAL	4.0
1	C	364	ILE	3.9
1	A	40	ALA	3.9
1	A	353	ILE	3.9
1	C	430	SER	3.8
1	A	340	GLN	3.7
1	B	418	LYS	3.7
1	A	337	THR	3.6
1	B	174	ASN	3.6
1	C	324	THR	3.6
1	A	360	GLY	3.3
1	B	283	THR	3.3
1	B	384	ALA	3.3
1	B	205	GLN	3.3
1	B	242	PHE	3.3
1	C	93	ALA	3.2
1	A	418	LYS	3.2
1	B	163	LEU	3.2
1	A	373	VAL	3.2
1	C	131	SER	3.2
1	C	198	LEU	3.2
1	B	282	GLY	3.1
1	C	132	LEU	3.1
1	A	23	VAL	3.1
1	C	325	VAL	3.1
1	C	423	LEU	3.1
1	A	188	VAL	3.1
1	C	127	ALA	3.0
1	A	37	TYR	3.0
1	C	118	GLY	3.0
1	A	227	VAL	3.0
1	C	192	LEU	3.0
1	C	117	LEU	3.0
1	A	294	GLU	2.9
1	B	129	PRO	2.9
1	C	263	PHE	2.9
1	A	420	GLU	2.8
1	B	263	PHE	2.8
1	A	375	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	322	GLY	2.8
1	C	260	PRO	2.8
1	C	355	THR	2.8
1	C	287	THR	2.8
1	C	229	PRO	2.8
1	C	398	ASP	2.7
1	A	110	ASN	2.7
1	B	11	ASP	2.7
1	A	257	GLY	2.7
1	C	424	ASP	2.7
1	C	320	TYR	2.7
1	A	32	ALA	2.7
1	B	14	VAL	2.7
1	B	310	ALA	2.7
1	B	296	GLY	2.6
1	B	188	VAL	2.6
1	C	237	VAL	2.6
1	A	300	GLY	2.6
1	B	213	ALA	2.6
1	B	311	THR	2.6
1	C	262	LYS	2.5
1	B	133	VAL	2.5
1	B	261	ILE	2.4
1	C	255	VAL	2.4
1	A	343	VAL	2.4
1	C	264	ILE	2.4
1	A	338	LEU	2.4
1	B	428	TRP	2.4
1	A	41	VAL	2.4
1	C	106	GLY	2.4
1	C	397	LEU	2.4
1	C	261	ILE	2.3
1	C	321	GLN	2.3
1	C	233	VAL	2.3
1	A	196	MET	2.3
1	A	186	LEU	2.3
1	B	256	PHE	2.3
1	C	293	GLU	2.2
1	C	428	TRP	2.2
1	A	281	SER	2.2
1	A	22	LEU	2.2
1	B	402	THR	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	385	LEU	2.2
1	C	124	ALA	2.2
1	B	312	ILE	2.1
1	C	252	LEU	2.1
1	C	96	ALA	2.1
1	B	238	TYR	2.1
1	A	192	LEU	2.1
1	A	229	PRO	2.1
1	A	425	GLU	2.1
1	B	221	GLU	2.1
1	B	425	GLU	2.1
1	C	116	ASN	2.1
1	C	278	ARG	2.1
1	B	127	ALA	2.1
1	B	363	ALA	2.1
1	A	130	PRO	2.1
1	B	153	VAL	2.1
1	B	389	MET	2.1
1	B	284	LEU	2.0
1	C	104	ILE	2.0
1	B	338	LEU	2.0
1	B	204	MET	2.0
1	A	419	THR	2.0
1	C	221	GLU	2.0
1	A	336	LEU	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 ⓘ

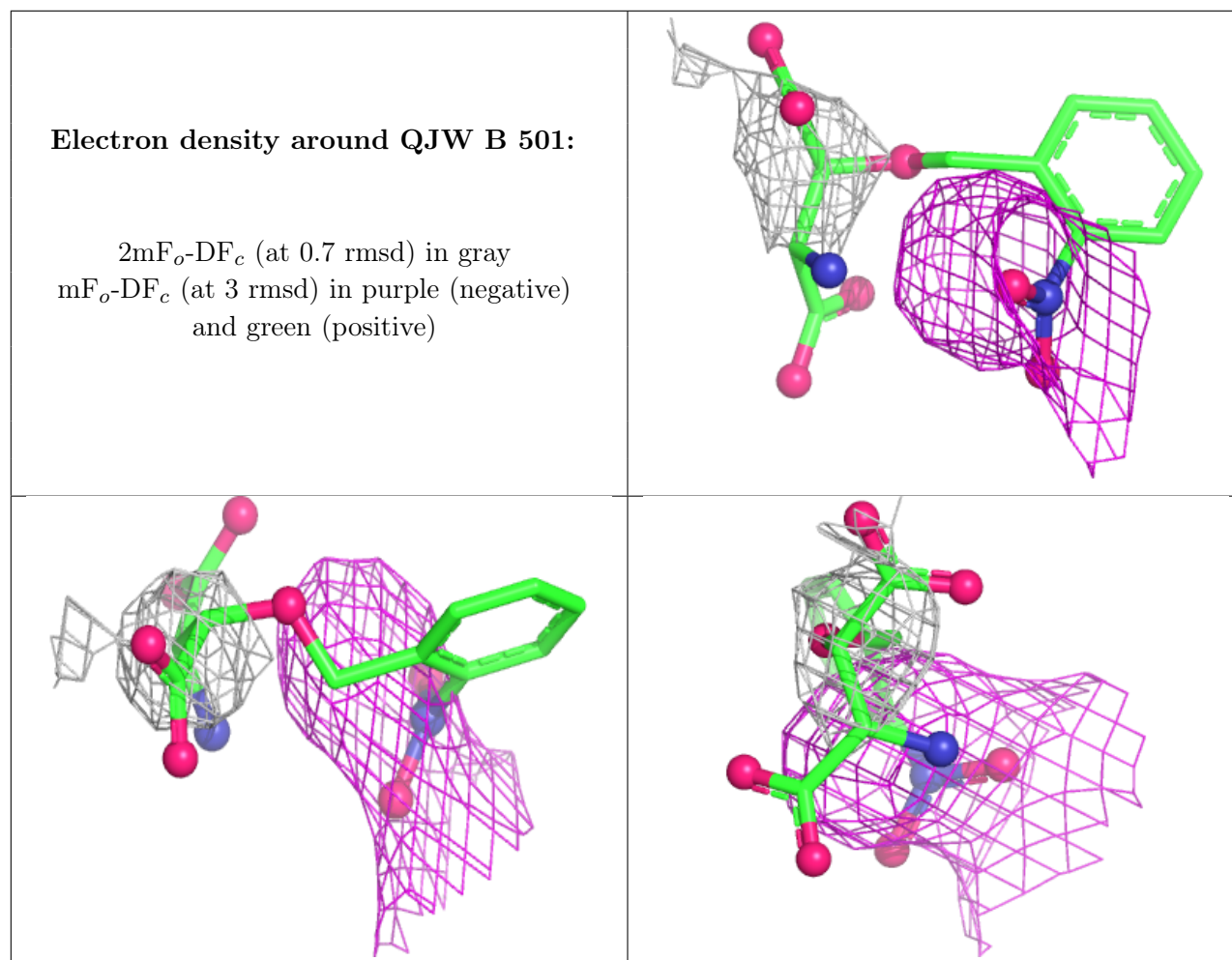
There are no oligosaccharides in this entry.

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.

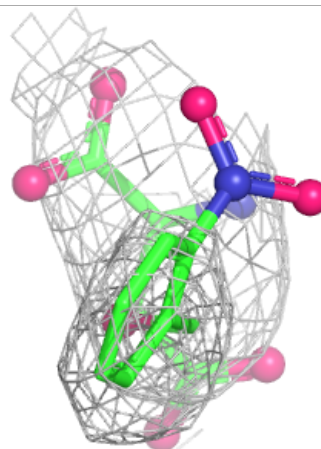
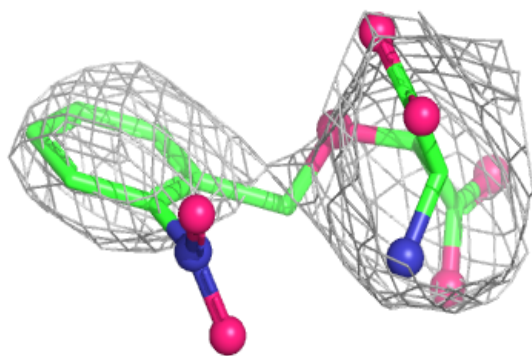
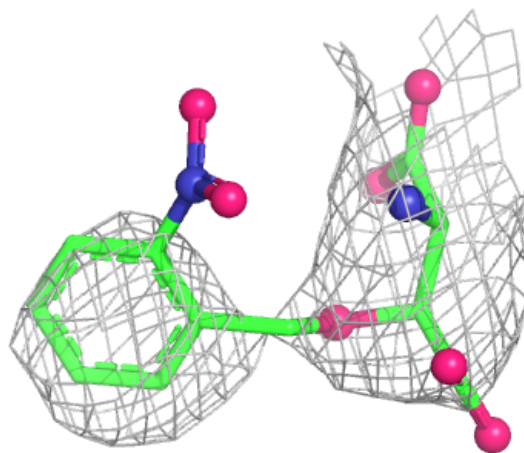
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	QJW	B	501	20/20	0.62	0.16	169,188,202,209	0
2	QJW	C	501	20/20	0.63	0.15	160,201,211,212	0
4	PGE	C	502	10/10	0.64	0.10	144,171,193,207	0
2	QJW	A	501	20/20	0.74	0.16	204,219,235,238	0
3	PEG	B	502	7/7	0.80	0.11	160,165,181,185	0
3	PEG	B	503	7/7	0.81	0.57	176,192,229,239	0
3	PEG	C	503	7/7	0.89	0.41	138,187,205,233	0
3	PEG	A	502	7/7	0.90	0.34	123,151,189,190	0

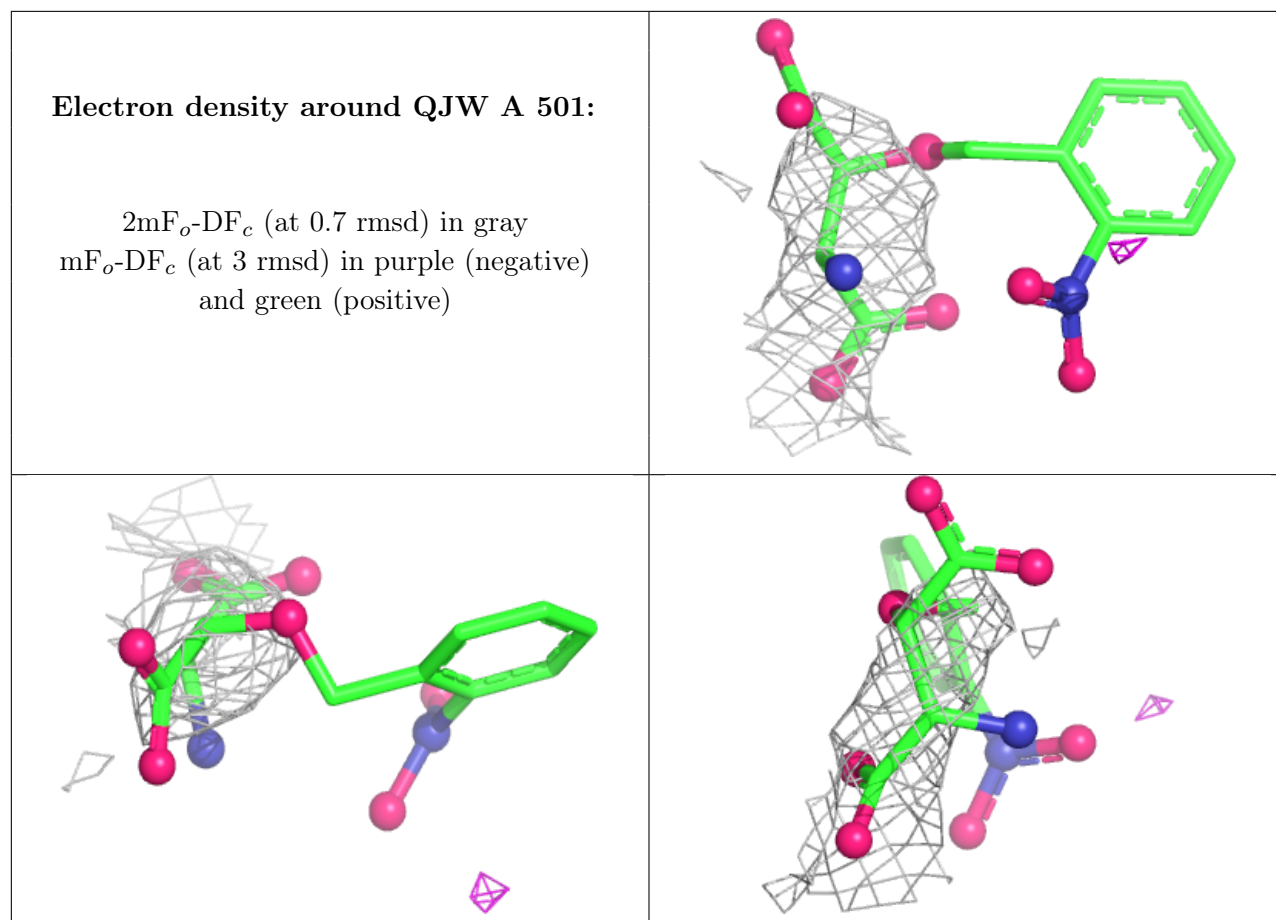
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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



Electron density around QJW C 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 ⓘ

There are no such residues in this entry.