



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 07:51 PM UTC

PDB ID : 1Q4L / pdb_00001q4l
Title : GSK-3 Beta complexed with Inhibitor I-5
Authors : Bertrand, J.A.; Thieffine, S.; Vulpetti, A.; Cristiani, C.; Valsasina, B.; Knapp, S.; Kalisz, H.M.; Flocco, M.
Deposited on : 2003-08-04
Resolution : 2.77 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

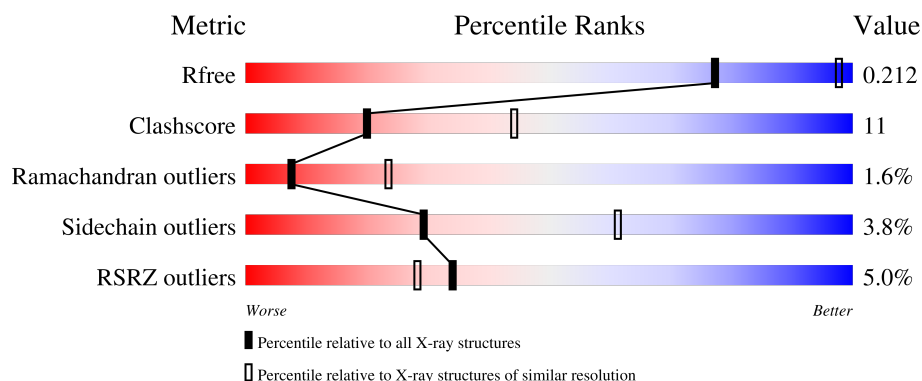
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.77 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	5248 (2.80-2.76)
Clashscore	190562	5693 (2.80-2.76)
Ramachandran outliers	187476	5590 (2.80-2.76)
Sidechain outliers	187428	5592 (2.80-2.76)
RSRZ outliers	180081	5251 (2.80-2.76)

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	424	4% 59% 19% • 19%
1	B	424	4% 58% 19% • 21%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 5515 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.

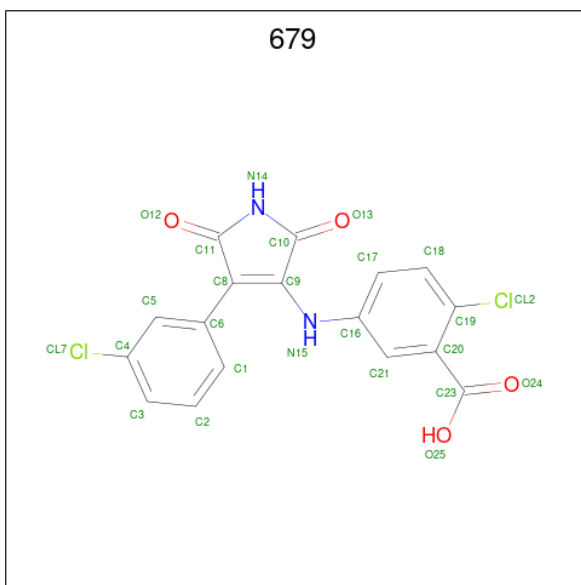
- Molecule 1 is a protein called GLYCOGEN SYNTHASE KINASE-3 BETA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	342	Total	C	N	O	S	0	0	0
			2728	1753	470	494	11			
1	B	337	Total	C	N	O	S	0	0	0
			2690	1726	461	492	11			

There are 10 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-3	GLY	-	cloning artifact	UNP P49841
A	-2	PRO	-	cloning artifact	UNP P49841
A	-1	LEU	-	cloning artifact	UNP P49841
A	0	GLY	-	cloning artifact	UNP P49841
A	1	SER	-	cloning artifact	UNP P49841
B	-3	GLY	-	cloning artifact	UNP P49841
B	-2	PRO	-	cloning artifact	UNP P49841
B	-1	LEU	-	cloning artifact	UNP P49841
B	0	GLY	-	cloning artifact	UNP P49841
B	1	SER	-	cloning artifact	UNP P49841

- Molecule 2 is 2-CHLORO-5-[4-(3-CHLORO-PHENYL)-2,5-DIOXO-2,5-DIHYDRO-1H-PYRROL-3-YLAMINO]-BENZOIC ACID (CCD ID: 679) (formula: C₁₇H₁₀Cl₂N₂O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	Cl	N	O	0	0
			25	17	2	2	4		
2	B	1	Total	C	Cl	N	O	0	0
			25	17	2	2	4		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	17	Total	O	0	0
			17	17		
3	B	30	Total	O	0	0
			30	30		

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	84.17Å 86.66Å 178.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	20.00 – 2.77 20.00 – 2.77	Depositor EDS
% Data completeness (in resolution range)	98.7 (20.00-2.77) 98.5 (20.00-2.77)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.88 (at 2.79Å)	Xtriage
Refinement program	CNX 2000	Depositor
R, R_{free}	0.212 , 0.251 0.208 , 0.212	Depositor DCC
R_{free} test set	1704 reflections (5.09%)	wwPDB-VP
Wilson B-factor (Å ²)	50.5	Xtriage
Anisotropy	0.596	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.023 for k,h,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5515	wwPDB-VP
Average B, all atoms (Å ²)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.20% 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: 679

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	0.55	0/2794	1.00	14/3800 (0.4%)
1	B	0.56	0/2755	1.04	14/3748 (0.4%)
All	All	0.56	0/5549	1.02	28/7548 (0.4%)

There are no bond length outliers.

All (28) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	135	VAL	CA-C-N	8.85	129.41	119.32
1	B	135	VAL	C-N-CA	8.85	129.41	119.32
1	A	135	VAL	CA-C-N	7.95	127.87	119.05
1	A	135	VAL	C-N-CA	7.95	127.87	119.05
1	B	190	ASP	N-CA-C	-6.58	99.05	109.04
1	B	376	ILE	CB-CA-C	-6.49	105.07	111.30
1	A	376	ILE	CB-CA-C	-6.47	105.09	111.30
1	A	150	LYS	N-CA-C	6.39	120.66	112.86
1	B	309	THR	CA-C-N	6.28	126.85	120.38
1	B	309	THR	C-N-CA	6.28	126.85	120.38
1	A	304	VAL	N-CA-C	6.12	116.90	110.72
1	B	92	ARG	N-CA-C	-6.08	104.24	112.26
1	A	136	PRO	N-CA-C	5.95	121.80	113.53
1	A	307	PRO	N-CA-C	-5.93	101.17	111.32
1	B	371	PRO	N-CA-C	5.83	117.81	110.70
1	A	190	ASP	N-CA-C	-5.82	100.20	109.04
1	A	371	PRO	N-CA-C	5.61	117.54	110.70
1	A	97	GLU	N-CA-C	-5.44	105.43	111.36
1	B	379	PRO	CA-C-N	5.38	126.57	119.84
1	B	379	PRO	C-N-CA	5.38	126.57	119.84
1	B	89	GLN	N-CA-C	5.28	117.57	109.07
1	B	192	ASP	N-CA-C	5.25	117.08	111.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	379	PRO	CA-C-N	5.11	126.23	119.84
1	A	379	PRO	C-N-CA	5.11	126.23	119.84
1	A	192	ASP	N-CA-C	5.10	116.92	111.36
1	B	190	ASP	CA-C-N	5.08	124.52	119.24
1	B	190	ASP	C-N-CA	5.08	124.52	119.24
1	A	119	SER	N-CA-C	5.06	117.38	110.55

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	2728	0	2755	61	0
1	B	2690	0	2707	64	0
2	A	25	0	9	1	0
2	B	25	0	9	2	0
3	A	17	0	0	0	0
3	B	30	0	0	0	0
All	All	5515	0	5480	125	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 11.

All (125) 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:383:ARG:HA	1:B:383:ARG:HE	1.08	1.08
1:B:89:GLN:HE22	1:B:95:ASN:HB2	1.38	0.89
1:B:383:ARG:HA	1:B:383:ARG:NE	1.89	0.87
1:B:383:ARG:HE	1:B:383:ARG:CA	1.89	0.85
1:B:62:ILE:HG21	1:B:72:GLN:HB2	1.64	0.79
1:A:98:LEU:O	1:A:102:ARG:HG3	1.86	0.75
1:A:162:MET:HG3	1:A:247:LEU:HD13	1.73	0.70
1:A:91:LYS:HA	1:A:91:LYS:HE2	1.74	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:110:VAL:HG23	1:B:133:ASP:HB2	1.76	0.68
1:B:370:ASN:HD22	1:B:372:PRO:HD2	1.58	0.68
1:A:60:LYS:HE2	1:A:72:GLN:NE2	2.08	0.67
1:B:205:LYS:NZ	1:B:213:ASN:OD1	2.28	0.67
1:A:162:MET:HE2	1:A:247:LEU:HB2	1.78	0.64
1:A:370:ASN:HD22	1:A:372:PRO:HD2	1.61	0.64
1:B:308:ARG:HH11	1:B:308:ARG:HG2	1.62	0.64
1:A:284:MET:O	1:A:285:ASN:HB2	1.98	0.63
1:A:205:LYS:NZ	1:A:213:ASN:OD1	2.30	0.63
1:B:96:ARG:CZ	1:B:205:LYS:HD2	2.30	0.61
1:B:162:MET:HG3	1:B:247:LEU:HD13	1.84	0.59
1:A:370:ASN:HD22	1:A:370:ASN:C	2.10	0.59
1:B:306:ARG:HG2	1:B:309:THR:HG23	1.83	0.59
1:B:103:LYS:O	1:B:103:LYS:HG2	2.03	0.58
1:A:62:ILE:HG12	1:A:70:VAL:O	2.04	0.58
1:B:193:THR:O	1:B:357:PRO:HG3	2.03	0.58
1:B:208:VAL:HB	1:B:211:GLU:OE1	2.04	0.58
1:B:62:ILE:HG21	1:B:72:GLN:CB	2.31	0.58
1:B:370:ASN:ND2	1:B:372:PRO:HD2	2.18	0.58
1:B:370:ASN:HD22	1:B:370:ASN:C	2.11	0.57
1:B:98:LEU:O	1:B:102:ARG:HG3	2.04	0.57
1:B:162:MET:HE2	1:B:247:LEU:HB2	1.86	0.57
1:A:220:ARG:O	1:A:221:TYR:HB2	2.05	0.56
1:A:208:VAL:HB	1:A:211:GLU:OE1	2.05	0.56
1:B:62:ILE:HG13	1:B:62:ILE:O	2.05	0.55
1:B:115:PHE:HA	1:B:129:ASN:O	2.06	0.55
1:A:370:ASN:ND2	1:A:372:PRO:HD2	2.21	0.55
1:A:276:PRO:HG3	1:A:323:TYR:CZ	2.42	0.55
1:A:149:ALA:HB1	1:A:151:GLN:NE2	2.22	0.55
1:B:63:GLY:HA3	2:B:452:679:CL2	2.44	0.55
1:A:307:PRO:O	1:A:308:ARG:CB	2.54	0.54
1:A:36:LYS:HG2	1:A:37:VAL:N	2.22	0.54
1:B:308:ARG:HG2	1:B:308:ARG:NH1	2.23	0.54
1:A:196:LEU:C	1:A:196:LEU:HD23	2.33	0.53
1:B:371:PRO:HB2	1:B:372:PRO:HD3	1.91	0.53
1:A:49:ASP:O	1:A:51:PRO:HD3	2.09	0.53
1:A:106:HIS:HE1	1:A:108:ASN:HD22	1.57	0.53
1:B:220:ARG:O	1:B:221:TYR:HB2	2.09	0.53
1:A:86:LYS:HG2	1:A:127:TYR:HD2	1.74	0.52
1:A:220:ARG:O	1:A:221:TYR:CB	2.58	0.52
1:A:149:ALA:HB1	1:A:151:GLN:HE22	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:57:THR:O	1:A:58:ASP:HB2	2.09	0.52
1:B:196:LEU:C	1:B:196:LEU:HD23	2.34	0.52
1:A:96:ARG:CZ	1:A:205:LYS:HD2	2.41	0.51
1:A:110:VAL:HG21	1:A:199:CYS:HB3	1.93	0.50
1:A:307:PRO:O	1:A:308:ARG:HB2	2.11	0.50
1:B:85:LYS:HD2	2:B:452:679:CL7	2.49	0.49
1:B:370:ASN:ND2	1:B:370:ASN:C	2.70	0.49
1:A:371:PRO:HB2	1:A:372:PRO:HD3	1.94	0.49
1:A:97:GLU:HG3	1:A:201:PHE:C	2.36	0.49
1:A:63:GLY:HA3	2:A:451:679:CL2	2.50	0.48
1:B:42:ALA:HB1	1:B:114:TYR:HB3	1.95	0.48
1:A:280:GLN:O	1:A:284:MET:HG3	2.12	0.48
1:A:301:TRP:O	1:A:304:VAL:HB	2.14	0.48
1:A:365:GLN:HE21	1:A:365:GLN:HA	1.79	0.48
1:B:306:ARG:CG	1:B:309:THR:HG23	2.44	0.47
1:A:349:LYS:HE2	1:A:355:ASP:OD1	2.14	0.47
1:A:268:GLU:OE2	1:A:268:GLU:HA	2.14	0.47
1:A:372:PRO:O	1:A:375:THR:HG23	2.14	0.47
1:B:62:ILE:CG2	1:B:72:GLN:CB	2.92	0.47
1:A:149:ALA:CB	1:A:151:GLN:NE2	2.77	0.47
1:B:72:GLN:HG2	1:B:73:ALA:N	2.30	0.47
1:A:62:ILE:HD11	1:A:70:VAL:HG12	1.97	0.47
1:B:136:PRO:HG2	1:B:191:PRO:HD3	1.97	0.46
1:B:268:GLU:OE2	1:B:268:GLU:HA	2.15	0.46
1:A:307:PRO:O	1:A:308:ARG:HG2	2.16	0.46
1:A:125:GLU:N	1:A:125:GLU:OE1	2.48	0.45
1:A:307:PRO:O	1:A:308:ARG:CG	2.64	0.45
1:A:252:LEU:HG	1:A:305:PHE:CE1	2.52	0.45
1:B:323:TYR:O	1:B:325:PRO:HD3	2.16	0.45
1:A:80:GLU:CD	1:A:113:ARG:HH12	2.25	0.45
1:B:217:ILE:O	1:B:218:CYS:CB	2.65	0.45
1:B:220:ARG:O	1:B:221:TYR:CB	2.65	0.45
1:B:251:LEU:HD11	1:B:313:ALA:HB1	1.97	0.45
1:B:88:LEU:HD12	1:B:88:LEU:HA	1.86	0.44
1:B:124:ASP:OD1	1:B:125:GLU:N	2.51	0.44
1:B:349:LYS:HE2	1:B:355:ASP:OD1	2.17	0.44
1:B:357:PRO:O	1:B:359:LEU:HG	2.17	0.44
1:A:370:ASN:C	1:A:370:ASN:ND2	2.71	0.44
1:B:66:SER:HB3	1:B:67:PHE:CD1	2.53	0.44
1:A:238:ILE:HG13	1:A:239:ASP:N	2.32	0.44
1:B:152:THR:OG1	1:B:306:ARG:NH1	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:365:GLN:HE21	1:B:365:GLN:HA	1.82	0.43
1:B:372:PRO:O	1:B:375:THR:HG23	2.18	0.43
1:B:214:VAL:HB	1:B:216:TYR:CE2	2.53	0.43
1:A:106:HIS:CE1	1:A:108:ASN:HD22	2.36	0.43
1:A:144:ARG:HH12	1:A:148:ARG:NH1	2.17	0.43
1:B:308:ARG:O	1:B:309:THR:C	2.61	0.43
1:A:281:ILE:HA	1:A:284:MET:CE	2.49	0.43
1:A:357:PRO:O	1:A:359:LEU:HG	2.19	0.42
1:A:284:MET:O	1:A:285:ASN:CB	2.64	0.42
1:B:90:ASP:HB3	1:B:93:PHE:HD1	1.84	0.42
1:B:288:TYR:CD1	1:B:288:TYR:C	2.97	0.42
1:A:96:ARG:O	1:A:96:ARG:HG2	2.19	0.42
1:B:215:SER:HB3	1:B:231:ALA:O	2.19	0.42
1:B:60:LYS:HE2	1:B:60:LYS:HB3	1.81	0.42
1:B:65:GLY:O	1:B:66:SER:C	2.62	0.42
1:B:124:ASP:O	1:B:125:GLU:O	2.37	0.42
1:A:217:ILE:O	1:A:218:CYS:CB	2.68	0.41
1:A:214:VAL:HB	1:A:216:TYR:CE2	2.55	0.41
1:B:217:ILE:O	1:B:218:CYS:HB3	2.20	0.41
1:A:193:THR:O	1:A:194:ALA:HB3	2.20	0.41
1:A:72:GLN:HG2	1:A:73:ALA:N	2.34	0.41
1:A:217:ILE:O	1:A:218:CYS:HB3	2.20	0.41
1:B:116:PHE:CD1	1:B:116:PHE:C	2.99	0.41
1:A:45:GLY:HA3	1:A:112:LEU:O	2.21	0.41
1:A:323:TYR:O	1:A:325:PRO:HD3	2.20	0.41
1:B:91:LYS:HD3	1:B:91:LYS:HA	1.75	0.41
1:B:156:ILE:HG23	1:B:157:TYR:N	2.36	0.41
1:A:160:LEU:HD11	1:A:350:LEU:CD2	2.51	0.41
1:B:238:ILE:HG13	1:B:239:ASP:N	2.34	0.41
1:B:345:ASP:HA	1:B:346:PRO:HD3	1.90	0.41
1:B:152:THR:O	1:B:153:LEU:C	2.64	0.40
1:A:308:ARG:HG2	1:A:308:ARG:NH1	2.37	0.40
1:B:219:SER:O	1:B:223:ARG:HG2	2.22	0.40
1:B:252:LEU:HG	1:B:305:PHE:CE1	2.56	0.40
1:A:91:LYS:HE2	1:A:91:LYS:CA	2.48	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	336/424 (79%)	311 (93%)	17 (5%)	8 (2%)	4	15
1	B	331/424 (78%)	309 (93%)	19 (6%)	3 (1%)	14	37
All	All	667/848 (79%)	620 (93%)	36 (5%)	11 (2%)	7	23

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	149	ALA
1	B	66	SER
1	B	125	GLU
1	A	49	ASP
1	A	221	TYR
1	A	308	ARG
1	A	77	ASP
1	B	221	TYR
1	A	218	CYS
1	A	300	PRO
1	A	294	PRO

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	303/366 (83%)	292 (96%)	11 (4%)	31	63
1	B	300/366 (82%)	288 (96%)	12 (4%)	28	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
All	All	603/732 (82%)	580 (96%)	23 (4%)	29	61

All (23) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	46	GLN
1	A	61	VAL
1	A	66	SER
1	A	125	GLU
1	A	132	LEU
1	A	217	ILE
1	A	279	GLU
1	A	285	ASN
1	A	306	ARG
1	A	316	LEU
1	A	375	THR
1	B	90	ASP
1	B	91	LYS
1	B	101	MET
1	B	132	LEU
1	B	147	SER
1	B	155	VAL
1	B	217	ILE
1	B	279	GLU
1	B	301	TRP
1	B	316	LEU
1	B	375	THR
1	B	383	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	72	GLN
1	A	108	ASN
1	A	151	GLN
1	A	365	GLN
1	A	370	ASN
1	B	89	GLN
1	B	365	GLN
1	B	370	ASN

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 ⓘ

2 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	679	A	451	-	26,27,27	2.44	14 (53%)	34,39,39	1.66	7 (20%)
2	679	B	452	-	26,27,27	2.55	16 (61%)	34,39,39	1.70	7 (20%)

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	679	A	451	-	-	4/12/28/28	0/3/3/3
2	679	B	452	-	-	4/12/28/28	0/3/3/3

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	452	679	C20-C23	-5.99	1.36	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	451	679	C20-C23	-5.70	1.37	1.49
2	A	451	679	C20-C19	4.08	1.45	1.39
2	B	452	679	C5-C6	3.95	1.45	1.39
2	B	452	679	C20-C19	3.46	1.44	1.39
2	A	451	679	C6-C8	-3.42	1.43	1.49
2	B	452	679	C5-C4	3.33	1.43	1.38
2	B	452	679	C8-C11	-3.11	1.42	1.49
2	A	451	679	C21-C20	3.05	1.44	1.39
2	A	451	679	C17-C16	2.91	1.44	1.39
2	B	452	679	C21-C20	2.89	1.44	1.39
2	B	452	679	C1-C6	2.86	1.43	1.39
2	A	451	679	C8-C11	-2.76	1.42	1.49
2	A	451	679	C1-C6	2.73	1.43	1.39
2	B	452	679	C9-N15	2.72	1.42	1.35
2	B	452	679	C17-C16	2.68	1.43	1.39
2	B	452	679	C2-C1	2.64	1.43	1.38
2	A	451	679	C9-N15	2.59	1.41	1.35
2	A	451	679	C5-C6	2.56	1.43	1.39
2	A	451	679	C5-C4	2.50	1.42	1.38
2	A	451	679	C3-C4	2.44	1.42	1.38
2	A	451	679	C21-C16	2.36	1.43	1.39
2	B	452	679	C3-C4	2.35	1.42	1.38
2	B	452	679	C2-C3	2.35	1.42	1.38
2	B	452	679	C6-C8	-2.27	1.45	1.49
2	B	452	679	C8-C9	2.17	1.44	1.40
2	B	452	679	C10-N14	-2.16	1.33	1.38
2	A	451	679	C19-CL2	-2.15	1.68	1.73
2	B	452	679	C11-N14	-2.02	1.33	1.38
2	A	451	679	C2-C1	2.01	1.42	1.38

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	452	679	C8-C11-N14	6.51	110.54	106.64
2	A	451	679	C8-C11-N14	5.78	110.10	106.64
2	A	451	679	C18-C19-CL2	-3.23	112.06	118.42
2	A	451	679	C20-C19-CL2	3.00	125.44	121.01
2	A	451	679	O25-C23-C20	2.74	123.06	115.28
2	B	452	679	C16-N15-C9	2.72	134.70	127.89
2	A	451	679	C16-N15-C9	2.66	134.54	127.89
2	B	452	679	O25-C23-C20	2.41	122.13	115.28
2	A	451	679	O24-C23-C20	-2.39	116.26	121.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	452	679	C18-C19-CL2	-2.33	113.83	118.42
2	B	452	679	O24-C23-C20	-2.32	116.43	121.97
2	B	452	679	C6-C5-C4	2.23	121.57	119.17
2	A	451	679	C11-N14-C10	-2.06	109.17	111.36
2	B	452	679	C6-C8-C9	2.05	131.63	126.97

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	452	679	C19-C20-C23-O25
2	A	451	679	C19-C20-C23-O24
2	A	451	679	C19-C20-C23-O25
2	B	452	679	C19-C20-C23-O24
2	A	451	679	C21-C20-C23-O24
2	B	452	679	C21-C20-C23-O24
2	A	451	679	C21-C20-C23-O25
2	B	452	679	C21-C20-C23-O25

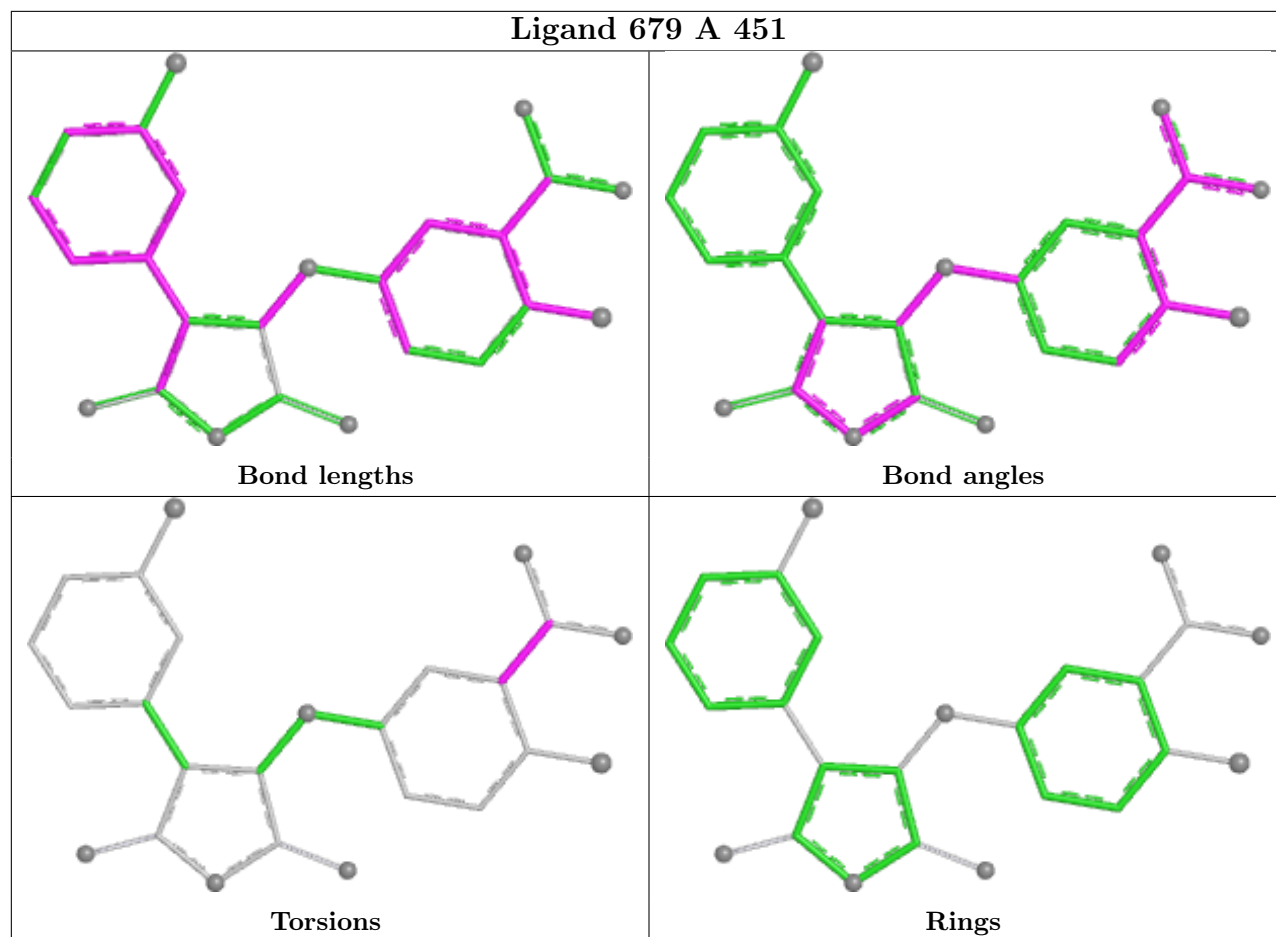
There are no ring outliers.

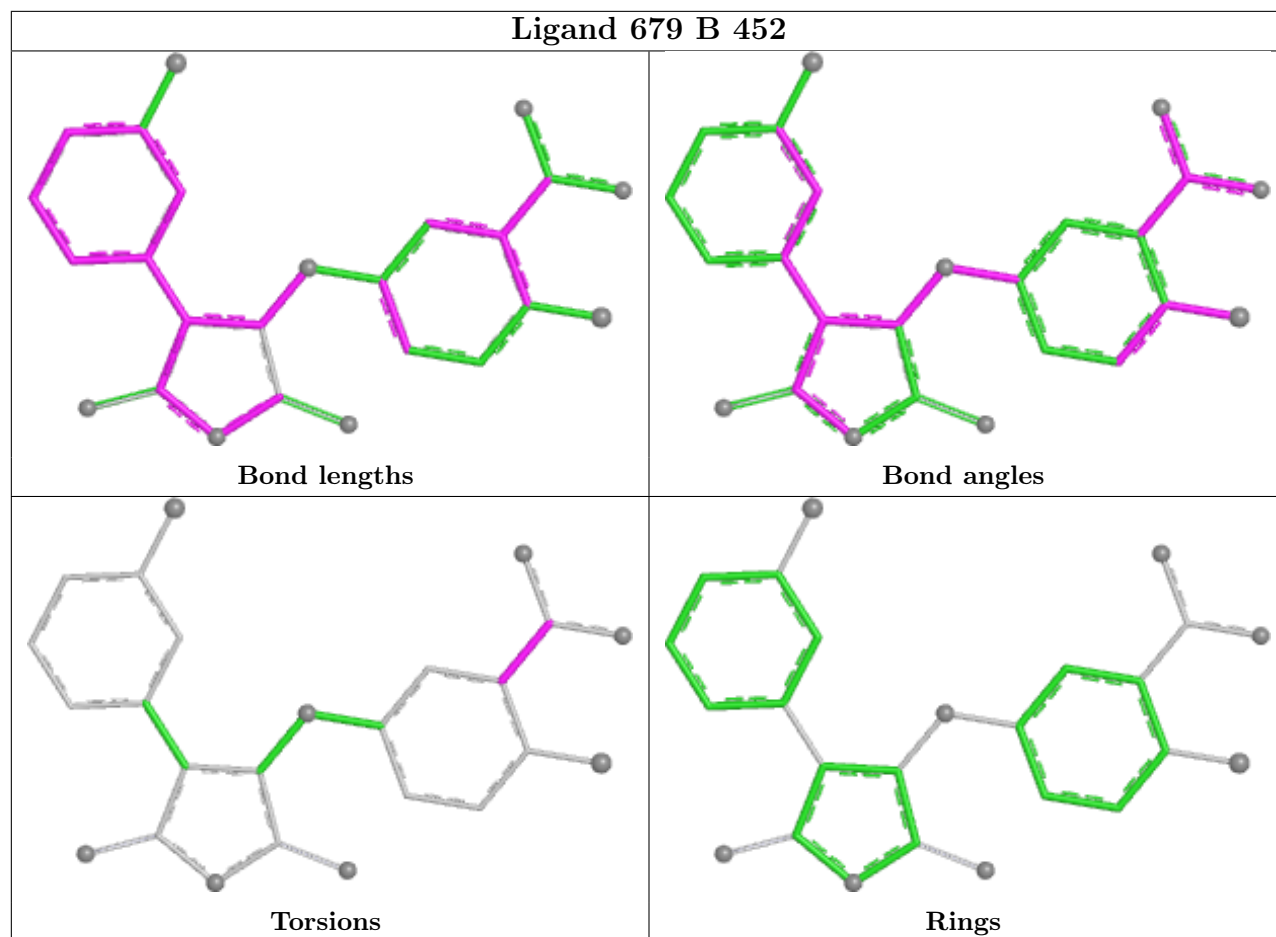
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	451	679	1	0
2	B	452	679	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.

Ligand 679 A 451





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	342/424 (80%)	-0.04	17 (4%) 34 28	25, 48, 109, 170	0
1	B	337/424 (79%)	-0.13	17 (5%) 34 28	23, 44, 101, 157	0
All	All	679/848 (80%)	-0.09	34 (5%) 34 28	23, 46, 108, 170	0

All (34) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	120	GLY	5.5
1	B	300	PRO	4.9
1	A	386	ALA	4.9
1	A	93	PHE	4.7
1	A	120	GLY	4.3
1	A	124	ASP	3.7
1	A	296	ILE	3.7
1	B	124	ASP	3.6
1	A	298	ALA	3.3
1	A	285	ASN	3.2
1	B	288	TYR	3.2
1	A	300	PRO	3.2
1	A	295	GLN	3.2
1	B	383	ARG	3.0
1	B	91	LYS	3.0
1	B	286	PRO	2.9
1	B	92	ARG	2.9
1	A	94	LYS	2.9
1	A	293	PHE	2.9
1	A	90	ASP	2.8
1	A	385	GLN	2.7
1	B	308	ARG	2.7
1	A	308	ARG	2.6
1	A	35	SER	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	93	PHE	2.5
1	B	278	ARG	2.4
1	B	125	GLU	2.3
1	B	62	ILE	2.3
1	B	64	ASN	2.2
1	B	303	LYS	2.2
1	A	299	HIS	2.1
1	A	302	THR	2.1
1	B	279	GLU	2.1
1	B	94	LYS	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 oligosaccharides in this entry.

6.4 Ligands [i](#)

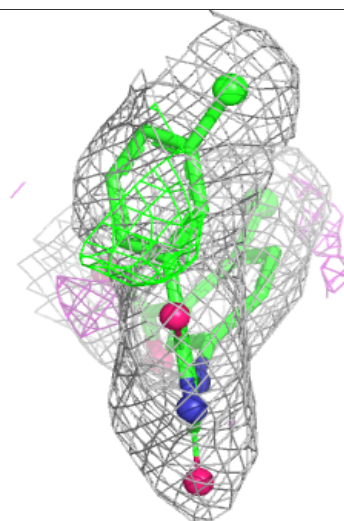
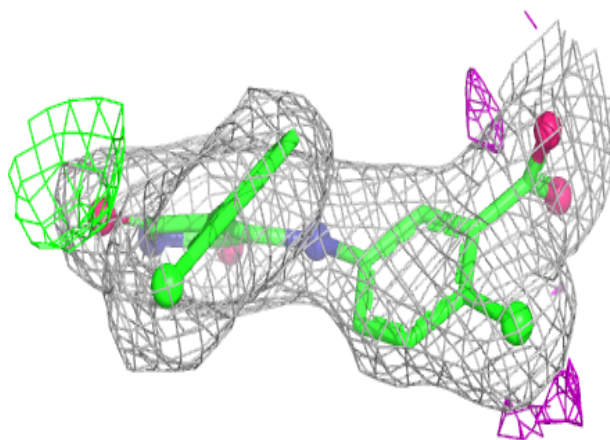
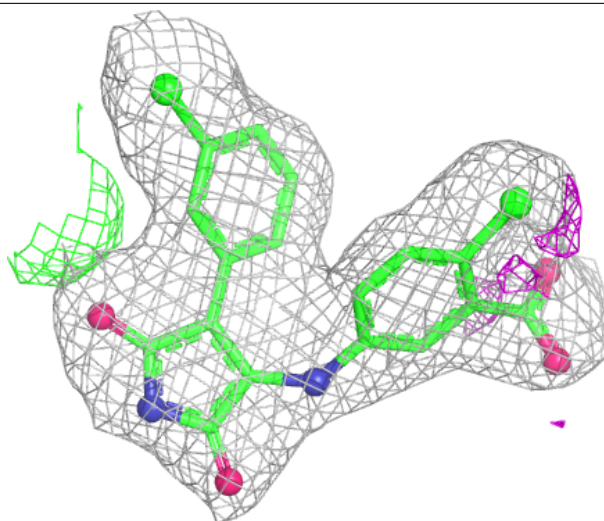
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	679	A	451	25/25	0.95	0.09	47,47,47,47	0
2	679	B	452	25/25	0.95	0.08	43,43,43,43	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.

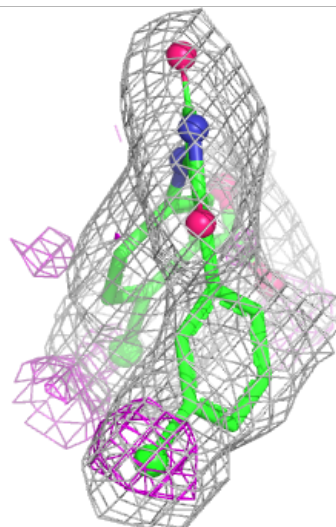
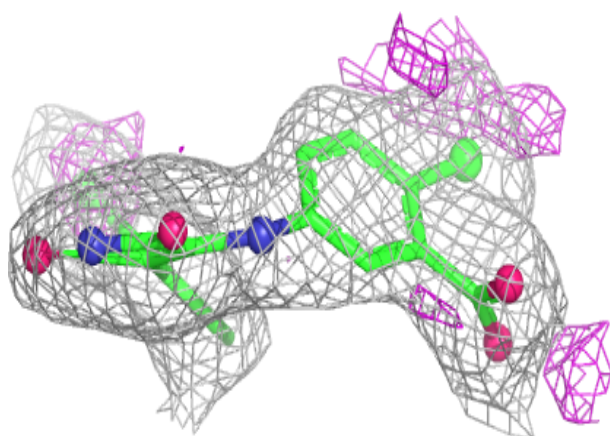
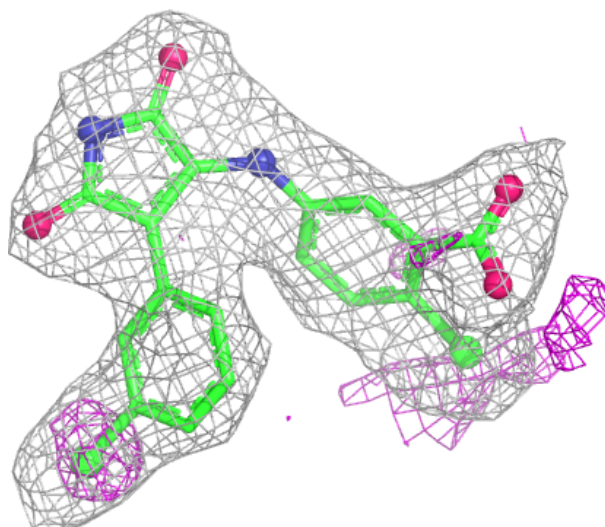
Electron density around 679 A 451:

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



Electron density around 679 B 452:

$2mF_o-DF_c$ (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.