



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 08:39 PM UTC

PDB ID : 3KYR / pdb_00003kyr
Title : Bace-1 in complex with a norstatine type inhibitor
Authors : Lindberg, J.D.; Borkakoti, N.; Derbyshire, D.; Nystrom, S.
Deposited on : 2009-12-07
Resolution : 2.60 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 : 4-5-2 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

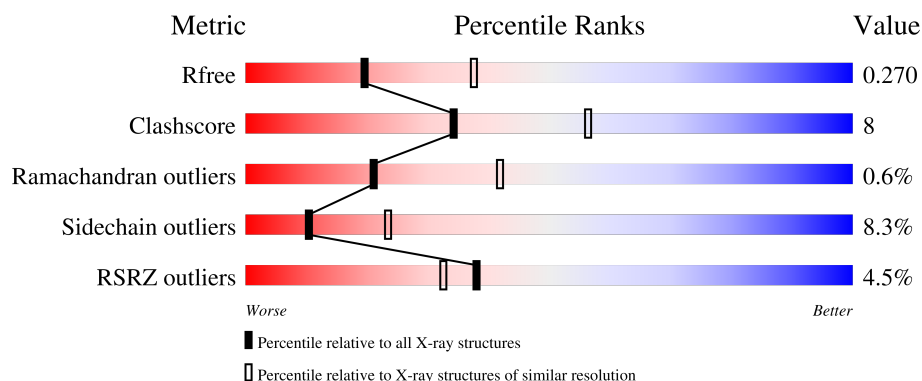
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.60 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}	180053	4008 (2.60-2.60)
Clashscore	190562	4347 (2.60-2.60)
Ramachandran outliers	187476	4277 (2.60-2.60)
Sidechain outliers	187428	4277 (2.60-2.60)
RSRZ outliers	180081	4008 (2.60-2.60)

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	405	3% 70% 17% • 10%
1	B	405	3% 70% 17% • 10%
1	C	405	5% 67% 19% • 11%

2 Entry composition [i](#)

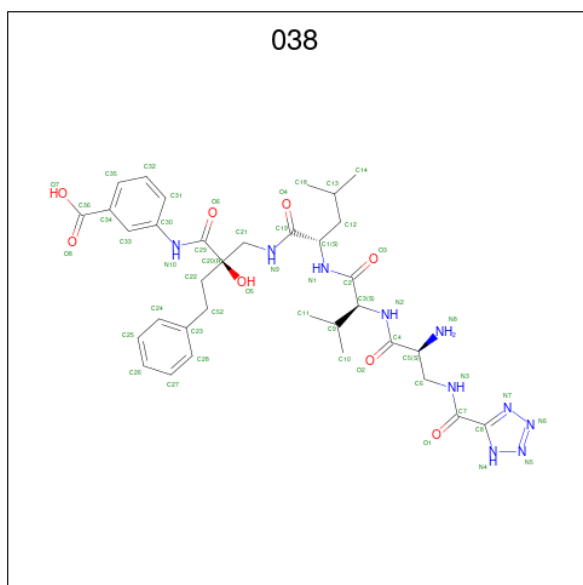
There are 3 unique types of molecules in this entry. The entry contains 8802 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Beta-secretase 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	365	Total	C	N	O	S	0	0	0
			2872	1841	478	539	14			
1	B	363	Total	C	N	O	S	0	0	0
			2857	1829	476	538	14			
1	C	360	Total	C	N	O	S	0	0	0
			2841	1824	474	529	14			

- Molecule 2 is 3-[[[(2S)-2-[[[(2S)-2-[[[(2S)-2-azanyl-3-(1H-1,2,3,4-tetrazol-5-ylcarbonylamino)propanoyl]amino]-3-methyl-butanoyl]amino]-4-methyl-pentanoyl]amino]methyl]-2-hydroxy-4-phenyl-butanoyl]amino]benzoic acid (CCD ID: 038) (formula: C₃₄H₄₆N₁₀O₈).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			52	34	10	8		
2	B	1	Total	C	N	O	0	0
			52	34	10	8		

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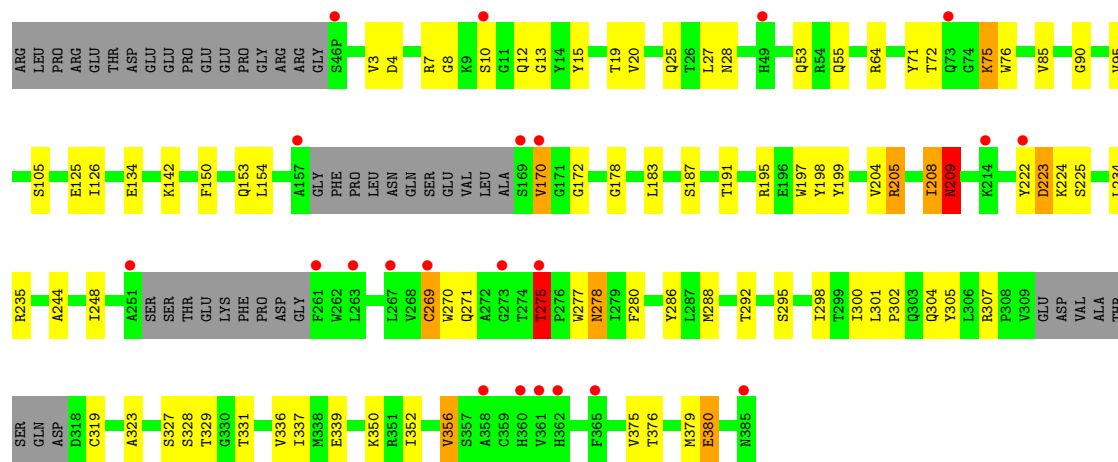
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			52	34	10	8		

- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	24	Total	O	0	0
			24	24		
3	B	26	Total	O	0	0
			26	26		
3	C	26	Total	O	0	0
			26	26		

- Molecule 1: Beta-secretase 1





4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	81.76Å 102.77Å 101.43Å 90.00° 102.90° 90.00°	Depositor
Resolution (Å)	99.01 – 2.60 98.87 – 2.60	Depositor EDS
% Data completeness (in resolution range)	100.0 (99.01-2.60) 91.1 (98.87-2.60)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.11	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.94 (at 2.62Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.207 , 0.269 0.208 , 0.270	Depositor DCC
R_{free} test set	2320 reflections (5.05%)	wwPDB-VP
Wilson B-factor (Å ²)	29.0	Xtriage
Anisotropy	0.111	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 34.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	8802	wwPDB-VP
Average B, all atoms (Å ²)	24.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.98% 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: 038

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	0.90	1/2943 (0.0%)	1.00	1/3996 (0.0%)
1	B	0.91	0/2927	1.03	4/3974 (0.1%)
1	C	0.91	1/2912 (0.0%)	1.06	11/3953 (0.3%)
All	All	0.91	2/8782 (0.0%)	1.03	16/11923 (0.1%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	356	VAL	CA-CB	5.96	1.61	1.54
1	A	356	VAL	CA-CB	5.78	1.60	1.54

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	90	GLY	CA-C-N	-7.92	111.85	119.85
1	C	90	GLY	C-N-CA	-7.92	111.85	119.85
1	C	178	GLY	N-CA-C	7.81	121.43	110.74
1	C	209	ASN	CA-CB-CG	6.96	119.56	112.60
1	B	48(P)	VAL	CB-CA-C	-5.96	104.09	112.14
1	C	170	VAL	N-CA-C	5.67	115.74	108.82
1	A	190	TYR	N-CA-C	5.63	118.90	109.95
1	B	90	GLY	CA-C-N	-5.60	114.83	120.31
1	B	90	GLY	C-N-CA	-5.60	114.83	120.31
1	C	208	ILE	CA-C-N	5.44	130.13	122.46
1	C	208	ILE	C-N-CA	5.44	130.13	122.46
1	B	149	LEU	N-CA-CB	-5.40	101.80	110.77
1	C	275	THR	CA-C-N	5.29	126.45	119.84
1	C	275	THR	C-N-CA	5.29	126.45	119.84
1	C	13	GLY	N-CA-C	5.26	119.31	112.68
1	C	150	PHE	N-CA-C	-5.18	101.19	109.07

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	2872	0	2790	47	0
1	B	2857	0	2773	38	0
1	C	2841	0	2768	41	0
2	A	52	0	45	1	0
2	B	52	0	45	1	0
2	C	52	0	45	2	0
3	A	24	0	0	2	0
3	B	26	0	0	4	0
3	C	26	0	0	1	0
All	All	8802	0	8466	129	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 8.

All (129) 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:A:8:GLY:HA3	1:A:170:VAL:HG12	1.40	1.03
2:C:500:038:O6	2:C:500:038:H33	1.57	1.03
1:A:8:GLY:CA	1:A:170:VAL:HG12	1.93	0.99
1:C:269:CYS:HG	1:C:319:CYS:HG	1.19	0.91
1:C:295:SER:HB3	1:C:379:MET:CE	2.02	0.89
1:A:8:GLY:HA3	1:A:170:VAL:CG1	2.07	0.83
1:C:288:MET:HE2	1:C:379:MET:HB3	1.59	0.82
1:B:381:ASP:N	1:B:381:ASP:OD1	2.15	0.79
1:A:224:LYS:HE2	1:A:329:THR:HG21	1.65	0.77
1:C:295:SER:HB3	1:C:379:MET:HE1	1.68	0.76
1:C:204:VAL:HG11	1:C:379:MET:HG2	1.67	0.74
1:C:235:ARG:HB3	1:C:327:SER:HB2	1.69	0.74
1:C:75:LYS:HE2	3:C:403:HOH:O	1.87	0.74
2:C:500:038:O6	2:C:500:038:C33	2.32	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:260:GLY:HA3	1:B:266:GLN:HE21	1.54	0.71
1:A:73:GLN:HG2	1:A:73:GLN:O	1.91	0.68
1:A:235:ARG:HB3	1:A:327:SER:HB2	1.78	0.66
1:B:241:PHE:O	1:B:245:VAL:HG23	1.94	0.66
1:A:222:TYR:O	1:A:223:ASP:CB	2.44	0.65
1:C:125:GLU:OE2	1:C:195:ARG:NH2	2.29	0.65
1:A:215:MET:HE3	1:A:239:LYS:HE2	1.81	0.62
1:B:231:THR:CG2	3:B:391:HOH:O	2.47	0.62
2:A:500:038:O6	2:A:500:038:H33	2.00	0.60
1:B:228:ASP:OD2	1:B:231:THR:HB	2.01	0.60
1:B:288:MET:HE1	1:B:379:MET:HA	1.82	0.60
1:A:199:TYR:HB3	1:A:352:ILE:HD11	1.83	0.59
1:C:278:ASN:N	1:C:278:ASN:HD22	2.01	0.59
1:C:244:ALA:O	1:C:248:ILE:HG13	2.04	0.57
1:B:221:ASN:O	1:B:222:TYR:C	2.47	0.57
1:B:231:THR:HG21	3:B:391:HOH:O	2.04	0.57
1:B:288:MET:HE1	1:B:379:MET:N	2.20	0.57
1:B:42:ALA:CB	1:B:101:ALA:HB1	2.34	0.56
1:C:222:TYR:O	1:C:223:ASP:HB3	2.06	0.56
1:A:222:TYR:O	1:A:223:ASP:HB2	2.06	0.56
1:A:261:PHE:CE1	1:A:268:VAL:HG22	2.41	0.56
1:A:300:ILE:HD12	1:A:337:ILE:CD1	2.36	0.56
1:A:95:VAL:HG11	1:A:140:LEU:HA	1.88	0.55
1:A:232:THR:O	1:A:336:VAL:HB	2.06	0.55
1:C:198:TYR:CE1	1:C:224:LYS:HE3	2.41	0.55
1:B:282:VAL:HG12	1:B:301:LEU:HD23	1.87	0.55
1:A:8:GLY:N	1:A:170:VAL:HG12	2.22	0.54
1:A:197:TRP:CG	1:A:198:TYR:H	2.25	0.54
1:A:252:SER:HB2	1:A:279:ILE:HD12	1.88	0.54
1:B:7:ARG:HB2	1:B:15:TYR:CE1	2.42	0.54
1:B:30:LEU:HD23	1:B:118:ILE:HD12	1.89	0.54
1:B:259:ASP:N	1:B:259:ASP:OD1	2.42	0.53
1:B:288:MET:HE1	1:B:379:MET:CA	2.38	0.53
1:B:260:GLY:HA3	1:B:266:GLN:NE2	2.23	0.53
1:A:174:MET:HE2	1:A:176:ILE:CG1	2.39	0.52
1:B:222:TYR:CG	1:B:223:ASP:N	2.76	0.51
1:B:225:SER:HA	1:B:331:THR:O	2.11	0.51
1:A:7:ARG:CG	3:A:402:HOH:O	2.59	0.50
1:C:288:MET:HA	1:C:379:MET:HE2	1.93	0.50
1:C:199:TYR:HB3	1:C:352:ILE:HD11	1.94	0.50
1:A:180:ASP:OD2	1:B:77:GLU:OE2	2.29	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:307:ARG:HG2	1:C:323:ALA:HB2	1.94	0.49
1:A:197:TRP:CD1	1:A:198:TYR:H	2.31	0.49
1:B:198:TYR:CE1	1:B:224:LYS:HE3	2.48	0.49
1:C:225:SER:HA	1:C:331:THR:O	2.13	0.49
1:B:46(P):SER:HA	3:B:411:HOH:O	2.12	0.49
1:B:276:PRO:O	1:B:279:ILE:HG12	2.12	0.48
2:B:500:038:H33	2:B:500:038:O6	2.12	0.48
1:B:189:TRP:O	1:B:353:GLY:HA2	2.13	0.48
1:C:20:VAL:HG12	1:C:85:VAL:HG22	1.94	0.48
1:A:7:ARG:HG2	3:A:402:HOH:O	2.13	0.48
1:A:344:VAL:O	1:A:352:ILE:HA	2.14	0.48
1:A:13:GLY:HA3	1:A:30:LEU:HD11	1.96	0.48
1:B:290:GLU:HB2	3:B:408:HOH:O	2.14	0.48
1:A:174:MET:HE2	1:A:176:ILE:HG12	1.97	0.47
1:A:78:GLY:HA3	1:A:101:ALA:O	2.13	0.47
1:A:297:ARG:NH2	1:A:371:GLU:OE1	2.46	0.47
1:A:221:ASN:O	1:A:223:ASP:N	2.48	0.47
1:A:271:GLN:O	1:A:272:ALA:C	2.56	0.47
1:A:224:LYS:CE	1:A:329:THR:HG21	2.41	0.46
1:C:301:LEU:HB3	1:C:302:PRO:HD2	1.97	0.46
1:A:71:TYR:O	1:A:72:THR:C	2.59	0.45
1:A:156:GLY:HA3	1:A:339:GLU:OE2	2.16	0.45
1:C:280:PHE:HB3	1:C:302:PRO:HB3	1.98	0.45
1:B:380:GLU:N	1:B:380:GLU:CD	2.74	0.45
1:B:45:HIS:HB3	1:B:48:LEU:HG	1.99	0.45
1:C:376:THR:HB	1:C:379:MET:HE3	1.97	0.45
1:A:297:ARG:NE	1:A:371:GLU:OE1	2.48	0.45
1:C:208:ILE:O	1:C:209:ASN:ND2	2.46	0.45
1:B:239:LYS:HD3	1:B:239:LYS:HA	1.57	0.45
1:C:302:PRO:HA	1:C:305:TYR:CE2	2.52	0.45
1:C:154:LEU:O	1:C:339:GLU:HA	2.17	0.44
1:A:17:GLU:HG2	1:A:88:PRO:HG2	1.99	0.44
1:A:228:ASP:OD2	1:A:231:THR:HB	2.18	0.44
1:C:205:ARG:HB2	1:C:286:TYR:CD1	2.53	0.44
1:B:47(P):PHE:CZ	1:B:178:GLY:HA3	2.52	0.44
1:B:235:ARG:HA	1:B:325:SER:O	2.18	0.44
1:A:223:ASP:OD2	1:A:329:THR:HG22	2.18	0.44
1:C:380:GLU:H	1:C:380:GLU:HG2	1.58	0.44
1:C:222:TYR:O	1:C:223:ASP:CB	2.65	0.43
1:C:270:TRP:CE3	1:C:275:THR:HG23	2.53	0.43
1:C:8:GLY:HA3	1:C:170:VAL:HG23	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:76:TRP:HA	1:C:105:SER:HA	2.00	0.43
1:B:235:ARG:HB3	1:B:327:SER:HB2	2.00	0.43
1:C:15:TYR:CD1	1:C:28:ASN:HB3	2.52	0.43
1:A:343:VAL:HA	1:A:353:GLY:O	2.18	0.43
1:B:259:ASP:HA	1:B:262:TRP:HD1	1.83	0.43
1:B:2:MET:HG2	1:B:90:GLY:HA2	2.01	0.43
1:C:153:GLN:OE1	1:C:183:LEU:HD22	2.19	0.42
1:A:82:THR:OG1	1:A:96:ARG:NH1	2.52	0.42
1:B:300:ILE:HD11	1:B:305:TYR:HD2	1.84	0.42
1:C:300:ILE:HD13	1:C:337:ILE:HD13	2.00	0.42
1:C:126:ILE:HG23	1:C:197:TRP:HB2	2.01	0.42
1:C:3:VAL:O	1:C:4:ASP:HB2	2.18	0.42
1:A:125:GLU:O	1:A:125:GLU:HG3	2.18	0.42
1:A:22:SER:O	1:A:57:SER:HA	2.20	0.42
1:A:307:ARG:O	1:A:320:TYR:HA	2.20	0.42
1:A:237:PRO:HG3	1:A:330:GLY:HA2	2.02	0.41
1:C:71:TYR:O	1:C:72:THR:C	2.63	0.41
1:C:19:THR:HA	1:C:25:GLN:O	2.19	0.41
1:C:234:LEU:HD22	1:C:337:ILE:HD11	2.01	0.41
1:B:12:GLN:HE21	1:B:113:SER:HA	1.84	0.41
1:B:197:TRP:CG	1:B:198:TYR:H	2.39	0.41
1:B:380:GLU:CD	1:B:380:GLU:H	2.28	0.41
1:C:4:ASP:HA	1:C:172:GLY:O	2.21	0.41
1:A:19:THR:HA	1:A:25:GLN:O	2.21	0.41
1:B:234:LEU:O	1:B:324:ILE:HA	2.19	0.41
1:C:53:GLN:HE21	1:C:55:GLN:NE2	2.18	0.41
1:C:298:ILE:O	1:C:298:ILE:HG13	2.21	0.41
1:A:231:THR:HG21	1:A:235:ARG:HH11	1.85	0.40
1:C:134:GLU:OE2	1:C:142:LYS:HD3	2.22	0.40
1:A:113:SER:O	1:A:114:ASN:HB3	2.21	0.40
1:A:357:SER:O	1:A:360:HIS:HB3	2.21	0.40
1:A:4:ASP:HA	1:A:172:GLY:O	2.21	0.40
1:B:189:TRP:HB3	1:B:296:PHE:CD1	2.57	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	357/405 (88%)	341 (96%)	13 (4%)	3 (1%)	16	34
1	B	355/405 (88%)	333 (94%)	21 (6%)	1 (0%)	36	58
1	C	352/405 (87%)	325 (92%)	25 (7%)	2 (1%)	21	42
All	All	1064/1215 (88%)	999 (94%)	59 (6%)	6 (1%)	21	42

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	ASP
1	B	222	TYR
1	A	222	TYR
1	C	223	ASP
1	C	277	TRP
1	A	238	LYS

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	311/346 (90%)	289 (93%)	22 (7%)	13	31
1	B	310/346 (90%)	279 (90%)	31 (10%)	7	16
1	C	307/346 (89%)	283 (92%)	24 (8%)	11	26
All	All	928/1038 (89%)	851 (92%)	77 (8%)	10	23

All (77) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	64	ARG
1	A	107	LYS
1	A	125	GLU
1	A	142	LYS
1	A	149	LEU
1	A	170	VAL
1	A	203	ILE
1	A	214	LYS
1	A	224	LYS
1	A	231	THR
1	A	239	LYS
1	A	267	LEU
1	A	271	GLN
1	A	298	ILE
1	A	300	ILE
1	A	329	THR
1	A	336	VAL
1	A	356	VAL
1	A	362	HIS
1	A	364	GLU
1	A	367	THR
1	A	380	GLU
1	B	9	LYS
1	B	20	VAL
1	B	22	SER
1	B	64	ARG
1	B	87	ILE
1	B	94	THR
1	B	95	VAL
1	B	104	GLU
1	B	114	ASN
1	B	149	LEU
1	B	169	SER
1	B	202	ILE
1	B	231	THR
1	B	239	LYS
1	B	254	THR
1	B	259	ASP
1	B	263	LEU
1	B	267	LEU
1	B	300	ILE
1	B	307	ARG

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Mol	Chain	Res	Type
1	B	328	SER
1	B	336	VAL
1	B	356	VAL
1	B	361	VAL
1	B	364	GLU
1	B	367	THR
1	B	375	VAL
1	B	377	LEU
1	B	380	GLU
1	B	381	ASP
1	B	382	CYS
1	C	7	ARG
1	C	10	SER
1	C	12	GLN
1	C	27	LEU
1	C	64	ARG
1	C	75	LYS
1	C	95	VAL
1	C	187	SER
1	C	191	THR
1	C	205	ARG
1	C	209	ASN
1	C	269	CYS
1	C	271	GLN
1	C	275	THR
1	C	278	ASN
1	C	292	THR
1	C	304	GLN
1	C	328	SER
1	C	329	THR
1	C	336	VAL
1	C	350	LYS
1	C	356	VAL
1	C	375	VAL
1	C	380	GLU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (24) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	12	GLN
1	A	28	ASN
1	A	89	HIS

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Mol	Chain	Res	Type
1	A	181	HIS
1	A	233	ASN
1	A	266	GLN
1	A	293	ASN
1	A	304	GLN
1	B	12	GLN
1	B	28	ASN
1	B	55	GLN
1	B	98	ASN
1	B	209	ASN
1	B	266	GLN
1	B	326	GLN
1	C	12	GLN
1	C	28	ASN
1	C	53	GLN
1	C	73	GLN
1	C	278	ASN
1	C	293	ASN
1	C	326	GLN
1	C	360	HIS
1	C	385	ASN

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	038	A	500	-	51,54,54	1.33	4 (7%)	66,74,74	1.25	6 (9%)
2	038	C	500	-	51,54,54	1.65	4 (7%)	66,74,74	1.72	12 (18%)
2	038	B	500	-	51,54,54	1.37	3 (5%)	66,74,74	1.67	14 (21%)

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	038	A	500	-	-	5/62/63/63	0/3/3/3
2	038	C	500	-	-	8/62/63/63	0/3/3/3
2	038	B	500	-	-	10/62/63/63	0/3/3/3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	500	038	N4-N5	6.63	1.43	1.35
2	C	500	038	N7-N6	5.04	1.43	1.36
2	B	500	038	N4-N5	4.92	1.41	1.35
2	A	500	038	N4-N5	4.20	1.40	1.35
2	B	500	038	N7-N6	3.67	1.41	1.36
2	B	500	038	C4-N2	-3.64	1.26	1.34
2	A	500	038	N7-N6	3.53	1.41	1.36
2	C	500	038	C4-N2	-3.26	1.27	1.34
2	A	500	038	C30-N10	-3.15	1.35	1.41
2	A	500	038	C4-N2	-3.04	1.27	1.34
2	C	500	038	C30-N10	-3.02	1.35	1.41

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	500	038	C6-N3-C7	5.40	130.19	122.06
2	B	500	038	C21-N9-C19	4.58	129.83	122.91
2	B	500	038	C6-N3-C7	4.43	128.73	122.06
2	C	500	038	C30-N10-C29	-4.35	119.12	126.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	500	038	O5-C20-C29	-4.11	101.43	108.87
2	A	500	038	C6-N3-C7	3.88	127.89	122.06
2	C	500	038	O5-C20-C29	-3.80	102.00	108.87
2	C	500	038	C20-C29-N10	-3.63	110.79	114.66
2	C	500	038	C7-C8-N4	3.49	126.57	123.53
2	B	500	038	C7-C8-N4	3.44	126.53	123.53
2	A	500	038	C6-C5-C4	3.39	115.80	108.70
2	A	500	038	C21-N9-C19	3.09	127.58	122.91
2	C	500	038	O6-C29-C20	3.03	125.78	119.91
2	C	500	038	C12-C1-C19	-2.99	103.51	110.59
2	B	500	038	C9-C3-N2	-2.95	104.30	111.44
2	C	500	038	C6-C5-C4	2.95	114.87	108.70
2	C	500	038	O5-C20-C22	2.93	113.57	108.88
2	B	500	038	N7-N6-N5	-2.83	107.12	110.50
2	B	500	038	O5-C20-C22	2.72	113.23	108.88
2	B	500	038	C8-N7-N6	2.68	107.58	105.34
2	A	500	038	C7-C8-N4	2.61	125.80	123.53
2	B	500	038	O5-C20-C21	-2.45	102.55	108.21
2	B	500	038	C12-C1-C19	-2.37	104.96	110.59
2	B	500	038	C6-C5-C4	2.33	113.59	108.70
2	C	500	038	C12-C1-N1	-2.30	105.39	110.58
2	B	500	038	C21-C20-C29	2.29	116.63	110.34
2	C	500	038	C5-C6-N3	-2.22	107.62	112.30
2	B	500	038	N4-N5-N6	2.18	109.78	106.68
2	C	500	038	C1-C19-N9	2.14	121.14	116.54
2	A	500	038	C35-C34-C33	2.11	121.69	119.25
2	B	500	038	C35-C34-C36	-2.09	116.23	120.37
2	A	500	038	C12-C1-N1	-2.01	106.03	110.58

There are no chirality outliers.

All (23) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	500	038	O1-C7-C8-N4
2	B	500	038	O1-C7-C8-N4
2	C	500	038	O1-C7-C8-N4
2	C	500	038	O5-C20-C22-C52
2	C	500	038	C21-C20-C22-C52
2	C	500	038	C29-C20-C22-C52
2	B	500	038	C33-C34-C36-O7
2	C	500	038	C20-C22-C52-C23
2	B	500	038	C35-C34-C36-O7

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Mol	Chain	Res	Type	Atoms
2	B	500	038	C2-C3-C9-C11
2	B	500	038	C33-C34-C36-O8
2	B	500	038	N1-C1-C19-O4
2	B	500	038	N1-C1-C19-N9
2	B	500	038	C35-C34-C36-O8
2	A	500	038	C28-C23-C52-C22
2	B	500	038	C24-C23-C52-C22
2	C	500	038	C24-C23-C52-C22
2	B	500	038	C28-C23-C52-C22
2	C	500	038	C28-C23-C52-C22
2	A	500	038	C24-C23-C52-C22
2	C	500	038	O2-C4-C5-N8
2	A	500	038	N1-C1-C19-O4
2	A	500	038	N1-C1-C19-N9

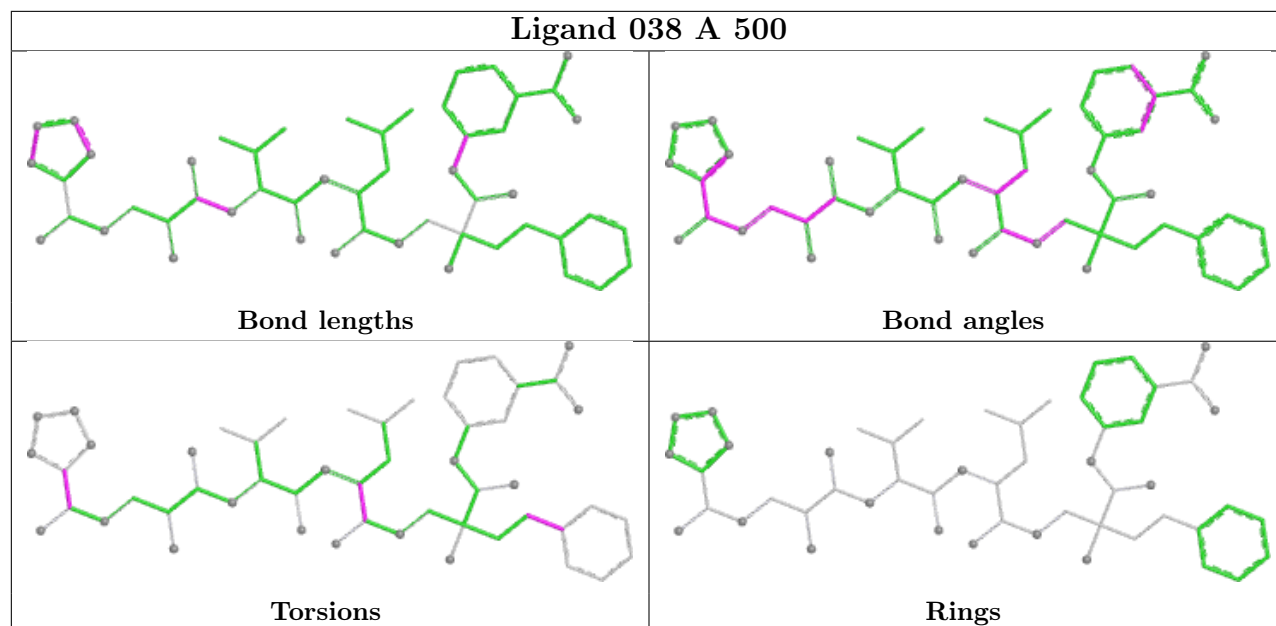
There are no ring outliers.

3 monomers are involved in 4 short contacts:

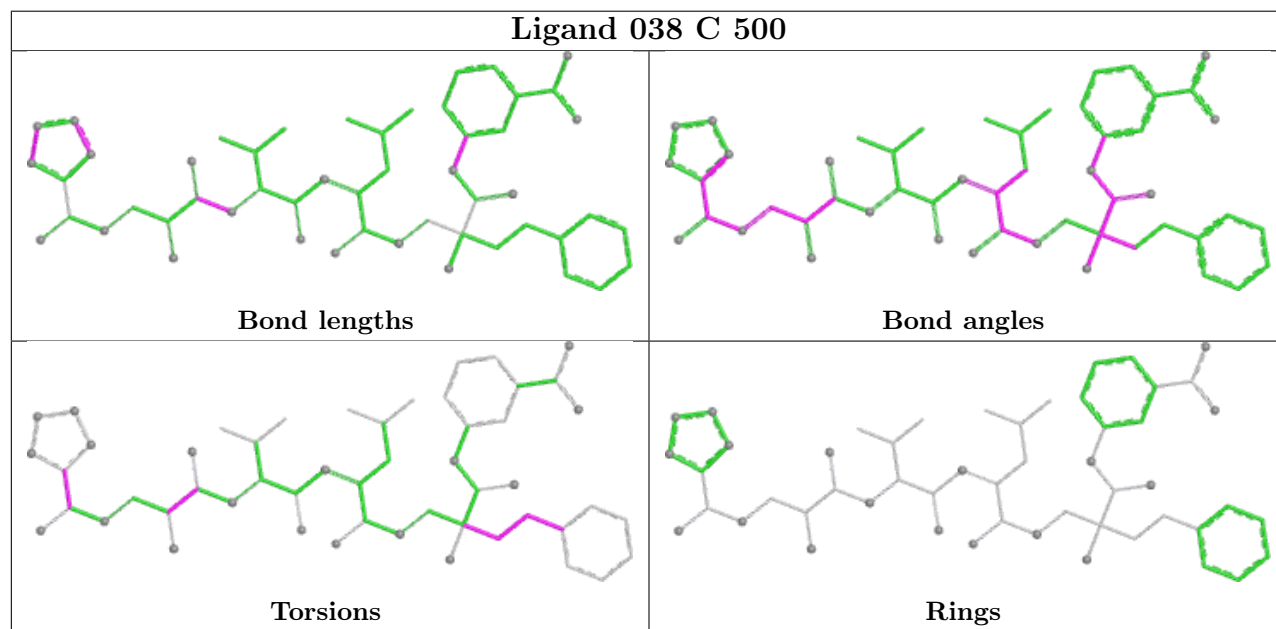
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	500	038	1	0
2	C	500	038	2	0
2	B	500	038	1	0

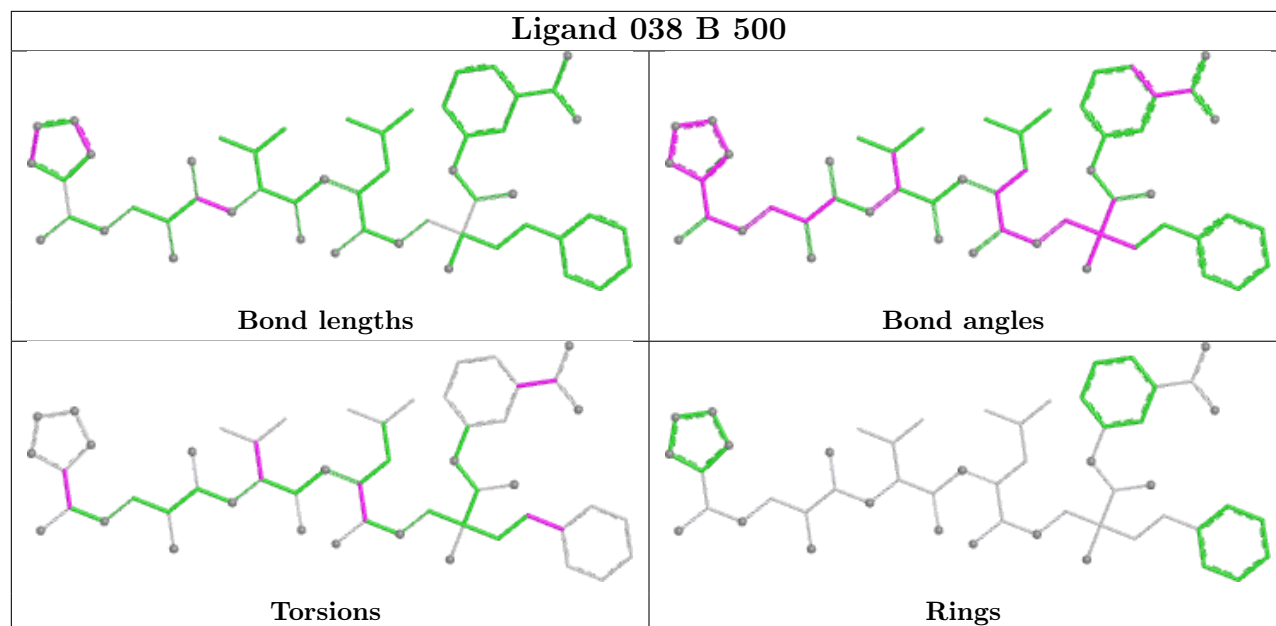
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

Ligand 038 A 500



Ligand 038 C 500





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	365/405 (90%)	0.05	13 (3%) 46 40	7, 24, 40, 50	0
1	B	363/405 (89%)	-0.03	14 (3%) 43 38	6, 21, 42, 53	0
1	C	360/405 (88%)	0.16	22 (6%) 27 22	4, 23, 54, 64	0
All	All	1088/1215 (89%)	0.06	49 (4%) 38 32	4, 22, 45, 64	0

All (49) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	157	ALA	4.1
1	C	46(P)	SER	3.9
1	C	361	VAL	3.7
1	C	251	ALA	3.6
1	B	359	CYS	3.5
1	A	170	VAL	3.5
1	B	217	CYS	3.3
1	C	10	SER	3.1
1	B	46(P)	SER	3.1
1	A	73	GLN	3.0
1	C	169	SER	3.0
1	A	266	GLN	2.9
1	C	214	LYS	2.9
1	B	362	HIS	2.8
1	C	360	HIS	2.8
1	C	365	PHE	2.8
1	B	259	ASP	2.7
1	A	8	GLY	2.7
1	A	364	GLU	2.7
1	A	269	CYS	2.6
1	C	273	GLY	2.6
1	C	263	LEU	2.6
1	C	362	HIS	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	265	GLU	2.5
1	B	382	CYS	2.5
1	C	269	CYS	2.5
1	B	264	GLY	2.5
1	C	170	VAL	2.5
1	C	267	LEU	2.4
1	A	384	TYR	2.4
1	C	261	PHE	2.4
1	B	380	GLU	2.4
1	A	267	LEU	2.3
1	B	222	TYR	2.3
1	B	273	GLY	2.3
1	C	222	TYR	2.3
1	A	317	ASP	2.2
1	B	361	VAL	2.2
1	C	275	THR	2.2
1	C	358	ALA	2.1
1	A	214	LYS	2.1
1	B	169	SER	2.1
1	B	269	CYS	2.1
1	A	260	GLY	2.1
1	C	73	GLN	2.1
1	C	385	ASN	2.1
1	A	130	ASP	2.0
1	A	9	LYS	2.0
1	C	49	HIS	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](#)

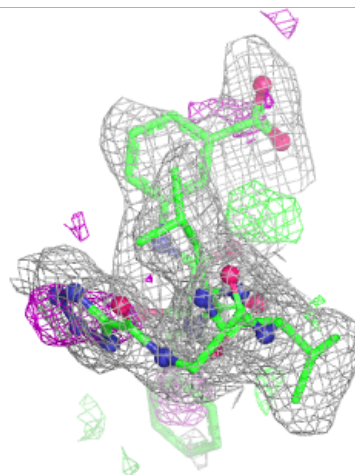
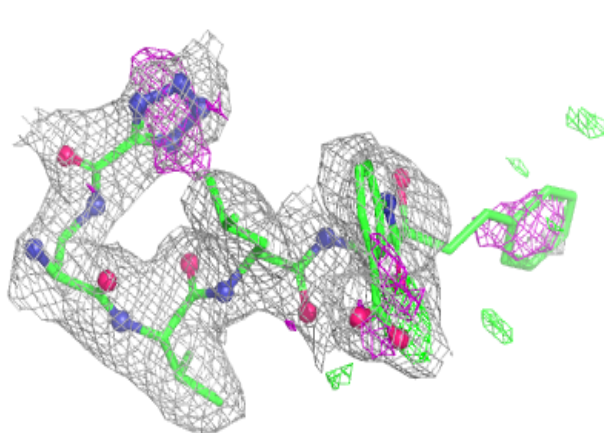
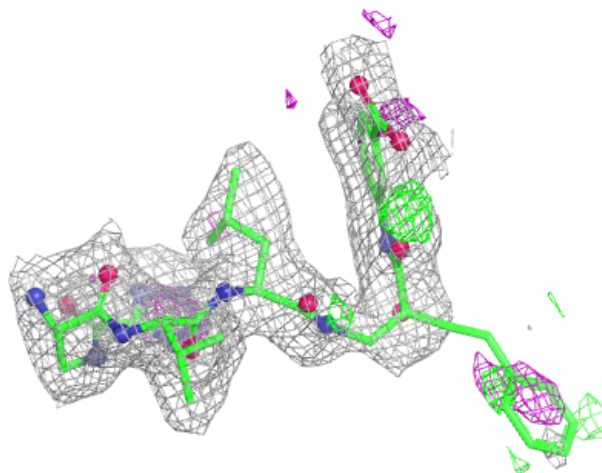
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists 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	038	C	500	52/52	0.90	0.14	4,24,52,54	0
2	038	A	500	52/52	0.93	0.10	8,16,38,40	0
2	038	B	500	52/52	0.95	0.09	7,17,36,38	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.

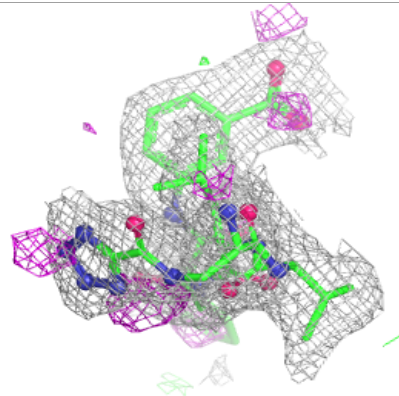
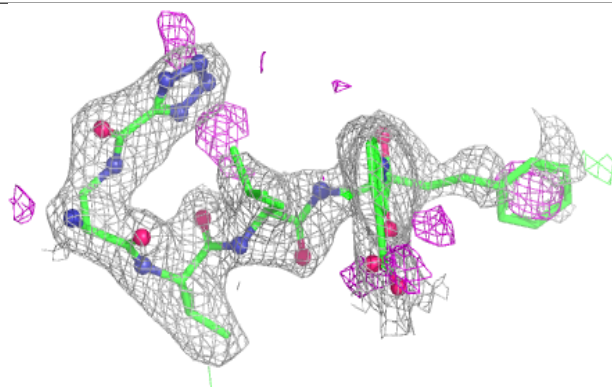
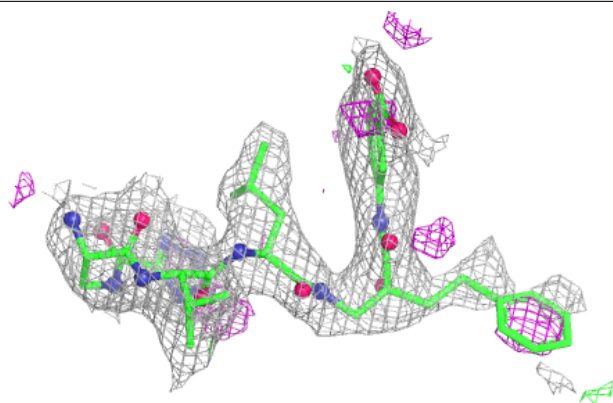
Electron density around 038 C 500:

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

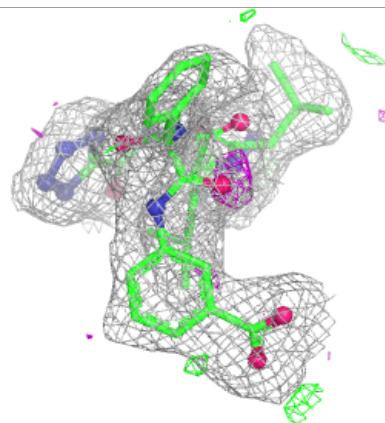
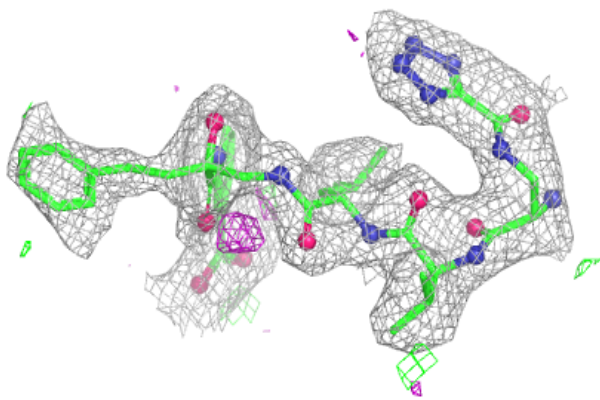
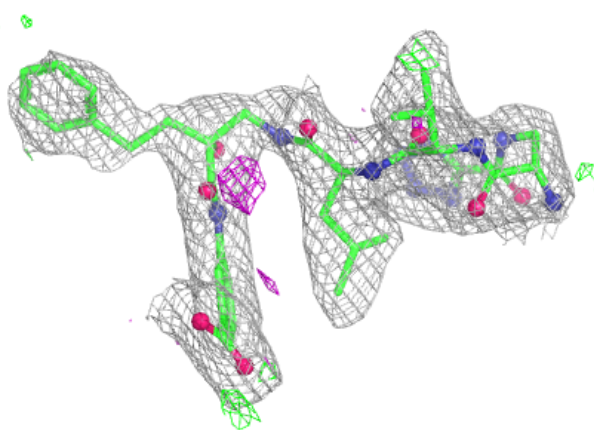


Electron density around 038 A 500:

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

**Electron density around 038 B 500:**

$2mF_o-DF_c$ (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.