



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:57 AM UTC

PDB ID : 3CIC / pdb_00003cic
Title : Structure of BACE Bound to SCH709583
Authors : Strickland, C.; Cumming, J.
Deposited on : 2008-03-11
Resolution : 1.75 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

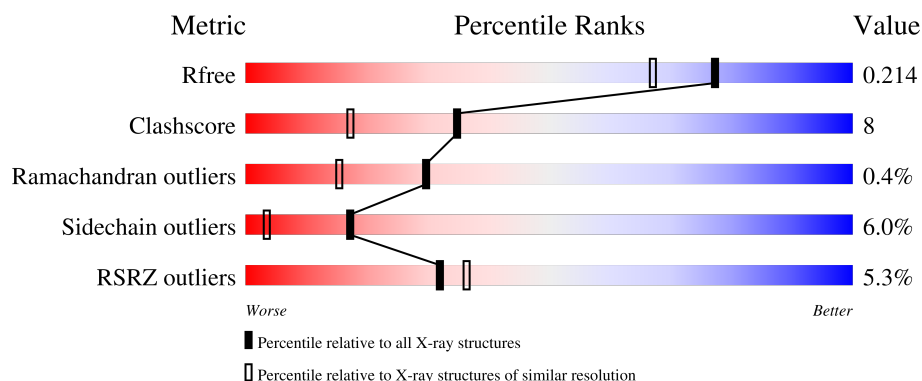
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.75 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	3183 (1.76-1.76)
Clashscore	190562	3299 (1.76-1.76)
Ramachandran outliers	187476	3274 (1.76-1.76)
Sidechain outliers	187428	3274 (1.76-1.76)
RSRZ outliers	180081	3183 (1.76-1.76)

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	390	6% 78% 19% .
1	B	390	4% 77% 20% .

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
3	TAR	A	552	X	-	-	-
3	TAR	B	553	X	-	-	-

2 Entry composition [i](#)

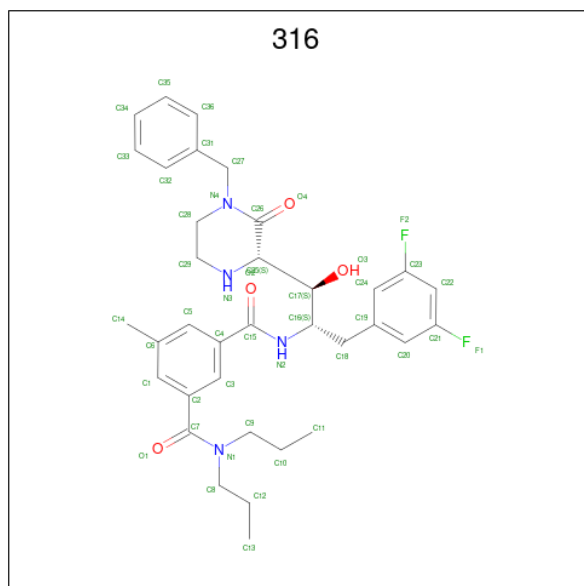
There are 4 unique types of molecules in this entry. The entry contains 7191 atoms, of which 0 are hydrogens and 0 are deuteriums.

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.

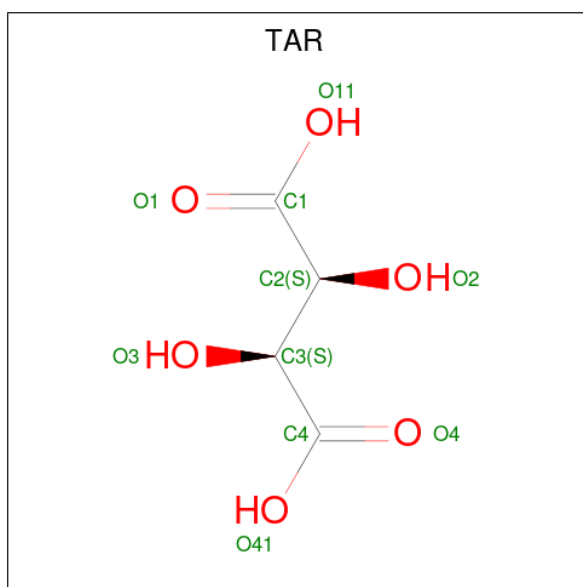
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	390	Total	C	N	O	S	0	0	0
			3060	1959	508	579	14			
1	B	389	Total	C	N	O	S	0	0	0
			3052	1953	507	578	14			

- Molecule 2 is N'-[(1S,2S)-2-[(2S)-4-benzyl-3-oxopiperazin-2-yl]-1-(3,5-difluorobenzyl)-2-hydroxyethyl]-5-methyl-N,N-dipropylbenzene-1,3-dicarboxamide (CCD ID: 316) (formula: C₃₅H₄₂F₂N₄O₄).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	F	N	O	0	0
			45	35	2	4	4		
2	B	1	Total	C	F	N	O	0	0
			45	35	2	4	4		

- Molecule 3 is D(-)-TARTARIC ACID (CCD ID: TAR) (formula: C₄H₆O₆).



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

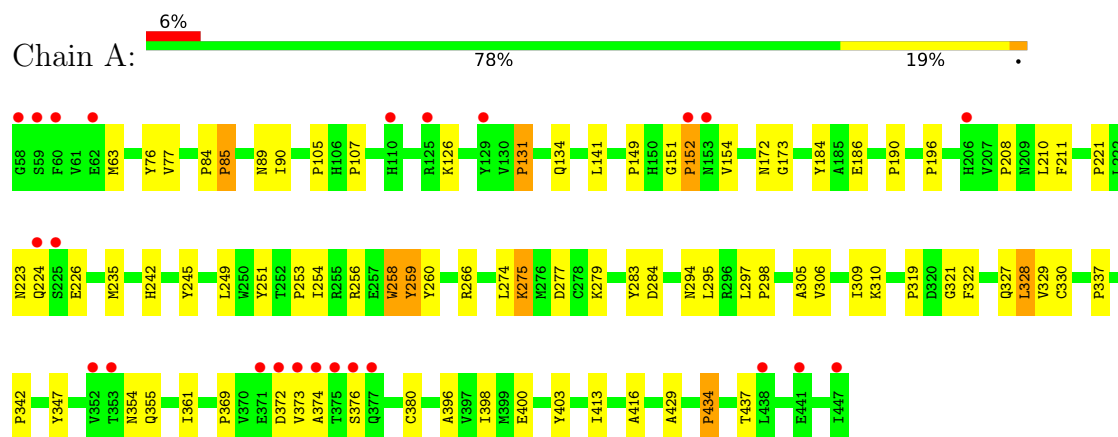
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	504	Total	O	0	0
			504	504		
4	B	465	Total	O	0	0
			465	465		

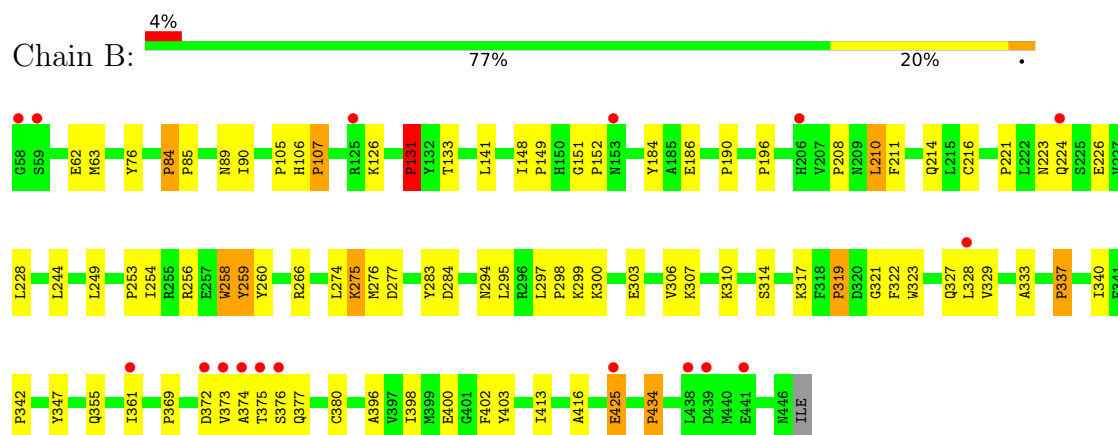
3 Residue-property plots [i](#)

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: Beta-secretase 1



• Molecule 1: Beta-secretase 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	86.40Å 89.04Å 130.70Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 1.75 50.00 – 1.75	Depositor EDS
% Data completeness (in resolution range)	99.6 (50.00-1.75) 99.6 (50.00-1.75)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.84 (at 1.75Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.199 , 0.224 0.188 , 0.214	Depositor DCC
R_{free} test set	5076 reflections (4.97%)	wwPDB-VP
Wilson B-factor (Å ²)	18.9	Xtriage
Anisotropy	0.459	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 47.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.000 for k,h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7191	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 51.19 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 5.8080e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 316, TAR

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	0.48	0/3138	1.09	17/4267 (0.4%)
1	B	0.48	0/3130	1.11	19/4256 (0.4%)
All	All	0.48	0/6268	1.10	36/8523 (0.4%)

There are no bond length outliers.

All (36) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	294	ASN	N-CA-C	7.92	121.24	110.55
1	A	295	LEU	N-CA-C	-7.75	97.39	109.25
1	B	294	ASN	N-CA-C	7.61	120.83	110.55
1	A	259	TYR	N-CA-C	-7.40	99.87	110.59
1	B	403	TYR	N-CA-C	-6.86	98.06	108.96
1	B	295	LEU	N-CA-C	-6.83	97.41	108.41
1	B	259	TYR	N-CA-C	-6.56	100.19	110.36
1	A	254	ILE	N-CA-C	-6.54	98.10	107.98
1	A	403	TYR	N-CA-C	-6.54	98.57	108.96
1	A	277	ASP	N-CA-C	-6.47	100.45	110.10
1	A	184	TYR	N-CA-C	6.30	119.06	110.55
1	B	184	TYR	N-CA-C	6.19	118.90	110.55
1	A	134	GLN	N-CA-C	6.15	118.90	111.40
1	B	254	ILE	N-CA-C	-6.12	98.74	107.98
1	B	275	LYS	N-CA-C	6.09	119.82	111.54
1	A	275	LYS	N-CA-C	5.96	119.78	111.74
1	B	277	ASP	N-CA-C	-5.85	101.39	110.10
1	B	274	LEU	N-CA-C	-5.84	105.42	112.54
1	A	251	TYR	N-CA-C	5.74	118.83	109.59
1	A	274	LEU	N-CA-C	-5.57	105.75	112.54
1	B	84	PRO	CA-C-N	5.46	125.77	119.93
1	B	84	PRO	C-N-CA	5.46	125.77	119.93

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	297	LEU	CA-C-N	5.42	125.43	119.90
1	A	297	LEU	C-N-CA	5.42	125.43	119.90
1	B	90	ILE	N-CA-C	5.37	115.58	107.75
1	A	258	TRP	N-CA-C	-5.25	99.62	110.80
1	A	429	ALA	N-CA-C	-5.17	103.70	110.53
1	B	216	CYS	N-CA-C	5.17	117.14	107.99
1	A	90	ILE	N-CA-C	5.12	115.23	107.75
1	B	297	LEU	CA-C-N	5.08	125.08	119.90
1	B	297	LEU	C-N-CA	5.08	125.08	119.90
1	A	85	PRO	N-CA-C	5.06	119.51	111.26
1	B	258	TRP	N-CA-C	-5.04	100.06	110.80
1	B	148	ILE	CA-C-N	5.03	125.06	119.32
1	B	148	ILE	C-N-CA	5.03	125.06	119.32
1	B	402	PHE	N-CA-C	5.01	116.81	109.24

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	3060	0	2970	41	0
1	B	3052	0	2959	48	0
2	A	45	0	42	2	0
2	B	45	0	42	2	0
3	A	10	0	4	0	0
3	B	10	0	4	0	0
4	A	504	0	0	2	0
4	B	465	0	0	0	0
All	All	7191	0	6021	92	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 (92) 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:361:ILE:HD13	1:B:398:ILE:HD12	1.36	1.04
1:A:249:LEU:HD23	1:A:416:ALA:HB2	1.47	0.96
1:B:249:LEU:HD23	1:B:416:ALA:HB2	1.62	0.81
1:A:63:MET:HG2	1:A:151:GLY:HA2	1.63	0.79
1:B:361:ILE:CD1	1:B:398:ILE:HD12	2.18	0.72
1:B:126:LYS:HE3	1:B:141:LEU:HD12	1.79	0.64
1:B:355:GLN:HG3	1:B:434:PRO:HB2	1.80	0.63
1:B:63:MET:HG2	1:B:151:GLY:HA2	1.83	0.61
1:B:425:GLU:N	1:B:425:GLU:OE1	2.33	0.60
1:A:249:LEU:HD23	1:A:416:ALA:CB	2.28	0.60
1:A:361:ILE:HD13	1:A:398:ILE:HD12	1.83	0.60
1:A:260:TYR:HB3	1:A:413:ILE:HD11	1.85	0.59
1:B:62:GLU:H	1:B:62:GLU:CD	2.11	0.59
1:A:355:GLN:HG3	1:A:434:PRO:HB2	1.84	0.58
1:A:321:GLY:C	1:A:327:GLN:HG2	2.29	0.57
1:B:321:GLY:C	1:B:327:GLN:HG2	2.29	0.57
1:B:372:ASP:HB2	1:B:380:CYS:SG	2.44	0.57
1:B:186:GLU:OE2	1:B:256:ARG:NH2	2.38	0.56
1:B:375:THR:HG22	1:B:375:THR:O	2.05	0.56
1:B:275:LYS:O	1:B:275:LYS:HG2	2.06	0.55
1:B:361:ILE:HD13	1:B:398:ILE:CD1	2.23	0.55
1:A:63:MET:CG	1:A:151:GLY:HA2	2.36	0.55
1:A:258:TRP:CG	1:A:259:TYR:H	2.26	0.54
1:B:260:TYR:HB3	1:B:413:ILE:HD11	1.90	0.54
1:A:210:LEU:C	1:A:210:LEU:HD23	2.32	0.54
1:A:210:LEU:HD23	1:A:211:PHE:N	2.23	0.53
1:B:223:ASN:OD1	1:B:226:GLU:HG3	2.08	0.53
1:A:306:VAL:CG1	1:A:310:LYS:HE3	2.38	0.52
1:A:306:VAL:HG12	1:A:310:LYS:HE3	1.90	0.52
1:B:210:LEU:HD23	1:B:211:PHE:N	2.24	0.52
2:A:501:316:H9	2:A:501:316:C3	2.39	0.52
1:B:319:PRO:HG3	1:B:327:GLN:NE2	2.25	0.52
1:B:131:PRO:HG2	1:B:131:PRO:O	2.10	0.52
2:B:501:316:H9	2:B:501:316:C3	2.39	0.52
1:A:131:PRO:O	1:A:131:PRO:HG2	2.10	0.52
1:B:396:ALA:O	1:B:400:GLU:HG3	2.09	0.52
1:B:210:LEU:HD23	1:B:210:LEU:C	2.35	0.51
1:A:224:GLN:HG3	4:A:924:HOH:O	2.09	0.51
1:B:214:GLN:OE1	1:B:244:LEU:HD22	2.11	0.51
1:A:396:ALA:O	1:A:400:GLU:HG3	2.12	0.50
1:B:258:TRP:CG	1:B:259:TYR:H	2.30	0.50
1:B:306:VAL:HG12	1:B:310:LYS:HE3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:372:ASP:HB2	1:A:380:CYS:SG	2.52	0.50
1:A:372:ASP:C	1:A:374:ALA:H	2.20	0.50
1:B:126:LYS:HE3	1:B:141:LEU:CD1	2.42	0.50
1:A:361:ILE:HD13	1:A:398:ILE:CD1	2.42	0.49
1:B:306:VAL:CG1	1:B:310:LYS:HE3	2.41	0.49
1:B:372:ASP:OD2	1:B:374:ALA:HB3	2.12	0.49
1:A:126:LYS:HD2	1:A:141:LEU:HD12	1.94	0.49
1:B:425:GLU:H	1:B:425:GLU:CD	2.21	0.49
1:B:355:GLN:CG	1:B:434:PRO:HB2	2.42	0.49
1:A:186:GLU:OE2	1:A:256:ARG:NH2	2.46	0.48
1:A:275:LYS:HG2	1:A:275:LYS:O	2.12	0.48
1:A:266:ARG:HB3	1:A:347:TYR:HB2	1.95	0.48
1:B:276:MET:CE	1:B:300:LYS:HG2	2.43	0.48
1:A:279:LYS:NZ	4:A:817:HOH:O	2.47	0.48
1:B:299:LYS:O	1:B:303:GLU:HG3	2.14	0.47
1:B:303:GLU:O	1:B:307:LYS:HG3	2.15	0.46
1:A:76:TYR:CD1	1:A:89:ASN:HB3	2.51	0.46
1:A:372:ASP:OD2	1:A:374:ALA:HB3	2.16	0.46
1:B:322:PHE:CD1	1:B:329:VAL:HG23	2.51	0.45
1:A:328:LEU:HD12	1:A:328:LEU:O	2.17	0.45
1:B:283:TYR:HA	1:B:284:ASP:HA	1.73	0.45
1:B:276:MET:HE1	1:B:300:LYS:HG2	1.98	0.45
1:A:372:ASP:C	1:A:374:ALA:N	2.73	0.45
1:A:242:HIS:CE1	1:A:245:TYR:HH	2.33	0.45
1:A:258:TRP:CD1	1:A:259:TYR:H	2.35	0.45
1:A:152:PRO:HG2	1:A:154:VAL:HG22	1.99	0.44
1:A:354:ASN:HA	1:A:437:THR:O	2.17	0.44
1:A:172:ASN:HD22	1:A:173:GLY:N	2.16	0.44
1:A:328:LEU:HD12	1:A:328:LEU:C	2.42	0.44
1:A:373:VAL:O	1:A:373:VAL:HG12	2.17	0.44
1:B:106:HIS:CG	1:B:107:PRO:HD2	2.53	0.43
1:B:373:VAL:HG12	1:B:373:VAL:O	2.19	0.43
1:B:314:SER:O	1:B:317:LYS:NZ	2.52	0.42
1:A:283:TYR:HA	1:A:284:ASP:HA	1.77	0.42
1:B:337:PRO:O	1:B:340:ILE:HG12	2.19	0.42
1:B:266:ARG:HB3	1:B:347:TYR:HB2	2.01	0.42
1:B:76:TYR:CD1	1:B:89:ASN:HB3	2.55	0.42
1:B:372:ASP:C	1:B:374:ALA:H	2.27	0.42
1:A:223:ASN:OD1	1:A:226:GLU:HG3	2.20	0.42
1:A:305:ALA:O	1:A:309:ILE:HG13	2.20	0.41
1:A:328:LEU:HD13	1:A:330:CYS:SG	2.60	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:77:VAL:HG11	1:A:235:MET:HE1	2.03	0.41
1:B:224:GLN:O	1:B:228:LEU:HG	2.20	0.41
1:B:372:ASP:C	1:B:374:ALA:N	2.79	0.41
1:A:322:PHE:CD1	1:A:329:VAL:HG13	2.56	0.41
1:B:310:LYS:HE2	1:B:323:TRP:CD1	2.55	0.40
1:B:333:ALA:HB2	1:B:377:GLN:O	2.21	0.40
1:B:133:THR:HB	2:B:501:316:H5	2.04	0.40
2:A:501:316:H16	2:A:501:316:O4	2.22	0.40
1:B:258:TRP:CD1	1:B:259:TYR:H	2.39	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	388/390 (100%)	376 (97%)	11 (3%)	1 (0%)	36	21
1	B	387/390 (99%)	377 (97%)	8 (2%)	2 (0%)	24	11
All	All	775/780 (99%)	753 (97%)	19 (2%)	3 (0%)	30	15

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	376	SER
1	B	376	SER
1	B	131	PRO

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	332/332 (100%)	313 (94%)	19 (6%)	18	4
1	B	331/332 (100%)	310 (94%)	21 (6%)	16	3
All	All	663/664 (100%)	623 (94%)	40 (6%)	17	3

All (40) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	84	PRO
1	A	85	PRO
1	A	105	PRO
1	A	107	PRO
1	A	131	PRO
1	A	149	PRO
1	A	152	PRO
1	A	190	PRO
1	A	196	PRO
1	A	208	PRO
1	A	221	PRO
1	A	253	PRO
1	A	298	PRO
1	A	319	PRO
1	A	328	LEU
1	A	337	PRO
1	A	342	PRO
1	A	369	PRO
1	A	434	PRO
1	B	84	PRO
1	B	85	PRO
1	B	105	PRO
1	B	107	PRO
1	B	131	PRO
1	B	149	PRO
1	B	152	PRO
1	B	190	PRO
1	B	196	PRO
1	B	208	PRO
1	B	210	LEU
1	B	221	PRO
1	B	253	PRO
1	B	298	PRO

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Mol	Chain	Res	Type
1	B	319	PRO
1	B	328	LEU
1	B	337	PRO
1	B	342	PRO
1	B	369	PRO
1	B	425	GLU
1	B	434	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (15) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	73	GLN
1	A	114	GLN
1	A	134	GLN
1	A	172	ASN
1	A	294	ASN
1	A	354	ASN
1	A	387	GLN
1	A	423	HIS
1	B	89	ASN
1	B	134	GLN
1	B	172	ASN
1	B	294	ASN
1	B	332	GLN
1	B	423	HIS
1	B	446	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

4 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
3	TAR	A	552	-	9,9,9	1.15	2 (22%)	12,12,12	0.98	0
3	TAR	B	553	-	9,9,9	1.16	2 (22%)	12,12,12	0.95	0
2	316	A	501	-	47,48,48	1.67	18 (38%)	58,66,66	1.06	4 (6%)
2	316	B	501	-	47,48,48	1.68	18 (38%)	58,66,66	1.09	5 (8%)

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
3	TAR	B	553	-	2/2/4/4	0/12/12/12	-
2	316	A	501	-	-	1/38/52/52	0/4/4/4
3	TAR	A	552	-	2/2/4/4	0/12/12/12	-
2	316	B	501	-	-	0/38/52/52	0/4/4/4

All (40) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	501	316	C24-C23	3.30	1.43	1.37
2	B	501	316	C24-C23	3.17	1.42	1.37
2	A	501	316	C20-C21	3.15	1.42	1.37
2	B	501	316	C20-C21	3.10	1.42	1.37
2	B	501	316	C22-C23	3.09	1.42	1.37
2	B	501	316	C22-C21	3.09	1.42	1.37
2	A	501	316	C22-C21	2.92	1.42	1.37
2	A	501	316	C5-C6	2.71	1.43	1.39
2	A	501	316	C3-C2	2.69	1.43	1.39
2	A	501	316	C22-C23	2.68	1.42	1.37
2	B	501	316	C5-C6	2.65	1.43	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	501	316	C3-C2	2.63	1.43	1.39
2	B	501	316	C5-C4	2.57	1.43	1.39
2	A	501	316	C5-C4	2.45	1.43	1.39
2	A	501	316	C24-C19	2.38	1.43	1.39
2	B	501	316	C33-C32	2.36	1.42	1.38
2	B	501	316	C1-C6	2.36	1.42	1.39
3	B	553	TAR	O11-C1	-2.32	1.23	1.30
2	A	501	316	C35-C36	2.32	1.42	1.38
2	B	501	316	C35-C36	2.31	1.42	1.38
2	A	501	316	C33-C32	2.30	1.42	1.38
3	A	552	TAR	O11-C1	-2.29	1.23	1.30
2	A	501	316	C35-C34	2.28	1.43	1.38
2	B	501	316	C35-C34	2.27	1.43	1.38
2	A	501	316	C1-C6	2.27	1.42	1.39
2	A	501	316	C3-C4	2.24	1.42	1.39
2	A	501	316	C20-C19	2.24	1.43	1.39
2	B	501	316	C34-C33	2.24	1.43	1.38
2	B	501	316	C3-C4	2.21	1.42	1.39
2	B	501	316	C24-C19	2.18	1.43	1.39
2	B	501	316	C36-C31	2.17	1.43	1.38
2	A	501	316	C1-C2	2.17	1.42	1.39
3	B	553	TAR	O41-C4	-2.17	1.23	1.30
2	B	501	316	C1-C2	2.15	1.42	1.39
2	A	501	316	C34-C33	2.12	1.42	1.38
2	B	501	316	C20-C19	2.11	1.42	1.39
3	A	552	TAR	O41-C4	-2.09	1.24	1.30
2	B	501	316	C32-C31	2.08	1.43	1.38
2	A	501	316	C32-C31	2.04	1.42	1.38
2	A	501	316	C36-C31	2.04	1.42	1.38

All (9) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	316	C22-C21-C20	-2.88	120.00	123.50
2	A	501	316	C24-C23-C22	-2.76	120.15	123.50
2	A	501	316	C23-C22-C21	2.73	120.06	116.08
2	B	501	316	C24-C23-C22	-2.66	120.27	123.50
2	A	501	316	C22-C21-C20	-2.62	120.31	123.50
2	B	501	316	C23-C22-C21	2.57	119.83	116.08
2	B	501	316	C16-N2-C15	-2.24	118.87	122.94
2	A	501	316	C16-N2-C15	-2.13	119.06	122.94
2	B	501	316	C31-C27-N4	-2.06	109.92	113.15

All (4) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
3	A	552	TAR	C3
3	A	552	TAR	C2
3	B	553	TAR	C3
3	B	553	TAR	C2

All (1) torsion outliers are listed below:

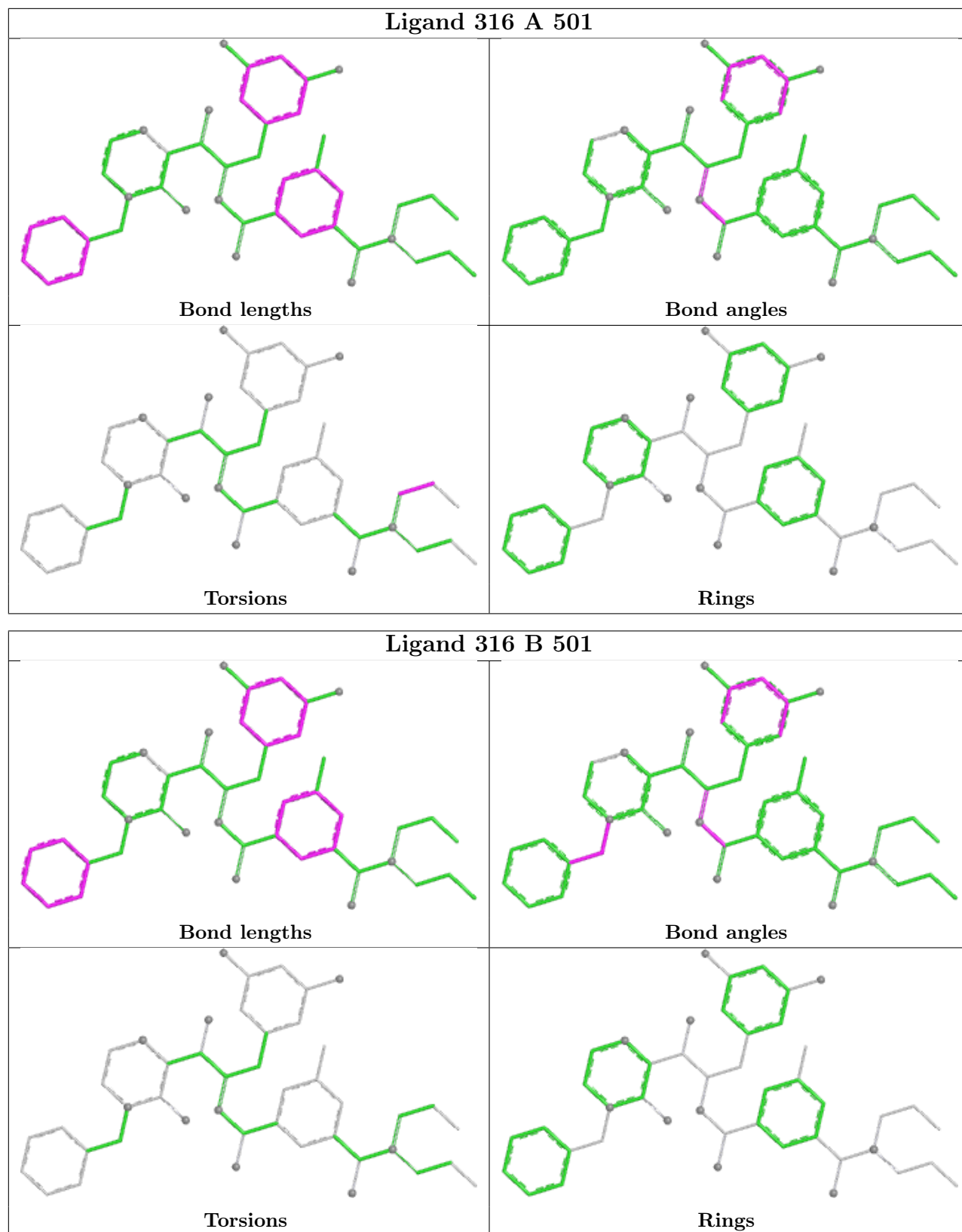
Mol	Chain	Res	Type	Atoms
2	A	501	316	C13-C12-C8-N1

There are no ring outliers.

2 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	501	316	2	0
2	B	501	316	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 ⓘ

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	390/390 (100%)	0.18	24 (6%) 26 30	12, 18, 35, 69	0
1	B	389/390 (99%)	0.10	17 (4%) 39 45	10, 17, 34, 64	0
All	All	779/780 (99%)	0.14	41 (5%) 32 36	10, 17, 35, 69	0

All (41) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	373	VAL	8.3
1	A	373	VAL	7.5
1	A	447	ILE	6.4
1	A	375	THR	6.0
1	B	374	ALA	5.8
1	B	375	THR	5.6
1	A	374	ALA	5.3
1	A	58	GLY	4.5
1	B	425	GLU	4.0
1	A	441	GLU	3.8
1	B	372	ASP	3.5
1	A	59	SER	3.5
1	B	441	GLU	3.2
1	A	376	SER	3.2
1	A	225	SER	3.2
1	A	110	HIS	3.2
1	B	59	SER	3.1
1	A	224	GLN	2.9
1	B	58	GLY	2.8
1	B	206	HIS	2.7
1	B	376	SER	2.7
1	A	353	THR	2.6
1	B	224	GLN	2.6
1	A	125	ARG	2.6

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Mol	Chain	Res	Type	RSRZ
1	A	438	LEU	2.5
1	A	153	ASN	2.4
1	B	328	LEU	2.3
1	A	62	GLU	2.3
1	A	129	TYR	2.3
1	A	371	GLU	2.3
1	A	352	VAL	2.3
1	A	206	HIS	2.2
1	B	361	ILE	2.2
1	B	439	ASP	2.1
1	A	372	ASP	2.1
1	A	377	GLN	2.1
1	A	152	PRO	2.1
1	B	153	ASN	2.0
1	B	438	LEU	2.0
1	A	60	PHE	2.0
1	B	125	ARG	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.

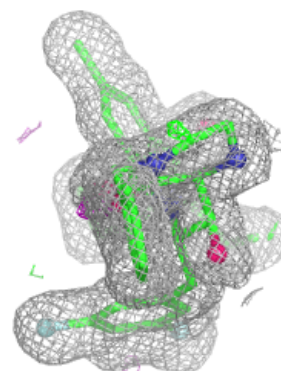
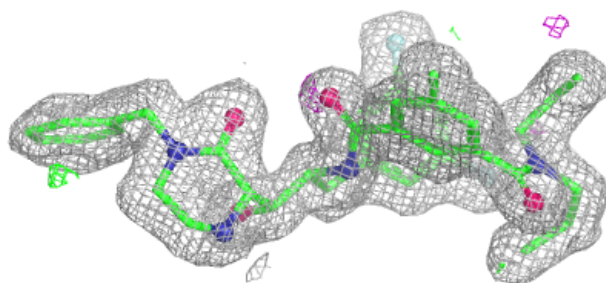
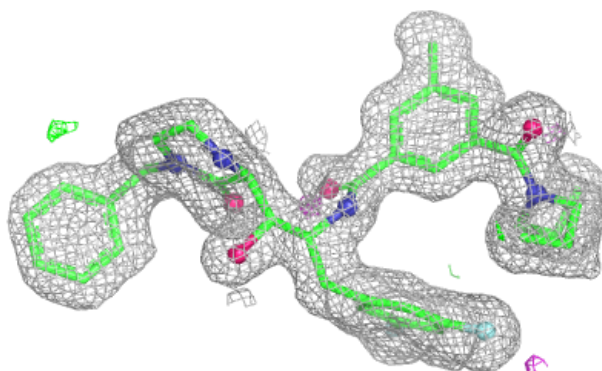
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
3	TAR	A	552	10/10	0.88	0.09	25,34,37,37	0
3	TAR	B	553	10/10	0.93	0.07	25,29,33,33	0
2	316	A	501	45/45	0.94	0.07	13,18,22,26	0
2	316	B	501	45/45	0.95	0.07	12,16,21,23	0

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.

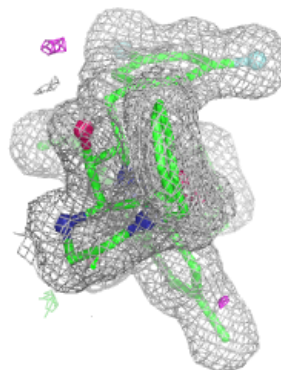
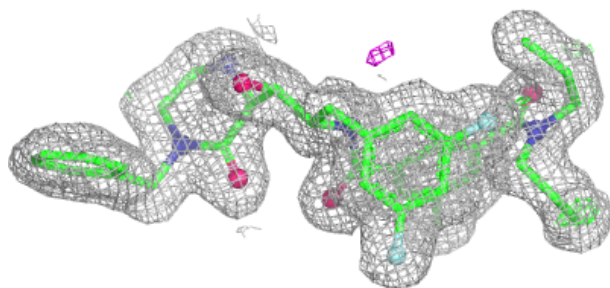
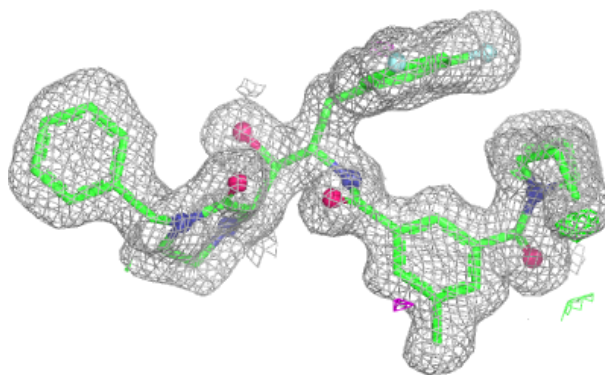
Electron density around 316 A 501:

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



Electron density around 316 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.