Full wwPDB X-ray Structure Validation Report (i)

Oct 31, 2021 – 11:37 AM EDT

PDB ID	:	3CKP
Title	:	Crystal structure of BACE-1 in complex with inhibitor
Authors	:	Min, K.
Deposited on	:	2008-03-16
Resolution	:	2.30 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 (i) symbol.

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

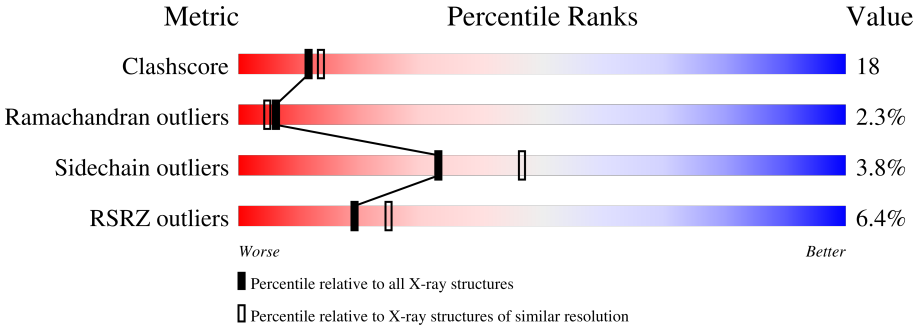
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.23.2
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.23.2

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 2.30 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))
Clashscore	141614	5643 (2.30-2.30)
Ramachandran outliers	138981	5575 (2.30-2.30)
Sidechain outliers	138945	5575 (2.30-2.30)
RSRZ outliers	127900	4938 (2.30-2.30)

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 <=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	412	3% 63% 28% • 8%
1	B	412	7% 62% 27% • 9%
1	C	412	8% 47% 40% • 8%

2 Entry composition (i)

There are 4 unique types of molecules in this entry. The entry contains 9210 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
			Total	C	N	O	S			
1	A	379	2974	1904	496	560	14	0	0	0
1	B	376	2956	1894	492	556	14	0	0	0
1	C	377	2967	1900	494	559	14	0	0	0

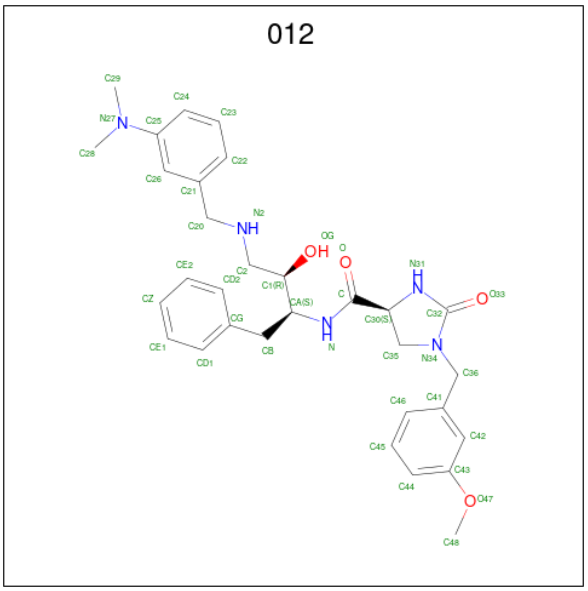
There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-6	LYS	ARG	engineered mutation	UNP P56817
A	-5	LYS	ARG	engineered mutation	UNP P56817
B	-6	LYS	ARG	engineered mutation	UNP P56817
B	-5	LYS	ARG	engineered mutation	UNP P56817
C	-6	LYS	ARG	engineered mutation	UNP P56817
C	-5	LYS	ARG	engineered mutation	UNP P56817

- Molecule 2 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
			Total	Cl		
2	A	5	5	5	0	0
2	B	2	2	2	0	0
2	C	2	2	2	0	0

- Molecule 3 is (4S)-N-[(1S,2R)-1-benzyl-3-{[3-(dimethylamino)benzyl]amino}-2-hydroxy propyl]-1-(3-methoxybenzyl)-2-oxoimidazolidine-4-carboxamide (three-letter code: 012) (formula: $C_{31}H_{39}N_5O_4$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			40	31	5	4		
3	B	1	Total	C	N	O	0	0
			40	31	5	4		
3	C	1	Total	C	N	O	0	0
			40	31	5	4		

- Molecule 4 is water.

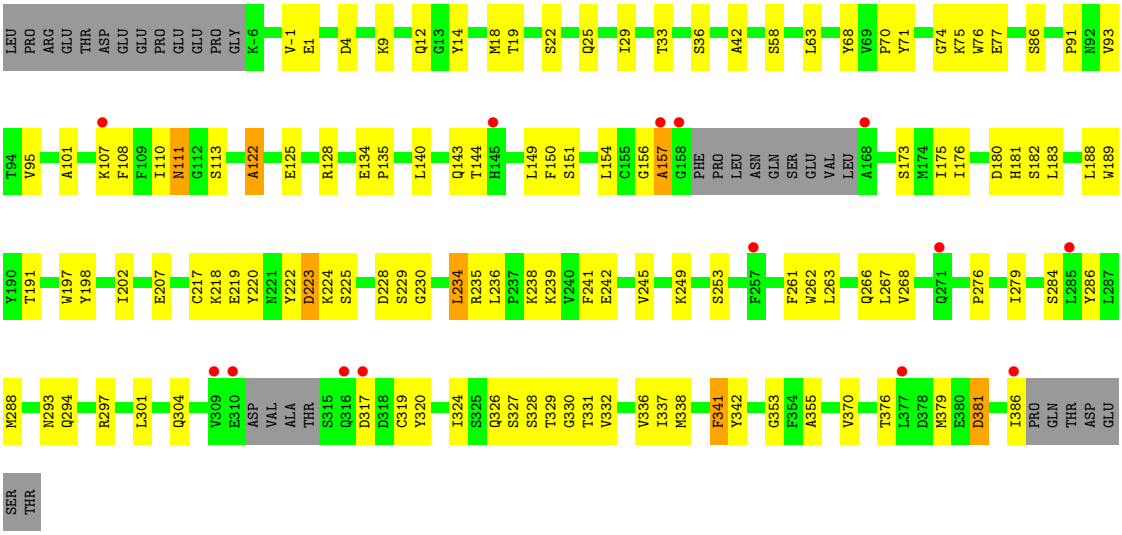
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	81	Total	O	0	0
			81	81		
4	B	64	Total	O	0	0
			64	64		
4	C	39	Total	O	0	0
			39	39		

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.

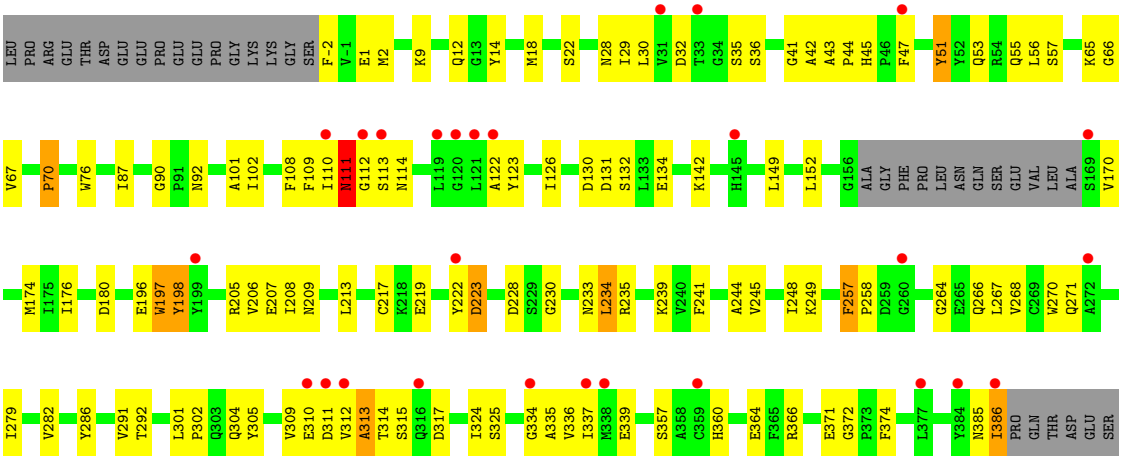
• Molecule 1: Beta-secretase 1

Chain A: 3% 63% 28% • 8%



• Molecule 1: Beta-secretase 1

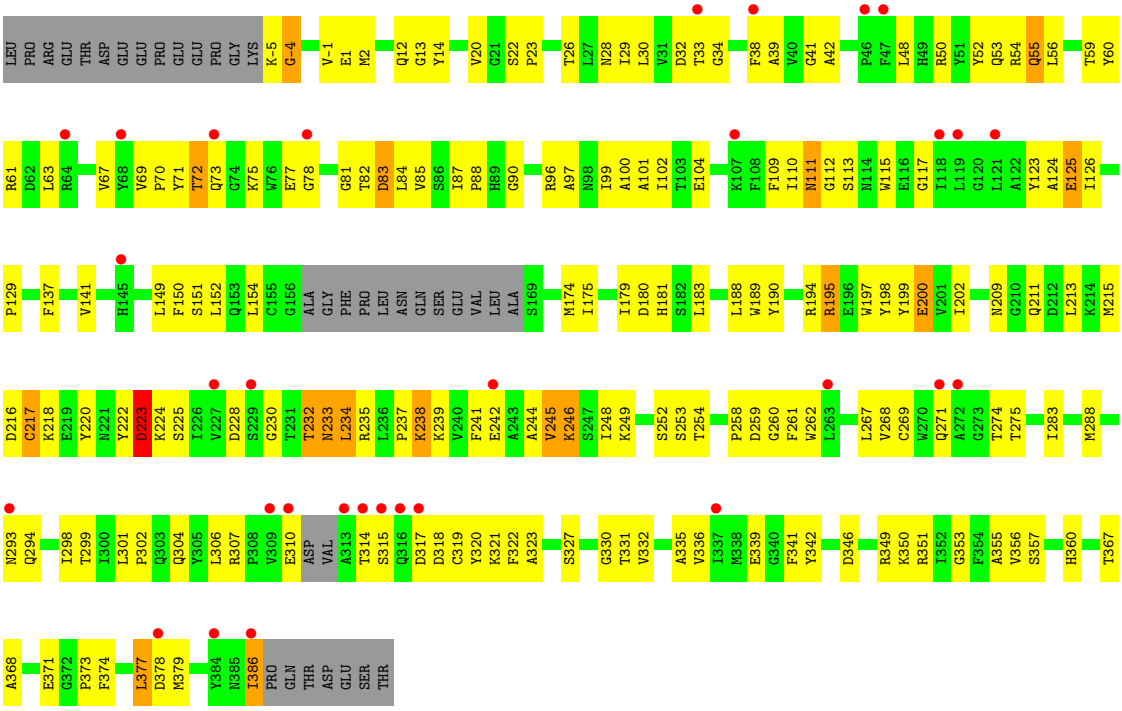
Chain B: 7% 62% 27% • 9%



THR

- Molecule 1: Beta-secretase 1

Chain C:



4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	224.06Å 105.65Å 63.70Å 90.00° 101.47° 90.00°	Depositor
Resolution (Å)	19.97 – 2.30 29.98 – 2.30	Depositor EDS
% Data completeness (in resolution range)	87.3 (19.97-2.30) 87.2 (29.98-2.30)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.31 (at 2.29Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.245 , 0.304 0.240 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å^2)	30.8	Xtriage
Anisotropy	0.761	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.31 , 41.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	9210	wwPDB-VP
Average B, all atoms (Å^2)	44.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.04% of the height of the origin peak. No significant pseudotranslation is detected.*

[1]Intensities estimated from amplitudes.

[2]Theoretical values of $< |L| >$, $< L^2 >$ 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: CL, 012

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	0.46	0/3048	0.72	2/4138 (0.0%)
1	B	0.43	0/3031	0.71	1/4119 (0.0%)
1	C	0.43	0/3041	0.70	2/4129 (0.0%)
All	All	0.44	0/9120	0.71	5/12386 (0.0%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	C	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	223	ASP	N-CA-C	-6.58	93.24	111.00
1	B	198	TYR	N-CA-C	-5.77	95.43	111.00
1	C	198	TYR	N-CA-C	-5.65	95.74	111.00
1	A	198	TYR	N-CA-C	-5.64	95.78	111.00
1	A	342	TYR	N-CA-C	-5.42	96.36	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	52	TYR	Sidechain

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	2974	0	2889	85	0
1	B	2956	0	2865	99	0
1	C	2967	0	2886	134	0
2	A	5	0	0	1	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0
3	A	40	0	39	5	0
3	B	40	0	39	1	0
3	C	40	0	39	6	0
4	A	81	0	0	3	0
4	B	64	0	0	2	0
4	C	39	0	0	2	0
All	All	9210	0	8757	313	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 18.

All (313) 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:53:GLN:HB3	1:B:55:GLN:HE22	1.27	0.96
1:C:55:GLN:H	1:C:55:GLN:HE21	1.11	0.95
1:B:234:LEU:HB2	1:B:336:VAL:HG21	1.47	0.94
1:C:55:GLN:HG2	1:C:56:LEU:HD12	1.53	0.91
1:A:4:ASP:H	1:A:173:SER:HB3	1.39	0.88
1:C:225:SER:OG	1:C:331:THR:HB	1.75	0.87
1:B:53:GLN:HB3	1:B:55:GLN:NE2	1.91	0.85
1:C:246:LYS:HA	1:C:246:LYS:HE2	1.56	0.85
1:C:110:ILE:HB	1:C:113:SER:HB3	1.59	0.84
1:C:20:VAL:HG12	1:C:85:VAL:HG22	1.59	0.84
1:B:271:GLN:CD	1:B:271:GLN:H	1.81	0.83
1:B:9:LYS:HD3	1:B:12:GLN:OE1	1.81	0.81
1:A:301:LEU:H	1:A:304:GLN:NE2	1.80	0.80
1:A:301:LEU:H	1:A:304:GLN:HE21	1.25	0.80
1:A:68:TYR:HB2	1:A:77:GLU:HG2	1.67	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:180:ASP:OD2	1:A:182:SER:HB3	1.86	0.76
1:B:310:GLU:HG3	1:B:311:ASP:N	2.01	0.76
1:C:125:GLU:HG2	1:C:197:TRP:HB2	1.68	0.75
1:B:55:GLN:HE21	1:B:56:LEU:HG	1.51	0.75
1:C:188:LEU:HD23	1:C:355:ALA:HB2	1.67	0.75
1:C:194:ARG:HB3	1:C:200:GLU:HG2	1.69	0.75
1:B:241:PHE:O	1:B:245:VAL:HG23	1.88	0.74
1:A:238:LYS:O	1:A:242:GLU:HG3	1.87	0.74
1:B:234:LEU:HB2	1:B:336:VAL:CG2	2.18	0.73
1:B:301:LEU:H	1:B:304:GLN:NE2	1.86	0.73
1:A:110:ILE:HB	1:A:113:SER:HB3	1.71	0.72
1:C:82:THR:O	1:C:83:ASP:HB2	1.89	0.72
1:C:41:GLY:HA2	1:C:102:ILE:HB	1.71	0.72
1:C:55:GLN:H	1:C:55:GLN:NE2	1.86	0.72
1:C:314:THR:HG22	1:C:315:SER:N	2.07	0.70
1:A:241:PHE:O	1:A:245:VAL:HG23	1.90	0.70
1:B:279:ILE:HG22	1:C:211:GLN:HE21	1.56	0.69
1:B:245:VAL:HG12	1:B:249:LYS:HE2	1.74	0.69
1:C:-5:LYS:HG2	1:C:-4:GLY:H	1.57	0.68
1:B:2:MET:HG2	1:B:90:GLY:HA2	1.77	0.67
1:B:310:GLU:HG3	1:B:311:ASP:H	1.60	0.67
1:C:55:GLN:HE21	1:C:55:GLN:N	1.90	0.66
1:C:225:SER:HA	1:C:331:THR:O	1.95	0.66
1:C:111:ASN:HD22	1:C:112:GLY:N	1.94	0.66
1:C:261:PHE:CE1	1:C:322:PHE:HB2	2.32	0.65
1:B:219:GLU:OE1	1:B:239:LYS:HD2	1.96	0.64
1:B:335:ALA:O	1:B:339:GLU:HG3	1.98	0.64
1:C:20:VAL:CG1	1:C:85:VAL:HG22	2.28	0.64
1:B:385:ASN:O	1:B:386:ILE:HG22	1.98	0.64
1:C:314:THR:HG22	1:C:315:SER:H	1.63	0.64
1:C:-5:LYS:HG2	1:C:-4:GLY:N	2.13	0.63
1:C:222:TYR:O	1:C:223:ASP:HB2	1.98	0.63
1:A:68:TYR:CB	1:A:77:GLU:HG2	2.29	0.63
1:C:302:PRO:O	1:C:306:LEU:HB2	1.98	0.63
1:A:276:PRO:O	1:A:279:ILE:HG12	1.98	0.63
1:B:311:ASP:C	1:B:313:ALA:H	2.01	0.63
1:A:74:GLY:HA2	1:A:107:LYS:HB2	1.80	0.62
1:B:241:PHE:HE1	1:B:324:ILE:O	1.81	0.62
1:B:309:VAL:HG23	1:B:309:VAL:O	1.98	0.62
1:A:267:LEU:HD13	1:A:319:CYS:HB3	1.80	0.62
1:C:149:LEU:HD23	1:C:149:LEU:C	2.20	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:234:LEU:HB2	1:C:336:VAL:HG21	1.81	0.62
1:B:386:ILE:HD13	1:B:386:ILE:O	2.00	0.61
1:C:97:ALA:O	1:C:99:ILE:HD12	2.01	0.61
1:A:293:ASN:HA	1:A:376:THR:O	2.01	0.60
1:C:234:LEU:HB2	1:C:336:VAL:CG2	2.31	0.60
1:B:14:TYR:CE2	1:B:170:VAL:HB	2.37	0.60
1:B:301:LEU:HB3	1:B:302:PRO:HD2	1.83	0.60
1:A:238:LYS:HG3	1:A:326:GLN:NE2	2.16	0.59
1:C:137:PHE:O	1:C:141:VAL:HG23	2.03	0.59
1:C:241:PHE:O	1:C:245:VAL:HG23	2.03	0.59
1:A:149:LEU:HD23	1:A:149:LEU:C	2.23	0.58
1:A:151:SER:OG	1:A:175:ILE:HB	2.04	0.58
1:C:301:LEU:H	1:C:304:GLN:HE21	1.52	0.58
1:A:218:LYS:HE3	4:A:640:HOH:O	2.04	0.58
1:C:238:LYS:HE2	1:C:242:GLU:OE2	2.03	0.58
1:C:271:GLN:HA	1:C:271:GLN:HE21	1.66	0.58
1:A:4:ASP:N	1:A:173:SER:HB3	2.16	0.57
1:C:14:TYR:CG	1:C:154:LEU:HD22	2.40	0.57
1:C:298:ILE:HB	1:C:341:PHE:CZ	2.40	0.57
1:B:149:LEU:C	1:B:149:LEU:HD23	2.25	0.57
1:A:14:TYR:CG	1:A:154:LEU:HD22	2.40	0.56
1:B:206:VAL:HG11	1:B:213:LEU:HD22	1.87	0.56
1:B:267:LEU:HD22	1:B:309:VAL:HG21	1.87	0.56
1:C:110:ILE:HD11	3:C:503:012:H45	1.87	0.56
1:B:205:ARG:HB3	1:B:286:TYR:HB2	1.87	0.56
1:B:65:LYS:HD3	1:B:66:GLY:N	2.21	0.56
1:C:34:GLY:HA3	1:C:228:ASP:OD1	2.05	0.56
1:C:72:THR:HG22	1:C:73:GLN:N	2.20	0.56
1:A:183:LEU:HA	4:A:678:HOH:O	2.05	0.56
1:B:311:ASP:C	1:B:313:ALA:N	2.58	0.56
1:C:179:ILE:HG23	1:C:342:TYR:HE2	1.71	0.56
1:B:14:TYR:O	1:B:30:LEU:HD22	2.06	0.55
1:B:205:ARG:NE	1:B:207:GLU:OE2	2.37	0.55
1:C:83:ASP:O	1:C:96:ARG:HA	2.06	0.55
1:B:228:ASP:OD1	1:B:230:GLY:N	2.34	0.55
1:C:30:LEU:HD21	3:C:503:012:H48A	1.89	0.55
1:A:286:TYR:CZ	1:A:297:ARG:HD3	2.41	0.55
1:C:77:GLU:HB3	1:C:104:GLU:HB2	1.88	0.55
1:B:314:THR:O	1:B:315:SER:HB3	2.07	0.55
1:B:111:ASN:C	1:B:111:ASN:HD22	2.10	0.55
1:B:12:GLN:HE21	1:B:110:ILE:HG21	1.72	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:55:GLN:HG2	1:C:56:LEU:CD1	2.34	0.55
1:C:222:TYR:O	1:C:223:ASP:CB	2.54	0.54
1:A:42:ALA:CB	1:A:101:ALA:HB1	2.37	0.54
1:C:14:TYR:CD2	1:C:154:LEU:HD22	2.42	0.54
1:C:53:GLN:HB3	1:C:56:LEU:HD13	1.88	0.54
1:A:180:ASP:HB3	1:A:183:LEU:HG	1.89	0.54
1:B:310:GLU:CG	1:B:311:ASP:H	2.18	0.54
1:C:367:THR:HG23	1:C:368:ALA:O	2.08	0.54
1:A:238:LYS:CG	1:A:326:GLN:NE2	2.70	0.54
1:C:33:THR:OG1	1:C:228:ASP:HA	2.08	0.54
1:B:244:ALA:O	1:B:248:ILE:HG13	2.07	0.54
1:C:29:ILE:HD12	1:C:117:GLY:HA3	1.89	0.54
1:B:55:GLN:NE2	1:B:56:LEU:HG	2.20	0.53
1:A:207:GLU:HB2	1:A:284:SER:HB2	1.91	0.53
1:C:202:ILE:HD12	1:C:288:MET:HE3	1.88	0.53
1:C:268:VAL:O	1:C:319:CYS:HA	2.07	0.53
1:C:217:CYS:HA	1:C:220:TYR:CD1	2.43	0.53
1:C:314:THR:CG2	1:C:315:SER:N	2.72	0.53
1:C:12:GLN:HG2	1:C:110:ILE:HD13	1.91	0.52
1:C:87:ILE:N	4:C:642:HOH:O	2.40	0.52
1:B:271:GLN:H	1:B:271:GLN:NE2	2.07	0.52
1:B:264:GLY:HA2	4:B:615:HOH:O	2.09	0.52
1:C:237:PRO:HD3	1:C:331:THR:OG1	2.09	0.52
1:C:30:LEU:HD11	3:C:503:012:H48A	1.90	0.52
1:A:149:LEU:HD23	1:A:150:PHE:N	2.25	0.52
1:C:97:ALA:O	1:C:99:ILE:CD1	2.58	0.52
1:C:48:LEU:HD21	1:C:109:PHE:CD2	2.45	0.51
1:C:149:LEU:HD23	1:C:150:PHE:N	2.24	0.51
1:A:217:CYS:HA	1:A:220:TYR:CD1	2.44	0.51
1:A:235:ARG:HB3	1:A:327:SER:HB2	1.92	0.51
1:B:205:ARG:HB3	1:B:286:TYR:CG	2.46	0.51
1:B:301:LEU:H	1:B:304:GLN:HE21	1.57	0.51
1:B:42:ALA:CB	1:B:101:ALA:HB1	2.40	0.51
1:C:349:ARG:NH1	1:C:351:ARG:NH2	2.59	0.51
1:B:130:ASP:OD2	1:B:132:SER:HB2	2.10	0.51
1:C:314:THR:CG2	1:C:315:SER:H	2.22	0.51
1:A:225:SER:OG	1:A:331:THR:HB	2.11	0.51
1:C:70:PRO:HA	1:C:75:LYS:HB3	1.92	0.51
1:C:230:GLY:O	3:C:503:012:H48B	2.11	0.51
1:C:151:SER:OG	1:C:175:ILE:HB	2.11	0.51
1:C:307:ARG:HH22	1:C:321:LYS:HE3	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:195:ARG:HB3	1:C:197:TRP:CD1	2.46	0.50
1:A:234:LEU:HD13	1:A:234:LEU:O	2.11	0.50
1:B:357:SER:HB3	1:B:360:HIS:HB3	1.93	0.50
1:A:219:GLU:HG3	1:A:239:LYS:HD3	1.93	0.50
1:C:235:ARG:HB2	1:C:332:VAL:HB	1.93	0.50
1:A:241:PHE:HE1	1:A:324:ILE:O	1.94	0.50
1:B:230:GLY:O	3:B:502:012:H48B	2.12	0.50
1:A:36:SER:OG	1:A:122:ALA:HB3	2.12	0.49
1:A:143:GLN:HG3	1:C:1:GLU:OE1	2.11	0.49
1:A:341:PHE:HB3	1:A:355:ALA:O	2.12	0.49
1:B:47:PHE:CD1	1:B:109:PHE:O	2.65	0.49
1:B:43:ALA:HB1	1:B:44:PRO:HD2	1.93	0.49
1:A:95:VAL:HG11	1:A:140:LEU:HA	1.94	0.49
1:A:228:ASP:OD1	1:A:230:GLY:N	2.42	0.49
1:B:42:ALA:HB2	1:B:101:ALA:HB1	1.94	0.49
1:C:113:SER:HB2	1:C:115:TRP:NE1	2.28	0.49
1:C:213:LEU:HB3	1:C:220:TYR:OH	2.13	0.49
1:A:218:LYS:HG3	1:A:381:ASP:O	2.12	0.49
1:C:32:ASP:OD1	1:C:230:GLY:HA3	2.12	0.49
1:A:234:LEU:N	1:A:336:VAL:HG11	2.28	0.48
1:A:188:LEU:HD23	1:A:355:ALA:HB2	1.95	0.48
1:A:235:ARG:HB2	1:A:332:VAL:HB	1.95	0.48
1:B:174:MET:SD	1:B:176:ILE:HD11	2.53	0.48
1:A:234:LEU:HB2	1:A:336:VAL:CG1	2.43	0.48
1:A:93:VAL:HG21	1:A:144:THR:HG21	1.95	0.48
1:C:71:TYR:O	1:C:72:THR:C	2.52	0.48
1:A:261:PHE:CD1	1:A:268:VAL:HG23	2.48	0.48
1:C:301:LEU:HB3	1:C:302:PRO:HD2	1.95	0.48
1:C:26:THR:HG22	1:C:50:ARG:NH1	2.29	0.48
1:C:215:MET:HE3	1:C:239:LYS:HG2	1.96	0.48
1:B:28:ASN:O	1:B:29:ILE:HD13	2.14	0.48
1:B:205:ARG:HB3	1:B:286:TYR:CB	2.44	0.47
1:C:59:THR:HG21	1:C:84:LEU:HD12	1.96	0.47
1:A:110:ILE:HD11	3:A:501:012:H45	1.96	0.47
1:C:224:LYS:O	1:C:331:THR:N	2.47	0.47
1:C:294:GLN:N	1:C:379:MET:HE1	2.29	0.47
1:A:337:ILE:HG22	1:A:338:MET:N	2.29	0.47
1:B:257:PHE:CB	1:B:258:PRO:HD2	2.44	0.47
1:A:297:ARG:O	1:A:370:VAL:HA	2.15	0.47
1:B:209:ASN:ND2	1:C:209:ASN:HB3	2.29	0.47
1:B:282:VAL:HG13	1:B:366:ARG:NH1	2.30	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:47:PHE:HD1	1:B:109:PHE:O	1.98	0.47
1:B:268:VAL:HG13	1:B:270:TRP:CZ3	2.49	0.47
1:C:238:LYS:O	1:C:242:GLU:HG3	2.15	0.47
1:A:14:TYR:CZ	1:A:154:LEU:HB3	2.50	0.46
1:A:238:LYS:HA	1:A:326:GLN:HG3	1.96	0.46
1:A:128:ARG:NH2	3:A:501:012:H28B	2.29	0.46
1:B:305:TYR:HB2	1:B:324:ILE:HG13	1.96	0.46
1:C:200:GLU:HA	1:C:225:SER:O	2.16	0.46
1:B:1:GLU:HG3	1:B:2:MET:HG3	1.98	0.46
1:C:216:ASP:OD2	1:C:218:LYS:HB2	2.16	0.46
1:C:244:ALA:O	1:C:248:ILE:HG13	2.15	0.46
1:B:1:GLU:CG	1:B:2:MET:H	2.29	0.46
1:B:18:MET:HG2	1:B:87:ILE:HG12	1.96	0.46
1:B:257:PHE:N	1:B:257:PHE:CD1	2.84	0.46
1:A:222:TYR:O	1:A:223:ASP:CB	2.63	0.46
1:B:197:TRP:CG	1:B:198:TYR:N	2.84	0.46
1:A:18:MET:SD	1:A:29:ILE:HG13	2.55	0.46
1:B:180:ASP:C	1:B:180:ASP:OD2	2.55	0.46
1:B:207:GLU:O	1:B:208:ILE:HD13	2.16	0.46
1:A:-1:VAL:HG12	1:A:1:GLU:OE1	2.16	0.45
1:B:67:VAL:HG13	1:B:76:TRP:HZ3	1.81	0.45
1:B:111:ASN:C	1:B:111:ASN:ND2	2.69	0.45
1:C:216:ASP:O	1:C:218:LYS:N	2.49	0.45
1:C:252:SER:O	1:C:254:THR:N	2.50	0.45
1:C:283:ILE:O	1:C:299:THR:HA	2.16	0.45
1:A:71:TYR:CG	3:A:501:012:HD2	2.52	0.45
1:C:69:VAL:O	1:C:75:LYS:HB2	2.17	0.45
1:C:189:TRP:O	1:C:353:GLY:HA2	2.16	0.45
1:B:41:GLY:HA2	1:B:102:ILE:HB	1.97	0.45
1:C:110:ILE:CD1	3:C:503:012:H45	2.47	0.45
1:B:112:GLY:O	1:B:113:SER:C	2.54	0.45
1:C:386:ILE:HD13	1:C:386:ILE:C	2.36	0.45
1:A:249:LYS:HD3	1:A:262:TRP:CD1	2.52	0.45
1:B:271:GLN:CD	1:B:271:GLN:N	2.60	0.45
1:B:12:GLN:NE2	1:B:110:ILE:HG21	2.31	0.45
1:B:208:ILE:O	1:B:209:ASN:C	2.55	0.45
1:B:336:VAL:CG2	1:B:337:ILE:N	2.80	0.45
1:C:20:VAL:HG12	1:C:85:VAL:HG13	1.99	0.45
1:A:230:GLY:O	3:A:501:012:H48B	2.16	0.45
1:C:152:LEU:HD23	1:C:174:MET:HA	1.98	0.45
1:A:19:THR:OG1	1:A:86:SER:HB2	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:22:SER:O	1:B:57:SER:HA	2.17	0.44
1:B:152:LEU:HD23	1:B:174:MET:HA	1.98	0.44
1:C:233:ASN:HB3	1:C:323:ALA:O	2.17	0.44
1:A:202:ILE:HB	1:A:288:MET:HE3	1.98	0.44
1:C:59:THR:HG21	1:C:84:LEU:CD1	2.47	0.44
1:C:180:ASP:HB3	1:C:183:LEU:HD12	1.99	0.44
1:C:274:THR:O	1:C:275:THR:C	2.53	0.44
1:B:257:PHE:HB3	1:B:258:PRO:HD2	1.99	0.44
1:A:110:ILE:HG22	1:A:111:ASN:N	2.33	0.44
1:C:42:ALA:CB	1:C:101:ALA:HB1	2.48	0.44
1:A:301:LEU:N	1:A:304:GLN:HE21	2.05	0.44
1:C:269:CYS:HA	1:C:318:ASP:O	2.18	0.44
1:B:45:HIS:HE1	1:B:47:PHE:CD1	2.36	0.44
1:B:108:PHE:O	1:B:110:ILE:HD12	2.18	0.44
1:B:233:ASN:HA	1:B:336:VAL:HG13	1.99	0.44
1:C:13:GLY:HA3	1:C:30:LEU:HD11	1.99	0.44
1:C:190:TYR:CG	1:C:351:ARG:HD2	2.53	0.44
1:C:271:GLN:HA	1:C:271:GLN:NE2	2.31	0.43
1:A:63:LEU:O	1:C:181:HIS:HD2	2.00	0.43
1:C:356:VAL:HG23	4:C:612:HOH:O	2.17	0.43
1:A:75:LYS:HD3	2:A:607:CL:CL	2.54	0.43
1:C:327:SER:OG	1:C:330:GLY:O	2.36	0.43
1:A:191:THR:HA	1:A:288:MET:O	2.19	0.43
1:C:28:ASN:N	1:C:50:ARG:HH21	2.16	0.43
1:C:232:THR:HB	1:C:233:ASN:H	1.61	0.43
1:B:222:TYR:O	1:B:223:ASP:CB	2.66	0.43
1:A:22:SER:HB2	1:A:58:SER:OG	2.17	0.43
1:B:291:VAL:HG12	1:B:292:THR:N	2.34	0.43
1:C:26:THR:HG22	1:C:50:ARG:HH12	1.83	0.43
1:C:267:LEU:HB2	1:C:320:TYR:O	2.19	0.43
1:C:293:ASN:OD1	1:C:377:LEU:HA	2.19	0.43
1:A:9:LYS:HB2	1:A:12:GLN:OE1	2.19	0.43
1:A:71:TYR:CD1	3:A:501:012:HD2	2.54	0.43
1:B:266:GLN:HG3	4:B:635:HOH:O	2.19	0.42
1:A:235:ARG:HG2	1:A:235:ARG:HH21	1.82	0.42
1:B:134:GLU:OE1	1:B:142:LYS:HE3	2.19	0.42
1:B:314:THR:O	1:B:315:SER:CB	2.66	0.42
1:C:22:SER:HA	1:C:23:PRO:C	2.39	0.42
1:C:188:LEU:HD23	1:C:355:ALA:CB	2.44	0.42
1:B:51:TYR:CD1	1:B:51:TYR:N	2.88	0.42
1:C:63:LEU:HG	1:C:81:GLY:HA2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:124:ALA:O	1:C:126:ILE:N	2.52	0.42
1:C:249:LYS:HG3	1:C:262:TRP:CE2	2.54	0.42
1:A:134:GLU:HA	1:A:135:PRO:HD3	1.91	0.42
1:B:32:ASP:OD1	1:B:230:GLY:HA3	2.19	0.42
1:A:234:LEU:HB2	1:A:336:VAL:HG13	2.01	0.42
1:A:267:LEU:C	1:A:267:LEU:HD12	2.39	0.42
1:B:92:ASN:OD1	1:B:92:ASN:O	2.38	0.42
1:C:71:TYR:CG	3:C:503:012:HD2	2.55	0.42
1:C:357:SER:HB3	1:C:360:HIS:HB3	2.01	0.42
1:A:224:LYS:O	1:A:330:GLY:HA3	2.20	0.42
1:B:235:ARG:HA	1:B:325:SER:O	2.20	0.42
1:A:234:LEU:HD13	1:A:236:LEU:HG	2.02	0.42
1:A:320:TYR:N	1:A:320:TYR:CD1	2.88	0.42
1:C:61:ARG:HB2	1:C:82:THR:OG1	2.20	0.42
1:C:232:THR:O	1:C:335:ALA:N	2.51	0.42
1:B:123:TYR:CZ	1:B:196:GLU:HG2	2.55	0.42
1:C:67:VAL:HG23	1:C:129:PRO:HG3	2.02	0.42
1:C:294:GLN:HG2	1:C:373:PRO:HB2	2.02	0.42
1:C:258:PRO:O	1:C:260:GLY:N	2.54	0.41
1:A:267:LEU:HB2	1:A:320:TYR:O	2.20	0.41
1:C:28:ASN:O	1:C:29:ILE:HD13	2.19	0.41
1:C:202:ILE:CD1	1:C:288:MET:HE3	2.49	0.41
1:A:14:TYR:CD1	1:A:154:LEU:HD22	2.55	0.41
1:A:70:PRO:HD2	1:A:128:ARG:NH1	2.35	0.41
1:B:-2:PHE:CD1	1:B:-2:PHE:N	2.87	0.41
1:A:19:THR:HA	1:A:25:GLN:O	2.20	0.41
1:B:336:VAL:HG23	1:B:337:ILE:N	2.36	0.41
1:B:364:GLU:OE2	1:C:374:PHE:HB3	2.20	0.41
1:B:372:GLY:HA2	1:B:374:PHE:CE1	2.56	0.41
1:A:294:GLN:N	1:A:379:MET:HE1	2.35	0.41
1:B:35:SER:O	1:B:122:ALA:HB3	2.21	0.41
1:A:76:TRP:HD1	1:A:108:PHE:CE1	2.39	0.41
1:A:157:ALA:HA	4:A:668:HOH:O	2.21	0.41
1:C:335:ALA:O	1:C:339:GLU:HG3	2.21	0.41
1:C:111:ASN:HD22	1:C:111:ASN:C	2.21	0.41
1:A:91:PRO:HD3	1:A:176:ILE:HB	2.03	0.41
1:B:36:SER:OG	1:B:126:ILE:HG13	2.21	0.41
1:B:76:TRP:HB2	1:B:102:ILE:HG23	2.02	0.41
1:A:189:TRP:O	1:A:353:GLY:HA2	2.21	0.41
1:A:218:LYS:NZ	1:A:381:ASP:O	2.45	0.41
1:C:54:ARG:HD2	1:C:60:TYR:CZ	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:39:ALA:HB2	1:C:100:ALA:HB3	2.03	0.40
1:B:270:TRP:O	1:B:317:ASP:HB3	2.21	0.40
1:B:309:VAL:O	1:B:309:VAL:CG2	2.66	0.40
1:C:2:MET:HG2	1:C:90:GLY:HA2	2.04	0.40
1:C:123:TYR:HE1	1:C:199:TYR:CE2	2.40	0.40
1:C:77:GLU:N	1:C:104:GLU:O	2.44	0.40
1:B:42:ALA:O	1:B:51:TYR:HD2	2.04	0.40
1:A:33:THR:HG23	1:A:229:SER:OG	2.21	0.40
1:A:261:PHE:C	1:A:263:LEU:H	2.24	0.40
1:C:78:GLY:HA3	1:C:101:ALA:O	2.22	0.40
1:C:125:GLU:HG2	1:C:197:TRP:CB	2.43	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	373/412 (90%)	341 (91%)	27 (7%)	5 (1%)	12	12
1	B	372/412 (90%)	329 (88%)	35 (9%)	8 (2%)	6	5
1	C	371/412 (90%)	324 (87%)	34 (9%)	13 (4%)	3	2
All	All	1116/1236 (90%)	994 (89%)	96 (9%)	26 (2%)	6	5

All (26) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	223	ASP
1	B	223	ASP
1	C	125	GLU
1	C	223	ASP
1	C	233	ASN
1	B	312	VAL

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Mol	Chain	Res	Type
1	C	72	THR
1	C	238	LYS
1	C	253	SER
1	C	259	ASP
1	B	111	ASN
1	B	313	ALA
1	B	334	GLY
1	C	83	ASP
1	C	217	CYS
1	C	232	THR
1	A	253	SER
1	C	350	LYS
1	A	122	ALA
1	A	157	ALA
1	B	131	ASP
1	B	217	CYS
1	C	-4	GLY
1	A	156	GLY
1	C	346	ASP
1	B	70	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	321/353 (91%)	309 (96%)	12 (4%)	34	48
1	B	319/353 (90%)	310 (97%)	9 (3%)	43	60
1	C	322/353 (91%)	306 (95%)	16 (5%)	24	34
All	All	962/1059 (91%)	925 (96%)	37 (4%)	33	47

All (37) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	111	ASN
1	A	125	GLU

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Mol	Chain	Res	Type
1	A	181	HIS
1	A	197	TRP
1	A	234	LEU
1	A	266	GLN
1	A	317	ASP
1	A	328	SER
1	A	329	THR
1	A	341	PHE
1	A	381	ASP
1	A	386	ILE
1	B	51	TYR
1	B	70	PRO
1	B	111	ASN
1	B	114	ASN
1	B	197	TRP
1	B	234	LEU
1	B	257	PHE
1	B	371	GLU
1	B	386	ILE
1	C	-1	VAL
1	C	38	PHE
1	C	55	GLN
1	C	88	PRO
1	C	111	ASN
1	C	195	ARG
1	C	200	GLU
1	C	234	LEU
1	C	245	VAL
1	C	246	LYS
1	C	310	GLU
1	C	317	ASP
1	C	371	GLU
1	C	377	LEU
1	C	378	ASP
1	C	386	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	28	ASN
1	A	111	ASN
1	A	304	GLN

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Mol	Chain	Res	Type
1	A	326	GLN
1	B	28	ASN
1	B	55	GLN
1	B	73	GLN
1	B	92	ASN
1	B	111	ASN
1	B	304	GLN
1	B	316	GLN
1	C	28	ASN
1	C	55	GLN
1	C	73	GLN
1	C	111	ASN
1	C	181	HIS
1	C	211	GLN
1	C	266	GLN
1	C	271	GLN
1	C	304	GLN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

Of 12 ligands modelled in this entry, 9 are monoatomic - leaving 3 for Mogul analysis.

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	012	B	502	-	42,43,43	1.41	4 (9%)	54,58,58	2.47	7 (12%)
3	012	C	503	-	42,43,43	1.52	6 (14%)	54,58,58	2.45	6 (11%)
3	012	A	501	-	42,43,43	1.42	5 (11%)	54,58,58	2.50	8 (14%)

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	012	B	502	-	-	10/32/44/44	0/4/4/4
3	012	C	503	-	-	9/32/44/44	0/4/4/4
3	012	A	501	-	-	3/32/44/44	0/4/4/4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	503	012	C32-N31	4.23	1.41	1.35
3	B	502	012	C32-N31	3.91	1.40	1.35
3	A	501	012	C32-N31	3.38	1.40	1.35
3	C	503	012	C32-N34	3.17	1.42	1.37
3	A	501	012	C32-N34	3.16	1.42	1.37
3	C	503	012	C36-N34	2.95	1.51	1.46
3	B	502	012	C36-N34	2.95	1.51	1.46
3	B	502	012	C32-N34	2.58	1.41	1.37
3	A	501	012	C24-C25	2.33	1.43	1.39
3	A	501	012	C44-C43	2.15	1.42	1.38
3	C	503	012	C42-C41	2.11	1.42	1.39
3	A	501	012	C36-N34	2.09	1.50	1.46
3	C	503	012	C44-C43	2.06	1.42	1.38
3	C	503	012	C24-C25	2.06	1.43	1.39
3	B	502	012	C42-C43	2.02	1.42	1.38

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	501	012	C30-N31-C32	-10.98	99.65	113.02
3	C	503	012	C30-N31-C32	-10.30	100.47	113.02
3	B	502	012	C30-N31-C32	-9.96	100.89	113.02
3	B	502	012	C35-N34-C32	-9.51	98.98	111.44
3	C	503	012	N31-C32-N34	9.10	117.45	108.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	A	501	012	N31-C32-N34	8.95	117.30	108.33
3	B	502	012	N31-C32-N34	8.46	116.81	108.33
3	C	503	012	C35-N34-C32	-8.42	100.41	111.44
3	A	501	012	C35-N34-C32	-8.30	100.56	111.44
3	B	502	012	C41-C36-N34	4.86	120.94	113.13
3	C	503	012	C41-C36-N34	4.34	120.10	113.13
3	A	501	012	C41-C36-N34	4.14	119.78	113.13
3	A	501	012	O33-C32-N31	-3.68	119.94	126.90
3	C	503	012	O33-C32-N31	-3.63	120.03	126.90
3	B	502	012	O33-C32-N31	-3.47	120.34	126.90
3	A	501	012	C36-N34-C35	-2.71	117.61	121.75
3	C	503	012	C36-N34-C35	-2.38	118.11	121.75
3	A	501	012	O-C-N	2.31	127.20	122.93
3	B	502	012	C36-N34-C35	-2.20	118.38	121.75
3	A	501	012	C30-C-N	-2.07	112.15	116.70
3	B	502	012	CB-CA-N	-2.06	107.07	110.07

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	502	012	OG-C1-C2-N2
3	C	503	012	OG-C1-C2-N2
3	B	502	012	C24-C25-N27-C28
3	B	502	012	C24-C25-N27-C29
3	B	502	012	C26-C25-N27-C28
3	B	502	012	C26-C25-N27-C29
3	C	503	012	C24-C25-N27-C29
3	A	501	012	C44-C43-O47-C48
3	C	503	012	C26-C25-N27-C28
3	C	503	012	C42-C43-O47-C48
3	A	501	012	C42-C43-O47-C48
3	C	503	012	C44-C43-O47-C48
3	B	502	012	C42-C43-O47-C48
3	B	502	012	C44-C43-O47-C48
3	C	503	012	C24-C25-N27-C28
3	C	503	012	C26-C25-N27-C29
3	B	502	012	CA-C1-C2-N2
3	C	503	012	CA-C1-C2-N2
3	B	502	012	C41-C36-N34-C35
3	B	502	012	O-C-C30-N31
3	C	503	012	C41-C36-N34-C35

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Mol	Chain	Res	Type	Atoms
3	A	501	012	C41-C36-N34-C35

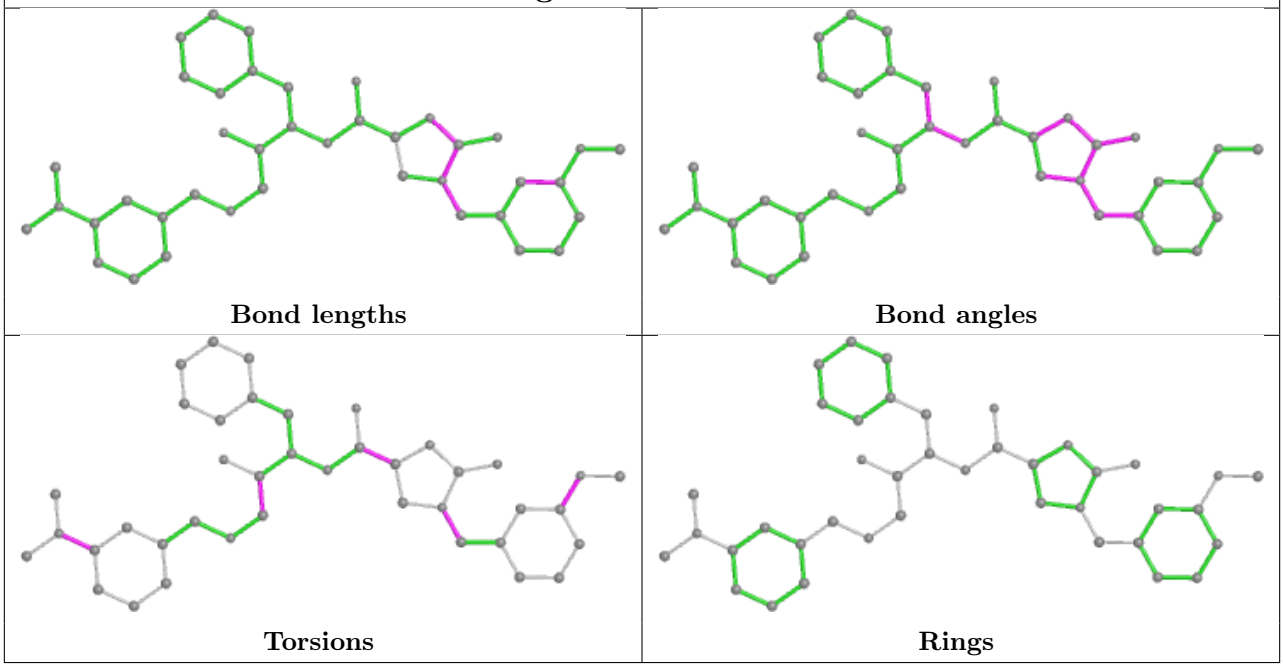
There are no ring outliers.

3 monomers are involved in 12 short contacts:

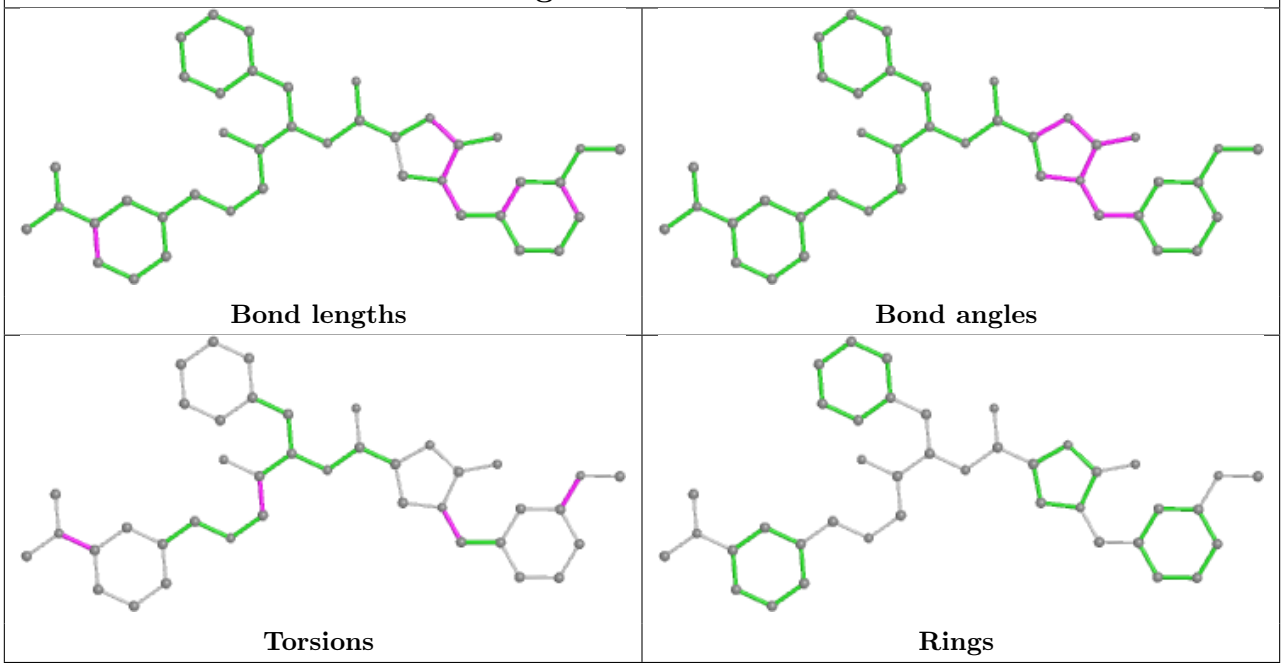
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	012	1	0
3	C	503	012	6	0
3	A	501	012	5	0

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 then 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.

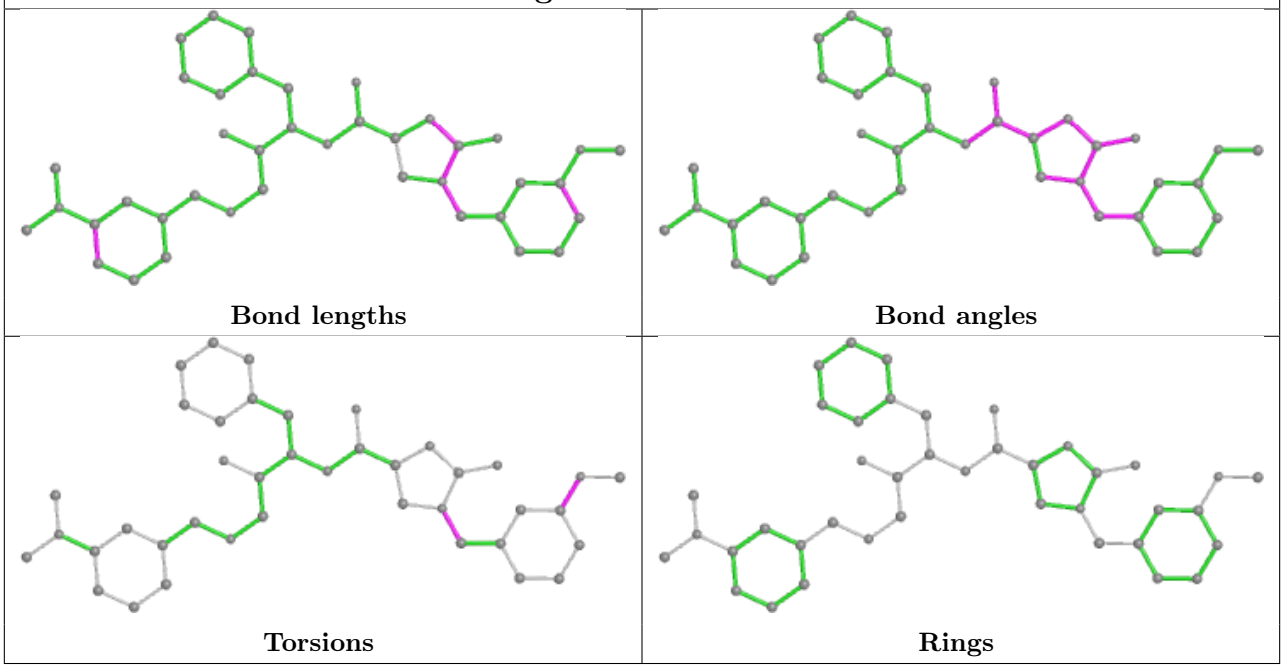
Ligand 012 B 502



Ligand 012 C 503



Ligand 012 A 501



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 (i)

6.1 Protein, DNA and RNA chains (i)

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	379/412 (91%)	0.21	14 (3%)	41	48	18, 35, 61, 91	0
1	B	376/412 (91%)	0.43	27 (7%)	15	20	22, 40, 68, 89	0
1	C	377/412 (91%)	0.58	31 (8%)	11	15	25, 50, 74, 105	0
All	All	1132/1236 (91%)	0.41	72 (6%)	19	25	18, 41, 69, 105	0

All (72) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	311	ASP	5.5
1	B	312	VAL	5.1
1	B	145	HIS	4.1
1	A	168	ALA	4.1
1	B	113	SER	4.0
1	B	386	ILE	3.8
1	A	316	GLN	3.8
1	C	73	GLN	3.6
1	C	317	ASP	3.5
1	B	384	TYR	3.4
1	C	64	ARG	3.3
1	C	384	TYR	3.3
1	C	310	GLU	3.2
1	A	386	ILE	3.1
1	B	112	GLY	3.1
1	B	120	GLY	3.1
1	B	119	LEU	3.0
1	C	315	SER	3.0
1	C	314	THR	3.0
1	B	121	LEU	2.9
1	B	169	SER	2.9
1	C	107	LYS	2.8
1	C	263	LEU	2.8

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Mol	Chain	Res	Type	RSRZ
1	C	119	LEU	2.8
1	C	145	HIS	2.7
1	B	260	GLY	2.7
1	C	386	ILE	2.7
1	C	378	ASP	2.6
1	B	316	GLN	2.6
1	B	222	TYR	2.6
1	A	158	GLY	2.6
1	C	47	PHE	2.5
1	B	31	VAL	2.5
1	A	157	ALA	2.5
1	B	47	PHE	2.5
1	C	33	THR	2.5
1	C	316	GLN	2.5
1	C	337	ILE	2.4
1	B	122	ALA	2.4
1	B	199	TYR	2.4
1	C	293	ASN	2.4
1	A	107	LYS	2.4
1	C	313	ALA	2.3
1	B	33	THR	2.3
1	C	121	LEU	2.3
1	A	257	PHE	2.3
1	B	334	GLY	2.3
1	B	359	CYS	2.3
1	B	377	LEU	2.3
1	A	310	GLU	2.3
1	C	78	GLY	2.2
1	B	337	ILE	2.2
1	C	118	ILE	2.2
1	B	338	MET	2.2
1	A	271	GLN	2.2
1	B	272	ALA	2.1
1	C	272	ALA	2.1
1	C	229	SER	2.1
1	C	68	TYR	2.1
1	C	46	PRO	2.1
1	A	145	HIS	2.1
1	C	271	GLN	2.1
1	B	110	ILE	2.1
1	A	309	VAL	2.1
1	C	309	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	C	38	PHE	2.1
1	A	317	ASP	2.0
1	A	377	LEU	2.0
1	C	242	GLU	2.0
1	C	227	VAL	2.0
1	A	285	LEU	2.0
1	B	310	GLU	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

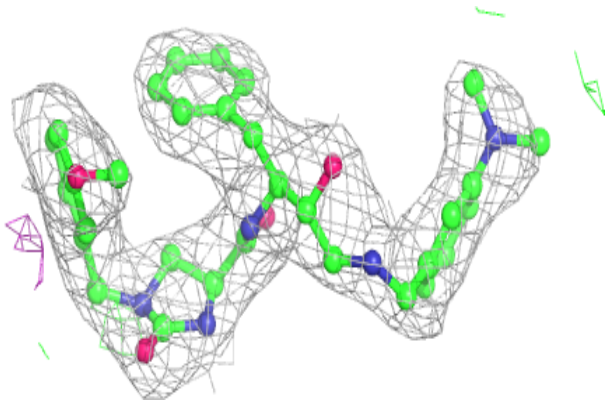
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

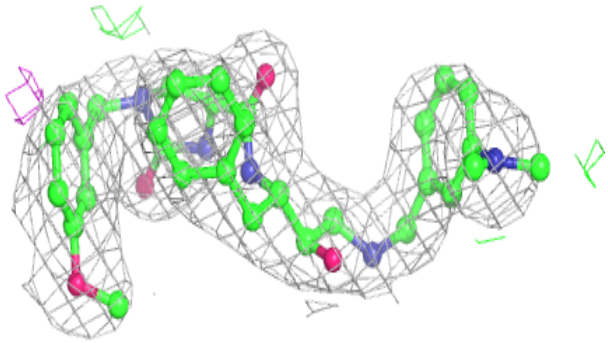
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
3	012	B	502	40/40	0.91	0.19	36,43,50,50	0
3	012	C	503	40/40	0.91	0.19	40,45,58,58	0
3	012	A	501	40/40	0.93	0.15	30,37,45,45	0
2	CL	C	609	1/1	0.96	0.06	43,43,43,43	0
2	CL	A	608	1/1	0.96	0.07	39,39,39,39	0
2	CL	B	602	1/1	0.97	0.17	23,23,23,23	0
2	CL	C	604	1/1	0.98	0.18	32,32,32,32	0
2	CL	A	607	1/1	0.98	0.09	34,34,34,34	0
2	CL	A	601	1/1	0.98	0.27	12,12,12,12	0
2	CL	A	605	1/1	0.98	0.21	32,32,32,32	0
2	CL	B	606	1/1	0.98	0.07	36,36,36,36	0
2	CL	A	603	1/1	0.99	0.16	21,21,21,21	0

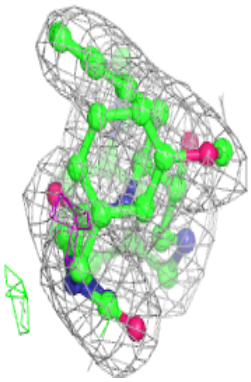
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around 012 B 502:

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

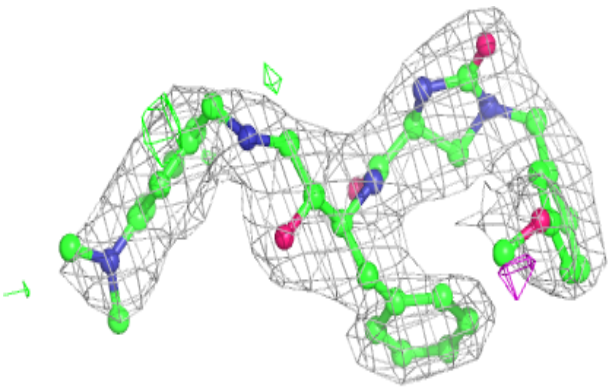


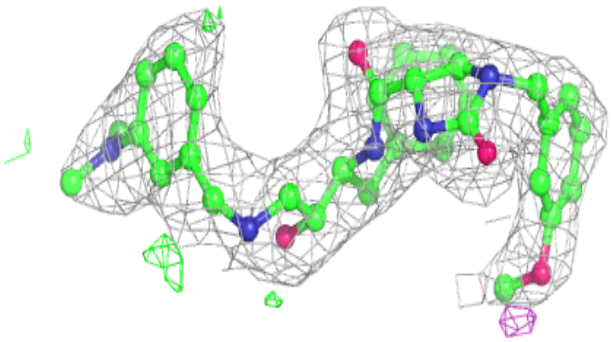


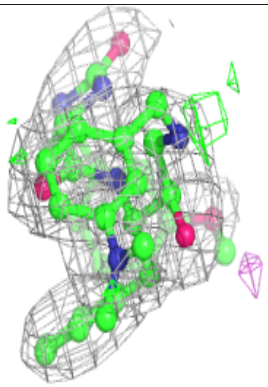


Electron density around 012 C 503:

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

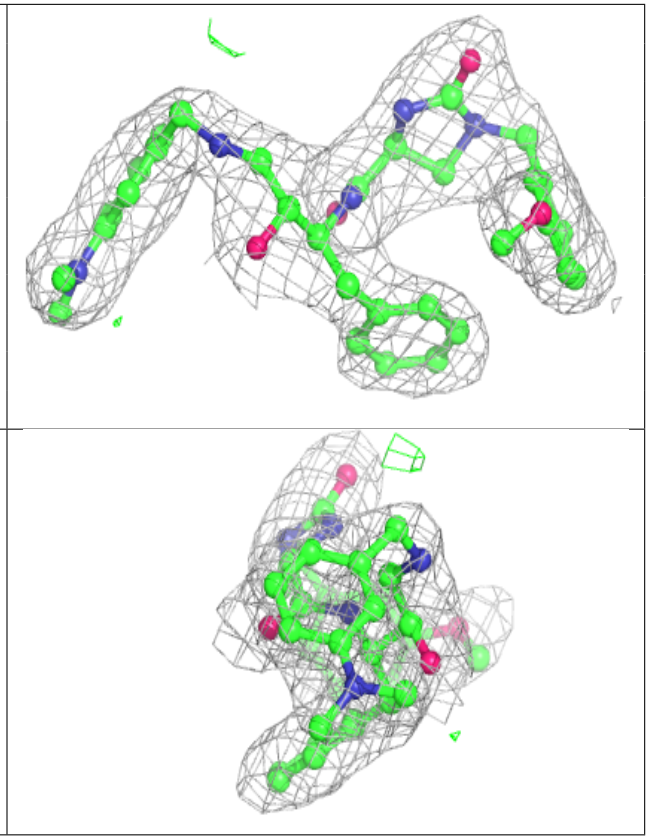






Electron density around 012 A 501:

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



6.5 Other polymers (i)

There are no such residues in this entry.