



Full wwPDB X-ray Structure Validation Report ⓘ

May 16, 2020 – 02:56 am BST

PDB ID : 2AOA
Title : Crystal structures of a high-affinity macrocyclic peptide mimetic in complex with the Grb2 SH2 domain
Authors : Phan, J.; Shi, Z.D.; Burke, T.R.; Waugh, D.S.
Deposited on : 2005-08-12
Resolution : 1.99 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 following versions of software and data (see [references ⓘ](#)) 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 : 2.11
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) : 2.11

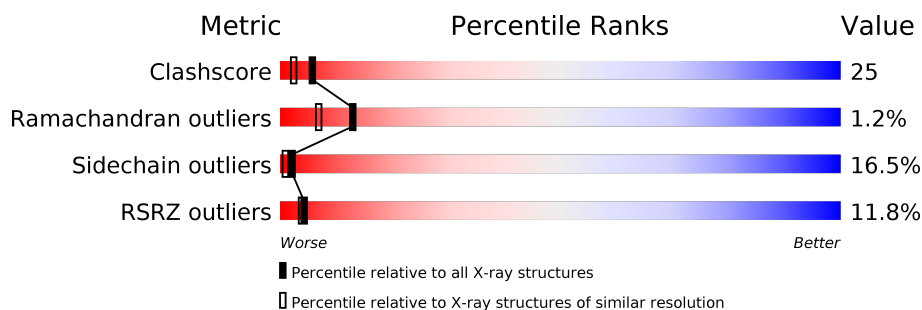
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.99 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	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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 on 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	99	<div> <div>11%</div> <div>41%</div> <div>33%</div> <div>16%</div> <div>6%</div> </div>
1	B	99	<div> <div>9%</div> <div>36%</div> <div>35%</div> <div>6%</div> <div>22%</div> </div>

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
2	S1S	A	201	X	-	-	-
2	S1S	A	401	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	S1S	B	301	X	-	-	-

2 Entry composition [i](#)

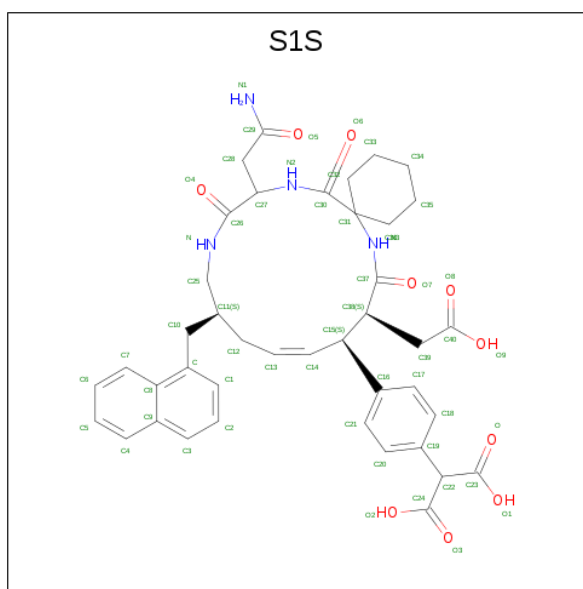
There are 4 unique types of molecules in this entry. The entry contains 1592 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Growth factor receptor-bound protein 2.

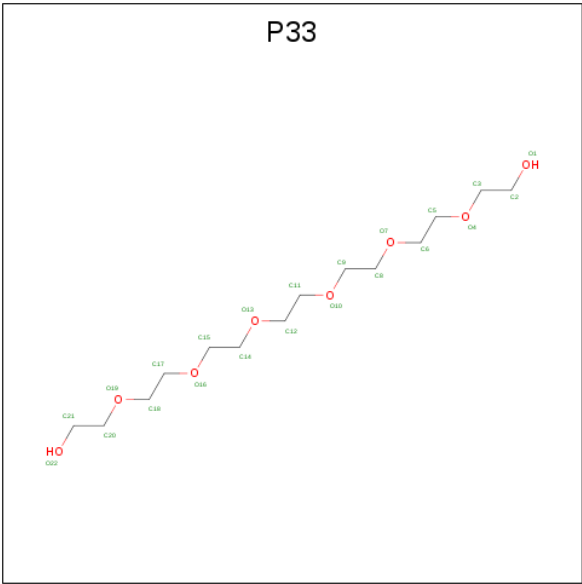
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
1	A	93	Total	C	N	O	0	0	0
			712	458	125	129			
1	B	77	Total	C	N	O	0	0	0
			590	379	103	108			

- Molecule 2 is 2-(4-((9S,10S,14S,Z)-18-(2-AMINO-2-OXOETHYL)-9-(CARBOXYMETHYL)-14-(NAPHTHALEN-1-YLMETHYL)-8,17,20-TRIOXO-7,16,19-TRIAZASPIRO[5.14]ICOS-11-EN-10-YL)PHENYL)MALONIC ACID (three-letter code: S1S) (formula: C₄₁H₄₆N₄O₁₀).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			55	41	4	10		
2	A	1	Total	C	N	O	0	0
			55	41	4	10		
2	B	1	Total	C	N	O	0	0
			55	41	4	10		

- Molecule 3 is 3,6,9,12,15,18-HEXAOSAICOSANE-1,20-DIOL (three-letter code: P33) (formula: C₁₄H₃₀O₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			22	14	8		

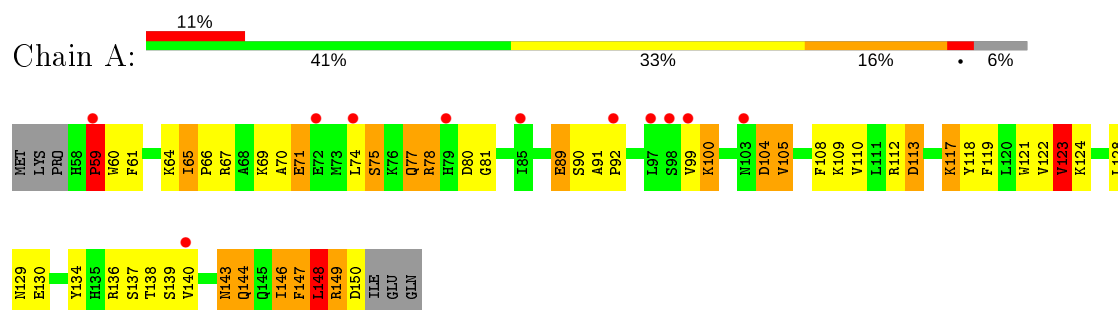
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	67	Total	O	0	0
			67	67		
4	B	36	Total	O	0	0
			36	36		

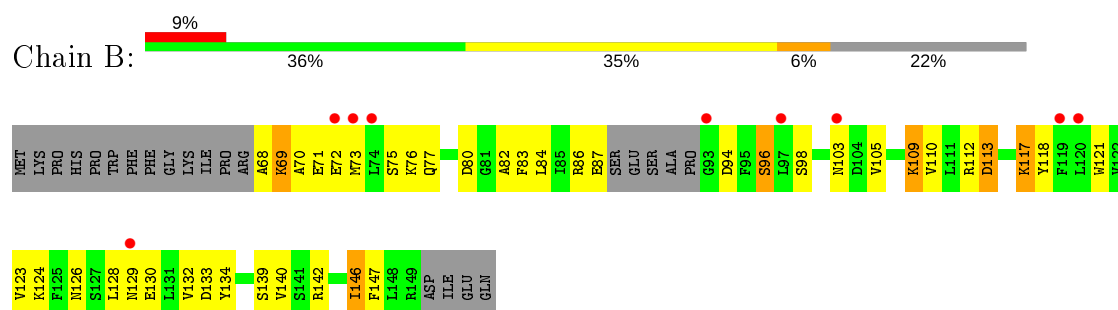
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA 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: Growth factor receptor-bound protein 2



- Molecule 1: Growth factor receptor-bound protein 2



4 Data and refinement statistics

Property	Value	Source
Space group	F 2 2 2	Depositor
Cell constants a, b, c, α , β , γ	88.17Å 102.66Å 107.24Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	56.80 – 1.99 19.66 – 1.99	Depositor EDS
% Data completeness (in resolution range)	94.0 (56.80-1.99) 89.0 (19.66-1.99)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.07 (at 1.99Å)	Xtriage
Refinement program	REFMAC 5.1.24	Depositor
R, R_{free}	0.246 , 0.307 0.253 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	37.3	Xtriage
Anisotropy	0.230	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.40 , 84.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.032 for -h,l,k	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	1592	wwPDB-VP
Average B, all atoms (Å ²)	45.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.26% 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: S1S, P33

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	2.18	27/730 (3.7%)	1.68	16/987 (1.6%)
1	B	2.05	11/602 (1.8%)	1.63	7/812 (0.9%)
All	All	2.12	38/1332 (2.9%)	1.66	23/1799 (1.3%)

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	A	0	1

All (38) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	123	VAL	CB-CG1	-9.05	1.33	1.52
1	A	149	ARG	CA-CB	-8.87	1.34	1.53
1	B	130	GLU	CD-OE1	8.41	1.34	1.25
1	A	112	ARG	NE-CZ	-8.29	1.22	1.33
1	A	134	TYR	CB-CG	-8.22	1.39	1.51
1	A	129	ASN	CA-CB	8.04	1.74	1.53
1	A	134	TYR	CE1-CZ	-7.82	1.28	1.38
1	B	139	SER	N-CA	-7.64	1.31	1.46
1	A	147	PHE	CA-CB	7.39	1.70	1.53
1	A	150	ASP	CA-CB	6.95	1.69	1.53
1	A	146	ILE	CA-CB	6.92	1.70	1.54
1	A	130	GLU	CD-OE1	6.87	1.33	1.25
1	A	108	PHE	CD1-CE1	-6.81	1.25	1.39
1	A	61	PHE	CE1-CZ	-6.74	1.24	1.37
1	B	110	VAL	CB-CG1	-6.42	1.39	1.52
1	A	139	SER	CA-CB	-6.38	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	60	TRP	CE3-CZ3	6.36	1.49	1.38
1	A	70	ALA	CA-CB	6.24	1.65	1.52
1	B	110	VAL	CB-CG2	6.06	1.65	1.52
1	B	130	GLU	CG-CD	5.99	1.60	1.51
1	A	89	GLU	CD-OE2	5.89	1.32	1.25
1	B	129	ASN	C-O	-5.84	1.12	1.23
1	A	119	PHE	CE1-CZ	5.83	1.48	1.37
1	A	139	SER	CB-OG	5.72	1.49	1.42
1	A	71	GLU	CD-OE1	-5.67	1.19	1.25
1	A	148	LEU	N-CA	5.56	1.57	1.46
1	A	59	PRO	CB-CG	5.50	1.77	1.50
1	B	139	SER	CB-OG	5.50	1.49	1.42
1	A	99	VAL	CB-CG1	-5.45	1.41	1.52
1	A	61	PHE	CG-CD1	-5.28	1.30	1.38
1	B	140	VAL	CB-CG1	-5.27	1.41	1.52
1	A	121	TRP	CB-CG	-5.18	1.41	1.50
1	B	112	ARG	N-CA	-5.17	1.36	1.46
1	A	134	TYR	CD1-CE1	-5.11	1.31	1.39
1	A	118	TYR	CD1-CE1	-5.11	1.31	1.39
1	B	121	TRP	CB-CG	5.10	1.59	1.50
1	A	149	ARG	CA-C	5.09	1.66	1.52
1	B	118	TYR	CD1-CE1	5.07	1.47	1.39

All (23) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	112	ARG	NE-CZ-NH1	-10.12	115.24	120.30
1	A	147	PHE	N-CA-C	9.15	135.71	111.00
1	B	113	ASP	CB-CG-OD1	9.15	126.54	118.30
1	A	67	ARG	NE-CZ-NH1	9.12	124.86	120.30
1	A	149	ARG	N-CA-C	9.12	135.61	111.00
1	A	112	ARG	NE-CZ-NH2	9.11	124.86	120.30
1	B	80	ASP	CB-CG-OD2	8.60	126.04	118.30
1	A	113	ASP	CB-CG-OD2	8.21	125.69	118.30
1	A	147	PHE	O-C-N	-7.26	111.09	122.70
1	A	100	LYS	CD-CE-NZ	7.01	127.83	111.70
1	B	69	LYS	CB-CA-C	6.85	124.10	110.40
1	A	112	ARG	CB-CA-C	-6.83	96.75	110.40
1	B	146	ILE	CG1-CB-CG2	-6.69	96.69	111.40
1	B	86	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	A	136	ARG	NE-CZ-NH2	-6.43	117.09	120.30
1	A	80	ASP	CB-CG-OD2	6.39	124.06	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	80	ASP	CB-CG-OD1	-6.30	112.63	118.30
1	A	104	ASP	CB-CG-OD2	6.16	123.84	118.30
1	A	67	ARG	NE-CZ-NH2	-5.77	117.41	120.30
1	B	132	VAL	CA-CB-CG1	5.71	119.47	110.90
1	B	68	ALA	N-CA-C	-5.63	95.81	111.00
1	A	136	ARG	NE-CZ-NH1	5.43	123.01	120.30
1	A	74	LEU	CB-CG-CD1	5.00	119.50	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	148	LEU	Peptide

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	712	0	655	52	0
1	B	590	0	539	37	0
2	A	110	0	80	10	0
2	B	55	0	41	3	0
3	B	22	0	30	3	0
4	A	67	0	0	2	0
4	B	36	0	0	5	0
All	All	1592	0	1345	72	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 25.

All (72) 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:117:LYS:NZ	1:B:124:LYS:HB2	1.10	1.39
1:A:59:PRO:CB	1:A:59:PRO:CG	1.77	1.38

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:117:LYS:HZ3	1:B:124:LYS:CB	1.51	1.23
1:A:117:LYS:NZ	1:B:124:LYS:CB	2.04	1.19
1:A:117:LYS:HZ2	2:A:401:S1S:H20	0.98	1.08
1:B:77:GLN:O	4:B:529:HOH:O	1.81	0.98
1:A:117:LYS:NZ	2:A:401:S1S:H20	1.81	0.95
3:B:501:P33:H141	4:B:517:HOH:O	1.66	0.93
1:A:148:LEU:O	4:A:446:HOH:O	1.87	0.92
1:A:123:VAL:HG11	1:B:123:VAL:HG21	1.53	0.91
1:A:117:LYS:HZ2	2:A:401:S1S:C20	1.83	0.91
1:A:117:LYS:HZ1	1:B:124:LYS:HB2	1.07	0.89
1:A:89:GLU:OE2	2:A:201:S1S:H22	1.78	0.83
1:A:117:LYS:CE	1:B:124:LYS:HB2	2.13	0.78
1:A:123:VAL:HG11	1:B:123:VAL:CG2	2.15	0.77
1:A:138:THR:OG1	4:A:431:HOH:O	2.04	0.75
1:A:65:ILE:HD12	1:A:66:PRO:HD2	1.67	0.75
1:A:65:ILE:HD11	1:A:69:LYS:CB	2.18	0.74
1:B:76:LYS:O	4:B:525:HOH:O	2.07	0.72
1:A:117:LYS:HZ3	1:B:124:LYS:HB2	0.89	0.72
1:B:70:ALA:HB1	1:B:84:LEU:HD21	1.71	0.72
1:A:77:GLN:O	1:A:100:LYS:HE2	1.93	0.69
1:A:78:ARG:O	1:A:100:LYS:HE3	1.92	0.68
1:B:69:LYS:O	1:B:72:GLU:N	2.27	0.68
1:B:87:GLU:OE1	1:B:87:GLU:N	2.28	0.67
1:B:109:LYS:CE	2:B:301:S1S:O3	2.43	0.66
1:A:65:ILE:HD12	1:A:66:PRO:CD	2.25	0.66
1:A:149:ARG:CB	1:B:82:ALA:HA	2.26	0.65
3:B:501:P33:H172	4:B:517:HOH:O	1.95	0.65
1:B:109:LYS:NZ	2:B:301:S1S:O3	2.32	0.63
1:A:117:LYS:NZ	2:A:401:S1S:C20	2.52	0.63
1:A:123:VAL:CG1	1:B:123:VAL:CG2	2.77	0.62
1:B:69:LYS:O	1:B:73:MET:N	2.28	0.62
1:A:117:LYS:HZ3	1:B:124:LYS:CG	2.13	0.60
1:B:94:ASP:OD2	1:B:109:LYS:NZ	2.36	0.59
1:A:89:GLU:HG2	2:A:201:S1S:O2	2.03	0.59
1:A:122:VAL:HG12	1:A:124:LYS:HG3	1.86	0.57
1:A:71:GLU:HG2	1:A:105:VAL:CG1	2.36	0.56
1:A:117:LYS:HZ3	1:B:124:LYS:CD	2.17	0.56
1:A:117:LYS:HZ1	1:B:124:LYS:CB	1.95	0.55
1:A:71:GLU:HG2	1:A:105:VAL:HG11	1.90	0.53
1:A:149:ARG:CB	1:B:83:PHE:HD2	2.20	0.53
1:A:149:ARG:CB	1:B:83:PHE:CD2	2.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:147:PHE:O	1:A:148:LEU:CB	2.56	0.53
1:A:77:GLN:O	1:A:100:LYS:CE	2.57	0.52
1:A:110:VAL:HG11	1:B:128:LEU:HD11	1.94	0.50
1:B:71:GLU:HG2	1:B:105:VAL:HB	1.93	0.50
1:A:109:LYS:HG3	2:A:201:S1S:H14	1.95	0.49
1:B:109:LYS:HE3	2:B:301:S1S:O3	2.13	0.48
1:A:143:ASN:ND2	1:A:144:GLN:HG2	2.30	0.47
1:A:91:ALA:HA	1:A:92:PRO:HD3	1.79	0.47
1:B:117:LYS:NZ	4:B:532:HOH:O	2.46	0.46
1:B:69:LYS:O	1:B:70:ALA:C	2.54	0.45
3:B:501:P33:H172	3:B:501:P33:H141	1.71	0.45
1:A:90:SER:OG	2:A:201:S1S:O2	2.24	0.45
1:B:133:ASP:O	1:B:134:TYR:C	2.50	0.45
1:A:65:ILE:CD1	1:A:66:PRO:HD2	2.42	0.44
1:A:81:GLY:HA3	1:B:147:PHE:O	2.18	0.44
1:A:117:LYS:NZ	1:B:124:LYS:CD	2.81	0.43
1:A:146:ILE:HD13	1:A:146:ILE:HG21	1.67	0.43
1:A:65:ILE:CD1	1:A:69:LYS:CB	2.95	0.42
1:A:124:LYS:NZ	1:B:113:ASP:OD2	2.48	0.42
1:A:123:VAL:CG1	1:B:123:VAL:HB	2.50	0.42
1:A:143:ASN:HD22	1:A:144:GLN:HG2	1.84	0.42
1:A:113:ASP:OD2	2:A:401:S1S:O	2.38	0.41
1:B:96:SER:OG	1:B:109:LYS:HE3	2.20	0.41
1:A:143:ASN:ND2	1:A:143:ASN:H	2.19	0.41
1:B:146:ILE:HD13	1:B:146:ILE:HG21	1.54	0.41
1:A:71:GLU:O	1:A:75:SER:HB2	2.21	0.41
2:A:401:S1S:HC7	2:A:401:S1S:H102	1.88	0.41
1:A:149:ARG:CB	1:B:83:PHE:H	2.33	0.40
1:A:123:VAL:HG22	1:A:123:VAL:O	2.22	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	91/99 (92%)	83 (91%)	7 (8%)	1 (1%)	14	8
1	B	73/99 (74%)	70 (96%)	2 (3%)	1 (1%)	11	5
All	All	164/198 (83%)	153 (93%)	9 (6%)	2 (1%)	13	7

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	78	ARG
1	B	75	SER

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	69/88 (78%)	55 (80%)	14 (20%)	1	0
1	B	58/88 (66%)	51 (88%)	7 (12%)	5	2
All	All	127/176 (72%)	106 (84%)	21 (16%)	2	1

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	59	PRO
1	A	64	LYS
1	A	65	ILE
1	A	75	SER
1	A	77	GLN
1	A	104	ASP
1	A	105	VAL
1	A	117	LYS
1	A	123	VAL
1	A	128	LEU
1	A	137	SER
1	A	140	VAL
1	A	143	ASN
1	A	144	GLN

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Mol	Chain	Res	Type
1	B	96	SER
1	B	98	SER
1	B	103	ASN
1	B	109	LYS
1	B	117	LYS
1	B	126	ASN
1	B	142	ARG

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	77	GLN
1	A	106	GLN
1	A	143	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 carbohydrates in this entry.

5.6 Ligand geometry [i](#)

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	P33	B	501	-	21,21,21	1.04	1 (4%)	20,20,20	0.99	1 (5%)
2	S1S	B	301	-	48,59,59	2.46	19 (39%)	63,83,83	3.65	26 (41%)
2	S1S	A	201	-	48,59,59	1.87	14 (29%)	63,83,83	4.05	32 (50%)
2	S1S	A	401	-	48,59,59	1.99	9 (18%)	63,83,83	4.02	27 (42%)

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	P33	B	501	-	-	9/19/19/19	-
2	S1S	B	301	-	1/1/13/18	7/56/76/76	0/4/5/5
2	S1S	A	201	-	2/2/13/18	15/56/76/76	0/4/5/5
2	S1S	A	401	-	2/2/13/18	13/56/76/76	0/4/5/5

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	S1S	C36-C31	-6.38	1.45	1.54
2	B	301	S1S	C28-C29	-6.09	1.35	1.51
2	A	401	S1S	C31-N3	5.97	1.57	1.46
2	A	401	S1S	C16-C15	-5.95	1.45	1.52
2	B	301	S1S	C28-C27	-4.92	1.43	1.53
2	A	201	S1S	O6-C30	-4.67	1.14	1.22
2	B	301	S1S	C20-C19	4.44	1.46	1.39
2	A	201	S1S	C28-C29	4.14	1.62	1.51
2	B	301	S1S	C25-N	3.97	1.57	1.46
2	B	301	S1S	C36-C35	3.91	1.62	1.52
2	B	301	S1S	C-C8	3.87	1.51	1.42
2	A	201	S1S	C6-C7	3.85	1.45	1.36
2	A	401	S1S	O6-C30	3.39	1.28	1.22
2	A	201	S1S	C27-C26	-3.32	1.44	1.52
2	B	301	S1S	C38-C37	-3.30	1.46	1.51
2	B	301	S1S	C2-C1	3.23	1.45	1.38
2	A	201	S1S	C-C8	3.14	1.49	1.42
2	B	301	S1S	C30-N2	-3.10	1.27	1.34
2	A	401	S1S	C1-C	3.09	1.43	1.37
2	A	401	S1S	C12-C13	3.08	1.59	1.50
2	A	201	S1S	C31-C30	3.01	1.60	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	S1S	C7-C8	2.93	1.48	1.42
2	B	301	S1S	C6-C7	2.86	1.43	1.36
2	A	401	S1S	C28-C27	2.85	1.59	1.53
2	A	201	S1S	C16-C15	-2.79	1.49	1.52
2	B	301	S1S	C32-C31	2.79	1.57	1.54
2	A	201	S1S	C8-C9	-2.76	1.37	1.43
2	A	201	S1S	C18-C17	-2.70	1.33	1.38
2	B	301	S1S	C4-C9	2.52	1.48	1.41
2	B	301	S1S	C31-C30	-2.47	1.48	1.53
2	A	201	S1S	C19-C22	-2.46	1.49	1.53
2	A	201	S1S	C38-C37	2.38	1.55	1.51
2	B	301	S1S	C16-C15	-2.31	1.49	1.52
2	B	301	S1S	C39-C38	2.27	1.57	1.54
2	B	301	S1S	C27-C26	2.22	1.58	1.52
3	B	501	P33	O16-C17	2.20	1.51	1.42
2	B	301	S1S	O6-C30	-2.12	1.19	1.22
2	A	201	S1S	C12-C13	2.07	1.56	1.50
2	A	401	S1S	C3-C9	-2.06	1.37	1.41
2	A	201	S1S	C32-C33	2.04	1.57	1.52
2	A	401	S1S	C15-C14	2.03	1.57	1.51
2	A	401	S1S	C27-C26	-2.03	1.47	1.52
2	A	201	S1S	O5-C29	2.01	1.30	1.24

All (86) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	S1S	O7-C37-C38	-14.15	104.68	121.73
2	A	201	S1S	C39-C38-C15	12.66	130.48	110.15
2	A	401	S1S	C38-C37-N3	12.59	133.47	116.25
2	B	301	S1S	C38-C37-N3	12.31	133.09	116.25
2	A	201	S1S	C27-C28-C29	-11.97	88.44	112.24
2	A	201	S1S	O7-C37-C38	-10.85	108.66	121.73
2	A	401	S1S	C28-C27-N2	9.80	129.79	110.60
2	B	301	S1S	O7-C37-C38	-9.30	110.52	121.73
2	A	201	S1S	C28-C27-N2	8.86	127.96	110.60
2	B	301	S1S	C27-N2-C30	8.83	138.37	121.50
2	A	201	S1S	C27-N2-C30	8.80	138.33	121.50
2	B	301	S1S	C39-C38-C15	8.06	123.09	110.15
2	A	401	S1S	C39-C38-C15	7.99	122.97	110.15
2	B	301	S1S	C32-C31-N3	-7.79	94.72	109.59
2	B	301	S1S	C27-C28-C29	-7.55	97.23	112.24
2	B	301	S1S	C11-C25-N	-7.50	98.60	112.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	401	S1S	C33-C32-C31	-7.31	101.53	112.41
2	A	201	S1S	C38-C37-N3	6.95	125.75	116.25
2	A	401	S1S	C17-C18-C19	6.67	127.91	121.20
2	A	401	S1S	C36-C31-C32	6.43	117.46	109.30
2	A	401	S1S	C32-C31-N3	-6.40	97.37	109.59
2	B	301	S1S	C36-C31-C32	6.37	117.38	109.30
2	B	301	S1S	C26-C27-N2	6.20	128.04	111.16
2	A	201	S1S	C20-C21-C16	-6.13	115.03	121.20
2	A	401	S1S	C35-C36-C31	-5.86	103.69	112.41
2	A	401	S1S	C25-N-C26	-5.38	112.39	122.67
2	A	201	S1S	C25-N-C26	-5.38	112.40	122.67
2	A	201	S1S	C12-C11-C10	5.29	117.72	110.75
2	A	401	S1S	C20-C19-C18	-5.14	111.88	118.29
2	B	301	S1S	C21-C20-C19	-5.06	116.11	121.20
2	A	401	S1S	C27-N2-C30	5.02	131.09	121.50
2	A	201	S1S	C20-C19-C18	4.89	124.39	118.29
2	A	201	S1S	C17-C18-C19	-4.85	116.32	121.20
2	A	401	S1S	C7-C8-C9	4.81	124.11	117.89
2	A	201	S1S	C31-N3-C37	4.78	130.21	122.13
2	B	301	S1S	C27-C26-N	-4.71	107.05	116.54
2	A	401	S1S	O6-C30-C31	4.55	127.88	121.00
2	A	201	S1S	C16-C15-C14	-4.32	100.39	110.15
2	A	201	S1S	C36-C35-C34	-4.29	104.72	111.37
2	A	401	S1S	C20-C21-C16	4.23	125.45	121.20
2	A	201	S1S	C10-C-C8	4.22	127.42	120.76
2	A	201	S1S	C21-C16-C17	4.01	123.29	118.29
2	B	301	S1S	C35-C36-C31	4.00	118.37	112.41
2	A	401	S1S	C3-C9-C8	3.80	124.12	119.12
2	A	401	S1S	C31-C30-N2	-3.68	110.09	116.58
2	A	201	S1S	O5-C29-N1	-3.63	112.60	122.50
2	A	201	S1S	C15-C14-C13	3.50	133.88	126.01
2	A	201	S1S	C28-C27-C26	3.44	118.52	110.42
2	B	301	S1S	C12-C11-C10	-3.43	106.24	110.75
2	B	301	S1S	O4-C26-C27	3.36	127.53	120.45
2	B	301	S1S	O7-C37-N3	-3.32	116.05	123.14
2	A	201	S1S	O5-C29-C28	3.27	127.74	120.87
2	A	401	S1S	C30-C31-N3	-3.26	104.29	110.06
2	B	301	S1S	C31-N3-C37	3.16	127.48	122.13
2	A	201	S1S	C36-C31-C30	-3.14	100.55	108.96
2	A	401	S1S	C32-C31-C30	3.14	117.35	108.96
2	A	201	S1S	C4-C9-C3	-3.12	115.91	123.19
2	B	301	S1S	C20-C21-C16	3.06	124.28	121.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	201	S1S	C20-C19-C22	-3.05	114.32	120.98
2	A	201	S1S	C-C10-C11	-3.04	107.29	114.34
2	A	401	S1S	C20-C19-C22	3.04	127.62	120.98
2	B	301	S1S	C28-C27-N2	2.98	116.44	110.60
2	A	201	S1S	C17-C16-C15	-2.96	116.55	120.93
2	A	401	S1S	C21-C16-C17	-2.94	114.62	118.29
2	A	201	S1S	C10-C-C1	-2.83	115.04	119.86
2	A	201	S1S	C31-C30-N2	-2.78	111.68	116.58
2	A	401	S1S	C26-C27-N2	2.76	118.67	111.16
2	A	201	S1S	C4-C9-C8	2.71	122.69	119.12
2	A	401	S1S	C6-C7-C8	-2.66	117.20	120.89
2	A	201	S1S	C32-C31-C30	2.58	115.85	108.96
2	B	301	S1S	C33-C32-C31	2.58	116.24	112.41
3	B	501	P33	O13-C12-C11	-2.55	98.91	110.39
2	B	301	S1S	C6-C5-C4	2.53	123.98	120.44
2	B	301	S1S	C6-C7-C8	-2.51	117.42	120.89
2	B	301	S1S	C18-C17-C16	-2.48	118.70	121.20
2	A	201	S1S	C35-C36-C31	2.39	115.96	112.41
2	B	301	S1S	C18-C19-C22	-2.37	115.79	120.98
2	B	301	S1S	C36-C31-C30	2.37	115.30	108.96
2	B	301	S1S	C30-C31-N3	-2.30	105.98	110.06
2	A	201	S1S	C3-C2-C1	2.30	124.65	120.99
2	A	401	S1S	C31-N3-C37	2.28	125.99	122.13
2	A	401	S1S	C-C8-C9	-2.27	116.17	118.98
2	A	401	S1S	C27-C28-C29	2.24	116.69	112.24
2	A	401	S1S	C4-C9-C3	-2.09	118.31	123.19
2	A	201	S1S	C2-C3-C9	-2.08	117.19	120.44
2	B	301	S1S	C20-C19-C22	2.00	125.36	120.98

All (5) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	B	301	S1S	C27
2	A	201	S1S	C27
2	A	201	S1S	C38
2	A	401	S1S	C38
2	A	401	S1S	C27

All (44) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	301	S1S	N2-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
2	B	301	S1S	C26-C27-C28-C29
2	A	201	S1S	C15-C38-C39-C40
2	A	201	S1S	C37-C38-C39-C40
2	A	201	S1S	C16-C15-C38-C39
2	A	201	S1S	C14-C15-C38-C39
2	A	201	S1S	O7-C37-C38-C39
2	A	201	S1S	N3-C37-C38-C39
2	A	201	S1S	O7-C37-C38-C15
2	A	201	S1S	N3-C37-C38-C15
2	A	201	S1S	C25-C11-C12-C13
2	A	201	S1S	C10-C11-C12-C13
2	A	201	S1S	N2-C27-C28-C29
2	A	201	S1S	C26-C27-C28-C29
2	A	401	S1S	C37-C38-C39-C40
2	A	401	S1S	C16-C15-C38-C39
2	A	401	S1S	C16-C15-C38-C37
2	A	401	S1S	C14-C15-C38-C37
2	A	401	S1S	N2-C27-C28-C29
3	B	501	P33	C15-C14-O13-C12
3	B	501	P33	C14-C15-O16-C17
3	B	501	P33	C8-C9-O10-C11
2	B	301	S1S	C26-C27-N2-C30
3	B	501	P33	O13-C14-C15-O16
3	B	501	P33	C17-C18-O19-C20
3	B	501	P33	C18-C17-O16-C15
2	A	201	S1S	C13-C14-C15-C38
2	B	301	S1S	N3-C37-C38-C15
2	A	401	S1S	O7-C37-C38-C15
2	A	401	S1S	N3-C37-C38-C15
2	A	401	S1S	O6-C30-C31-C32
2	A	401	S1S	C14-C15-C16-C17
2	A	401	S1S	N2-C30-C31-C32
2	A	201	S1S	O4-C26-C27-C28
2	A	401	S1S	O4-C26-C27-C28
3	B	501	P33	C9-C8-O7-C6
2	B	301	S1S	N2-C30-C31-C32
2	A	401	S1S	C14-C15-C16-C21
2	A	201	S1S	C28-C27-N2-C30
2	B	301	S1S	C14-C15-C16-C21
3	B	501	P33	C12-C11-O10-C9
2	A	401	S1S	N-C26-C27-C28
2	B	301	S1S	O4-C26-C27-C28

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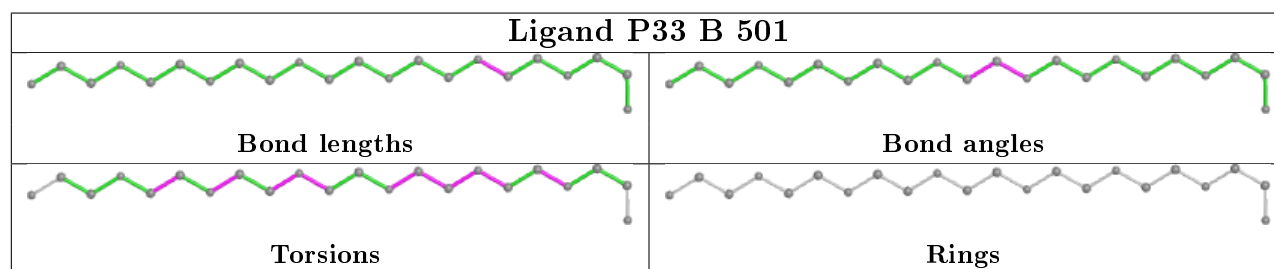
Mol	Chain	Res	Type	Atoms
3	B	501	P33	O4-C5-C6-O7

There are no ring outliers.

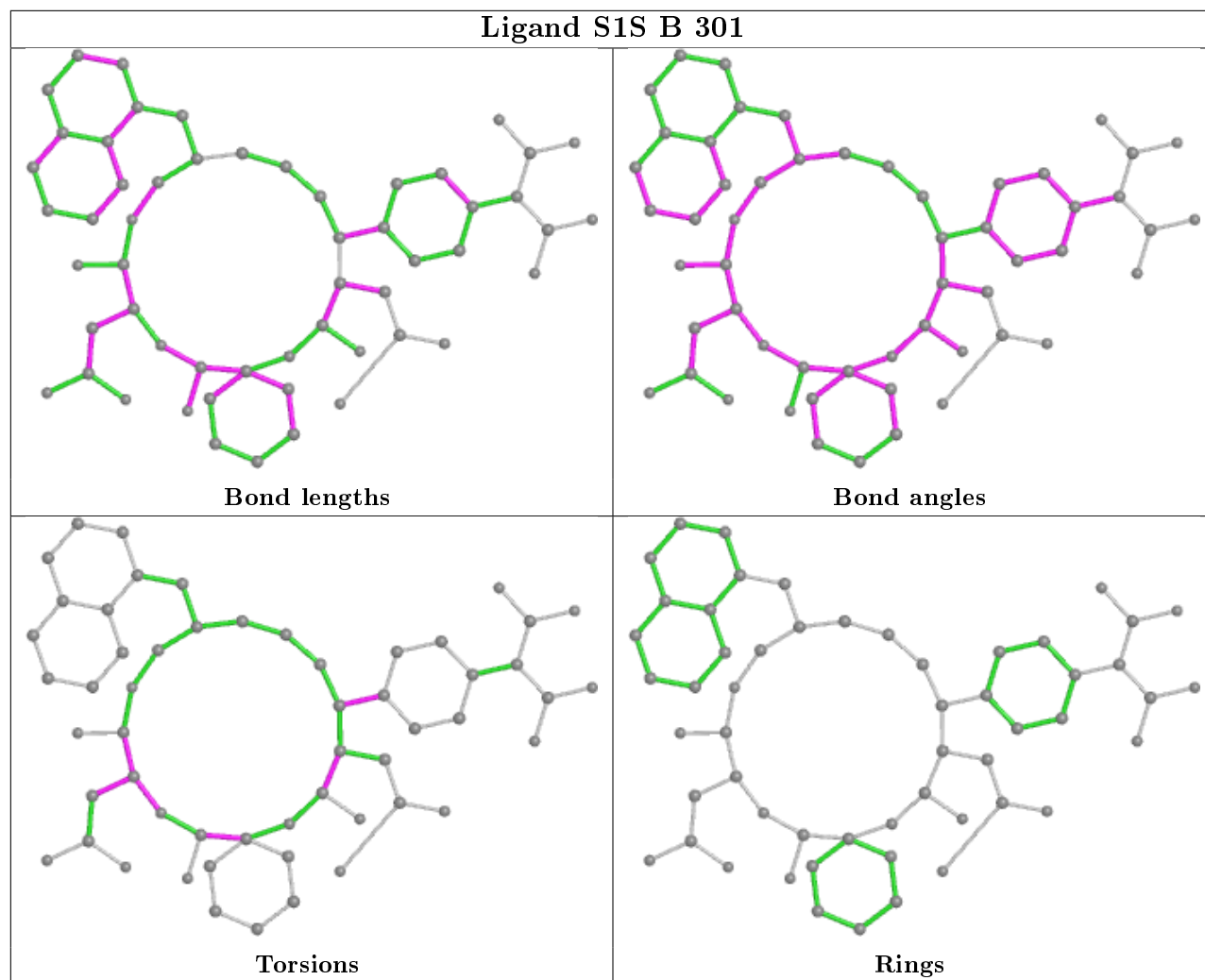
4 monomers are involved in 16 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	501	P33	3	0
2	B	301	S1S	3	0
2	A	201	S1S	4	0
2	A	401	S1S	6	0

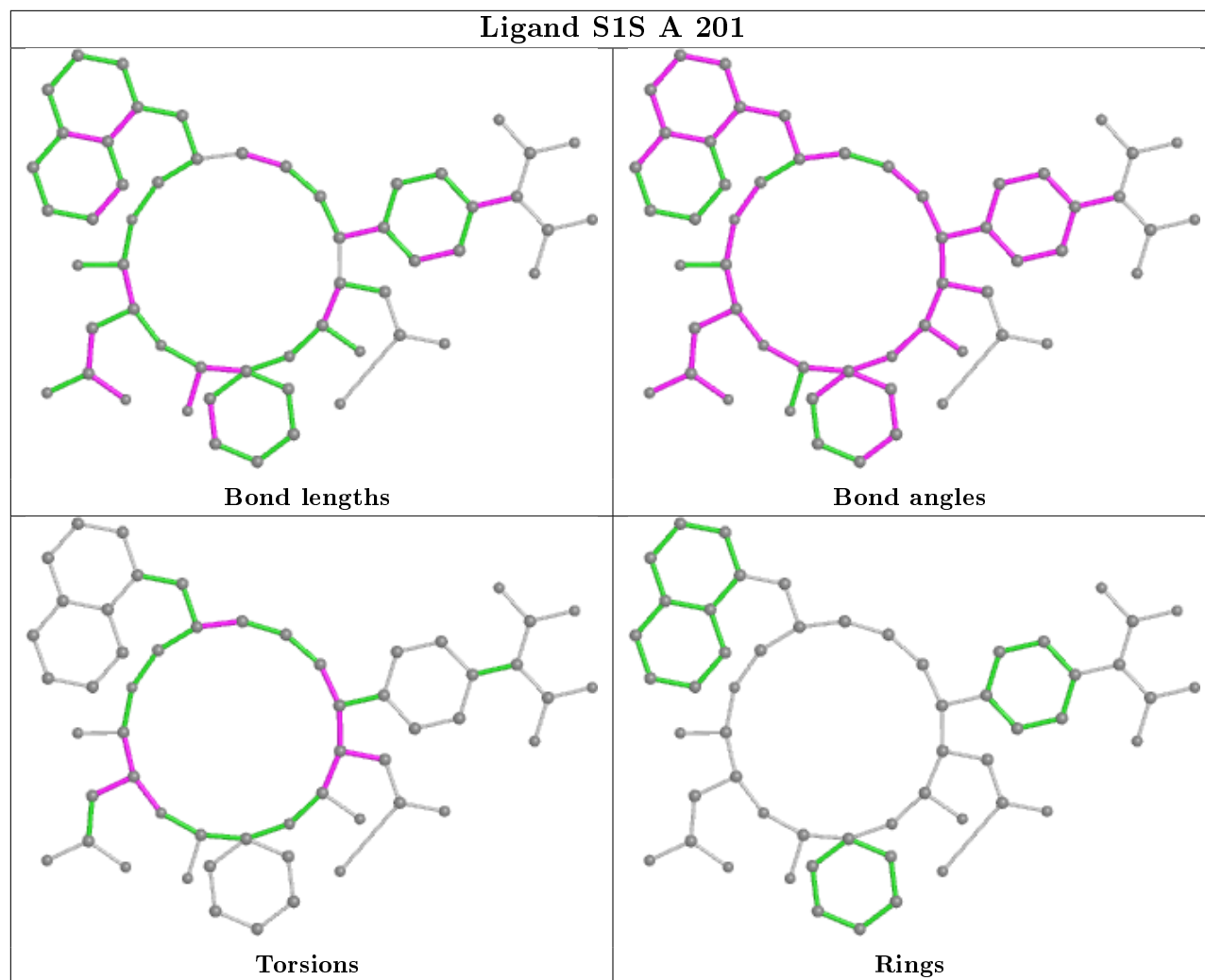
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

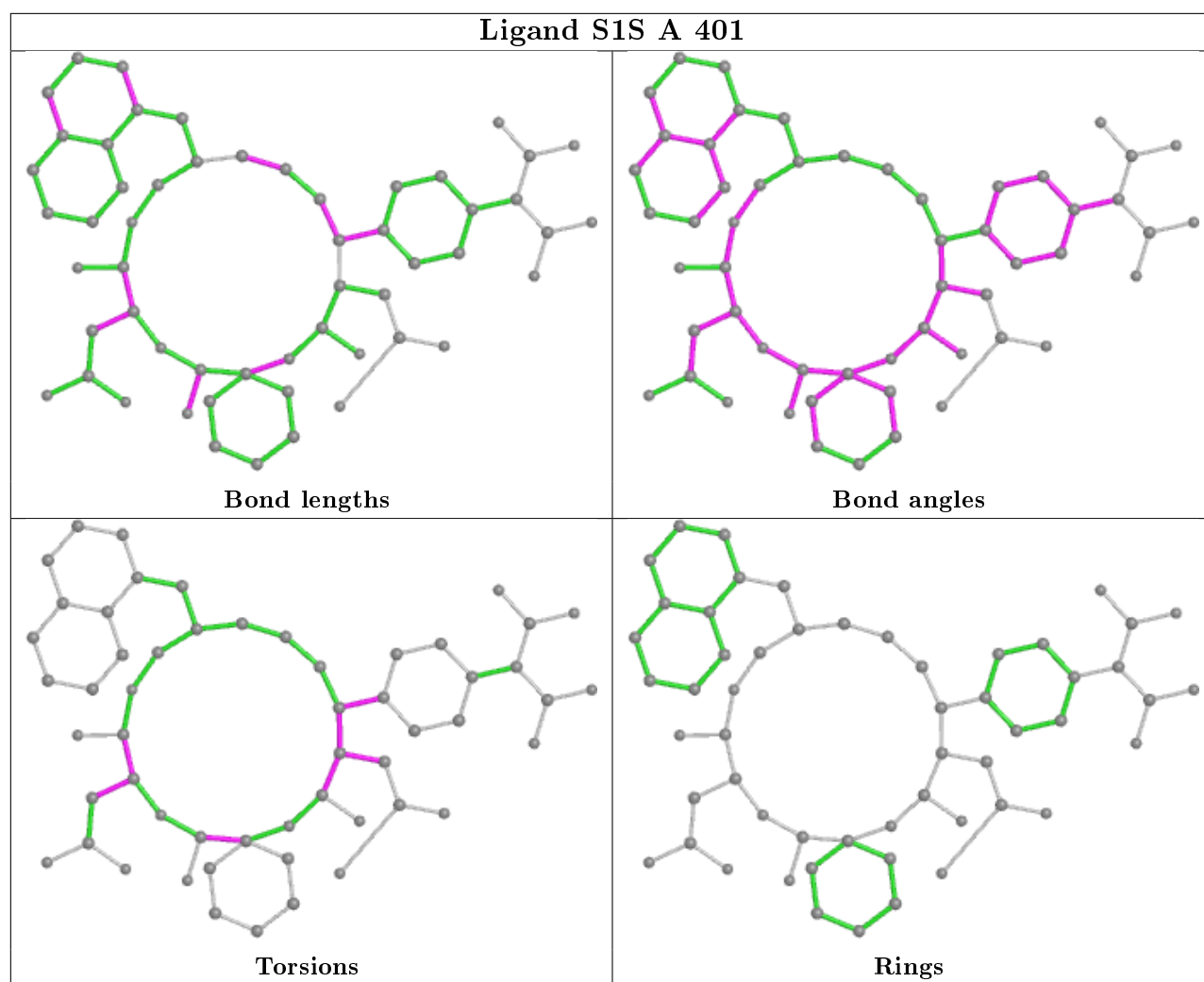


Ligand S1S B 301



Ligand S1S A 201





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	93/99 (93%)	0.80	11 (11%) 4 4	31, 44, 63, 66	0
1	B	77/99 (77%)	0.75	9 (11%) 4 4	27, 42, 69, 70	0
All	All	170/198 (85%)	0.78	20 (11%) 4 4	27, 44, 64, 70	0

All (20) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	97	LEU	5.1
1	B	103	ASN	4.0
1	B	72	GLU	3.9
1	A	85	ILE	3.7
1	A	92	PRO	3.4
1	B	93	GLY	3.1
1	A	79	HIS	2.9
1	A	99	VAL	2.6
1	A	74	LEU	2.5
1	B	73	MET	2.4
1	A	140	VAL	2.4
1	A	103	ASN	2.3
1	A	72	GLU	2.2
1	B	97	LEU	2.2
1	A	59	PRO	2.2
1	A	98	SER	2.2
1	B	129	ASN	2.1
1	B	120	LEU	2.1
1	B	119	PHE	2.1
1	B	74	LEU	2.1

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 carbohydrates in this entry.

6.4 Ligands [i](#)

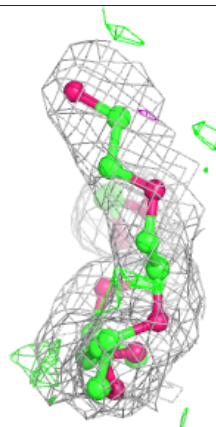
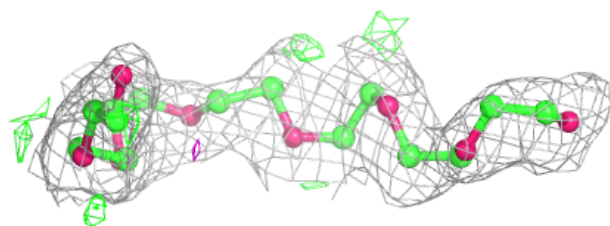
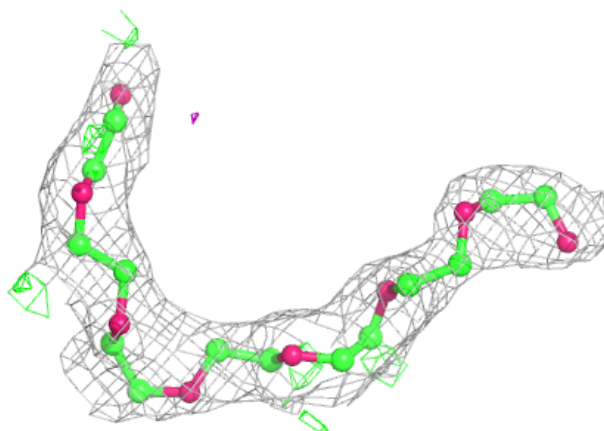
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
3	P33	B	501	22/22	0.85	0.13	48,67,74,76	0
2	S1S	A	401	55/55	0.88	0.14	26,37,49,66	0
2	S1S	A	201	55/55	0.90	0.14	34,47,57,64	0
2	S1S	B	301	55/55	0.93	0.12	19,34,58,71	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.

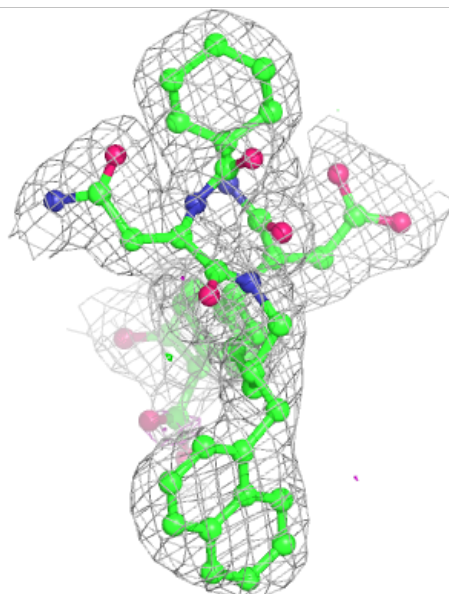
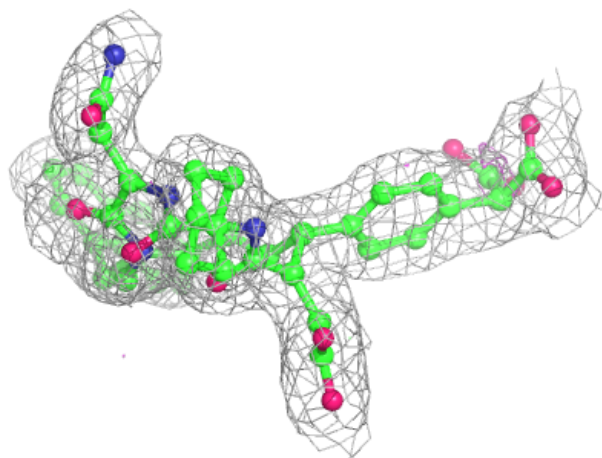
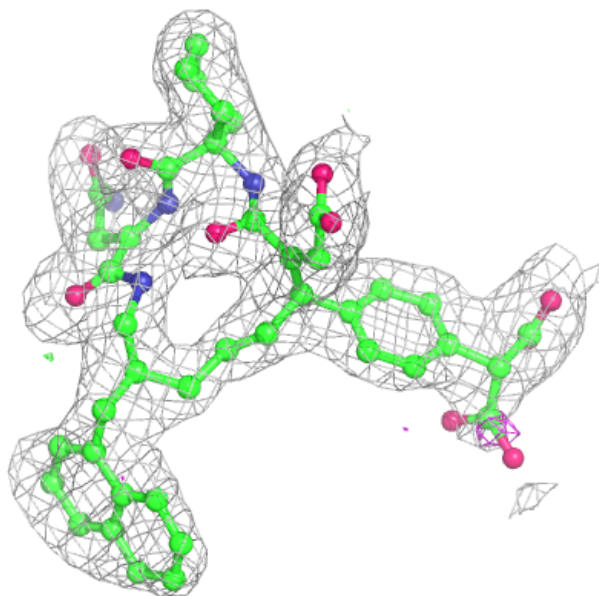
Electron density around P33 B 501:

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



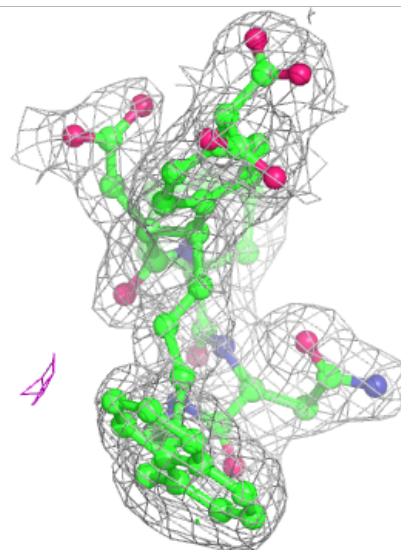
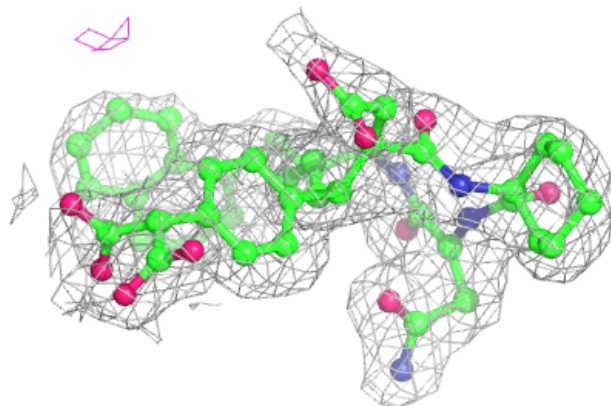
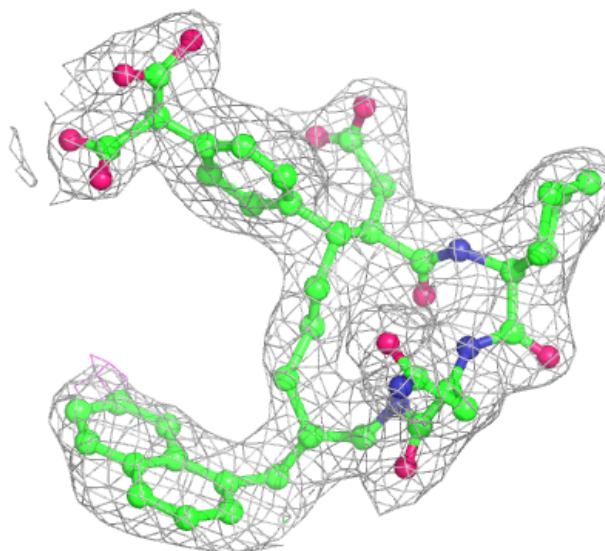
Electron density around S1S A 401:

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



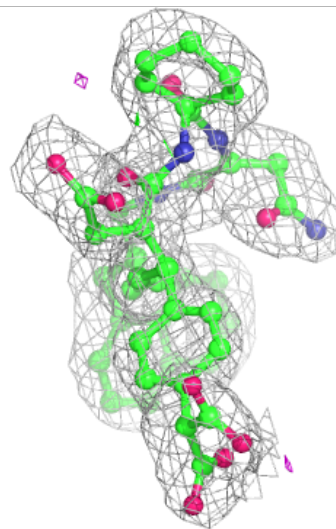
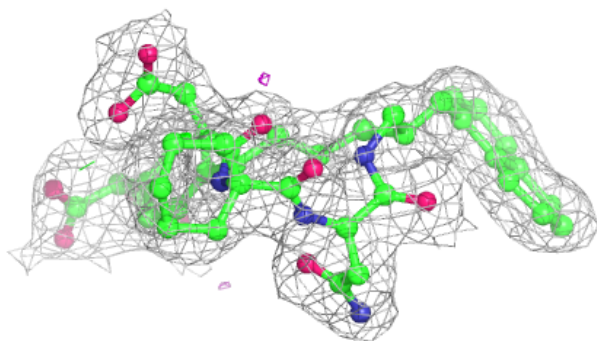
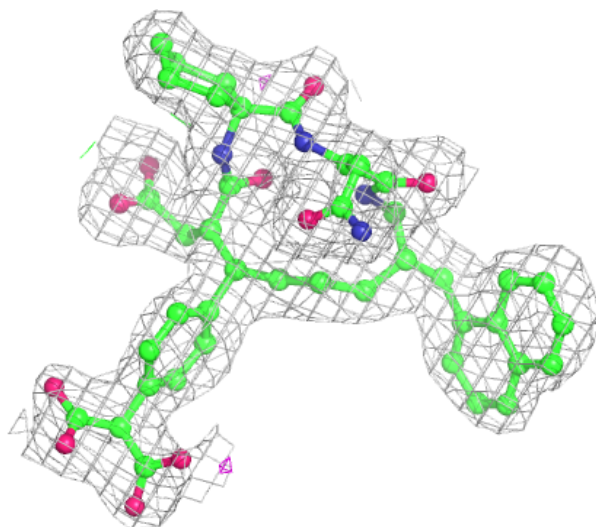
Electron density around S1S A 201:

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



Electron density around S1S B 301:

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



6.5 Other polymers ⓘ

There are no such residues in this entry.