



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 6, 2026 – 01:46 PM UTC

PDB ID : 7FQH / pdb_00007fqh
Title : Crystal Structure of human Legumain in complex with (2S)-N-[(3S)-5-amino-5-oxopent-1-yn-3-yl]-1-[1-[4-(cyclopropylmethoxy)phenyl]cyclopropanecarbon
yl]pyrrolidine-2-carboxamide
Authors : Ehler, A.; Benz, J.; Bartels, B.; Hewings-David, S.; Rudolph, M.G.
Deposited on : 2022-10-05
Resolution : 2.18 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

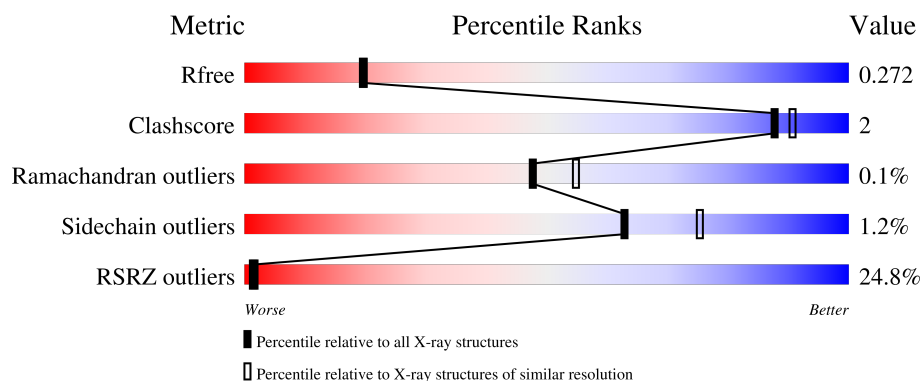
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.18 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	8975 (2.20-2.16)
Clashscore	190562	9786 (2.20-2.16)
Ramachandran outliers	187476	9664 (2.20-2.16)
Sidechain outliers	187428	9664 (2.20-2.16)
RSRZ outliers	180081	8979 (2.20-2.16)

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	444	2% 54% 5% 41%
1	B	444	5% 53% 6% 41%
1	D	444	37% 57% . 42%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6505 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 Legumain.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	262	Total	C	N	O	S	0	1	0
			2112	1337	357	403	15			
1	B	261	Total	C	N	O	S	0	0	0
			2094	1323	355	401	15			
1	D	259	Total	C	N	O	S	0	0	0
			2082	1316	353	399	14			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP Q99538
A	1	LYS	-	expression tag	UNP Q99538
A	2	LEU	-	expression tag	UNP Q99538
A	3	CYS	-	expression tag	UNP Q99538
A	4	ILE	-	expression tag	UNP Q99538
A	5	LEU	-	expression tag	UNP Q99538
A	6	LEU	-	expression tag	UNP Q99538
A	7	ALA	-	expression tag	UNP Q99538
A	8	VAL	-	expression tag	UNP Q99538
A	9	VAL	-	expression tag	UNP Q99538
A	10	ALA	-	expression tag	UNP Q99538
A	11	PHE	-	expression tag	UNP Q99538
A	12	VAL	-	expression tag	UNP Q99538
A	13	GLY	-	expression tag	UNP Q99538
A	14	LEU	-	expression tag	UNP Q99538
A	15	SER	-	expression tag	UNP Q99538
A	16	LEU	-	expression tag	UNP Q99538
A	17	GLY	-	expression tag	UNP Q99538
A	147	SNN	ASP	conflict	UNP Q99538
A	272	GLN	ASN	conflict	UNP Q99538
A	434	VAL	-	expression tag	UNP Q99538
A	435	ASP	-	expression tag	UNP Q99538
A	436	HIS	-	expression tag	UNP Q99538

Continued on next page...

Continued from previous page...

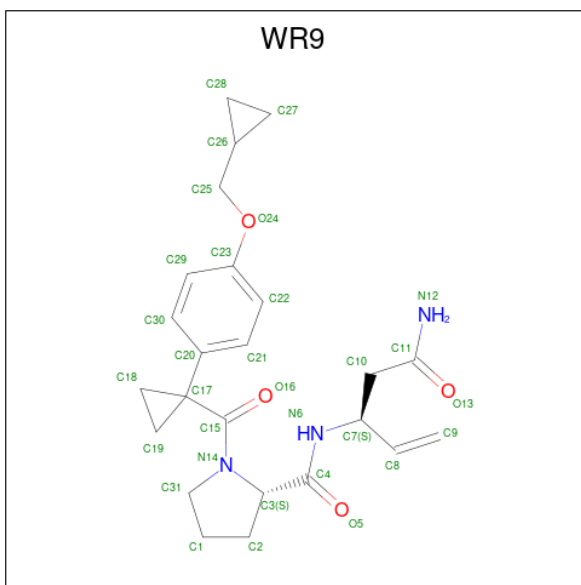
Chain	Residue	Modelled	Actual	Comment	Reference
A	437	HIS	-	expression tag	UNP Q99538
A	438	HIS	-	expression tag	UNP Q99538
A	439	HIS	-	expression tag	UNP Q99538
A	440	HIS	-	expression tag	UNP Q99538
A	441	HIS	-	expression tag	UNP Q99538
A	442	HIS	-	expression tag	UNP Q99538
A	443	HIS	-	expression tag	UNP Q99538
B	0	MET	-	initiating methionine	UNP Q99538
B	1	LYS	-	expression tag	UNP Q99538
B	2	LEU	-	expression tag	UNP Q99538
B	3	CYS	-	expression tag	UNP Q99538
B	4	ILE	-	expression tag	UNP Q99538
B	5	LEU	-	expression tag	UNP Q99538
B	6	LEU	-	expression tag	UNP Q99538
B	7	ALA	-	expression tag	UNP Q99538
B	8	VAL	-	expression tag	UNP Q99538
B	9	VAL	-	expression tag	UNP Q99538
B	10	ALA	-	expression tag	UNP Q99538
B	11	PHE	-	expression tag	UNP Q99538
B	12	VAL	-	expression tag	UNP Q99538
B	13	GLY	-	expression tag	UNP Q99538
B	14	LEU	-	expression tag	UNP Q99538
B	15	SER	-	expression tag	UNP Q99538
B	16	LEU	-	expression tag	UNP Q99538
B	17	GLY	-	expression tag	UNP Q99538
B	147	SNN	ASP	conflict	UNP Q99538
B	272	GLN	ASN	conflict	UNP Q99538
B	434	VAL	-	expression tag	UNP Q99538
B	435	ASP	-	expression tag	UNP Q99538
B	436	HIS	-	expression tag	UNP Q99538
B	437	HIS	-	expression tag	UNP Q99538
B	438	HIS	-	expression tag	UNP Q99538
B	439	HIS	-	expression tag	UNP Q99538
B	440	HIS	-	expression tag	UNP Q99538
B	441	HIS	-	expression tag	UNP Q99538
B	442	HIS	-	expression tag	UNP Q99538
B	443	HIS	-	expression tag	UNP Q99538
D	0	MET	-	initiating methionine	UNP Q99538
D	1	LYS	-	expression tag	UNP Q99538
D	2	LEU	-	expression tag	UNP Q99538
D	3	CYS	-	expression tag	UNP Q99538
D	4	ILE	-	expression tag	UNP Q99538

Continued on next page...

Continued from previous page...

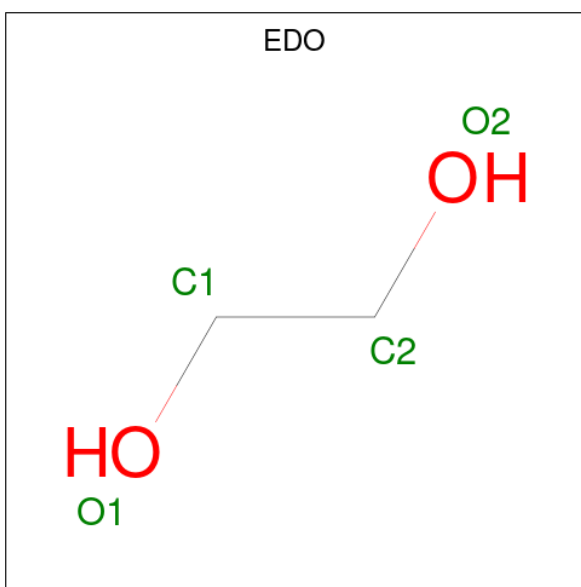
Chain	Residue	Modelled	Actual	Comment	Reference
D	5	LEU	-	expression tag	UNP Q99538
D	6	LEU	-	expression tag	UNP Q99538
D	7	ALA	-	expression tag	UNP Q99538
D	8	VAL	-	expression tag	UNP Q99538
D	9	VAL	-	expression tag	UNP Q99538
D	10	ALA	-	expression tag	UNP Q99538
D	11	PHE	-	expression tag	UNP Q99538
D	12	VAL	-	expression tag	UNP Q99538
D	13	GLY	-	expression tag	UNP Q99538
D	14	LEU	-	expression tag	UNP Q99538
D	15	SER	-	expression tag	UNP Q99538
D	16	LEU	-	expression tag	UNP Q99538
D	17	GLY	-	expression tag	UNP Q99538
D	147	SNN	ASP	conflict	UNP Q99538
D	272	GLN	ASN	conflict	UNP Q99538
D	434	VAL	-	expression tag	UNP Q99538
D	435	ASP	-	expression tag	UNP Q99538
D	436	HIS	-	expression tag	UNP Q99538
D	437	HIS	-	expression tag	UNP Q99538
D	438	HIS	-	expression tag	UNP Q99538
D	439	HIS	-	expression tag	UNP Q99538
D	440	HIS	-	expression tag	UNP Q99538
D	441	HIS	-	expression tag	UNP Q99538
D	442	HIS	-	expression tag	UNP Q99538
D	443	HIS	-	expression tag	UNP Q99538

- Molecule 2 is N-[(3S)-5-amino-5-oxopent-1-en-3-yl]-1-{1-[4-(cyclopropylmethoxy)phenyl]cyclopropane-1-carbonyl}-L-prolinamide (CCD ID: WR9) (formula: C₂₄H₃₁N₃O₄) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			31	24	3	4		
2	B	1	Total	C	N	O	0	0
			31	24	3	4		
2	D	1	Total	C	N	O	0	0
			31	24	3	4		

- Molecule 3 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		

Continued on next page...

Continued from previous page...

Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).

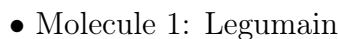
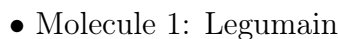


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
4	A	1	Total	C	N	O	0	0
			14	8	1	5		
4	B	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	43	Total	O	0	0
			43	43		
5	B	45	Total	O	0	0
			45	45		

- Molecule 1: Legumain



CYS	GLU	ILE	SER	S216	V132	Y70	MET
GLU	VAL	PRO	PRO	Y217	L133	Y71	LYS
LYS	SER	VAL	VAL	A218	K134	D72	LEU
PRO	LEU	PRO	PRO	C219	S135	D73	CYS
TYR	LEU	LEU	LEU	Y220	F142	I74	ILE
PRO	ALA	ALA	PRO	Y221	I143	A75	LEU
LEU	ALA	SER	PRO	D222	Y144	Y76	LEU
HIS	SER	GLU	VAL	E223	F145	S77	ALA
ARG	ILE	ALA	THR	K224	F145	E78	ALA
ILE	ALA	ALA	HIS	R225	S150	D79	VAL
LYS	GLU	GLU	LEU	S226	T151	N80	VAL
LEU	VAL	VAL	ASP	T227	G152	P81	ALA
SER	GLU	GLN	LEU	Y228	I153	T82	VAL
MET	GLN	LEU	THR	G230	V155	P83	GLY
ASP	LEU	LEU	PRO	L229	V156	G84	LEU
HIS	LEU	LEU	SER	D231	P157	V86	SER
VAL	SER	SER	PRO	W232	N158	N87	LEU
CYS	GLU	GLU	ASP	Y233	E159	N88	GLY
LEU	ARG	ARG	VAL	S234	D160	R89	VAL
GLY	ALA	ALA	PRO	W237	H161	P90	PRO
HIS	PRO	PRO	LEU	V243	V163	N91	ILE
TYR	LEU	THR	THR	E244	L166	G92	ASP
VAL	THR	ILE	ILE	D245	N167	T93	ASP
ASP	GLY	GLY	MET	L246	H170	D94	GLU
HIS	HIS	LYS	LYS	K253	I171	V95	ASP
HIS	SER	ARG	ARG	D247	Y172	Y96	GLY
HIS	CYS	LYS	LYS	L257	K101	V99	
HIS	PRO	LEU	LEU	V258	D102	P100	
HIS	PRO	MET	ASN	K259	Y174	K101	
HIS	GLU	ASN	THR	S260	H175	D102	
HIS	GLU	GLU	GLU	H261	H176	T104	
HIS	THR	SER	SER	T262	E106	G105	
HIS	THR	ARG	ARG	N263	Y179	E107	
CYS	GLN	GLN	GLN	T264	M182	V108	
PHE	LEU	LEU	LEU	S265	V183	P110	
ASN	THR	THR	THR	H266	F184	Q111	
TRP	GLU	GLU	GLU	V267	A188	Q112	
HIS	GLU	GLU	GLU	G271	G192	F113	
SER	ILE	ILE	ILE	Q272	S193	Y116	
PRO	GLN	GLN	GLN	K273	L117	L117	
THR	THR	ARG	ARG	T274	R118	R118	
TYR	TYR	HIS	HIS	I275	G119	G119	
GLU	GLU	LEU	LEU		D120	D120	
TYR	TYR	ASP	ASP		A121	A121	
ALA	ALA	ALA	ALA	V280	E122	E122	
LEU	LEU	ARG	ARG	M281	M201	M201	
ARG	ARG	HIS	HIS	Q282	V124	V124	
HIS	HIS	LEU	LEU	G285	K125	K125	
LEU	LEU	ILE	ILE		N203	N203	
TYR	TYR	GLU	GLU	MET	V204	V204	
VAL	VAL	LYS	LYS	LYS	G126	G126	
LEU	LEU	SER	SER	ARG	I127	I127	
VAL	VAL	VAL	VAL	LYS	G128	G128	
ASN	ASN	ASN	ASN	ALA	S129	S129	
LEU	LEU	LYS	LYS	SER	G130	G130	
					R213	R213	
					K131	K131	

4 Data and refinement statistics

Property	Value	Source
Space group	P 3 2 1	Depositor
Cell constants a, b, c, α , β , γ	117.80Å 117.80Å 102.81Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	51.46 – 2.18 51.46 – 2.18	Depositor EDS
% Data completeness (in resolution range)	65.1 (51.46-2.18) 65.5 (51.46-2.18)	Depositor EDS
R_{merge}	0.24	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.65 (at 2.18Å)	Xtriage
Refinement program	REFMAC 5.8.0267	Depositor
R, R_{free}	0.223 , 0.272 0.225 , 0.272	Depositor DCC
R_{free} test set	1465 reflections (3.35%)	wwPDB-VP
Wilson B-factor (Å ²)	34.6	Xtriage
Anisotropy	0.103	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.35 , 37.3	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.017 for -h,-k,l	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6505	wwPDB-VP
Average B, all atoms (Å ²)	41.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.11% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: EDO, WR9, NAG, SNN

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	0.97	0/2165	1.33	1/2936 (0.0%)
1	B	0.99	0/2143	1.35	0/2907
1	D	0.99	0/2131	1.35	0/2892
All	All	0.98	0/6439	1.34	1/8735 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	48	ASP	CA-CB-CG	6.20	118.80	112.60

There are no chirality outliers.

There are no planarity outliers.

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	2112	0	1993	11	0
1	B	2094	0	1971	14	0
1	D	2082	0	1960	0	0
2	A	31	0	0	0	0
2	B	31	0	0	0	0
2	D	31	0	0	0	0
3	A	4	0	6	0	0

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	B	4	0	6	0	0
4	A	14	0	13	1	0
4	B	14	0	13	0	0
5	A	43	0	0	0	0
5	B	45	0	0	1	0
All	All	6505	0	5962	25	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 2.

The worst 5 of 25 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:186:ILE:HD11	1:B:195:MET:HE3	1.87	0.56
1:A:199:PRO:HD3	4:A:503:NAG:O3	2.10	0.52
1:B:183:VAL:HA	1:B:205:TYR:O	2.10	0.51
1:B:90:PRO:HD3	1:B:220:TYR:CG	2.45	0.51
1:A:198:LEU:HD21	1:A:204:VAL:HG12	1.95	0.48

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	260/444 (59%)	250 (96%)	10 (4%)	0	100	100
1	B	258/444 (58%)	253 (98%)	5 (2%)	0	100	100
1	D	256/444 (58%)	237 (93%)	18 (7%)	1 (0%)	30	31
All	All	774/1332 (58%)	740 (96%)	33 (4%)	1 (0%)	48	55

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	D	94	ASP

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	229/396 (58%)	228 (100%)	1 (0%)	84	91
1	B	227/396 (57%)	224 (99%)	3 (1%)	61	74
1	D	226/396 (57%)	222 (98%)	4 (2%)	51	65
All	All	682/1188 (57%)	674 (99%)	8 (1%)	63	75

5 of 8 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	D	237	TRP
1	D	117	LEU
1	D	74	ILE
1	B	286	MET
1	D	109	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 15 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	254	GLN
1	D	197	HIS
1	B	269	GLN
1	D	211	ASN
1	D	46	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

3 non-standard protein/DNA/RNA residues 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
1	SNN	A	147	1	5,6,8	1.03	0	1,6,11	2.76	1 (100%)
1	SNN	B	147	1	5,6,8	0.99	0	1,6,11	2.77	1 (100%)
1	SNN	D	147	1	5,6,8	0.65	0	1,6,11	0.86	0

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
1	SNN	A	147	1	-	3/3/5/12	-
1	SNN	B	147	1	-	3/3/5/12	-
1	SNN	D	147	1	-	3/3/5/12	-

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	147	SNN	O5-C5-C4	-2.77	117.31	125.38
1	A	147	SNN	O5-C5-C4	-2.76	117.36	125.38

There are no chirality outliers.

5 of 9 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	147	SNN	O-C-CA-C4
1	A	147	SNN	C5-C4-CA-N
1	B	147	SNN	O-C-CA-C4
1	B	147	SNN	C5-C4-CA-N

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms
1	D	147	SNN	O-C-CA-C4

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

7 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	EDO	B	503	-	3,3,3	0.11	0	2,2,2	0.06	0
2	WR9	D	501	1	34,34,34	0.28	0	47,49,49	0.66	1 (2%)
4	NAG	B	502	1	14,14,15	0.46	0	17,19,21	0.76	0
2	WR9	B	501	1	34,34,34	0.29	0	47,49,49	0.80	1 (2%)
4	NAG	A	503	1	14,14,15	0.75	1 (7%)	17,19,21	0.83	0
3	EDO	A	502	-	3,3,3	0.17	0	2,2,2	0.25	0
2	WR9	A	501	1	34,34,34	0.30	0	47,49,49	0.70	1 (2%)

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	EDO	B	503	-	-	0/1/1/1	-
2	WR9	D	501	1	-	10/35/51/51	0/4/4/4
4	NAG	B	502	1	-	2/6/23/26	0/1/1/1

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	WR9	B	501	1	-	4/35/51/51	0/4/4/4
4	NAG	A	503	1	-	2/6/23/26	0/1/1/1
3	EDO	A	502	-	-	0/1/1/1	-
2	WR9	A	501	1	-	5/35/51/51	0/4/4/4

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	503	NAG	C1-C2	2.12	1.55	1.52

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	501	WR9	C18-C17-C20	4.67	124.02	118.58
2	A	501	WR9	C18-C17-C20	4.06	123.32	118.58
2	D	501	WR9	C18-C17-C20	3.47	122.63	118.58

There are no chirality outliers.

5 of 23 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	501	WR9	O24-C25-C26-C27
2	A	501	WR9	C22-C23-O24-C25
2	A	501	WR9	C29-C23-O24-C25
2	B	501	WR9	C22-C23-O24-C25
2	B	501	WR9	C29-C23-O24-C25

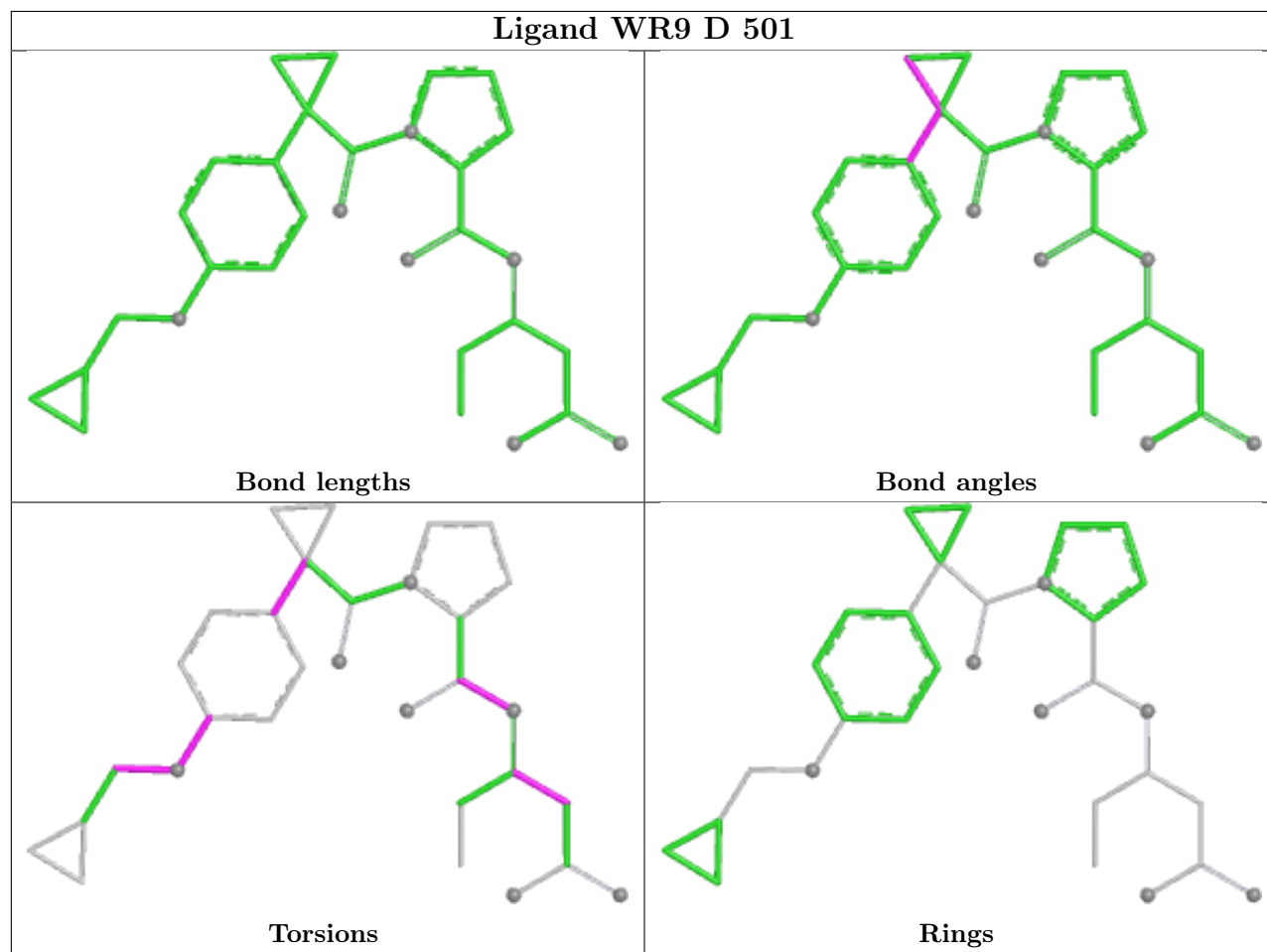
There are no ring outliers.

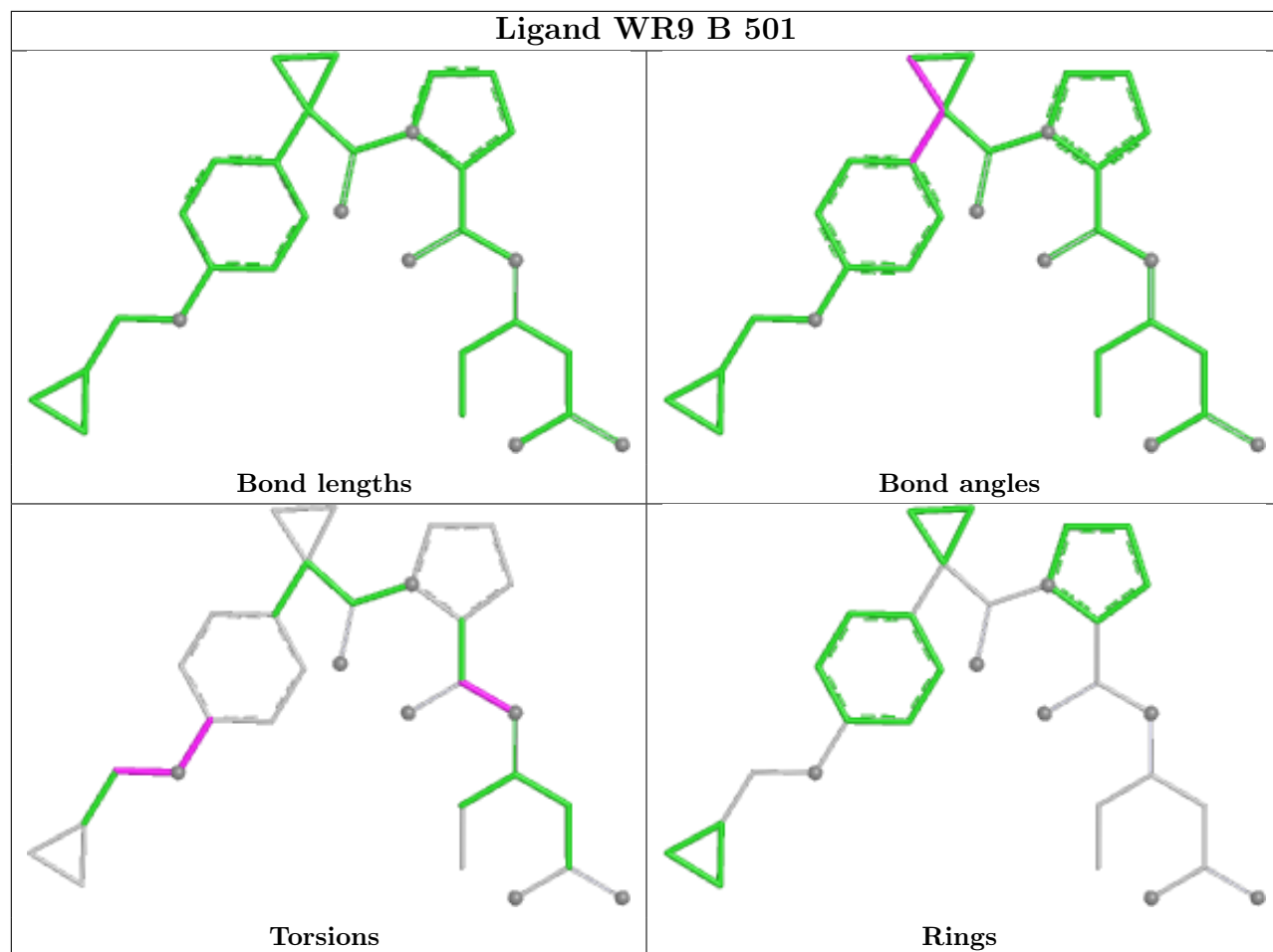
1 monomer is involved in 1 short contact:

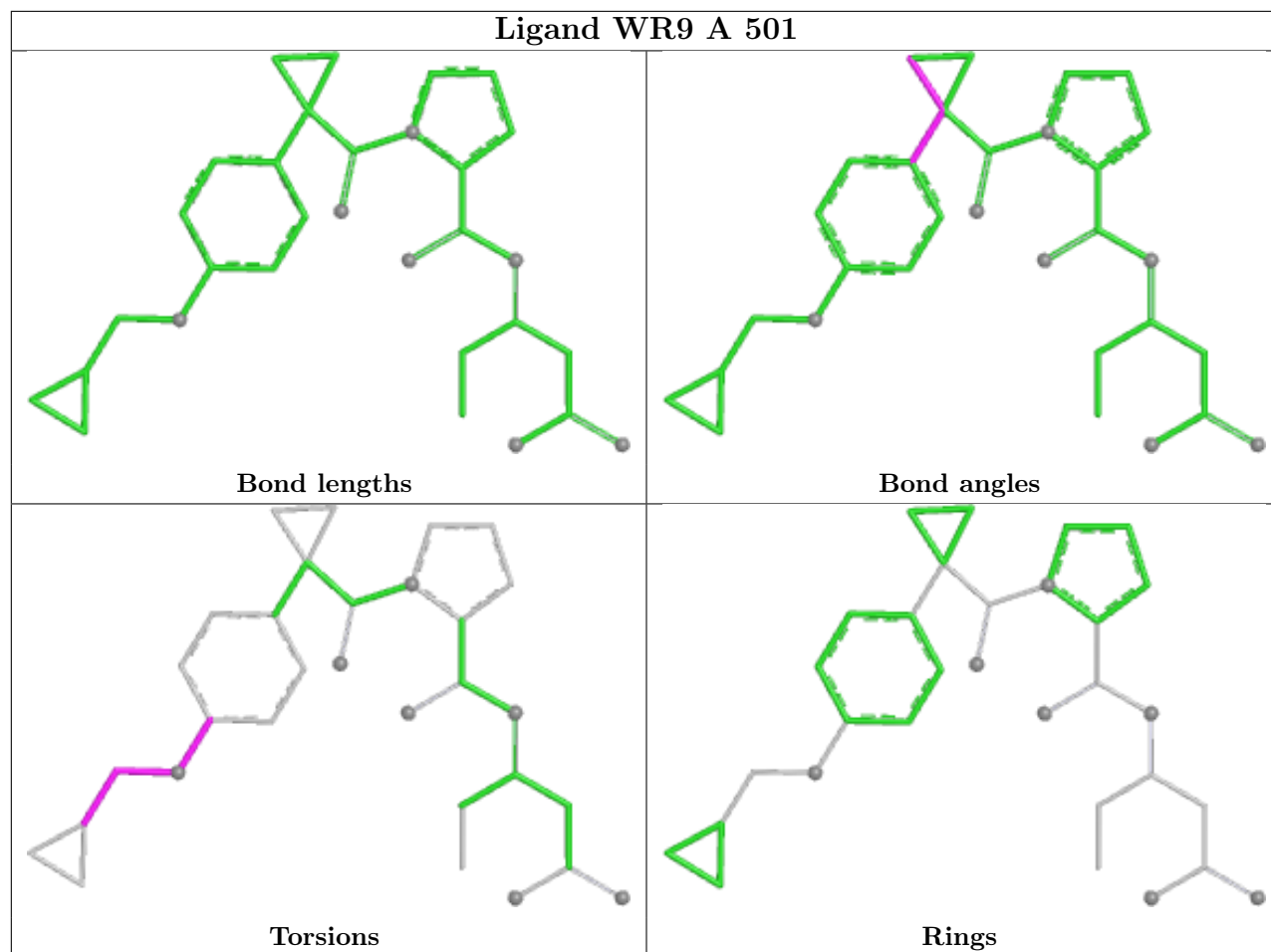
Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	503	NAG	1	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.







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	261/444 (58%)	0.49	8 (3%) 51 51	18, 36, 53, 72	1 (0%)
1	B	260/444 (58%)	0.51	20 (7%) 19 18	22, 36, 58, 83	0
1	D	258/444 (58%)	2.86	165 (63%) 0 0	10, 23, 40, 62	258 (100%)
All	All	779/1332 (58%)	1.28	193 (24%) 2 1	10, 33, 52, 83	259 (33%)

The worst 5 of 193 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	170	ILE	12.1
1	D	134	LYS	8.4
1	D	126	GLY	8.1
1	D	125	LYS	8.1
1	D	121	ALA	7.8

6.2 Non-standard residues in protein, DNA, RNA chains [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
1	SNN	D	147	7/8	0.84	0.09	26,27,28,28	7
1	SNN	B	147	7/8	0.89	0.11	23,27,30,34	0
1	SNN	A	147	7/8	0.94	0.09	15,17,18,18	0

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

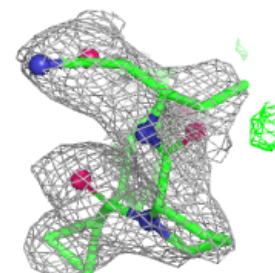
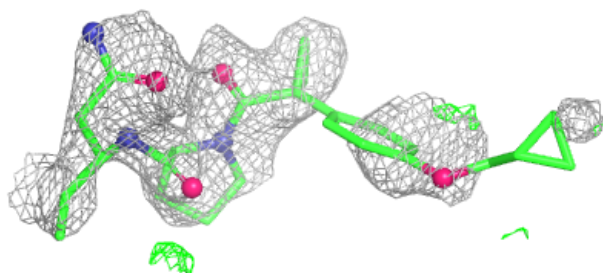
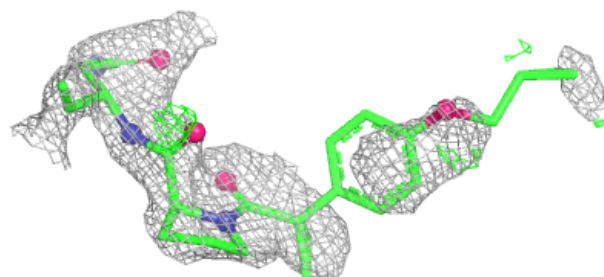
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q<0.9' lists 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
4	NAG	A	503	14/15	0.49	0.25	64,72,77,79	0
3	EDO	A	502	4/4	0.67	0.15	42,43,44,45	0
4	NAG	B	502	14/15	0.74	0.15	47,53,61,62	0
2	WR9	D	501	31/31	0.77	0.20	29,36,52,52	31
2	WR9	B	501	31/31	0.86	0.16	32,51,97,98	0
3	EDO	B	503	4/4	0.91	0.11	26,26,26,27	0
2	WR9	A	501	31/31	0.93	0.10	24,34,54,56	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.

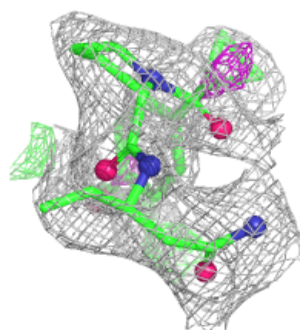
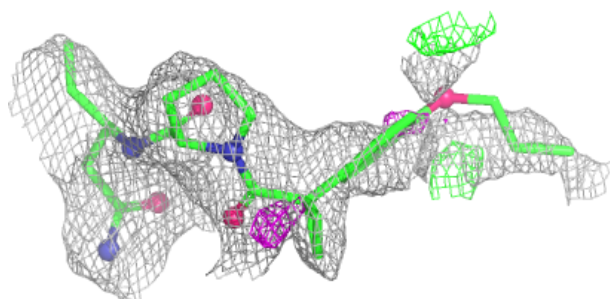
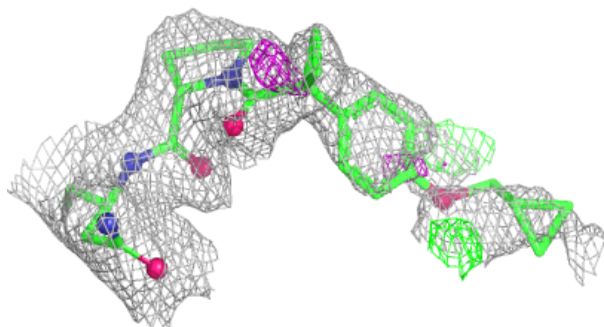
Electron density around WR9 D 501:

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

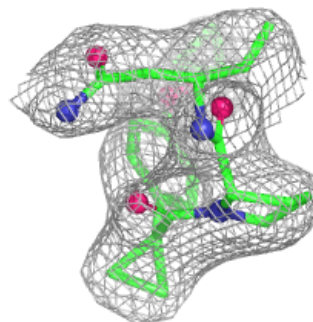
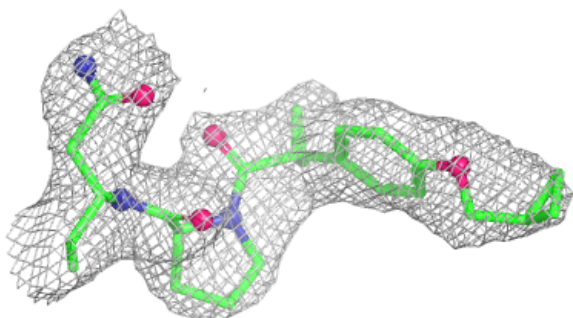
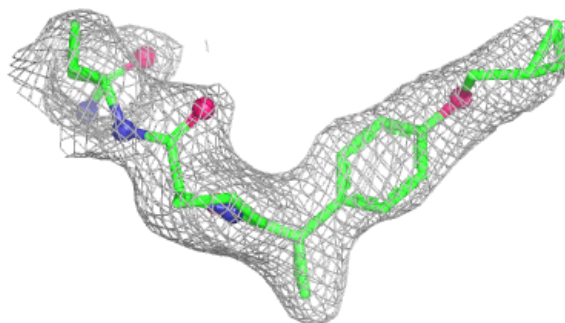


Electron density around WR9 B 501:

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

**Electron density around WR9 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.