



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 20, 2026 – 10:37 AM UTC

PDB ID : 8P1F / pdb_00008p1f
Title : X-ray structure of acetylcholine-binding protein (AChBP) in complex with FL001909.
Authors : Cederfelt, D.; Boronat, P.; Dobritsch, D.; Hennig, S.; Fitzgerald, E.A.; de Esch, I.J.P.; Danielson, U.H.
Deposited on : 2023-05-12
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

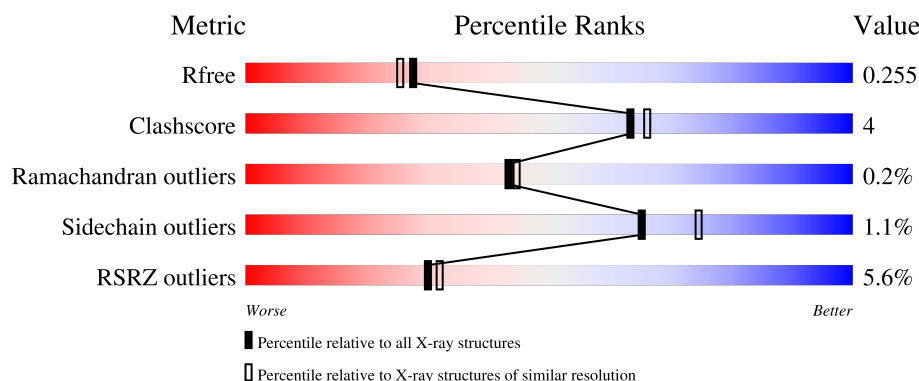
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 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.



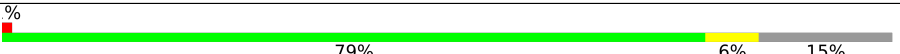
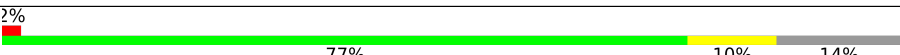
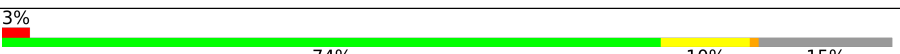
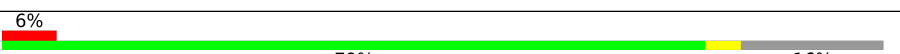
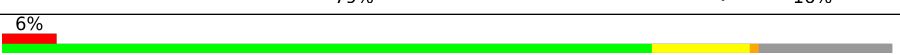
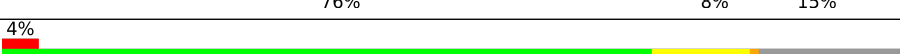
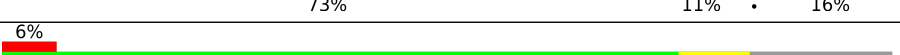
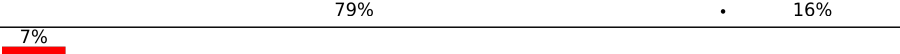
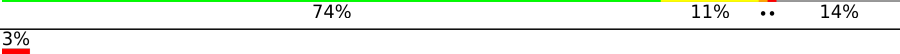
Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	180053	6658 (2.10-2.10)
Clashscore	190562	7164 (2.10-2.10)
Ramachandran outliers	187476	7099 (2.10-2.10)
Sidechain outliers	187428	7100 (2.10-2.10)
RSRZ outliers	180081	6662 (2.10-2.10)

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	237	
1	B	237	
1	C	237	
1	D	237	

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Mol	Chain	Length	Quality of chain
1	E	237	
1	F	237	
1	G	237	
1	H	237	
1	I	237	
1	J	237	
1	K	237	
1	L	237	
1	M	237	
1	N	237	
1	O	237	
1	P	237	
1	Q	237	
1	R	237	
1	S	237	
1	T	237	

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 33433 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 Acetylcholine-binding protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	200	Total	C	N	O	S	0	3	0
			1626	1018	280	323	5			
1	B	201	Total	C	N	O	S	0	3	0
			1632	1021	281	325	5			
1	C	202	Total	C	N	O	S	0	1	0
			1618	1016	276	321	5			
1	D	203	Total	C	N	O	S	0	0	0
			1623	1016	280	322	5			
1	E	202	Total	C	N	O	S	0	0	0
			1612	1010	276	321	5			
1	F	204	Total	C	N	O	S	0	0	0
			1628	1019	278	326	5			
1	G	204	Total	C	N	O	S	0	0	0
			1632	1021	279	327	5			
1	H	202	Total	C	N	O	S	0	0	0
			1613	1011	276	321	5			
1	I	205	Total	C	N	O	S	0	5	0
			1673	1044	289	335	5			
1	J	201	Total	C	N	O	S	0	2	0
			1629	1020	285	321	3			
1	K	200	Total	C	N	O	S	0	3	0
			1619	1018	277	319	5			
1	L	201	Total	C	N	O	S	0	0	0
			1606	1007	275	319	5			
1	M	201	Total	C	N	O	S	0	0	0
			1609	1009	275	320	5			
1	N	200	Total	C	N	O	S	0	4	0
			1633	1023	283	322	5			
1	O	200	Total	C	N	O	S	0	1	0
			1610	1010	277	318	5			
1	P	199	Total	C	N	O	S	0	1	0
			1601	1006	276	314	5			

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Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	Q	204	Total	C	N	O	S	0	0	0
			1632	1021	279	327	5			
1	R	201	Total	C	N	O	S	0	0	0
			1609	1009	275	320	5			
1	S	206	Total	C	N	O	S	0	0	0
			1647	1029	284	329	5			
1	T	203	Total	C	N	O	S	0	3	0
			1647	1029	286	327	5			

There are 160 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	230	GLY	-	expression tag	UNP P58154
A	231	SER	-	expression tag	UNP P58154
A	232	HIS	-	expression tag	UNP P58154
A	233	HIS	-	expression tag	UNP P58154
A	234	HIS	-	expression tag	UNP P58154
A	235	HIS	-	expression tag	UNP P58154
A	236	HIS	-	expression tag	UNP P58154
A	237	HIS	-	expression tag	UNP P58154
B	230	GLY	-	expression tag	UNP P58154
B	231	SER	-	expression tag	UNP P58154
B	232	HIS	-	expression tag	UNP P58154
B	233	HIS	-	expression tag	UNP P58154
B	234	HIS	-	expression tag	UNP P58154
B	235	HIS	-	expression tag	UNP P58154
B	236	HIS	-	expression tag	UNP P58154
B	237	HIS	-	expression tag	UNP P58154
C	230	GLY	-	expression tag	UNP P58154
C	231	SER	-	expression tag	UNP P58154
C	232	HIS	-	expression tag	UNP P58154
C	233	HIS	-	expression tag	UNP P58154
C	234	HIS	-	expression tag	UNP P58154
C	235	HIS	-	expression tag	UNP P58154
C	236	HIS	-	expression tag	UNP P58154
C	237	HIS	-	expression tag	UNP P58154
D	230	GLY	-	expression tag	UNP P58154
D	231	SER	-	expression tag	UNP P58154
D	232	HIS	-	expression tag	UNP P58154
D	233	HIS	-	expression tag	UNP P58154
D	234	HIS	-	expression tag	UNP P58154
D	235	HIS	-	expression tag	UNP P58154
D	236	HIS	-	expression tag	UNP P58154

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Chain	Residue	Modelled	Actual	Comment	Reference
D	237	HIS	-	expression tag	UNP P58154
E	230	GLY	-	expression tag	UNP P58154
E	231	SER	-	expression tag	UNP P58154
E	232	HIS	-	expression tag	UNP P58154
E	233	HIS	-	expression tag	UNP P58154
E	234	HIS	-	expression tag	UNP P58154
E	235	HIS	-	expression tag	UNP P58154
E	236	HIS	-	expression tag	UNP P58154
E	237	HIS	-	expression tag	UNP P58154
F	230	GLY	-	expression tag	UNP P58154
F	231	SER	-	expression tag	UNP P58154
F	232	HIS	-	expression tag	UNP P58154
F	233	HIS	-	expression tag	UNP P58154
F	234	HIS	-	expression tag	UNP P58154
F	235	HIS	-	expression tag	UNP P58154
F	236	HIS	-	expression tag	UNP P58154
F	237	HIS	-	expression tag	UNP P58154
G	230	GLY	-	expression tag	UNP P58154
G	231	SER	-	expression tag	UNP P58154
G	232	HIS	-	expression tag	UNP P58154
G	233	HIS	-	expression tag	UNP P58154
G	234	HIS	-	expression tag	UNP P58154
G	235	HIS	-	expression tag	UNP P58154
G	236	HIS	-	expression tag	UNP P58154
G	237	HIS	-	expression tag	UNP P58154
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I	234	HIS	-	expression tag	UNP P58154
I	235	HIS	-	expression tag	UNP P58154
I	236	HIS	-	expression tag	UNP P58154
I	237	HIS	-	expression tag	UNP P58154
J	230	GLY	-	expression tag	UNP P58154

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Chain	Residue	Modelled	Actual	Comment	Reference
J	231	SER	-	expression tag	UNP P58154
J	232	HIS	-	expression tag	UNP P58154
J	233	HIS	-	expression tag	UNP P58154
J	234	HIS	-	expression tag	UNP P58154
J	235	HIS	-	expression tag	UNP P58154
J	236	HIS	-	expression tag	UNP P58154
J	237	HIS	-	expression tag	UNP P58154
K	230	GLY	-	expression tag	UNP P58154
K	231	SER	-	expression tag	UNP P58154
K	232	HIS	-	expression tag	UNP P58154
K	233	HIS	-	expression tag	UNP P58154
K	234	HIS	-	expression tag	UNP P58154
K	235	HIS	-	expression tag	UNP P58154
K	236	HIS	-	expression tag	UNP P58154
K	237	HIS	-	expression tag	UNP P58154
L	230	GLY	-	expression tag	UNP P58154
L	231	SER	-	expression tag	UNP P58154
L	232	HIS	-	expression tag	UNP P58154
L	233	HIS	-	expression tag	UNP P58154
L	234	HIS	-	expression tag	UNP P58154
L	235	HIS	-	expression tag	UNP P58154
L	236	HIS	-	expression tag	UNP P58154
L	237	HIS	-	expression tag	UNP P58154
M	230	GLY	-	expression tag	UNP P58154
M	231	SER	-	expression tag	UNP P58154
M	232	HIS	-	expression tag	UNP P58154
M	233	HIS	-	expression tag	UNP P58154
M	234	HIS	-	expression tag	UNP P58154
M	235	HIS	-	expression tag	UNP P58154
M	236	HIS	-	expression tag	UNP P58154
M	237	HIS	-	expression tag	UNP P58154
N	230	GLY	-	expression tag	UNP P58154
N	231	SER	-	expression tag	UNP P58154
N	232	HIS	-	expression tag	UNP P58154
N	233	HIS	-	expression tag	UNP P58154
N	234	HIS	-	expression tag	UNP P58154
N	235	HIS	-	expression tag	UNP P58154
N	236	HIS	-	expression tag	UNP P58154
N	237	HIS	-	expression tag	UNP P58154
O	230	GLY	-	expression tag	UNP P58154
O	231	SER	-	expression tag	UNP P58154
O	232	HIS	-	expression tag	UNP P58154

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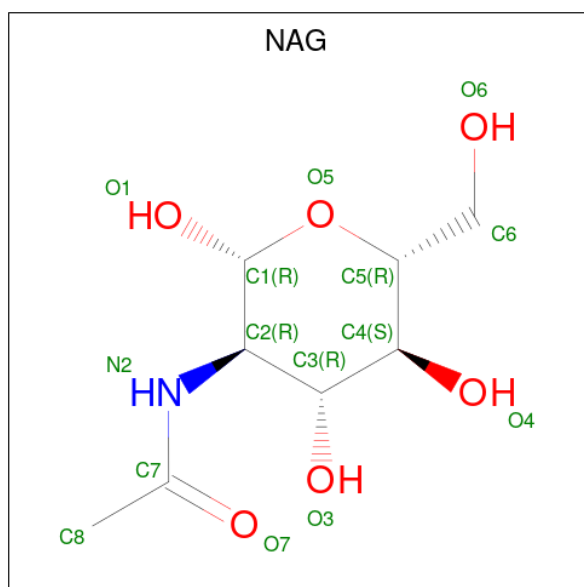
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O	234	HIS	-	expression tag	UNP P58154
O	235	HIS	-	expression tag	UNP P58154
O	236	HIS	-	expression tag	UNP P58154
O	237	HIS	-	expression tag	UNP P58154
P	230	GLY	-	expression tag	UNP P58154
P	231	SER	-	expression tag	UNP P58154
P	232	HIS	-	expression tag	UNP P58154
P	233	HIS	-	expression tag	UNP P58154
P	234	HIS	-	expression tag	UNP P58154
P	235	HIS	-	expression tag	UNP P58154
P	236	HIS	-	expression tag	UNP P58154
P	237	HIS	-	expression tag	UNP P58154
Q	230	GLY	-	expression tag	UNP P58154
Q	231	SER	-	expression tag	UNP P58154
Q	232	HIS	-	expression tag	UNP P58154
Q	233	HIS	-	expression tag	UNP P58154
Q	234	HIS	-	expression tag	UNP P58154
Q	235	HIS	-	expression tag	UNP P58154
Q	236	HIS	-	expression tag	UNP P58154
Q	237	HIS	-	expression tag	UNP P58154
R	230	GLY	-	expression tag	UNP P58154
R	231	SER	-	expression tag	UNP P58154
R	232	HIS	-	expression tag	UNP P58154
R	233	HIS	-	expression tag	UNP P58154
R	234	HIS	-	expression tag	UNP P58154
R	235	HIS	-	expression tag	UNP P58154
R	236	HIS	-	expression tag	UNP P58154
R	237	HIS	-	expression tag	UNP P58154
S	230	GLY	-	expression tag	UNP P58154
S	231	SER	-	expression tag	UNP P58154
S	232	HIS	-	expression tag	UNP P58154
S	233	HIS	-	expression tag	UNP P58154
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S	235	HIS	-	expression tag	UNP P58154
S	236	HIS	-	expression tag	UNP P58154
S	237	HIS	-	expression tag	UNP P58154
T	230	GLY	-	expression tag	UNP P58154
T	231	SER	-	expression tag	UNP P58154
T	232	HIS	-	expression tag	UNP P58154
T	233	HIS	-	expression tag	UNP P58154
T	234	HIS	-	expression tag	UNP P58154

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Chain	Residue	Modelled	Actual	Comment	Reference
T	235	HIS	-	expression tag	UNP P58154
T	236	HIS	-	expression tag	UNP P58154
T	237	HIS	-	expression tag	UNP P58154

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



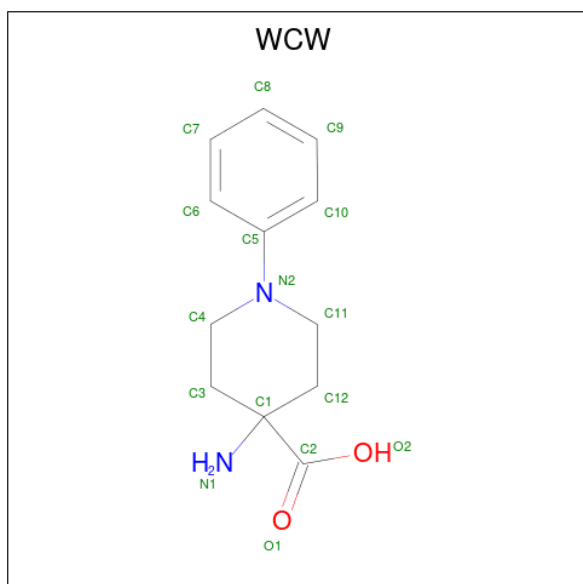
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	E	1	Total	C	N	O	0	0
			14	8	1	5		
2	F	1	Total	C	N	O	0	0
			14	8	1	5		
2	I	1	Total	C	N	O	0	0
			14	8	1	5		
2	J	1	Total	C	N	O	0	0
			14	8	1	5		
2	K	1	Total	C	N	O	0	0
			14	8	1	5		
2	L	1	Total	C	N	O	0	0
			14	8	1	5		
2	M	1	Total	C	N	O	0	0
			14	8	1	5		
2	N	1	Total	C	N	O	0	0
			14	8	1	5		

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Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	O	1	Total	C	N	O	0	0
			14	8	1	5		
2	Q	1	Total	C	N	O	0	0
			14	8	1	5		
2	R	1	Total	C	N	O	0	0
			14	8	1	5		
2	T	1	Total	C	N	O	0	0
			14	8	1	5		

- Molecule 3 is 4-azanyl-1-phenyl-piperidine-4-carboxylic acid (CCD ID: WCW) (formula: $C_{12}H_{16}N_2O_2$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	E	1	Total	C	N	O	0	0
			16	12	2	2		
3	G	1	Total	C	N	O	0	0
			16	12	2	2		
3	I	1	Total	C	N	O	0	0
			16	12	2	2		

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	31	Total	O	0	0
			31	31		
4	B	25	Total	O	0	0
			25	25		

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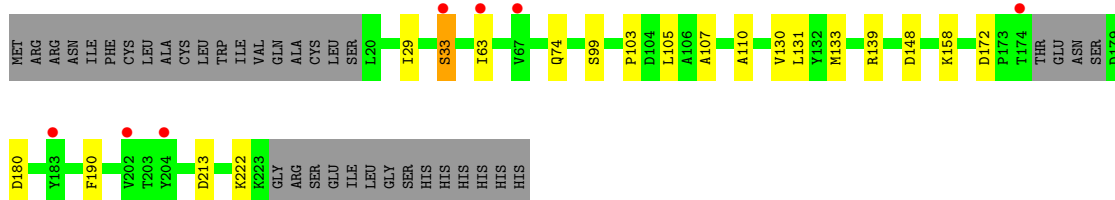
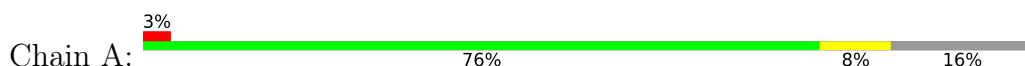
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	C	31	Total 31	O 31	0	0
4	D	37	Total 37	O 37	0	0
4	E	37	Total 37	O 37	0	0
4	F	50	Total 50	O 50	0	0
4	G	59	Total 60	O 60	0	1
4	H	55	Total 55	O 55	0	0
4	I	52	Total 52	O 52	0	0
4	J	56	Total 56	O 56	0	0
4	K	15	Total 15	O 15	0	0
4	L	15	Total 15	O 15	0	0
4	M	29	Total 29	O 29	0	0
4	N	36	Total 36	O 36	0	0
4	O	35	Total 35	O 35	0	0
4	P	17	Total 17	O 17	0	0
4	Q	28	Total 28	O 28	0	0
4	R	37	Total 37	O 37	0	0
4	S	31	Total 31	O 31	0	0
4	T	27	Total 27	O 27	0	0

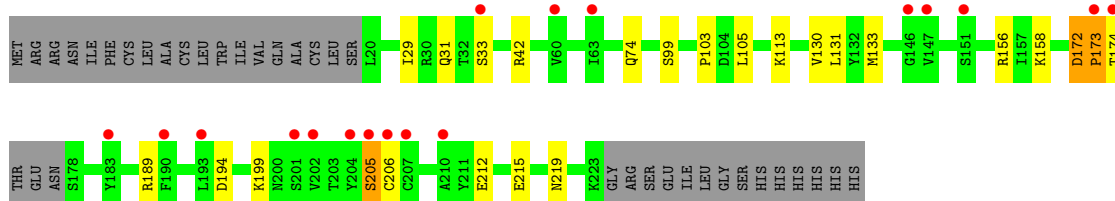
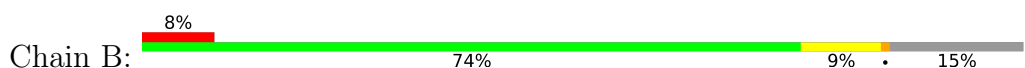
3 Residue-property plots [i](#)

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.

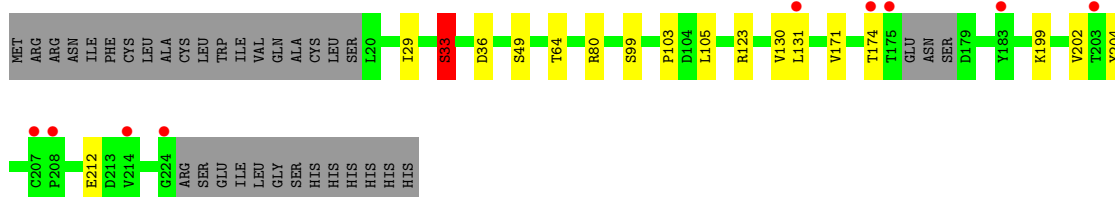
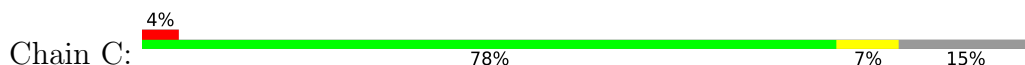
- Molecule 1: Acetylcholine-binding protein



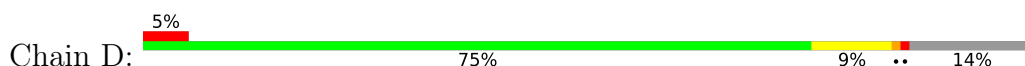
- Molecule 1: Acetylcholine-binding protein

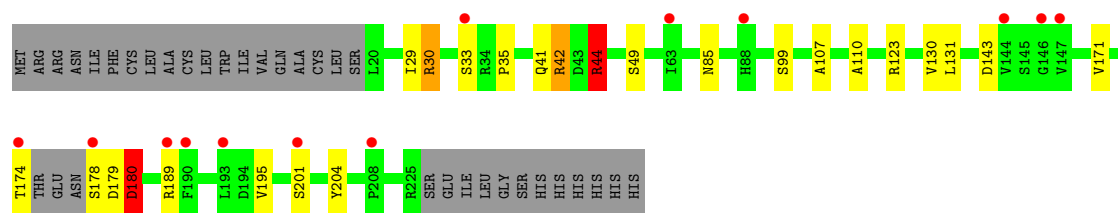


- Molecule 1: Acetylcholine-binding protein

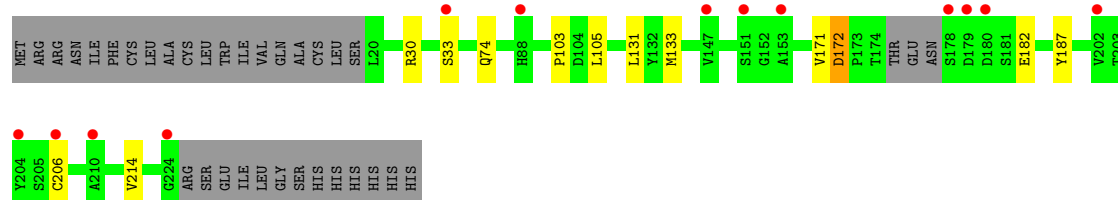
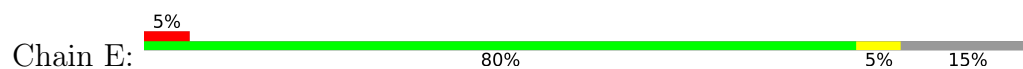


- Molecule 1: Acetylcholine-binding protein

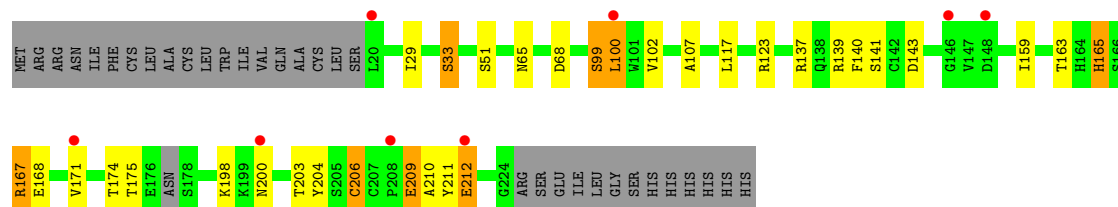




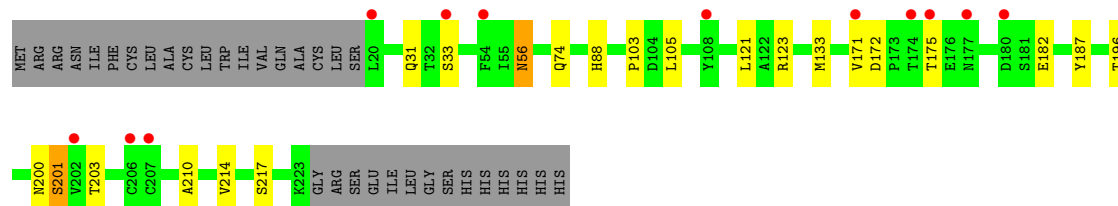
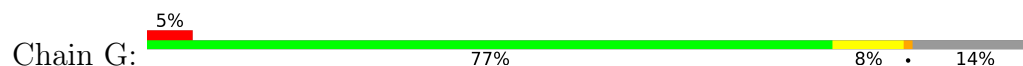
• Molecule 1: Acetylcholine-binding protein



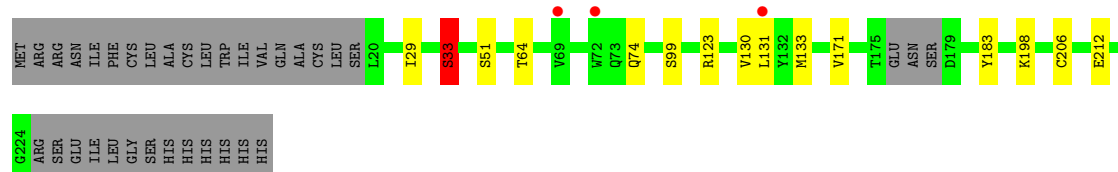
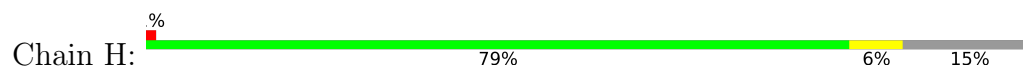
• Molecule 1: Acetylcholine-binding protein



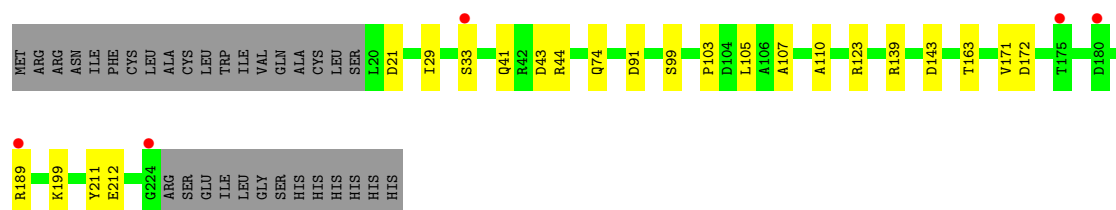
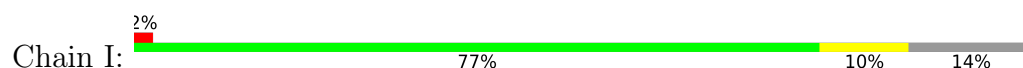
• Molecule 1: Acetylcholine-binding protein



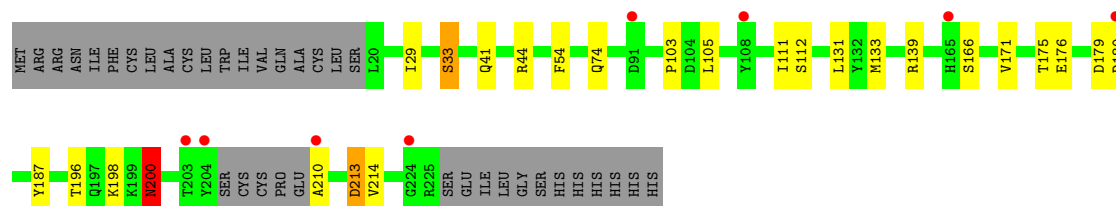
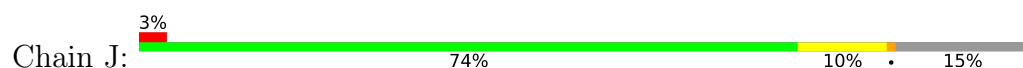
• Molecule 1: Acetylcholine-binding protein



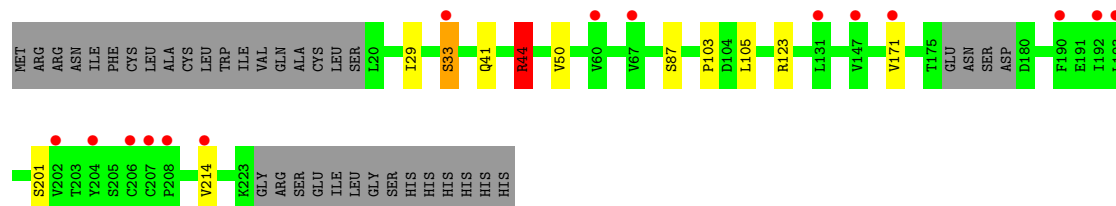
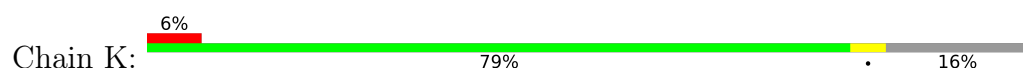
- Molecule 1: Acetylcholine-binding protein



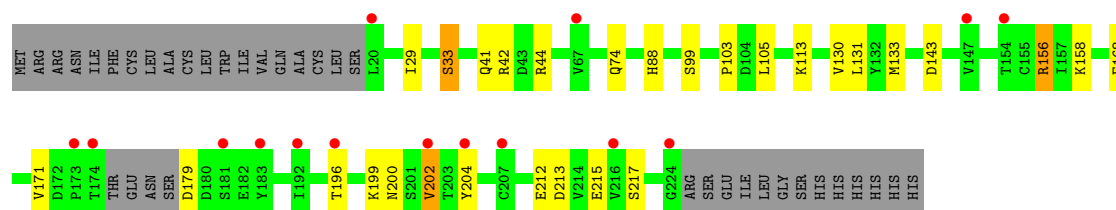
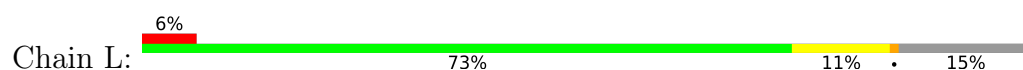
- Molecule 1: Acetylcholine-binding protein



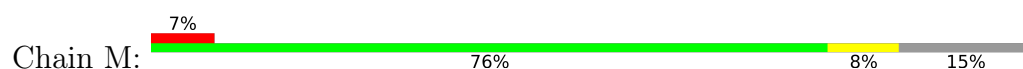
- Molecule 1: Acetylcholine-binding protein

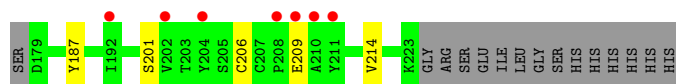


- Molecule 1: Acetylcholine-binding protein



- Molecule 1: Acetylcholine-binding protein

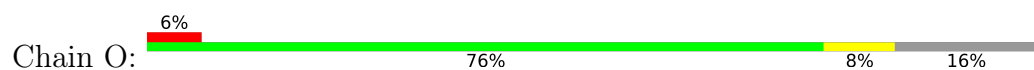




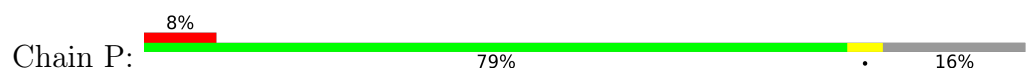
- Molecule 1: Acetylcholine-binding protein



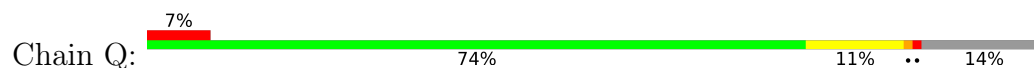
- Molecule 1: Acetylcholine-binding protein



- Molecule 1: Acetylcholine-binding protein

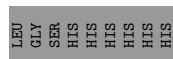
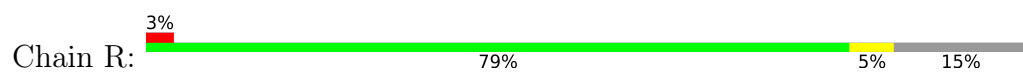


- Molecule 1: Acetylcholine-binding protein

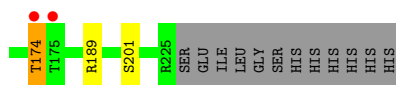
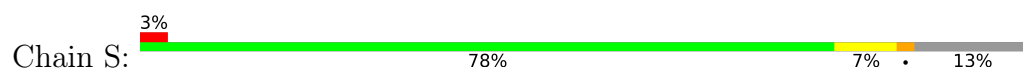


- Molecule 1: Acetylcholine-binding protein

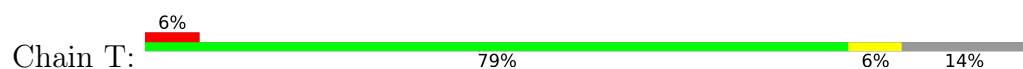




- Molecule 1: Acetylcholine-binding protein



- Molecule 1: Acetylcholine-binding protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	116.71Å 140.71Å 147.17Å 90.00° 109.68° 90.00°	Depositor
Resolution (Å)	49.37 – 2.10 49.37 – 2.10	Depositor EDS
% Data completeness (in resolution range)	99.7 (49.37-2.10) 99.7 (49.37-2.10)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.48 (at 2.10Å)	Xtriage
Refinement program	REFMAC 5.8.0238	Depositor
R, R_{free}	0.225 , 0.255 0.228 , 0.255	Depositor DCC
R_{free} test set	12970 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	50.2	Xtriage
Anisotropy	0.075	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 40.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	33433	wwPDB-VP
Average B, all atoms (Å ²)	62.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.40% 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: NAG, WCW

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	0/1661	1.21	1/2266 (0.0%)
1	B	1.00	1/1667 (0.1%)	1.26	4/2274 (0.2%)
1	C	0.98	0/1656	1.27	3/2259 (0.1%)
1	D	1.06	2/1658 (0.1%)	1.28	5/2260 (0.2%)
1	E	0.99	0/1647	1.25	2/2246 (0.1%)
1	F	1.13	2/1663 (0.1%)	1.33	6/2268 (0.3%)
1	G	1.11	5/1668 (0.3%)	1.37	6/2277 (0.3%)
1	H	1.01	0/1648	1.26	4/2248 (0.2%)
1	I	1.01	0/1715	1.24	1/2340 (0.0%)
1	J	1.05	2/1669 (0.1%)	1.30	3/2274 (0.1%)
1	K	0.96	1/1663 (0.1%)	1.22	1/2269 (0.0%)
1	L	0.97	0/1641	1.24	5/2238 (0.2%)
1	M	1.02	1/1644 (0.1%)	1.27	3/2243 (0.1%)
1	N	1.02	2/1671 (0.1%)	1.24	3/2279 (0.1%)
1	O	1.01	1/1648 (0.1%)	1.25	3/2248 (0.1%)
1	P	0.97	0/1639	1.21	2/2236 (0.1%)
1	Q	1.02	1/1668 (0.1%)	1.28	5/2277 (0.2%)
1	R	0.99	0/1644	1.25	1/2243 (0.0%)
1	S	1.06	1/1683 (0.1%)	1.28	6/2296 (0.3%)
1	T	0.97	0/1682	1.23	0/2293
All	All	1.02	19/33235 (0.1%)	1.26	64/45334 (0.1%)

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	B	0	2
1	D	0	3
1	E	0	1

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	F	0	2
1	G	0	1
1	J	0	1
1	M	0	1
1	N	0	2
1	Q	0	1
1	S	0	3
All	All	0	17

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	S	42	ARG	C-O	9.88	1.36	1.24
1	F	212	GLU	C-O	8.88	1.34	1.23
1	D	42	ARG	C-O	7.83	1.33	1.24
1	O	180	ASP	C-O	7.46	1.31	1.23
1	G	210	ALA	C-O	-7.15	1.15	1.24
1	B	173	PRO	C-O	-7.03	1.14	1.24
1	M	164	HIS	CE1-NE2	6.88	1.39	1.32
1	N	210	ALA	C-O	6.28	1.31	1.24
1	J	213	ASP	CG-OD1	5.94	1.36	1.25
1	N	41	GLN	N-CA	5.84	1.53	1.46
1	G	203	THR	C-O	-5.79	1.17	1.24
1	K	33	SER	CA-CB	-5.59	1.45	1.53
1	G	200	ASN	C-O	-5.54	1.17	1.23
1	Q	210	ALA	C-O	5.50	1.30	1.24
1	G	33	SER	CA-CB	-5.24	1.45	1.53
1	J	175	THR	C-O	5.22	1.30	1.24
1	D	42	ARG	N-CA	5.22	1.52	1.46
1	F	209	GLU	C-O	-5.21	1.17	1.23
1	G	201	SER	C-O	5.13	1.30	1.23

All (64) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	56	ASN	CA-CB-CG	15.10	127.70	112.60
1	Q	197	GLN	OE1-CD-NE2	-10.60	112.00	122.60
1	C	123	ARG	CG-CD-NE	-9.93	90.17	112.00
1	S	33	SER	N-CA-C	7.95	120.94	111.33
1	O	33	SER	N-CA-C	7.91	120.90	111.33
1	G	123	ARG	CG-CD-NE	-7.63	95.22	112.00
1	F	123	ARG	CG-CD-NE	-7.62	95.25	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	44	ARG	CA-C-O	7.57	126.61	119.72
1	J	200	ASN	CB-CA-C	7.31	122.93	109.70
1	J	33	SER	N-CA-C	7.28	120.14	111.33
1	D	44	ARG	O-C-N	-7.25	114.94	121.39
1	L	156	ARG	CG-CD-NE	-7.19	96.17	112.00
1	P	33	SER	N-CA-C	7.10	119.92	111.33
1	F	175	THR	N-CA-C	-6.68	104.61	112.89
1	O	180	ASP	CA-CB-CG	6.65	119.25	112.60
1	D	180	ASP	CA-CB-CG	6.62	119.22	112.60
1	Q	180	ASP	CA-C-O	-6.47	111.26	120.51
1	S	44	ARG	O-C-N	-6.46	115.64	121.39
1	L	33	SER	N-CA-C	6.34	119.00	111.33
1	Q	167	ARG	CG-CD-NE	6.09	125.41	112.00
1	D	44	ARG	CA-C-O	6.01	125.83	119.69
1	S	44	ARG	CA-C-O	5.97	125.78	119.69
1	J	179	ASP	CA-CB-CG	5.95	118.55	112.60
1	S	42	ARG	CB-CA-C	5.91	122.19	110.42
1	F	167	ARG	CB-CG-CD	5.83	124.71	111.30
1	C	33	SER	N-CA-C	5.83	117.63	111.28
1	B	173	PRO	CA-C-O	-5.79	110.06	120.60
1	G	201	SER	CA-C-O	-5.77	112.68	120.47
1	B	113	LYS	CA-CB-CG	5.76	125.62	114.10
1	M	33	SER	N-CA-C	-5.75	101.34	109.96
1	N	44	ARG	O-C-N	-5.71	115.05	121.79
1	K	44	ARG	CA-CB-CG	5.70	125.49	114.10
1	B	205	SER	CA-C-O	-5.68	112.61	119.49
1	N	174	THR	CA-C-O	-5.67	114.86	120.70
1	O	180	ASP	CB-CA-C	-5.62	102.94	112.00
1	H	33	SER	CA-C-O	-5.62	114.60	120.55
1	Q	113	LYS	CA-CB-CG	5.60	125.30	114.10
1	H	33	SER	N-CA-C	5.57	117.35	111.28
1	G	33	SER	N-CA-C	-5.57	101.61	109.96
1	F	99	SER	CA-C-O	-5.55	112.86	119.35
1	S	174	THR	CA-CB-OG1	-5.51	101.33	109.60
1	F	171	VAL	CA-CB-CG2	5.48	119.72	110.40
1	G	200	ASN	CA-CB-CG	5.38	117.98	112.60
1	R	33	SER	N-CA-C	5.37	117.88	111.71
1	E	172	ASP	CB-CA-C	5.36	116.92	108.88
1	D	180	ASP	N-CA-CB	5.33	117.90	110.07
1	A	180	ASP	CA-CB-CG	5.31	117.91	112.60
1	H	183	TYR	CA-C-N	5.30	128.40	120.87
1	H	183	TYR	C-N-CA	5.30	128.40	120.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	S	33	SER	CA-C-O	-5.27	114.94	120.63
1	P	33	SER	CA-C-O	-5.27	114.94	120.63
1	C	33	SER	CA-C-O	-5.25	114.98	120.55
1	I	172	ASP	CB-CA-C	5.24	116.75	108.88
1	M	166	SER	CA-CB-OG	-5.20	100.69	111.10
1	F	168	GLU	CB-CA-C	5.19	118.36	109.65
1	E	33	SER	N-CA-C	-5.18	102.18	109.96
1	D	42	ARG	CB-CA-C	5.16	120.68	110.42
1	L	179	ASP	CA-C-N	5.15	127.18	120.28
1	L	179	ASP	C-N-CA	5.15	127.18	120.28
1	Q	176	GLU	CB-CA-C	5.12	120.61	110.42
1	B	172	ASP	CA-CB-CG	5.12	117.72	112.60
1	L	33	SER	CA-C-O	-5.08	115.14	120.63
1	G	172	ASP	CB-CA-C	5.02	116.42	108.88
1	M	209	GLU	CA-C-O	-5.01	115.81	121.72

There are no chirality outliers.

All (17) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	205	SER	Mainchain
1	B	206	CYS	Peptide
1	D	41	GLN	Peptide
1	D	44	ARG	Peptide,Mainchain
1	E	206	CYS	Peptide
1	F	165	HIS	Peptide
1	F	206	CYS	Peptide
1	G	201	SER	Mainchain
1	J	200	ASN	Mainchain
1	M	206	CYS	Peptide
1	N	40	THR	Peptide
1	N	44	ARG	Peptide
1	Q	180	ASP	Mainchain
1	S	41	GLN	Peptide
1	S	44	ARG	Peptide,Mainchain

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	1626	0	1575	14	0
1	B	1632	0	1580	18	0
1	C	1618	0	1570	15	0
1	D	1623	0	1571	18	1
1	E	1612	0	1557	6	0
1	F	1628	0	1570	24	0
1	G	1632	0	1575	15	0
1	H	1613	0	1560	12	0
1	I	1673	0	1619	17	2
1	J	1629	0	1589	20	0
1	K	1619	0	1580	7	0
1	L	1606	0	1552	21	3
1	M	1609	0	1556	14	0
1	N	1633	0	1590	18	2
1	O	1610	0	1562	17	1
1	P	1601	0	1562	8	0
1	Q	1632	0	1574	18	0
1	R	1609	0	1556	11	2
1	S	1647	0	1591	16	2
1	T	1647	0	1595	15	1
2	C	14	0	13	0	0
2	E	14	0	13	0	0
2	F	14	0	13	1	0
2	I	14	0	13	0	0
2	J	14	0	13	0	0
2	K	14	0	13	2	0
2	L	14	0	13	0	0
2	M	14	0	13	0	0
2	N	14	0	13	0	0
2	O	14	0	13	0	0
2	Q	14	0	13	0	0
2	R	14	0	13	0	0
2	T	14	0	13	0	0
3	E	16	0	0	0	0
3	G	16	0	0	0	0
3	I	16	0	0	2	0
4	A	31	0	0	1	0
4	B	25	0	0	0	0
4	C	31	0	0	0	0
4	D	37	0	0	0	0
4	E	37	0	0	0	0
4	F	50	0	0	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	G	60	0	0	0	0
4	H	55	0	0	0	0
4	I	52	0	0	2	0
4	J	56	0	0	2	0
4	K	15	0	0	0	0
4	L	15	0	0	1	0
4	M	29	0	0	0	0
4	N	36	0	0	2	0
4	O	35	0	0	0	0
4	P	17	0	0	1	0
4	Q	28	0	0	1	0
4	R	37	0	0	0	0
4	S	31	0	0	1	0
4	T	27	0	0	0	0
All	All	33433	0	31653	257	7

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 4.

All (257) 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:Q:74:GLN:HB2	1:Q:133:MET:HE3	1.18	1.17
1:F:203:THR:HG21	1:N:182:GLU:HG3	1.30	1.11
1:Q:74:GLN:HB2	1:Q:133:MET:CE	1.89	1.02
1:O:150:GLU:HB2	1:S:150:GLU:HG3	1.50	0.93
1:Q:41:GLN:O	1:Q:44:ARG:HG2	1.67	0.92
1:L:41:GLN:O	1:L:44:ARG:HG2	1.68	0.92
1:Q:74:GLN:CB	1:Q:133:MET:HE3	1.99	0.91
1:K:41:GLN:O	1:K:44:ARG:HG3	1.73	0.89
1:J:166:SER:OG	1:J:210:ALA:HB3	1.74	0.87
1:F:206:CYS:SG	1:G:133:MET:HE1	2.17	0.84
1:N:34[B]:ARG:HH22	1:O:27:TYR:HB2	1.48	0.79
1:L:42:ARG:O	1:L:42:ARG:HG3	1.82	0.78
1:Q:51:SER:HA	1:Q:197:GLN:HE22	1.47	0.78
1:S:41:GLN:HG3	1:S:44:ARG:NH2	2.00	0.76
1:A:74:GLN:HB2	1:A:133:MET:HE2	1.68	0.74
1:F:51:SER:HB2	1:F:174:THR:HG22	1.69	0.74
1:F:165:HIS:ND1	1:F:210:ALA:O	2.19	0.73
1:E:171:VAL:HG12	1:E:214:VAL:HG23	1.72	0.72
1:B:219:ASN:OD1	1:T:44:ARG:HD3	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:29:ILE:O	1:N:33[A]:SER:HB3	1.90	0.71
1:D:29:ILE:O	1:D:33:SER:HB3	1.91	0.70
1:A:29:ILE:O	1:A:33[A]:SER:HB3	1.91	0.70
1:Q:29:ILE:O	1:Q:33:SER:HB3	1.91	0.70
1:A:148:ASP:OD1	1:A:222:LYS:HD2	1.91	0.69
1:N:42:ARG:HG3	1:N:43:ASP:N	2.07	0.69
1:B:29:ILE:O	1:B:33[B]:SER:HB3	1.92	0.69
1:F:33:SER:HB2	1:F:99:SER:O	1.94	0.68
1:F:29:ILE:O	1:F:33:SER:HB3	1.93	0.67
1:L:33:SER:HB3	4:L:410:HOH:O	1.93	0.67
1:J:33:SER:HB3	4:J:427:HOH:O	1.94	0.67
1:G:171:VAL:HG12	1:G:214:VAL:HG23	1.77	0.67
1:G:74:GLN:HB2	1:G:133:MET:HE2	1.76	0.67
1:J:166:SER:HG	1:J:210:ALA:HB3	1.60	0.66
1:I:29:ILE:O	1:I:33[A]:SER:HB2	1.98	0.64
1:G:74:GLN:HB2	1:G:133:MET:CE	2.29	0.63
1:M:74:GLN:HG3	1:M:133:MET:HE2	1.80	0.63
1:H:29:ILE:O	1:H:33:SER:HB3	1.99	0.63
1:J:74:GLN:HG3	1:J:133:MET:HE2	1.81	0.63
1:C:29:ILE:O	1:C:33:SER:HB3	1.99	0.62
1:I:41:GLN:O	1:I:44:ARG:HG2	1.99	0.62
1:S:41:GLN:HG3	1:S:44:ARG:HH22	1.62	0.62
1:I:29:ILE:O	1:I:33[B]:SER:HB3	1.99	0.62
1:S:74:GLN:HG3	1:S:133:MET:HE2	1.82	0.62
1:F:100:LEU:HD12	1:F:102:VAL:CG2	2.30	0.61
1:B:33[B]:SER:HB2	1:B:99:SER:O	1.99	0.61
1:Q:33:SER:HB2	1:Q:99:SER:O	2.00	0.61
1:F:203:THR:HG21	1:N:182:GLU:CG	2.21	0.61
1:D:143:ASP:HB2	1:E:187:TYR:CE1	2.36	0.60
1:S:29:ILE:O	1:S:33:SER:HB2	2.02	0.60
1:F:212:GLU:HB3	4:F:422:HOH:O	2.01	0.60
1:I:21:ASP:OD2	4:I:401:HOH:O	2.17	0.60
1:L:156:ARG:HD3	1:L:215:GLU:OE2	2.01	0.60
1:M:171:VAL:HG12	1:M:214:VAL:HG23	1.82	0.60
1:T:74:GLN:HG3	1:T:133:MET:HE2	1.83	0.60
1:E:74:GLN:HG3	1:E:133:MET:HE2	1.84	0.60
1:P:33:SER:HB3	4:P:311:HOH:O	2.01	0.59
1:T:29:ILE:O	1:T:33[A]:SER:HB2	2.03	0.59
1:B:42:ARG:NH1	1:G:88:HIS:CE1	2.71	0.59
1:R:29:ILE:O	1:R:33:SER:HB3	2.02	0.59
1:F:100:LEU:HD12	1:F:102:VAL:HG23	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:29:ILE:O	1:K:33:SER:HB3	2.03	0.58
1:L:74:GLN:HG3	1:L:133:MET:HE2	1.85	0.58
1:N:33[A]:SER:HB2	1:N:99:SER:O	2.03	0.58
1:Q:177:ASN:ND2	4:Q:401:HOH:O	2.36	0.58
1:A:33[A]:SER:HB2	1:A:99:SER:O	2.03	0.58
1:D:33:SER:HB2	1:D:99:SER:O	2.04	0.57
1:F:200:ASN:HA	1:M:201:SER:HB3	1.87	0.57
1:A:190:PHE:CE2	1:A:222:LYS:HG3	2.38	0.56
1:C:64:THR:HG22	1:D:189:ARG:NH1	2.21	0.56
1:C:202:VAL:HG11	1:C:204:TYR:CE2	2.41	0.56
1:O:29:ILE:O	1:O:33:SER:HB2	2.05	0.56
1:O:150:GLU:CB	1:S:150:GLU:HG3	2.31	0.55
1:R:202:VAL:HG11	1:R:204:TYR:CE2	2.41	0.55
1:I:139:ARG:NH1	4:I:402:HOH:O	2.40	0.55
1:P:29:ILE:O	1:P:33:SER:HB2	2.06	0.55
1:F:204:TYR:HA	1:G:182:GLU:OE1	2.06	0.55
1:L:202:VAL:CG1	1:L:204:TYR:CE2	2.90	0.55
1:L:29:ILE:O	1:L:33:SER:HB2	2.06	0.54
1:O:148:ASP:HB3	1:S:148:ASP:HB3	1.88	0.54
1:N:33[B]:SER:OG	1:N:99:SER:O	2.21	0.54
2:K:301:NAG:H3	2:K:301:NAG:C8	2.38	0.54
1:J:139[B]:ARG:NH1	4:J:401:HOH:O	2.40	0.54
1:S:86:SER:HA	1:S:89:SER:OG	2.08	0.54
2:K:301:NAG:H3	2:K:301:NAG:H83	1.89	0.54
1:B:130:VAL:C	1:B:131:LEU:HD12	2.34	0.53
1:T:130:VAL:C	1:T:131:LEU:HD12	2.34	0.53
1:L:158:LYS:HE3	1:L:213:ASP:OD2	2.08	0.53
1:R:64:THR:HG22	1:S:189:ARG:HD2	1.90	0.53
1:B:42:ARG:HH12	1:G:88:HIS:CE1	2.27	0.53
1:L:130:VAL:C	1:L:131:LEU:HD12	2.34	0.53
1:F:163:THR:HG21	1:G:121:LEU:HB2	1.91	0.53
1:O:130:VAL:C	1:O:131:LEU:HD12	2.34	0.53
1:C:130:VAL:C	1:C:131[A]:LEU:HD12	2.34	0.52
1:N:85:ASN:OD1	1:N:87:SER:OG	2.25	0.52
1:D:130:VAL:C	1:D:131:LEU:HD12	2.35	0.52
1:R:130:VAL:C	1:R:131:LEU:HD12	2.34	0.52
1:H:130:VAL:C	1:H:131:LEU:HD12	2.34	0.52
1:R:202:VAL:CG1	1:R:204:TYR:CE2	2.92	0.52
1:A:130:VAL:C	1:A:131:LEU:HD12	2.34	0.52
1:T:131:LEU:HD12	1:T:131:LEU:N	2.25	0.52
1:F:165:HIS:CG	1:F:209:GLU:HB3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:64:THR:HG22	1:I:189:ARG:HD3	1.92	0.51
1:B:131:LEU:HD12	1:B:131:LEU:N	2.25	0.51
1:C:202:VAL:CG1	1:C:204:TYR:CE2	2.93	0.51
1:C:36:ASP:OD2	1:D:30:ARG:NH1	2.43	0.51
1:L:42:ARG:O	1:L:42:ARG:CG	2.52	0.51
1:B:173:PRO:HG2	1:T:199:LYS:HD3	1.93	0.51
1:A:139:ARG:HD2	4:A:322:HOH:O	2.10	0.51
1:M:64:THR:HG22	1:N:189:ARG:HD2	1.92	0.50
1:R:33:SER:OG	1:R:99:SER:O	2.27	0.50
1:H:131:LEU:HD12	1:H:131:LEU:N	2.26	0.50
1:L:131:LEU:HD12	1:L:131:LEU:N	2.26	0.50
1:A:131:LEU:HD12	1:A:131:LEU:N	2.26	0.50
1:F:68:ASP:HB2	1:F:139:ARG:HH11	1.77	0.50
1:L:196:THR:CG2	1:L:217:SER:HB2	2.41	0.50
1:M:34:ARG:HD3	4:N:424:HOH:O	2.12	0.50
1:I:211:TYR:CZ	3:I:301:WCW:C12	2.95	0.50
1:R:131:LEU:HD12	1:R:131:LEU:N	2.27	0.50
1:J:29:ILE:O	1:J:33:SER:HB2	2.11	0.49
1:J:196:THR:CG2	1:J:198:LYS:HE3	2.43	0.49
1:F:165:HIS:HE1	1:F:211:TYR:CD2	2.30	0.49
1:D:131:LEU:HD12	1:D:131:LEU:N	2.27	0.49
1:D:204:TYR:HA	1:E:182:GLU:OE2	2.13	0.49
1:H:33:SER:OG	1:H:99:SER:O	2.28	0.48
1:I:33[B]:SER:HB2	1:I:99:SER:O	2.12	0.48
1:O:131:LEU:HD12	1:O:131:LEU:N	2.27	0.48
1:J:74:GLN:CG	1:J:133:MET:HE2	2.43	0.48
1:C:64:THR:HG22	1:D:189:ARG:CZ	2.43	0.48
1:Q:175:THR:O	1:Q:176:GLU:HB2	2.13	0.48
1:F:137:ARG:HD2	1:J:111:ILE:O	2.13	0.48
1:M:74:GLN:CG	1:M:133:MET:HE2	2.42	0.48
1:T:189:ARG:NH2	1:T:222:LYS:HE2	2.29	0.48
1:A:158:LYS:HE3	1:A:213:ASP:OD2	2.14	0.48
1:E:74:GLN:CG	1:E:133:MET:HE2	2.44	0.48
1:N:42:ARG:HG3	1:N:43:ASP:H	1.75	0.47
1:S:74:GLN:CG	1:S:133:MET:HE2	2.43	0.47
1:O:189:ARG:HB3	1:O:222:LYS:HE3	1.97	0.47
1:O:189:ARG:HE	1:O:222:LYS:HE3	1.79	0.47
1:Q:74:GLN:CG	1:Q:133:MET:HE3	2.44	0.47
1:A:29:ILE:O	1:A:33[B]:SER:HB3	2.14	0.47
1:F:141:SER:CB	1:G:56:ASN:HD21	2.28	0.47
1:H:206:CYS:HB2	1:I:74:GLN:OE1	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:T:74:GLN:CG	1:T:133:MET:HE2	2.43	0.47
1:A:63:ILE:HG22	1:B:189:ARG:HD3	1.97	0.47
1:P:143:ASP:HB2	1:Q:187:TYR:CE1	2.49	0.47
1:M:44:ARG:CG	1:M:45:PRO:HD2	2.44	0.47
1:K:50:VAL:HG13	1:K:214:VAL:HG11	1.96	0.46
1:L:74:GLN:CG	1:L:133:MET:HE2	2.44	0.46
1:M:143:ASP:HB2	1:N:187:TYR:CE1	2.51	0.46
1:N:199:LYS:NZ	4:N:401:HOH:O	2.48	0.46
1:P:34[B]:ARG:HH11	1:Q:23:ALA:HB1	1.81	0.46
1:T:29:ILE:O	1:T:33[B]:SER:HB3	2.16	0.46
1:O:103:PRO:HB2	1:O:105:LEU:HG	1.98	0.46
1:J:196:THR:HG21	1:J:198:LYS:HE3	1.98	0.45
1:D:49:SER:HB3	1:D:174:THR:HG22	1.98	0.45
1:H:171:VAL:O	1:H:171:VAL:HG23	2.17	0.45
1:C:171:VAL:O	1:C:171:VAL:HG23	2.16	0.45
1:G:196:THR:CG2	1:G:217:SER:HB2	2.46	0.45
1:J:171:VAL:HG23	1:J:214:VAL:HG23	1.98	0.45
1:M:34:ARG:NH1	1:N:23:ALA:HB1	2.31	0.45
1:B:31:GLN:HB3	1:G:31:GLN:HB3	1.98	0.45
1:A:148:ASP:OD1	1:A:222:LYS:CD	2.63	0.45
1:C:33:SER:OG	1:C:99:SER:O	2.29	0.45
1:I:143:ASP:HB2	1:J:187:TYR:CE1	2.52	0.45
1:T:171:VAL:HG23	1:T:171:VAL:O	2.16	0.45
1:R:171:VAL:O	1:R:171:VAL:HG23	2.17	0.44
1:C:80:ARG:HH22	2:F:301:NAG:H2	1.81	0.44
1:F:65:ASN:HB2	1:G:187:TYR:O	2.17	0.44
1:I:163:THR:HG22	3:I:301:WCW:C9	2.48	0.44
1:C:49:SER:HB3	1:C:174:THR:HG22	1.99	0.44
1:Q:103:PRO:HB2	1:Q:105:LEU:HG	2.00	0.44
1:B:156:ARG:NH1	1:B:215:GLU:OE1	2.50	0.44
1:J:54:PHE:O	1:J:180:ASP:OD2	2.35	0.44
1:B:103:PRO:HB2	1:B:105:LEU:HG	1.99	0.44
1:H:74:GLN:HG3	1:H:133:MET:HE2	2.00	0.44
1:O:171:VAL:HG23	1:O:171:VAL:O	2.17	0.44
1:P:205:SER:OG	1:Q:182:GLU:OE2	2.29	0.44
1:F:68:ASP:HB2	1:F:139:ARG:NH1	2.32	0.44
1:D:179:ASP:OD1	1:D:179:ASP:O	2.35	0.43
1:L:168:GLU:OE2	1:M:22:ARG:NH1	2.51	0.43
1:L:143:ASP:HB2	1:M:187:TYR:CE1	2.54	0.43
1:Q:51:SER:HB2	1:Q:174:THR:OG1	2.19	0.43
1:T:103:PRO:HB2	1:T:105:LEU:HG	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:GLN:HG3	1:B:133:MET:HE2	2.00	0.43
1:D:189:ARG:HG3	1:D:189:ARG:HH11	1.83	0.43
1:L:103:PRO:HB2	1:L:105:LEU:HG	2.01	0.43
1:D:171:VAL:O	1:D:171:VAL:HG23	2.19	0.43
1:G:103:PRO:HB2	1:G:105:LEU:HG	2.00	0.43
1:O:148:ASP:O	1:S:148:ASP:O	2.37	0.43
1:C:199:LYS:HE3	1:C:212:GLU:OE1	2.18	0.43
1:F:200:ASN:OD1	1:M:201:SER:C	2.62	0.43
1:G:74:GLN:HG3	1:G:133:MET:HE3	2.01	0.43
1:D:180:ASP:HB3	1:D:195:VAL:HB	2.01	0.43
1:J:171:VAL:HG23	1:J:171:VAL:O	2.19	0.43
1:B:219:ASN:OD1	1:T:44:ARG:CD	2.64	0.42
1:S:171:VAL:O	1:S:171:VAL:HG23	2.18	0.42
1:B:199:LYS:HE3	1:B:212:GLU:OE1	2.19	0.42
1:J:200:ASN:HB2	1:J:213:ASP:OD1	2.19	0.42
1:N:171:VAL:O	1:N:171:VAL:HG23	2.18	0.42
1:I:107:ALA:HB3	1:I:110:ALA:HB2	2.01	0.42
1:J:176:GLU:O	1:J:196:THR:HA	2.18	0.42
1:J:41:GLN:NE2	1:J:44:ARG:NH2	2.68	0.42
1:J:103:PRO:HB2	1:J:105:LEU:HG	2.01	0.42
1:K:103:PRO:HB2	1:K:105:LEU:HG	2.01	0.42
1:L:171:VAL:O	1:L:171:VAL:HG23	2.18	0.42
1:P:188:SER:O	1:P:223:LYS:CE	2.67	0.42
1:K:171:VAL:O	1:K:171:VAL:HG23	2.18	0.42
1:A:107:ALA:HB3	1:A:110:ALA:HB2	2.02	0.42
1:B:74:GLN:CG	1:B:133:MET:HE2	2.49	0.42
1:H:74:GLN:CG	1:H:133:MET:HE2	2.49	0.42
1:E:103:PRO:HB2	1:E:105:LEU:HG	2.00	0.42
1:O:179:ASP:OD1	1:O:179:ASP:O	2.38	0.42
1:C:64:THR:HA	1:D:189:ARG:HG3	2.01	0.42
1:L:171:VAL:HG22	1:L:212:GLU:HB3	2.02	0.42
1:O:199:LYS:HE3	1:O:212:GLU:OE1	2.19	0.42
1:S:107:ALA:HB3	1:S:110:ALA:HB2	2.01	0.42
1:I:171:VAL:HG23	1:I:171:VAL:O	2.18	0.42
1:K:123:ARG:HD2	1:K:123:ARG:HA	1.90	0.42
1:L:199:LYS:HE3	1:L:212:GLU:OE1	2.20	0.42
1:T:123:ARG:HD2	1:T:123:ARG:HA	1.91	0.42
1:H:171:VAL:HG22	1:H:212:GLU:HB3	2.01	0.42
1:I:103:PRO:HB2	1:I:105:LEU:HG	2.02	0.42
1:C:103:PRO:HB2	1:C:105:LEU:HG	2.02	0.41
1:D:107:ALA:HB3	1:D:110:ALA:HB2	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:R:171:VAL:HG22	1:R:212:GLU:HB3	2.02	0.41
1:B:194:ASP:HB2	1:T:44:ARG:HD2	2.02	0.41
1:A:103:PRO:HB2	1:A:105:LEU:HG	2.01	0.41
1:I:199:LYS:HE3	1:I:212:GLU:OE1	2.20	0.41
1:N:33[A]:SER:C	1:N:35:PRO:HD3	2.45	0.41
1:Q:156:ARG:NH1	1:Q:215:GLU:OE2	2.43	0.41
1:S:103:PRO:HB2	1:S:105:LEU:HG	2.02	0.41
1:K:50:VAL:CG1	1:K:214:VAL:HG11	2.51	0.41
1:D:33:SER:C	1:D:35:PRO:HD3	2.46	0.41
1:D:123:ARG:HA	1:D:123:ARG:HD2	1.91	0.41
1:F:117:LEU:HD22	1:J:112:SER:C	2.46	0.41
1:H:123:ARG:HA	1:H:123:ARG:HD2	1.91	0.41
1:L:33:SER:OG	1:L:99:SER:O	2.31	0.41
1:N:103:PRO:HB2	1:N:105:LEU:HG	2.03	0.41
1:N:143:ASP:HB2	1:O:187:TYR:CE1	2.55	0.41
1:P:188:SER:O	1:P:223:LYS:HE2	2.20	0.41
1:S:167:ARG:NH1	4:S:303:HOH:O	2.53	0.41
1:J:180:ASP:CG	1:J:180:ASP:O	2.63	0.41
1:F:107:ALA:HB1	1:F:140:PHE:HE2	1.86	0.40
1:O:107:ALA:HB3	1:O:110:ALA:HB2	2.03	0.40
1:H:64:THR:HG22	1:I:189:ARG:CD	2.51	0.40
1:L:196:THR:HG23	1:L:217:SER:HB2	2.04	0.40
1:M:163:THR:HG21	1:N:121:LEU:HB2	2.02	0.40
1:O:123:ARG:HD2	1:O:123:ARG:HA	1.90	0.40
1:R:64:THR:HA	1:S:189:ARG:HG3	2.04	0.40
1:B:158:LYS:HE2	1:B:215:GLU:OE1	2.22	0.40
1:F:143:ASP:HB2	1:G:187:TYR:CE1	2.56	0.40
1:M:123:ARG:HA	1:M:123:ARG:HD2	1.89	0.40
1:I:123:ARG:HA	1:I:123:ARG:HD2	1.90	0.40
1:P:189:ARG:HD2	1:T:64:THR:HG22	2.03	0.40
1:Q:143:ASP:HB2	1:R:187:TYR:CE1	2.56	0.40
1:Q:171:VAL:O	1:Q:171:VAL:HG23	2.21	0.40

All (7) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:L:200:ASN:OD1	1:R:201:SER:OG[2_657]	1.74	0.46
1:L:199:LYS:O	1:R:203:THR:OG1[2_657]	1.91	0.29
1:N:88:HIS:ND1	1:T:42:ARG:NH2[1_455]	1.92	0.28

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:I:43:ASP:OD2	1:N:42:ARG:O[2_556]	1.97	0.23
1:D:201:SER:OG	1:S:201:SER:OG[2_656]	2.02	0.18
1:O:42:ARG:NH2	1:S:88:HIS:NE2[1_455]	2.05	0.15
1:I:91:ASP:OD2	1:L:88:HIS:NE2[1_554]	2.18	0.02

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	199/237 (84%)	197 (99%)	2 (1%)	0	100	100
1	B	200/237 (84%)	194 (97%)	6 (3%)	0	100	100
1	C	199/237 (84%)	197 (99%)	2 (1%)	0	100	100
1	D	199/237 (84%)	196 (98%)	2 (1%)	1 (0%)	24	22
1	E	198/237 (84%)	196 (99%)	2 (1%)	0	100	100
1	F	200/237 (84%)	197 (98%)	3 (2%)	0	100	100
1	G	202/237 (85%)	199 (98%)	2 (1%)	1 (0%)	24	22
1	H	198/237 (84%)	196 (99%)	2 (1%)	0	100	100
1	I	208/237 (88%)	205 (99%)	3 (1%)	0	100	100
1	J	199/237 (84%)	196 (98%)	3 (2%)	0	100	100
1	K	199/237 (84%)	196 (98%)	3 (2%)	0	100	100
1	L	197/237 (83%)	195 (99%)	2 (1%)	0	100	100
1	M	197/237 (83%)	194 (98%)	3 (2%)	0	100	100
1	N	200/237 (84%)	199 (100%)	1 (0%)	0	100	100
1	O	197/237 (83%)	196 (100%)	1 (0%)	0	100	100
1	P	196/237 (83%)	195 (100%)	1 (0%)	0	100	100
1	Q	202/237 (85%)	197 (98%)	3 (2%)	2 (1%)	12	9
1	R	197/237 (83%)	195 (99%)	2 (1%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	S	204/237 (86%)	202 (99%)	0	2 (1%)	12	9
1	T	202/237 (85%)	199 (98%)	3 (2%)	0	100	100
All	All	3993/4740 (84%)	3941 (99%)	46 (1%)	6 (0%)	43	44

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	G	175	THR
1	S	174	THR
1	D	42	ARG
1	S	42	ARG
1	Q	180	ASP
1	Q	176	GLU

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	190/220 (86%)	187 (98%)	3 (2%)	55	64
1	B	191/220 (87%)	189 (99%)	2 (1%)	68	76
1	C	189/220 (86%)	188 (100%)	1 (0%)	81	88
1	D	189/220 (86%)	184 (97%)	5 (3%)	40	46
1	E	188/220 (86%)	185 (98%)	3 (2%)	55	64
1	F	190/220 (86%)	185 (97%)	5 (3%)	40	46
1	G	191/220 (87%)	191 (100%)	0	100	100
1	H	188/220 (86%)	185 (98%)	3 (2%)	55	64
1	I	196/220 (89%)	196 (100%)	0	100	100
1	J	189/220 (86%)	188 (100%)	1 (0%)	81	88
1	K	190/220 (86%)	187 (98%)	3 (2%)	55	64
1	L	187/220 (85%)	185 (99%)	2 (1%)	65	74
1	M	188/220 (86%)	186 (99%)	2 (1%)	65	74

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	N	191/220 (87%)	188 (98%)	3 (2%)	55	64
1	O	188/220 (86%)	188 (100%)	0	100	100
1	P	187/220 (85%)	184 (98%)	3 (2%)	55	64
1	Q	191/220 (87%)	187 (98%)	4 (2%)	47	54
1	R	188/220 (86%)	186 (99%)	2 (1%)	65	74
1	S	192/220 (87%)	191 (100%)	1 (0%)	81	88
1	T	192/220 (87%)	190 (99%)	2 (1%)	68	76
All	All	3795/4400 (86%)	3750 (99%)	45 (1%)	65	72

All (45) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33[A]	SER
1	A	33[B]	SER
1	A	172	ASP
1	B	172	ASP
1	B	174	THR
1	C	33	SER
1	D	30	ARG
1	D	44	ARG
1	D	85	ASN
1	D	178	SER
1	D	180	ASP
1	E	30	ARG
1	E	131	LEU
1	E	172	ASP
1	F	33	SER
1	F	100	LEU
1	F	159	ILE
1	F	167	ARG
1	F	198	LYS
1	H	33	SER
1	H	51	SER
1	H	198	LYS
1	J	131	LEU
1	K	44	ARG
1	K	87	SER
1	K	201	SER
1	L	113	LYS
1	L	202	VAL

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Mol	Chain	Res	Type
1	M	87	SER
1	M	123	ARG
1	N	20	LEU
1	N	87	SER
1	N	123	ARG
1	P	123	ARG
1	P	172	ASP
1	P	199	LYS
1	Q	33	SER
1	Q	43	ASP
1	Q	131	LEU
1	Q	178	SER
1	R	33	SER
1	R	123	ARG
1	S	131	LEU
1	T	33[A]	SER
1	T	33[B]	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (36) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	41	GLN
1	A	73	GLN
1	C	31	GLN
1	C	41	GLN
1	C	73	GLN
1	C	74	GLN
1	D	73	GLN
1	E	56	ASN
1	E	73	GLN
1	E	219	ASN
1	F	41	GLN
1	G	56	ASN
1	G	88	HIS
1	H	31	GLN
1	H	73	GLN
1	I	41	GLN
1	I	73	GLN
1	J	31	GLN
1	J	41	GLN
1	J	56	ASN
1	K	73	GLN

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Mol	Chain	Res	Type
1	L	74	GLN
1	L	219	ASN
1	M	41	GLN
1	M	73	GLN
1	N	56	ASN
1	N	73	GLN
1	O	56	ASN
1	O	73	GLN
1	P	73	GLN
1	Q	73	GLN
1	Q	74	GLN
1	Q	219	ASN
1	R	73	GLN
1	S	73	GLN
1	T	73	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

16 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
2	NAG	E	302	1	14,14,15	0.68	0	17,19,21	1.20	2 (11%)
2	NAG	M	301	1	14,14,15	0.88	0	17,19,21	2.23	5 (29%)
2	NAG	L	301	1	14,14,15	0.41	0	17,19,21	1.60	3 (17%)
2	NAG	R	301	1	14,14,15	0.66	0	17,19,21	1.28	1 (5%)
2	NAG	T	301	1	14,14,15	0.72	0	17,19,21	1.44	3 (17%)
3	WCW	I	301	-	15,17,17	0.71	1 (6%)	19,24,24	1.31	5 (26%)
2	NAG	C	301	1	14,14,15	0.61	0	17,19,21	1.23	2 (11%)
3	WCW	E	301	-	15,17,17	0.93	1 (6%)	19,24,24	1.21	2 (10%)
2	NAG	N	301	1	14,14,15	0.53	0	17,19,21	1.35	1 (5%)
2	NAG	Q	301	1	14,14,15	0.67	0	17,19,21	1.51	3 (17%)
2	NAG	I	302	1	14,14,15	0.71	0	17,19,21	1.66	5 (29%)
2	NAG	J	301	1	14,14,15	0.59	0	17,19,21	0.73	0
3	WCW	G	301	-	15,17,17	0.76	1 (6%)	19,24,24	1.36	2 (10%)
2	NAG	O	301	1	14,14,15	0.82	0	17,19,21	1.83	3 (17%)
2	NAG	K	301	1	14,14,15	0.97	1 (7%)	17,19,21	2.87	7 (41%)
2	NAG	F	301	1	14,14,15	0.57	0	17,19,21	1.80	3 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	E	302	1	-	0/6/23/26	0/1/1/1
2	NAG	M	301	1	-	1/6/23/26	0/1/1/1
2	NAG	L	301	1	-	0/6/23/26	0/1/1/1
2	NAG	R	301	1	-	0/6/23/26	0/1/1/1
2	NAG	T	301	1	-	2/6/23/26	0/1/1/1
3	WCW	I	301	-	-	4/9/22/22	0/2/2/2
2	NAG	C	301	1	-	0/6/23/26	0/1/1/1
3	WCW	E	301	-	-	0/9/22/22	0/2/2/2
2	NAG	N	301	1	-	2/6/23/26	0/1/1/1
2	NAG	Q	301	1	-	0/6/23/26	0/1/1/1
2	NAG	I	302	1	-	2/6/23/26	0/1/1/1
2	NAG	J	301	1	-	0/6/23/26	0/1/1/1
3	WCW	G	301	-	-	5/9/22/22	0/2/2/2
2	NAG	O	301	1	-	2/6/23/26	0/1/1/1
2	NAG	K	301	1	-	3/6/23/26	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	F	301	1	-	1/6/23/26	0/1/1/1

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	E	301	WCW	O2-C2	-2.50	1.21	1.30
3	G	301	WCW	O2-C2	-2.22	1.22	1.30
2	K	301	NAG	C1-C2	2.20	1.55	1.52
3	I	301	WCW	O2-C2	-2.14	1.22	1.30

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	K	301	NAG	C2-N2-C7	7.49	132.93	122.90
2	F	301	NAG	C1-O5-C5	6.00	120.22	112.19
2	M	301	NAG	C2-N2-C7	5.27	129.96	122.90
2	K	301	NAG	C8-C7-N2	5.05	124.49	116.12
2	N	301	NAG	C1-O5-C5	4.37	118.04	112.19
2	O	301	NAG	C1-C2-N2	4.29	117.19	110.43
2	M	301	NAG	C1-C2-N2	-4.25	103.73	110.43
2	O	301	NAG	C3-C4-C5	4.10	117.67	110.23
2	Q	301	NAG	C1-C2-N2	3.94	116.63	110.43
2	L	301	NAG	C1-C2-N2	-3.82	104.41	110.43
2	L	301	NAG	C3-C4-C5	3.61	116.77	110.23
2	T	301	NAG	O5-C1-C2	-3.55	105.80	111.29
2	K	301	NAG	C4-C3-C2	3.44	116.06	111.02
2	K	301	NAG	O5-C1-C2	3.38	116.53	111.29
2	C	301	NAG	C1-O5-C5	3.33	116.65	112.19
2	M	301	NAG	C4-C3-C2	3.28	115.83	111.02
2	O	301	NAG	C4-C3-C2	3.27	115.82	111.02
3	G	301	WCW	O2-C2-C1	3.26	122.39	113.69
2	R	301	NAG	O5-C5-C6	3.20	113.89	107.66
2	I	302	NAG	C2-N2-C7	3.02	126.95	122.90
3	G	301	WCW	O1-C2-C1	-3.01	114.94	122.73
2	T	301	NAG	C3-C4-C5	2.98	115.64	110.23
2	K	301	NAG	O7-C7-C8	-2.94	116.82	122.05
2	I	302	NAG	C3-C4-C5	2.79	115.28	110.23
2	I	302	NAG	C1-C2-N2	-2.77	106.07	110.43
3	E	301	WCW	O2-C2-C1	2.74	121.01	113.69
2	M	301	NAG	O5-C5-C4	-2.70	104.27	110.83
2	Q	301	NAG	C2-N2-C7	2.66	126.46	122.90
2	Q	301	NAG	C1-O5-C5	2.61	115.69	112.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	301	WCW	O2-C2-C1	2.58	120.56	113.69
3	I	301	WCW	C4-N2-C5	2.57	125.12	118.11
2	K	301	NAG	O5-C5-C4	-2.57	104.58	110.83
2	E	302	NAG	C2-N2-C7	2.57	126.34	122.90
3	I	301	WCW	O1-C2-C1	-2.56	116.11	122.73
2	F	301	NAG	C1-C2-N2	2.44	114.27	110.43
2	I	302	NAG	C8-C7-N2	2.33	119.97	116.12
2	M	301	NAG	C6-C5-C4	2.32	118.71	113.02
3	E	301	WCW	C4-N2-C5	2.28	124.31	118.11
3	I	301	WCW	C4-C3-C1	2.25	115.03	112.95
2	T	301	NAG	O3-C3-C2	2.21	114.00	109.40
2	I	302	NAG	O5-C5-C6	2.13	111.81	107.66
2	K	301	NAG	C1-C2-N2	-2.13	107.08	110.43
2	L	301	NAG	C4-C3-C2	2.11	114.11	111.02
2	E	302	NAG	O5-C5-C6	2.10	111.75	107.66
2	F	301	NAG	O5-C1-C2	-2.05	108.12	111.29
3	I	301	WCW	C11-N2-C5	2.04	123.67	118.11
2	C	301	NAG	O5-C5-C6	2.03	111.61	107.66

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	K	301	NAG	C3-C2-N2-C7
2	M	301	NAG	C3-C2-N2-C7
3	G	301	WCW	N1-C1-C2-O2
3	I	301	WCW	N1-C1-C2-O2
2	N	301	NAG	C4-C5-C6-O6
2	O	301	NAG	C4-C5-C6-O6
2	O	301	NAG	O5-C5-C6-O6
2	N	301	NAG	O5-C5-C6-O6
2	I	302	NAG	C8-C7-N2-C2
2	I	302	NAG	O7-C7-N2-C2
2	K	301	NAG	C8-C7-N2-C2
2	K	301	NAG	O7-C7-N2-C2
2	T	301	NAG	C4-C5-C6-O6
3	G	301	WCW	C10-C5-N2-C11
3	G	301	WCW	C6-C5-N2-C11
2	T	301	NAG	O5-C5-C6-O6
3	G	301	WCW	C6-C5-N2-C4
3	G	301	WCW	C10-C5-N2-C4
3	I	301	WCW	C12-C1-C2-O1

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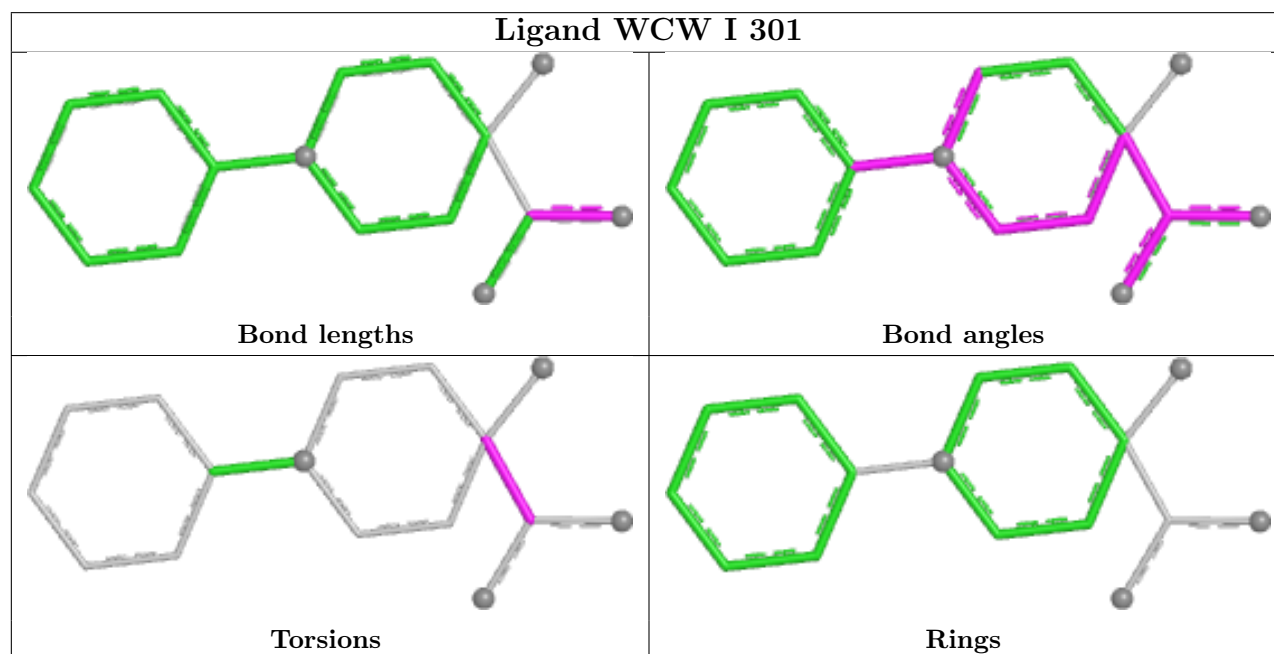
Mol	Chain	Res	Type	Atoms
3	I	301	WCW	C12-C1-C2-O2
2	F	301	NAG	C4-C5-C6-O6
3	I	301	WCW	C3-C1-C2-O2

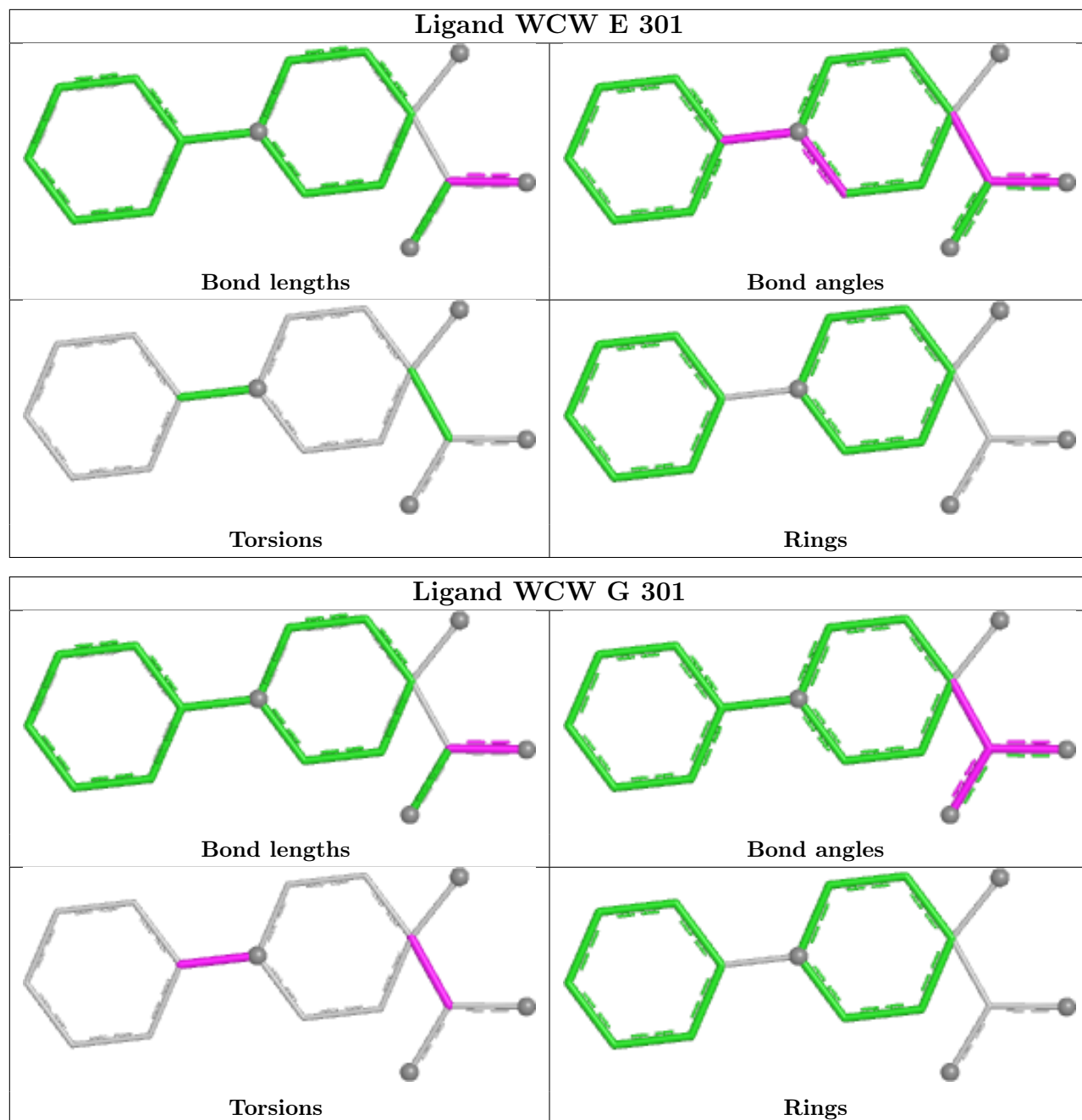
There are no ring outliers.

3 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	I	301	WCW	2	0
2	K	301	NAG	2	0
2	F	301	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 ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ > 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q < 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ > 2			OWAB(Å ²)	Q < 0.9
1	A	200/237 (84%)	0.57	7 (3%)	47	49	24, 56, 96, 117	3 (1%)
1	B	201/237 (84%)	0.85	18 (8%)	15	16	27, 59, 104, 145	3 (1%)
1	C	202/237 (85%)	0.64	9 (4%)	38	40	32, 59, 94, 120	1 (0%)
1	D	203/237 (85%)	0.59	13 (6%)	25	27	38, 58, 105, 148	0
1	E	202/237 (85%)	0.55	13 (6%)	25	27	39, 56, 97, 143	0
1	F	204/237 (86%)	0.56	8 (3%)	43	45	38, 53, 89, 106	0
1	G	204/237 (86%)	0.48	12 (5%)	28	30	37, 51, 87, 126	0
1	H	202/237 (85%)	0.28	3 (1%)	72	74	35, 49, 79, 112	0
1	I	205/237 (86%)	0.32	5 (2%)	59	62	21, 47, 78, 142	5 (2%)
1	J	201/237 (84%)	0.38	8 (3%)	42	44	26, 49, 85, 99	2 (0%)
1	K	200/237 (84%)	0.86	15 (7%)	20	21	30, 68, 119, 185	3 (1%)
1	L	201/237 (84%)	0.89	15 (7%)	20	21	44, 70, 110, 164	0
1	M	201/237 (84%)	0.77	16 (7%)	18	19	40, 62, 101, 128	0
1	N	200/237 (84%)	0.53	10 (5%)	34	36	25, 55, 89, 116	4 (2%)
1	O	200/237 (84%)	0.67	14 (7%)	22	24	27, 58, 106, 137	1 (0%)
1	P	199/237 (83%)	0.77	19 (9%)	14	14	27, 65, 105, 142	1 (0%)
1	Q	204/237 (86%)	0.82	16 (7%)	19	20	42, 60, 114, 144	0
1	R	201/237 (84%)	0.56	6 (2%)	52	55	40, 59, 92, 130	0
1	S	206/237 (86%)	0.42	6 (2%)	53	56	39, 54, 100, 128	0
1	T	203/237 (85%)	0.71	14 (6%)	23	24	24, 59, 109, 152	3 (1%)
All	All	4039/4740 (85%)	0.61	227 (5%)	30	32	21, 57, 100, 185	26 (0%)

All (227) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	M	211	TYR	5.9
1	B	204	TYR	5.8
1	T	210	ALA	4.7
1	M	210	ALA	4.7
1	Q	202	VAL	4.4
1	K	207	CYS	4.0
1	Q	175	THR	3.9
1	D	189	ARG	3.9
1	I	33[A]	SER	3.8
1	A	33[A]	SER	3.8
1	A	204	TYR	3.7
1	L	224	GLY	3.7
1	C	203	THR	3.6
1	T	202	VAL	3.6
1	I	175	THR	3.6
1	M	208	PRO	3.6
1	R	20	LEU	3.6
1	K	214	VAL	3.6
1	B	63	ILE	3.5
1	L	192	ILE	3.5
1	B	173	PRO	3.5
1	K	204	TYR	3.5
1	L	202	VAL	3.5
1	I	224	GLY	3.4
1	T	33[A]	SER	3.4
1	L	174	THR	3.4
1	J	108	TYR	3.4
1	P	131	LEU	3.3
1	K	208	PRO	3.2
1	R	175	THR	3.2
1	K	33	SER	3.2
1	M	33	SER	3.2
1	C	131[A]	LEU	3.2
1	F	100	LEU	3.1
1	Q	206	CYS	3.1
1	N	180	ASP	3.1
1	B	33[A]	SER	3.1
1	N	33[A]	SER	3.1
1	Q	207	CYS	3.1
1	K	131[A]	LEU	3.1
1	N	131	LEU	3.0
1	Q	214	VAL	3.0
1	G	207	CYS	3.0

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Mol	Chain	Res	Type	RSRZ
1	J	210	ALA	3.0
1	A	174	THR	2.9
1	Q	211	TYR	2.9
1	B	202	VAL	2.9
1	M	165	HIS	2.9
1	C	183	TYR	2.9
1	M	20	LEU	2.9
1	G	180	ASP	2.9
1	F	212	GLU	2.9
1	M	72	TRP	2.9
1	B	207	CYS	2.8
1	E	147	VAL	2.8
1	K	192	ILE	2.8
1	J	165	HIS	2.8
1	E	210	ALA	2.8
1	K	206	CYS	2.8
1	O	174	THR	2.8
1	R	207	CYS	2.8
1	P	208	PRO	2.8
1	T	211	TYR	2.8
1	M	209	GLU	2.8
1	Q	210	ALA	2.8
1	B	174	THR	2.8
1	L	147	VAL	2.8
1	M	63	ILE	2.8
1	H	72	TRP	2.8
1	R	63	ILE	2.7
1	M	204	TYR	2.7
1	E	33	SER	2.7
1	I	180	ASP	2.7
1	I	189	ARG	2.7
1	O	89	SER	2.7
1	O	57	ILE	2.7
1	Q	171	VAL	2.7
1	B	151	SER	2.6
1	E	178	SER	2.6
1	B	147	VAL	2.6
1	E	204	TYR	2.6
1	B	206	CYS	2.6
1	J	224	GLY	2.6
1	D	88	HIS	2.6
1	F	208	PRO	2.6

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Mol	Chain	Res	Type	RSRZ
1	P	183	TYR	2.6
1	T	174	THR	2.6
1	L	183	TYR	2.5
1	N	204	TYR	2.5
1	G	33	SER	2.5
1	Q	198	LYS	2.5
1	C	208	PRO	2.5
1	C	224	GLY	2.5
1	F	146	GLY	2.5
1	Q	197	GLN	2.5
1	C	175	THR	2.5
1	D	174	THR	2.5
1	D	201	SER	2.5
1	L	196	THR	2.5
1	N	203	THR	2.5
1	P	174	THR	2.5
1	A	202	VAL	2.4
1	K	202	VAL	2.4
1	O	204	TYR	2.4
1	P	207	CYS	2.4
1	E	151	SER	2.4
1	R	201	SER	2.4
1	S	175	THR	2.4
1	E	153	ALA	2.4
1	G	20	LEU	2.4
1	K	67	VAL	2.4
1	M	147	VAL	2.4
1	T	178	SER	2.4
1	B	193	LEU	2.4
1	E	88	HIS	2.4
1	G	177	ASN	2.4
1	K	147	VAL	2.4
1	K	171	VAL	2.4
1	O	144	VAL	2.4
1	Q	33	SER	2.4
1	C	207	CYS	2.4
1	L	207	CYS	2.4
1	O	153	ALA	2.4
1	Q	91	ASP	2.4
1	S	159	ILE	2.4
1	T	195	VAL	2.4
1	L	173	PRO	2.4

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Mol	Chain	Res	Type	RSRZ
1	T	206	CYS	2.4
1	O	20	LEU	2.3
1	O	58	LEU	2.3
1	T	20	LEU	2.3
1	Q	180	ASP	2.3
1	B	60	VAL	2.3
1	F	171	VAL	2.3
1	L	67	VAL	2.3
1	L	181	SER	2.3
1	P	171	VAL	2.3
1	L	204	TYR	2.3
1	T	204	TYR	2.3
1	A	63	ILE	2.3
1	D	144	VAL	2.3
1	G	171	VAL	2.3
1	M	202	VAL	2.3
1	O	202	VAL	2.3
1	J	203	THR	2.3
1	Q	201	SER	2.3
1	P	202	VAL	2.3
1	G	175	THR	2.3
1	P	154	THR	2.3
1	G	206	CYS	2.3
1	B	210	ALA	2.3
1	E	224	GLY	2.3
1	R	204	TYR	2.3
1	M	169	ILE	2.2
1	D	147	VAL	2.2
1	E	202	VAL	2.2
1	P	144	VAL	2.2
1	P	175	THR	2.2
1	F	200	ASN	2.2
1	O	180	ASP	2.2
1	M	166	SER	2.2
1	C	174	THR	2.2
1	P	63	ILE	2.2
1	J	91	ASP	2.2
1	T	43	ASP	2.2
1	A	183	TYR	2.2
1	B	201	SER	2.2
1	S	42	ARG	2.2
1	S	44	ARG	2.2

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Mol	Chain	Res	Type	RSRZ
1	P	214	VAL	2.2
1	N	58	LEU	2.2
1	O	206	CYS	2.2
1	G	108	TYR	2.2
1	E	179	ASP	2.2
1	J	180	ASP	2.2
1	S	174	THR	2.2
1	D	190	PHE	2.1
1	C	214	VAL	2.1
1	O	210	ALA	2.1
1	M	58	LEU	2.1
1	P	58	LEU	2.1
1	P	206	CYS	2.1
1	N	175	THR	2.1
1	T	173	PRO	2.1
1	D	63	ILE	2.1
1	M	192	ILE	2.1
1	P	220	PHE	2.1
1	Q	159	ILE	2.1
1	T	147	VAL	2.1
1	T	171	VAL	2.1
1	B	205	SER	2.1
1	F	20	LEU	2.1
1	H	131	LEU	2.1
1	N	20	LEU	2.1
1	F	148	ASP	2.1
1	J	204	TYR	2.1
1	Q	203	THR	2.1
1	G	54	PHE	2.1
1	G	202	VAL	2.1
1	P	147	VAL	2.1
1	E	180	ASP	2.1
1	O	179	ASP	2.1
1	G	174	THR	2.1
1	P	203	THR	2.1
1	P	204	TYR	2.1
1	N	63	ILE	2.1
1	A	67	VAL	2.1
1	B	190	PHE	2.1
1	K	60	VAL	2.1
1	K	190	PHE	2.1
1	L	216	VAL	2.1

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Mol	Chain	Res	Type	RSRZ
1	N	202	VAL	2.1
1	K	193	LEU	2.0
1	E	206	CYS	2.0
1	D	146	GLY	2.0
1	H	69	VAL	2.0
1	S	60	VAL	2.0
1	D	33	SER	2.0
1	D	178	SER	2.0
1	D	193	LEU	2.0
1	L	20	LEU	2.0
1	O	88	HIS	2.0
1	D	208	PRO	2.0
1	L	154	THR	2.0
1	P	196	THR	2.0
1	B	146	GLY	2.0
1	B	183	TYR	2.0

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

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

6.3 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

6.4 Ligands [i](#)

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

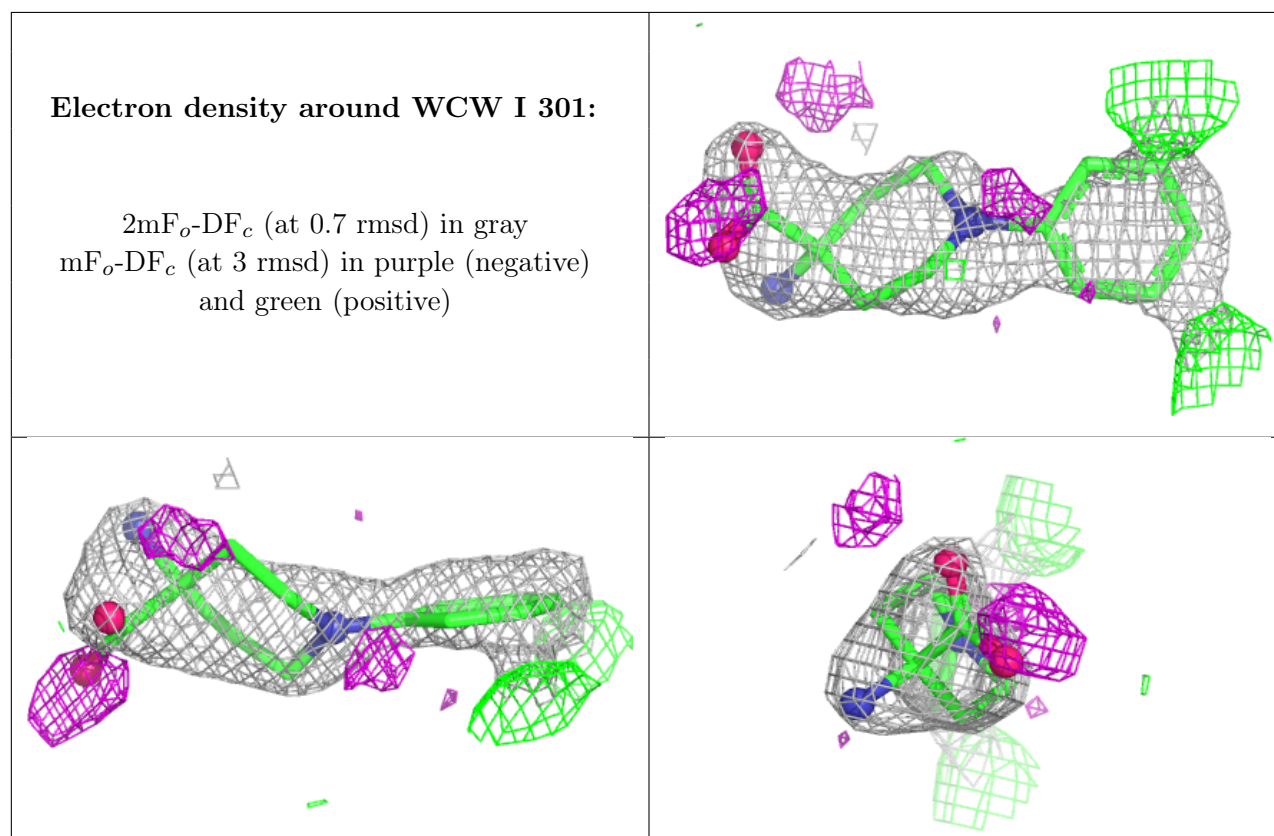
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	E	302	14/15	0.34	0.18	93,121,133,138	0
2	NAG	K	301	14/15	0.46	0.13	91,109,113,117	0
2	NAG	J	301	14/15	0.51	0.14	121,133,139,140	0
2	NAG	N	301	14/15	0.56	0.13	113,123,127,128	0
2	NAG	O	301	14/15	0.58	0.15	84,119,130,131	0
2	NAG	C	301	14/15	0.61	0.12	107,122,129,130	0
2	NAG	M	301	14/15	0.61	0.12	96,107,115,119	0

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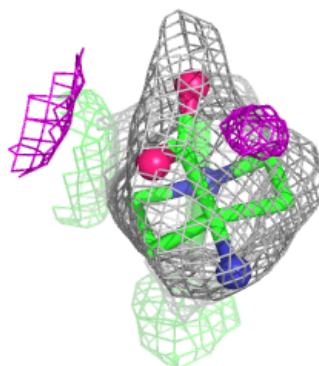
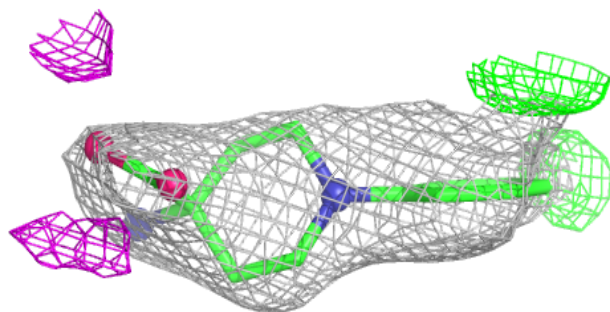
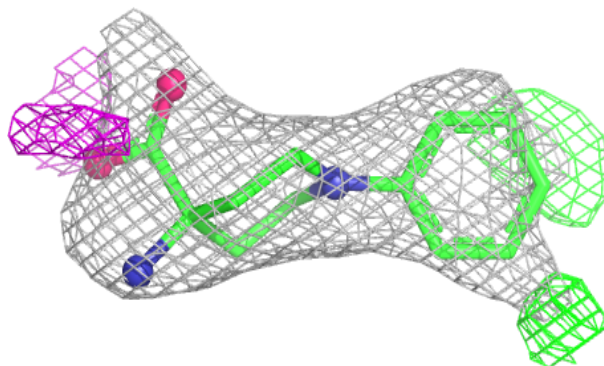
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	NAG	Q	301	14/15	0.61	0.13	100,117,121,124	0
2	NAG	T	301	14/15	0.61	0.15	96,125,133,135	0
2	NAG	R	301	14/15	0.64	0.13	88,118,124,125	0
2	NAG	I	302	14/15	0.67	0.13	82,106,111,119	0
2	NAG	F	301	14/15	0.70	0.12	84,96,107,108	0
2	NAG	L	301	14/15	0.70	0.12	100,119,125,125	0
3	WCW	I	301	16/16	0.80	0.21	72,87,97,117	0
3	WCW	G	301	16/16	0.83	0.19	78,85,95,104	0
3	WCW	E	301	16/16	0.84	0.18	72,95,114,115	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.

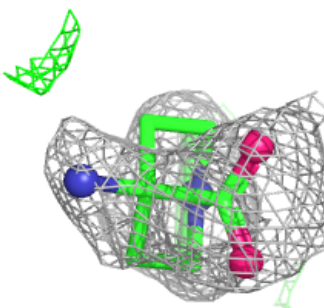
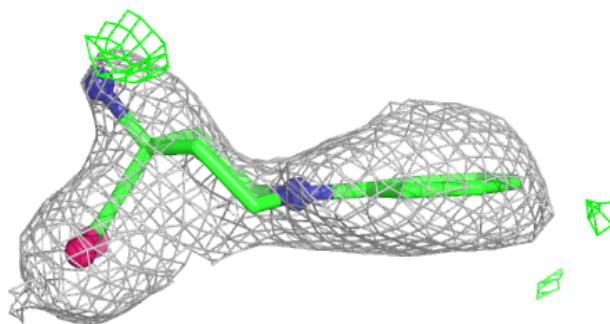
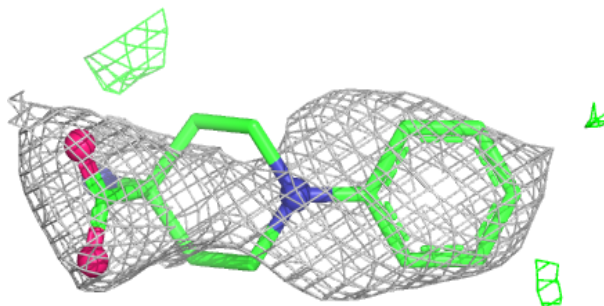


Electron density around WCW G 301:

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

**Electron density around WCW E 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 [i](#)

There are no such residues in this entry.