Full wwPDB X-ray Structure Validation Report (i)

Jul 11, 2023 – 08:38 PM JST

PDB ID	:	8HNJ
Title	:	Domain-stabilized glutamine-binding protein
Authors	:	Choi, S.H.; Park, J.H.; Seo, M.H.; Park, K.W.; Lee, W.K.
Deposited on	:	2022-12-08
Resolution	:	2.03 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the (i) symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

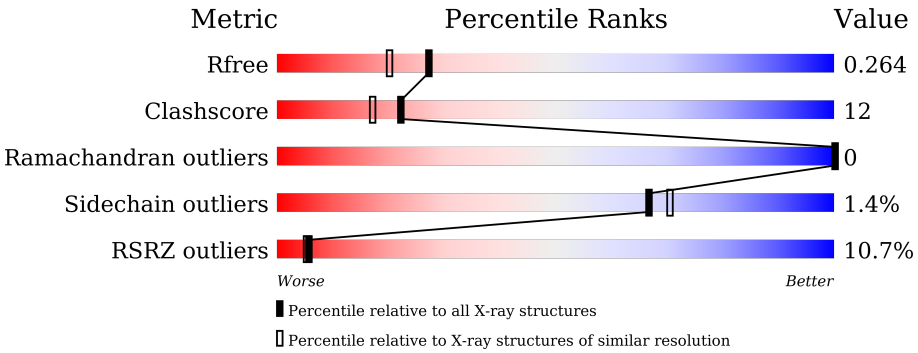
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.34
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.34

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 2.03 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}	130704	10434 (2.04-2.00)
Clashscore	141614	11643 (2.04-2.00)
Ramachandran outliers	138981	11493 (2.04-2.00)
Sidechain outliers	138945	11492 (2.04-2.00)
RSRZ outliers	127900	10220 (2.04-2.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	230	80% 13% • 5%
1	B	230	80% 13% • 5%
1	C	230	3% 82% 13% 5%
1	D	230	13% 70% 23% • 5%
1	E	230	40% 66% 28% • 5%
1	F	230	4% 80% 13% • 5%

2 Entry composition (i)

There are 3 unique types of molecules in this entry. The entry contains 20614 atoms, of which 9972 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 Glutamine ABC transporter, periplasmic glutamine-binding protein GlnH.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	219	Total	C	H	N	O	S	0	0	0
			3388	1089	1693	276	326	4			
1	B	219	Total	C	H	N	O	S	0	0	0
			3360	1083	1676	275	322	4			
1	C	219	Total	C	H	N	O	S	0	0	0
			3355	1082	1670	274	325	4			
1	D	219	Total	C	H	N	O	S	0	0	0
			3309	1073	1635	272	325	4			
1	E	219	Total	C	H	N	O	S	0	0	0
			3173	1042	1554	263	310	4			
1	F	219	Total	C	H	N	O	S	0	0	0
			3379	1088	1684	274	329	4			

There are 90 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP V0VBD8
A	20	LEU	LYS	conflict	UNP V0VBD8
A	94	ASP	ASN	conflict	UNP V0VBD8
A	96	ASP	ASN	conflict	UNP V0VBD8
A	98	ILE	VAL	conflict	UNP V0VBD8
A	146	GLY	ASN	conflict	UNP V0VBD8
A	222	ALA	-	expression tag	UNP V0VBD8
A	223	LEU	-	expression tag	UNP V0VBD8
A	224	GLU	-	expression tag	UNP V0VBD8
A	225	HIS	-	expression tag	UNP V0VBD8
A	226	HIS	-	expression tag	UNP V0VBD8
A	227	HIS	-	expression tag	UNP V0VBD8
A	228	HIS	-	expression tag	UNP V0VBD8
A	229	HIS	-	expression tag	UNP V0VBD8
A	230	HIS	-	expression tag	UNP V0VBD8
B	1	MET	-	initiating methionine	UNP V0VBD8

Continued on next page...

Continued from previous page...

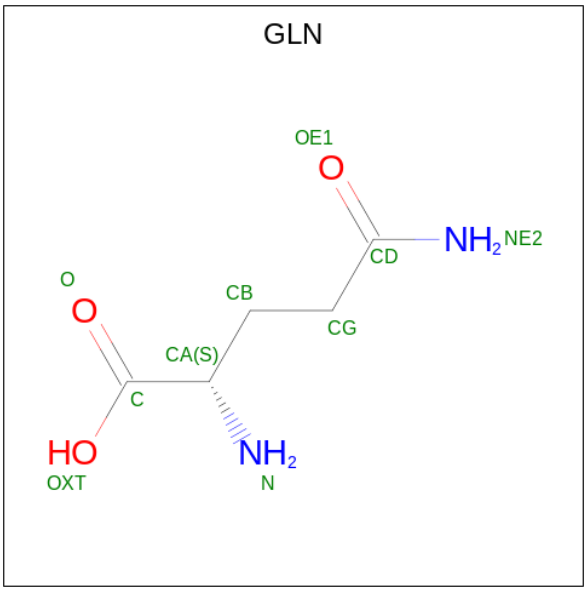
Chain	Residue	Modelled	Actual	Comment	Reference
B	20	LEU	LYS	conflict	UNP V0VBD8
B	94	ASP	ASN	conflict	UNP V0VBD8
B	96	ASP	ASN	conflict	UNP V0VBD8
B	98	ILE	VAL	conflict	UNP V0VBD8
B	146	GLY	ASN	conflict	UNP V0VBD8
B	222	ALA	-	expression tag	UNP V0VBD8
B	223	LEU	-	expression tag	UNP V0VBD8
B	224	GLU	-	expression tag	UNP V0VBD8
B	225	HIS	-	expression tag	UNP V0VBD8
B	226	HIS	-	expression tag	UNP V0VBD8
B	227	HIS	-	expression tag	UNP V0VBD8
B	228	HIS	-	expression tag	UNP V0VBD8
B	229	HIS	-	expression tag	UNP V0VBD8
B	230	HIS	-	expression tag	UNP V0VBD8
C	1	MET	-	initiating methionine	UNP V0VBD8
C	20	LEU	LYS	conflict	UNP V0VBD8
C	94	ASP	ASN	conflict	UNP V0VBD8
C	96	ASP	ASN	conflict	UNP V0VBD8
C	98	ILE	VAL	conflict	UNP V0VBD8
C	146	GLY	ASN	conflict	UNP V0VBD8
C	222	ALA	-	expression tag	UNP V0VBD8
C	223	LEU	-	expression tag	UNP V0VBD8
C	224	GLU	-	expression tag	UNP V0VBD8
C	225	HIS	-	expression tag	UNP V0VBD8
C	226	HIS	-	expression tag	UNP V0VBD8
C	227	HIS	-	expression tag	UNP V0VBD8
C	228	HIS	-	expression tag	UNP V0VBD8
C	229	HIS	-	expression tag	UNP V0VBD8
C	230	HIS	-	expression tag	UNP V0VBD8
D	1	MET	-	initiating methionine	UNP V0VBD8
D	20	LEU	LYS	conflict	UNP V0VBD8
D	94	ASP	ASN	conflict	UNP V0VBD8
D	96	ASP	ASN	conflict	UNP V0VBD8
D	98	ILE	VAL	conflict	UNP V0VBD8
D	146	GLY	ASN	conflict	UNP V0VBD8
D	222	ALA	-	expression tag	UNP V0VBD8
D	223	LEU	-	expression tag	UNP V0VBD8
D	224	GLU	-	expression tag	UNP V0VBD8
D	225	HIS	-	expression tag	UNP V0VBD8
D	226	HIS	-	expression tag	UNP V0VBD8
D	227	HIS	-	expression tag	UNP V0VBD8
D	228	HIS	-	expression tag	UNP V0VBD8

Continued on next page...

Continued from previous page...

Chain	Residue	Modelled	Actual	Comment	Reference
D	229	HIS	-	expression tag	UNP V0VBD8
D	230	HIS	-	expression tag	UNP V0VBD8
E	1	MET	-	initiating methionine	UNP V0VBD8
E	20	LEU	LYS	conflict	UNP V0VBD8
E	94	ASP	ASN	conflict	UNP V0VBD8
E	96	ASP	ASN	conflict	UNP V0VBD8
E	98	ILE	VAL	conflict	UNP V0VBD8
E	146	GLY	ASN	conflict	UNP V0VBD8
E	222	ALA	-	expression tag	UNP V0VBD8
E	223	LEU	-	expression tag	UNP V0VBD8
E	224	GLU	-	expression tag	UNP V0VBD8
E	225	HIS	-	expression tag	UNP V0VBD8
E	226	HIS	-	expression tag	UNP V0VBD8
E	227	HIS	-	expression tag	UNP V0VBD8
E	228	HIS	-	expression tag	UNP V0VBD8
E	229	HIS	-	expression tag	UNP V0VBD8
E	230	HIS	-	expression tag	UNP V0VBD8
F	1	MET	-	initiating methionine	UNP V0VBD8
F	20	LEU	LYS	conflict	UNP V0VBD8
F	94	ASP	ASN	conflict	UNP V0VBD8
F	96	ASP	ASN	conflict	UNP V0VBD8
F	98	ILE	VAL	conflict	UNP V0VBD8
F	146	GLY	ASN	conflict	UNP V0VBD8
F	222	ALA	-	expression tag	UNP V0VBD8
F	223	LEU	-	expression tag	UNP V0VBD8
F	224	GLU	-	expression tag	UNP V0VBD8
F	225	HIS	-	expression tag	UNP V0VBD8
F	226	HIS	-	expression tag	UNP V0VBD8
F	227	HIS	-	expression tag	UNP V0VBD8
F	228	HIS	-	expression tag	UNP V0VBD8
F	229	HIS	-	expression tag	UNP V0VBD8
F	230	HIS	-	expression tag	UNP V0VBD8

- Molecule 2 is GLUTAMINE (three-letter code: GLN) (formula: $C_5H_{10}N_2O_3$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total C H N O 20 5 10 2 3	0	0
2	B	1	Total C H N O 20 5 10 2 3	0	0
2	C	1	Total C H N O 20 5 10 2 3	0	0
2	D	1	Total C H N O 20 5 10 2 3	0	0
2	E	1	Total C H N O 20 5 10 2 3	0	0
2	F	1	Total C H N O 20 5 10 2 3	0	0

- Molecule 3 is water.

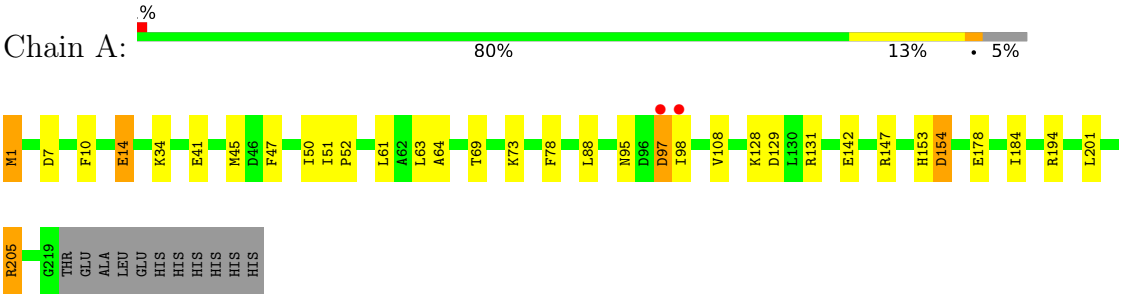
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	A	142	Total O 142 142	0	0
3	B	99	Total O 99 99	0	0
3	C	100	Total O 100 100	0	0
3	D	74	Total O 74 74	0	0
3	E	52	Total O 52 52	0	0
3	F	63	Total O 63 63	0	0

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.

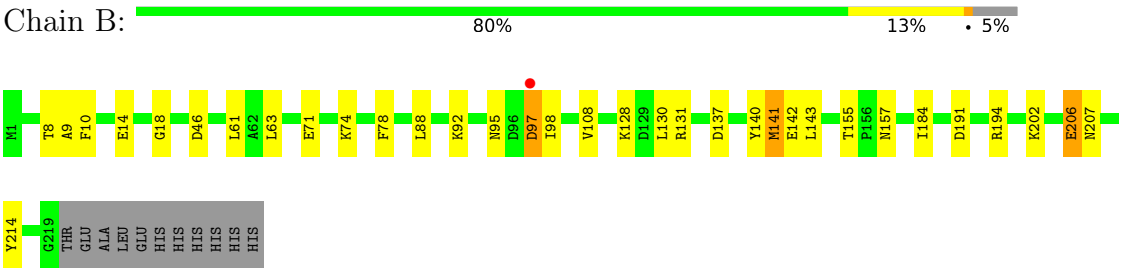
• Molecule 1: Glutamine ABC transporter, periplasmic glutamine-binding protein GlnH

Chain A:



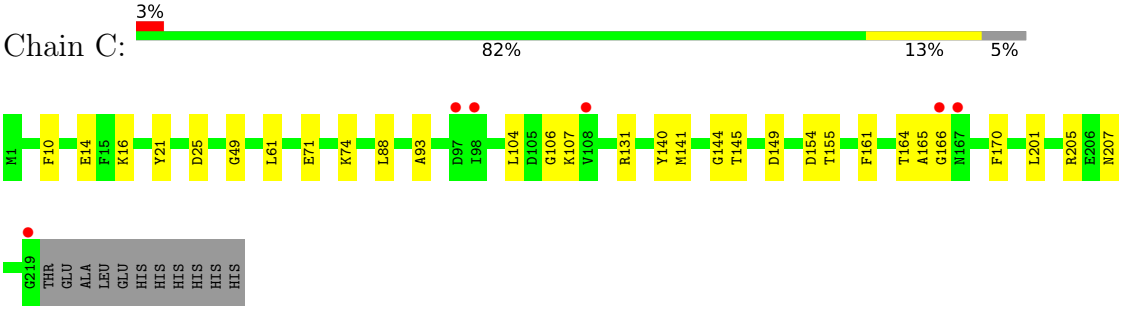
• Molecule 1: Glutamine ABC transporter, periplasmic glutamine-binding protein GlnH

Chain B:



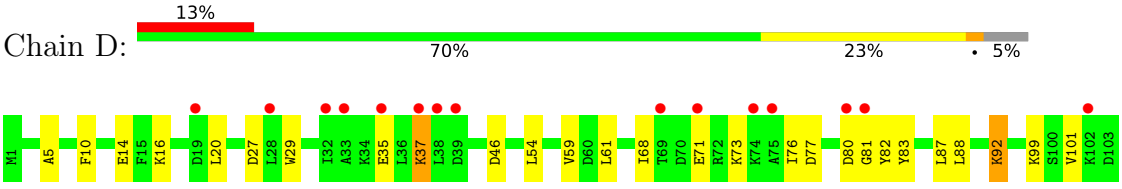
• Molecule 1: Glutamine ABC transporter, periplasmic glutamine-binding protein GlnH

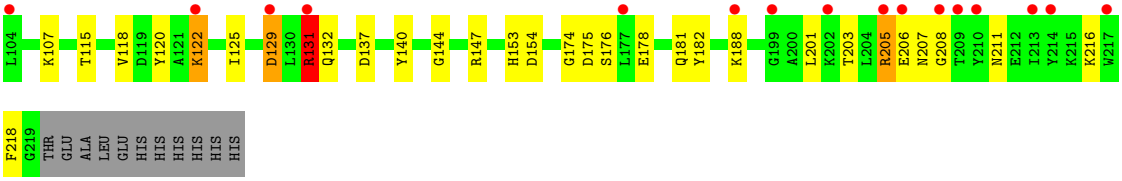
Chain C:



• Molecule 1: Glutamine ABC transporter, periplasmic glutamine-binding protein GlnH

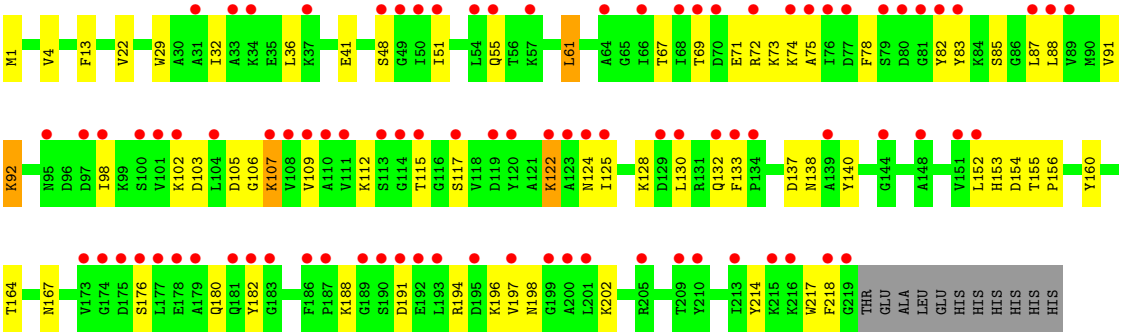
Chain D:





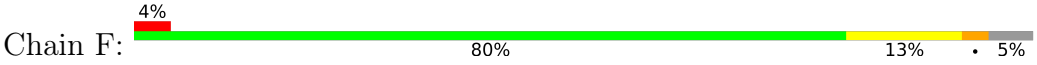
• Molecule 1: Glutamine ABC transporter, periplasmic glutamine-binding protein GlnH

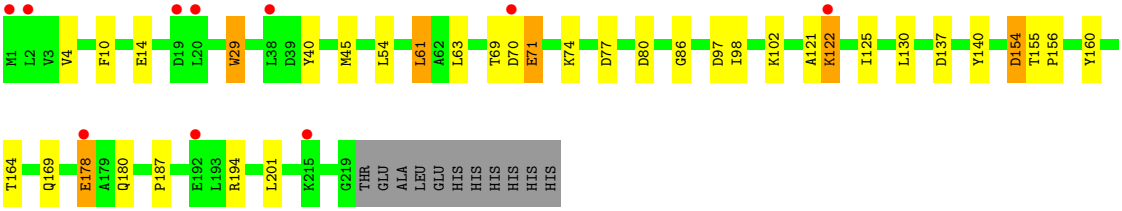
Chain E:



• Molecule 1: Glutamine ABC transporter, periplasmic glutamine-binding protein GlnH

Chain F:





4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	235.10Å 69.59Å 83.74Å 90.00° 90.71° 90.00°	Depositor
Resolution (Å)	28.79 – 2.03 29.39 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.7 (28.79-2.03) 95.0 (29.39-1.97)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.06 (at 1.96Å)	Xtriage
Refinement program	PHENIX 1.17.1_3660	Depositor
R, R_{free}	0.226 , 0.264 0.226 , 0.264	Depositor DCC
R_{free} test set	4777 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å^2)	32.0	Xtriage
Anisotropy	0.353	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.36 , 48.2	EDS
L-test for twinning[2]	$< \|L\| > = 0.48$, $< L^2 > = 0.32$	Xtriage
Estimated twinning fraction	0.000 for -h,-k,l	Xtriage
F_o,F_c correlation	0.95	EDS
Total number of atoms	20614	wwPDB-VP
Average B, all atoms (Å^2)	53.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 57.68 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 2.2848e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality (i)

5.1 Standard geometry (i)

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	0.71	1/1726 (0.1%)	0.97	8/2331 (0.3%)
1	B	0.84	3/1715 (0.2%)	0.87	5/2318 (0.2%)
1	C	0.64	0/1716	0.85	2/2321 (0.1%)
1	D	1.26	12/1704 (0.7%)	1.29	22/2307 (1.0%)
1	E	0.94	5/1648 (0.3%)	0.98	7/2237 (0.3%)
1	F	0.75	5/1726 (0.3%)	0.89	7/2333 (0.3%)
All	All	0.88	26/10235 (0.3%)	0.99	51/13847 (0.4%)

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	D	0	1

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	131	ARG	CG-CD	24.85	2.14	1.51
1	E	122	LYS	CD-CE	21.94	2.06	1.51
1	D	37	LYS	CD-CE	18.38	1.97	1.51
1	D	37	LYS	CE-NZ	15.63	1.88	1.49
1	B	206	GLU	CD-OE2	14.89	1.42	1.25
1	B	206	GLU	CD-OE1	14.52	1.41	1.25
1	D	131	ARG	CB-CG	11.68	1.84	1.52
1	F	122	LYS	CE-NZ	11.53	1.77	1.49
1	E	122	LYS	CB-CG	-10.99	1.22	1.52
1	D	92	LYS	CE-NZ	-10.09	1.23	1.49
1	F	122	LYS	CB-CG	9.04	1.76	1.52
1	D	92	LYS	CD-CE	8.60	1.72	1.51
1	E	107	LYS	CE-NZ	8.52	1.70	1.49
1	D	71	GLU	CB-CG	8.03	1.67	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	37	LYS	CG-CD	7.81	1.79	1.52
1	B	206	GLU	CG-CD	7.62	1.63	1.51
1	D	71	GLU	CG-CD	7.49	1.63	1.51
1	E	122	LYS	CE-NZ	6.92	1.66	1.49
1	E	107	LYS	CD-CE	5.90	1.66	1.51
1	D	122	LYS	CE-NZ	5.86	1.63	1.49
1	D	80	ASP	CB-CG	-5.76	1.39	1.51
1	F	122	LYS	CD-CE	5.74	1.65	1.51
1	D	71	GLU	CD-OE1	5.65	1.31	1.25
1	F	71	GLU	CD-OE1	-5.58	1.19	1.25
1	A	14	GLU	CG-CD	5.57	1.60	1.51
1	F	178	GLU	CB-CG	-5.11	1.42	1.52

All (51) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	131	ARG	NE-CZ-NH2	20.86	130.73	120.30
1	D	92	LYS	CD-CE-NZ	17.19	151.23	111.70
1	D	37	LYS	CD-CE-NZ	-15.09	76.99	111.70
1	E	122	LYS	CD-CE-NZ	-14.06	79.36	111.70
1	D	205	ARG	NE-CZ-NH2	-11.39	114.61	120.30
1	D	129	ASP	CB-CG-OD2	-11.37	108.07	118.30
1	F	201	LEU	CA-CB-CG	11.10	140.84	115.30
1	B	206	GLU	OE1-CD-OE2	10.36	135.73	123.30
1	E	191	ASP	CB-CG-OD2	10.17	127.46	118.30
1	D	205	ARG	NE-CZ-NH1	10.09	125.34	120.30
1	D	131	ARG	NH1-CZ-NH2	-9.94	108.47	119.40
1	E	191	ASP	N-CA-CB	-9.15	94.13	110.60
1	D	131	ARG	CG-CD-NE	-8.91	93.09	111.80
1	A	128	LYS	CD-CE-NZ	-8.81	91.44	111.70
1	D	205	ARG	CB-CG-CD	-8.69	89.00	111.60
1	D	131	ARG	CB-CG-CD	8.66	134.12	111.60
1	E	191	ASP	CB-CA-C	8.50	127.41	110.40
1	D	80	ASP	N-CA-CB	-8.45	95.39	110.60
1	F	122	LYS	CD-CE-NZ	-7.99	93.33	111.70
1	D	80	ASP	CB-CA-C	7.77	125.94	110.40
1	F	122	LYS	CB-CG-CD	-7.64	91.72	111.60
1	D	37	LYS	CA-CB-CG	-7.36	97.21	113.40
1	E	107	LYS	CA-CB-CG	7.26	129.38	113.40
1	D	80	ASP	CB-CG-OD2	6.99	124.59	118.30
1	A	34	LYS	CB-CA-C	-6.71	96.99	110.40
1	D	71	GLU	N-CA-CB	-6.52	98.87	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	178	GLU	CA-CB-CG	-6.45	99.21	113.40
1	F	71	GLU	CG-CD-OE2	-6.32	105.66	118.30
1	D	131	ARG	CD-NE-CZ	6.17	132.23	123.60
1	D	122	LYS	CD-CE-NZ	6.17	125.88	111.70
1	B	141	MET	CA-CB-CG	-6.14	102.86	113.30
1	A	205	ARG	NE-CZ-NH1	-6.10	117.25	120.30
1	A	88	LEU	CB-CG-CD2	-5.99	100.81	111.00
1	D	80	ASP	OD1-CG-OD2	-5.97	111.96	123.30
1	B	206	GLU	CG-CD-OE1	-5.93	106.43	118.30
1	E	191	ASP	OD1-CG-OD2	-5.90	112.09	123.30
1	D	92	LYS	CG-CD-CE	-5.69	94.83	111.90
1	D	80	ASP	CB-CG-OD1	5.67	123.40	118.30
1	B	97	ASP	CB-CG-OD2	5.66	123.39	118.30
1	A	97	ASP	CB-CA-C	5.65	121.71	110.40
1	A	34	LYS	CD-CE-NZ	-5.62	98.78	111.70
1	D	129	ASP	CB-CG-OD1	5.51	123.26	118.30
1	F	122	LYS	CA-CB-CG	5.40	125.28	113.40
1	E	122	LYS	CG-CD-CE	-5.35	95.85	111.90
1	C	201	LEU	CB-CG-CD1	-5.27	102.03	111.00
1	A	201	LEU	CA-CB-CG	5.22	127.31	115.30
1	C	25	ASP	CB-CG-OD1	5.19	122.97	118.30
1	F	29	TRP	CA-CB-CG	-5.05	104.10	113.70
1	A	88	LEU	CB-CG-CD1	5.04	119.57	111.00
1	D	175	ASP	CB-CG-OD1	-5.03	113.78	118.30
1	B	18	GLY	N-CA-C	-5.02	100.56	113.10

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	D	131	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1695	1693	1693	18	1

Continued on next page...

Continued from previous page...

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	B	1684	1676	1676	23	3
1	C	1685	1670	1670	33	1
1	D	1674	1635	1638	47	2
1	E	1619	1554	1537	77	0
1	F	1695	1684	1682	36	2
2	A	10	10	7	0	0
2	B	10	10	7	0	0
2	C	10	10	7	0	0
2	D	10	10	7	1	0
2	E	10	10	7	2	0
2	F	10	10	7	1	0
3	A	142	0	0	2	0
3	B	99	0	0	5	0
3	C	100	0	0	19	0
3	D	74	0	0	10	1
3	E	52	0	0	25	0
3	F	63	0	0	9	0
All	All	10642	9972	9938	234	5

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 12.

All (234) 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:F:122:LYS:CG	1:F:122:LYS:CB	1.77	1.61
1:D:37:LYS:CD	1:D:37:LYS:CG	1.79	1.55
1:E:107:LYS:NZ	1:E:107:LYS:CE	1.70	1.51
1:D:131:ARG:CG	1:D:131:ARG:CB	1.84	1.51
1:F:122:LYS:CE	1:F:122:LYS:NZ	1.77	1.47
1:D:37:LYS:CD	1:D:37:LYS:CE	1.97	1.42
1:D:37:LYS:CE	1:D:37:LYS:NZ	1.88	1.35
1:E:122:LYS:CE	1:E:122:LYS:CD	2.06	1.34
1:D:131:ARG:CG	1:D:131:ARG:CD	2.14	1.25
1:A:45:MET:SD	3:A:522:HOH:O	1.94	1.21
1:D:131:ARG:NH1	3:D:401:HOH:O	1.79	1.11
1:F:45:MET:SD	3:F:463:HOH:O	2.08	1.10
1:D:92:LYS:NZ	1:D:144:GLY:O	1.96	0.97
2:E:301:GLN:N	3:E:405:HOH:O	1.99	0.95
1:E:214:TYR:O	3:E:401:HOH:O	1.85	0.93
1:F:122:LYS:CB	1:F:122:LYS:CD	2.47	0.92

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:107:LYS:O	3:C:401:HOH:O	1.90	0.89
1:E:122:LYS:NZ	1:E:122:LYS:HG2	1.86	0.89
1:C:144:GLY:N	3:C:403:HOH:O	2.05	0.89
1:F:169:GLN:NE2	3:F:401:HOH:O	1.89	0.88
1:E:124:ASN:O	3:E:402:HOH:O	1.94	0.85
1:D:37:LYS:CD	1:D:37:LYS:NZ	2.39	0.85
1:E:122:LYS:CD	1:E:122:LYS:NZ	2.39	0.85
1:D:29:TRP:CZ2	1:D:29:TRP:CZ3	2.65	0.83
1:F:178:GLU:O	1:F:178:GLU:HG3	1.77	0.82
1:E:188:LYS:O	3:E:404:HOH:O	1.98	0.81
1:E:182:TYR:O	3:E:403:HOH:O	1.97	0.81
1:E:122:LYS:HG2	1:E:122:LYS:HZ3	1.46	0.81
1:E:130:LEU:HD13	1:E:132:GLN:NE2	1.95	0.80
1:C:149:ASP:O	3:C:402:HOH:O	1.98	0.80
1:E:130:LEU:HD13	1:E:132:GLN:HE21	1.45	0.80
1:E:122:LYS:NZ	1:E:122:LYS:CG	2.45	0.80
1:B:207:ASN:O	3:B:401:HOH:O	1.98	0.79
1:E:87:LEU:HD21	1:E:152:LEU:HD21	1.62	0.79
1:E:29:TRP:CZ2	1:E:29:TRP:CZ3	2.70	0.79
1:C:166:GLY:N	3:C:404:HOH:O	2.14	0.78
1:C:144:GLY:CA	3:C:403:HOH:O	2.33	0.77
1:E:167:ASN:OD1	3:E:406:HOH:O	2.02	0.77
1:E:82:TYR:N	3:E:403:HOH:O	2.09	0.76
1:E:122:LYS:CE	1:E:122:LYS:CG	2.63	0.75
1:D:46:ASP:OD2	3:D:402:HOH:O	2.05	0.75
1:F:77:ASP:OD2	3:F:402:HOH:O	2.04	0.74
1:F:122:LYS:NZ	1:F:122:LYS:CD	2.49	0.74
1:A:95:ASN:ND2	1:A:97:ASP:OD1	2.22	0.73
1:D:10:PHE:HB3	1:D:14:GLU:OE2	1.89	0.72
1:D:218:PHE:O	3:D:404:HOH:O	2.08	0.72
1:F:122:LYS:HE3	1:F:130:LEU:HD23	1.72	0.71
1:B:130:LEU:O	3:B:402:HOH:O	2.10	0.70
1:F:80:ASP:OD1	3:F:403:HOH:O	2.08	0.70
1:E:122:LYS:CD	1:E:122:LYS:HZ2	2.06	0.69
1:D:27:ASP:OD2	1:D:216:LYS:NZ	2.20	0.69
1:D:207:ASN:O	3:D:405:HOH:O	2.11	0.68
1:B:8:THR:O	3:B:403:HOH:O	2.11	0.68
1:D:107:LYS:NZ	3:D:403:HOH:O	2.05	0.67
1:D:54:LEU:HD23	1:D:59:VAL:HG23	1.77	0.67
1:F:10:PHE:HB3	1:F:14:GLU:OE2	1.95	0.66
1:E:105:ASP:OD1	3:E:407:HOH:O	2.13	0.66

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:131:ARG:HH11	1:C:131:ARG:HG2	1.60	0.66
1:F:194:ARG:NH2	3:F:402:HOH:O	2.28	0.66
1:E:55:GLN:NE2	1:E:75:ALA:HB1	2.12	0.65
1:E:32:ILE:HG21	1:E:197:VAL:HG13	1.78	0.65
1:B:88:LEU:HD22	1:B:155:THR:HG23	1.79	0.64
1:D:174:GLY:O	3:D:406:HOH:O	2.15	0.64
1:E:117:SER:HB3	1:E:152:LEU:CD1	2.28	0.63
1:F:4:VAL:HG22	1:F:61:LEU:HG	1.79	0.63
1:E:48:SER:OG	3:E:408:HOH:O	2.15	0.63
1:D:131:ARG:CG	1:D:131:ARG:NE	2.62	0.63
1:D:5:ALA:HB2	1:D:59:VAL:HG11	1.80	0.62
1:C:107:LYS:N	3:C:401:HOH:O	2.14	0.62
1:C:205:ARG:NH2	3:C:407:HOH:O	2.25	0.62
1:C:88:LEU:HD22	1:C:155:THR:HG23	1.82	0.61
1:C:165:ALA:N	3:C:404:HOH:O	2.34	0.60
1:E:107:LYS:NZ	1:E:107:LYS:CD	2.64	0.60
1:E:217:TRP:N	3:E:401:HOH:O	2.26	0.60
1:E:55:GLN:NE2	3:E:409:HOH:O	2.30	0.60
1:E:117:SER:HB3	1:E:152:LEU:HD11	1.82	0.59
1:E:112:LYS:O	1:E:115:THR:HG22	2.02	0.59
1:E:106:GLY:HA2	1:E:128:LYS:HB2	1.84	0.59
1:F:122:LYS:CD	1:F:122:LYS:HB3	2.33	0.59
1:D:37:LYS:NZ	1:D:37:LYS:HD3	2.18	0.58
1:F:4:VAL:HG22	1:F:61:LEU:CG	2.33	0.58
1:E:69:THR:OG1	1:E:72:ARG:HG3	2.03	0.58
1:A:178:GLU:OE1	3:A:401:HOH:O	2.16	0.58
1:F:4:VAL:HG22	1:F:61:LEU:CD2	2.33	0.58
1:E:87:LEU:HD23	1:E:87:LEU:C	2.25	0.57
1:E:91:VAL:CG2	3:E:416:HOH:O	2.53	0.56
1:C:205:ARG:NE	3:C:407:HOH:O	2.28	0.56
1:D:83:TYR:O	1:D:181:GLN:HA	2.05	0.56
1:D:129:ASP:OD2	1:D:131:ARG:HG2	2.07	0.55
1:E:83:TYR:HH	1:E:218:PHE:HE2	1.54	0.55
1:D:101:VAL:HG23	1:D:125:ILE:HD11	1.89	0.55
1:E:109:VAL:O	1:E:130:LEU:HA	2.07	0.55
1:F:97:ASP:OD2	1:F:98:ILE:HG13	2.07	0.54
1:C:49:GLY:HA3	3:C:447:HOH:O	2.08	0.54
1:F:4:VAL:HG22	1:F:61:LEU:HD21	1.88	0.54
1:E:55:GLN:OE1	3:E:409:HOH:O	2.19	0.54
1:D:82:TYR:HA	1:D:205:ARG:HH21	1.73	0.53
1:E:22:VAL:HG12	3:E:439:HOH:O	2.09	0.53

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:16:LYS:HA	1:D:20:LEU:O	2.09	0.53
1:B:140:TYR:OH	1:B:157:ASN:OD1	2.26	0.53
1:C:144:GLY:O	3:C:405:HOH:O	2.18	0.53
1:D:35:GLU:HA	1:D:35:GLU:OE2	2.09	0.53
1:B:202:LYS:O	1:B:206:GLU:OE2	2.27	0.53
1:A:47:PHE:HA	1:A:50:ILE:HD12	1.91	0.52
1:A:131:ARG:NE	1:A:142:GLU:OE2	2.39	0.52
1:A:14:GLU:HG2	1:A:14:GLU:O	2.09	0.52
1:E:36:LEU:HD11	1:E:196:LYS:O	2.09	0.52
1:B:131:ARG:NE	1:B:142:GLU:OE1	2.36	0.52
1:B:108:VAL:HG23	1:B:128:LYS:HD3	1.91	0.52
1:D:153:HIS:CG	1:D:154:ASP:H	2.28	0.52
1:C:165:ALA:C	3:C:404:HOH:O	2.46	0.52
1:E:137:ASP:HA	1:E:140:TYR:CD2	2.45	0.52
1:E:83:TYR:N	3:E:403:HOH:O	2.14	0.51
1:B:207:ASN:C	1:B:207:ASN:OD1	2.49	0.51
1:D:73:LYS:HB3	3:D:457:HOH:O	2.09	0.51
1:B:71:GLU:HA	1:B:74:LYS:HD3	1.92	0.51
1:E:91:VAL:HG22	3:E:416:HOH:O	2.11	0.51
1:F:69:THR:HG22	1:F:71:GLU:H	1.76	0.51
1:D:208:GLY:O	1:D:211:ASN:OD1	2.29	0.51
1:D:118:VAL:O	1:D:122:LYS:HG3	2.10	0.51
1:A:69:THR:O	1:A:73:LYS:HG3	2.11	0.50
1:E:133:PHE:CD2	1:E:138:ASN:HB3	2.46	0.50
1:B:92:LYS:HE2	1:B:143:LEU:O	2.12	0.50
1:C:71:GLU:OE2	1:C:74:LYS:NZ	2.42	0.50
1:C:141:MET:O	1:C:145:THR:HG23	2.12	0.50
1:D:101:VAL:HG12	3:D:415:HOH:O	2.11	0.50
1:A:1:MET:HE1	1:A:41:GLU:OE1	2.12	0.49
1:A:1:MET:SD	1:A:41:GLU:OE1	2.71	0.49
1:D:35:GLU:OE1	1:D:203:THR:HG21	2.11	0.49
1:D:101:VAL:CG2	1:D:125:ILE:HD11	2.42	0.49
1:E:36:LEU:HD11	1:E:196:LYS:C	2.33	0.49
1:B:214:TYR:OH	3:B:404:HOH:O	2.20	0.49
1:E:69:THR:HG1	1:E:72:ARG:HG3	1.76	0.49
1:E:78:PHE:O	1:E:194:ARG:HD2	2.12	0.49
1:B:95:ASN:ND2	1:B:97:ASP:OD1	2.45	0.49
1:F:14:GLU:HG2	1:F:14:GLU:O	2.13	0.49
1:B:10:PHE:HB3	1:B:14:GLU:OE1	2.12	0.49
1:B:63:LEU:HG	1:B:184:ILE:HG12	1.95	0.49
1:E:198:ASN:O	1:E:202:LYS:HG2	2.13	0.49

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:153:HIS:CD2	1:E:154:ASP:H	2.30	0.48
1:C:131:ARG:HG2	1:C:131:ARG:NH1	2.26	0.48
1:C:104:LEU:O	3:C:401:HOH:O	2.20	0.48
1:E:115:THR:OG1	2:E:301:GLN:HA	2.14	0.48
1:C:106:GLY:O	1:C:107:LYS:HD3	2.13	0.48
1:A:10:PHE:HB3	1:A:14:GLU:OE2	2.13	0.48
1:E:73:LYS:HE2	1:E:73:LYS:HB3	1.65	0.48
1:F:102:LYS:NZ	3:F:411:HOH:O	2.46	0.48
1:E:217:TRP:HB2	3:E:401:HOH:O	2.13	0.48
1:F:54:LEU:O	1:F:187:PRO:HB3	2.12	0.48
1:C:144:GLY:HA3	3:C:403:HOH:O	2.04	0.48
1:E:130:LEU:HD12	1:E:130:LEU:O	2.13	0.48
1:E:217:TRP:CA	3:E:401:HOH:O	2.62	0.48
1:E:67:THR:HG21	1:E:180:GLN:OE1	2.13	0.47
1:D:132:GLN:OE1	3:D:407:HOH:O	2.20	0.47
1:F:137:ASP:HA	1:F:140:TYR:CD2	2.50	0.47
1:C:164:THR:C	3:C:404:HOH:O	2.52	0.47
1:C:170:PHE:O	3:C:406:HOH:O	2.20	0.47
1:D:81:GLY:HA2	1:D:182:TYR:O	2.15	0.47
1:E:218:PHE:N	3:E:401:HOH:O	2.45	0.47
1:E:160:TYR:CZ	1:E:164:THR:HG21	2.50	0.47
1:F:121:ALA:HA	1:F:125:ILE:HG13	1.96	0.47
1:C:107:LYS:C	3:C:401:HOH:O	2.45	0.47
1:C:107:LYS:CA	3:C:401:HOH:O	2.61	0.46
1:E:160:TYR:CE1	1:E:164:THR:HG21	2.49	0.46
1:B:14:GLU:O	1:B:14:GLU:HG2	2.15	0.46
1:E:74:LYS:HB2	1:E:74:LYS:HE2	1.74	0.46
1:E:106:GLY:CA	1:E:128:LYS:HB2	2.46	0.46
1:D:129:ASP:OD2	1:D:131:ARG:CZ	2.63	0.46
1:A:7:ASP:HB2	1:A:64:ALA:HB1	1.98	0.46
1:C:93:ALA:HB1	3:D:462:HOH:O	2.16	0.45
1:C:106:GLY:C	1:C:107:LYS:HD3	2.37	0.45
1:D:137:ASP:HA	1:D:140:TYR:CD2	2.51	0.45
1:D:201:LEU:O	1:D:205:ARG:HG3	2.15	0.45
1:A:108:VAL:HG13	1:A:129:ASP:HB3	1.98	0.45
1:C:165:ALA:CA	3:C:404:HOH:O	2.64	0.45
1:D:37:LYS:CD	1:D:37:LYS:HZ3	2.29	0.45
1:D:115:THR:HA	2:D:301:GLN:O	2.16	0.45
1:E:125:ILE:HA	3:E:437:HOH:O	2.16	0.45
1:A:97:ASP:OD1	1:A:98:ILE:HG13	2.17	0.44
1:A:205:ARG:HH11	1:A:205:ARG:HD3	1.62	0.44

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:120:TYR:HD2	1:D:178:GLU:OE1	2.01	0.44
1:E:4:VAL:HG22	1:E:61:LEU:HG	1.99	0.44
1:F:29:TRP:HB2	1:F:63:LEU:HD22	2.00	0.44
1:A:51:ILE:HB	1:A:52:PRO:HD3	2.00	0.44
1:A:78:PHE:O	1:A:194:ARG:HD2	2.18	0.44
1:E:22:VAL:HA	3:E:439:HOH:O	2.17	0.44
1:D:87:LEU:O	1:D:176:SER:HA	2.18	0.44
1:F:69:THR:HG22	1:F:70:ASP:N	2.33	0.43
1:C:14:GLU:O	1:C:14:GLU:HG2	2.18	0.43
1:B:9:ALA:HB2	3:B:403:HOH:O	2.17	0.43
1:F:86:GLY:O	1:F:154:ASP:HA	2.17	0.43
1:F:160:TYR:CE1	1:F:164:THR:HG21	2.53	0.43
1:E:122:LYS:CG	1:E:122:LYS:HZ2	2.23	0.43
1:D:68:ILE:CG2	1:D:73:LYS:HE3	2.48	0.43
1:C:140:TYR:CE2	1:C:161:PHE:CD1	3.06	0.43
1:E:98:ILE:HD11	1:E:107:LYS:HG3	2.00	0.43
1:E:91:VAL:HG23	3:E:416:HOH:O	2.16	0.43
1:D:88:LEU:HD12	1:D:88:LEU:HA	1.94	0.43
1:E:91:VAL:HG22	1:E:92:LYS:N	2.34	0.43
1:F:102:LYS:HE3	3:F:411:HOH:O	2.19	0.42
1:F:154:ASP:OD2	2:F:301:GLN:N	2.51	0.42
1:E:155:THR:HG22	1:E:156:PRO:N	2.32	0.42
1:B:131:ARG:HG2	1:B:131:ARG:HH11	1.85	0.42
1:B:131:ARG:HG2	1:B:131:ARG:NH1	2.34	0.42
1:E:71:GLU:HA	1:E:74:LYS:HD3	2.01	0.42
1:E:22:VAL:CB	3:E:439:HOH:O	2.67	0.42
1:F:40:TYR:N	3:F:404:HOH:O	2.23	0.42
1:E:87:LEU:HG	1:E:88:LEU:N	2.35	0.42
1:E:67:THR:HG23	1:E:180:GLN:HB2	2.01	0.41
1:F:102:LYS:CE	3:F:411:HOH:O	2.67	0.41
1:A:153:HIS:CG	1:A:154:ASP:H	2.38	0.41
1:C:10:PHE:HB3	1:C:14:GLU:OE1	2.20	0.41
1:C:140:TYR:CD2	1:C:161:PHE:CE1	3.08	0.41
1:F:122:LYS:CE	1:F:122:LYS:HB3	2.50	0.41
1:B:78:PHE:O	1:B:194:ARG:HD3	2.19	0.41
1:C:93:ALA:HB3	1:D:206:GLU:O	2.20	0.41
1:B:191:ASP:OD1	1:B:194:ARG:NH2	2.53	0.41
1:D:73:LYS:HA	1:D:76:ILE:O	2.20	0.41
1:A:63:LEU:HG	1:A:184:ILE:HG12	2.02	0.41
1:E:1:MET:SD	1:E:41:GLU:HG3	2.60	0.41
1:E:51:ILE:O	1:E:55:GLN:HG3	2.20	0.41

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:102:LYS:CE	3:E:437:HOH:O	2.69	0.41
1:B:141:MET:O	1:B:141:MET:HG2	2.21	0.41
1:D:77:ASP:OD2	1:D:188:LYS:HA	2.20	0.41
1:E:85:SER:HB3	3:E:419:HOH:O	2.21	0.41
1:C:207:ASN:OD1	1:C:207:ASN:C	2.59	0.41
1:E:13:PHE:CZ	1:E:182:TYR:HE2	2.38	0.41
1:E:83:TYR:CE2	1:E:218:PHE:CZ	3.09	0.41
1:F:71:GLU:OE2	1:F:74:LYS:HE3	2.21	0.41
1:E:55:GLN:HE22	1:E:75:ALA:HB1	1.85	0.41
1:F:155:THR:HB	1:F:156:PRO:HD3	2.02	0.41
1:E:87:LEU:O	1:E:176:SER:HA	2.22	0.40
1:F:178:GLU:CG	1:F:180:GLN:HE21	2.35	0.40
1:B:97:ASP:OD1	1:B:98:ILE:HG13	2.22	0.40

All (5) 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:C:21:TYR:H	1:F:169:GLN:HE22[1_565]	1.20	0.40
1:B:137:ASP:OD2	1:D:147:ARG:HH22[1_556]	1.37	0.23
1:B:46:ASP:OD2	3:D:401:HOH:O[1_556]	2.09	0.11
1:A:147:ARG:HH22	1:F:137:ASP:OD2[4_556]	1.59	0.01
1:B:137:ASP:OD2	1:D:147:ARG:NH2[1_556]	2.19	0.01

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	217/230 (94%)	213 (98%)	4 (2%)	0	100	100
1	B	217/230 (94%)	212 (98%)	5 (2%)	0	100	100
1	C	217/230 (94%)	211 (97%)	6 (3%)	0	100	100

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	D	217/230 (94%)	211 (97%)	6 (3%)	0	100	100
1	E	217/230 (94%)	208 (96%)	9 (4%)	0	100	100
1	F	217/230 (94%)	211 (97%)	6 (3%)	0	100	100
All	All	1302/1380 (94%)	1266 (97%)	36 (3%)	0	100	100

There are no Ramachandran outliers to report.

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	177/189 (94%)	174 (98%)	3 (2%)	60	63
1	B	174/189 (92%)	173 (99%)	1 (1%)	86	89
1	C	174/189 (92%)	171 (98%)	3 (2%)	60	63
1	D	171/189 (90%)	169 (99%)	2 (1%)	71	75
1	E	153/189 (81%)	150 (98%)	3 (2%)	55	57
1	F	176/189 (93%)	174 (99%)	2 (1%)	73	77
All	All	1025/1134 (90%)	1011 (99%)	14 (1%)	67	70

All (14) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	1	MET
1	A	61	LEU
1	A	154	ASP
1	B	61	LEU
1	C	16	LYS
1	C	61	LEU
1	C	154	ASP
1	D	61	LEU
1	D	99	LYS
1	E	61	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
1	E	92	LYS
1	E	103	ASP
1	F	61	LEU
1	F	154	ASP

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

Mol	Chain	Res	Type
1	E	132	GLN
1	E	135	ASN
1	E	153	HIS

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 monosaccharides in this entry.

5.6 Ligand geometry

6 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	GLN	F	301	-	8,9,9	1.63	3 (37%)	10,11,11	1.42	2 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
2	GLN	D	301	-	8,9,9	1.47	1 (12%)	10,11,11	1.12	0
2	GLN	C	301	-	8,9,9	1.38	1 (12%)	10,11,11	1.50	1 (10%)
2	GLN	A	301	-	8,9,9	1.55	2 (25%)	10,11,11	1.46	1 (10%)
2	GLN	B	301	-	8,9,9	1.80	2 (25%)	10,11,11	1.44	3 (30%)
2	GLN	E	301	-	8,9,9	1.60	2 (25%)	10,11,11	1.18	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
2	GLN	F	301	-	-	3/9/9/9	-
2	GLN	D	301	-	-	1/9/9/9	-
2	GLN	C	301	-	-	0/9/9/9	-
2	GLN	A	301	-	-	0/9/9/9	-
2	GLN	B	301	-	-	0/9/9/9	-
2	GLN	E	301	-	-	1/9/9/9	-

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	301	GLN	CD-NE2	3.93	1.45	1.32
2	E	301	GLN	CD-NE2	3.60	1.44	1.32
2	D	301	GLN	CD-NE2	3.50	1.44	1.32
2	C	301	GLN	CD-NE2	3.30	1.43	1.32
2	A	301	GLN	CD-NE2	3.17	1.43	1.32
2	F	301	GLN	CD-NE2	3.13	1.42	1.32
2	E	301	GLN	O-C	2.37	1.29	1.22
2	F	301	GLN	OE1-CD	-2.24	1.17	1.24
2	A	301	GLN	OE1-CD	-2.20	1.17	1.24
2	F	301	GLN	O-C	2.02	1.28	1.22
2	B	301	GLN	O-C	2.02	1.28	1.22

All (7) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	F	301	GLN	CB-CG-CD	-3.04	102.27	112.59
2	C	301	GLN	CB-CA-C	-2.98	103.20	110.30
2	A	301	GLN	CB-CG-CD	-2.80	103.08	112.59
2	B	301	GLN	CB-CG-CD	-2.37	104.56	112.59

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	301	GLN	CG-CB-CA	-2.18	108.75	113.84
2	F	301	GLN	CG-CB-CA	-2.03	109.10	113.84
2	B	301	GLN	OXT-C-CA	2.01	120.24	113.38

There are no chirality outliers.

All (5) torsion outliers are listed below:

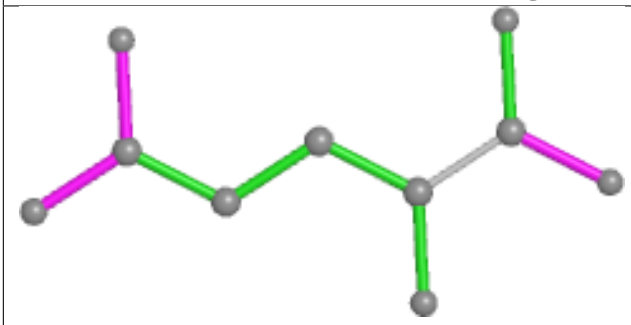
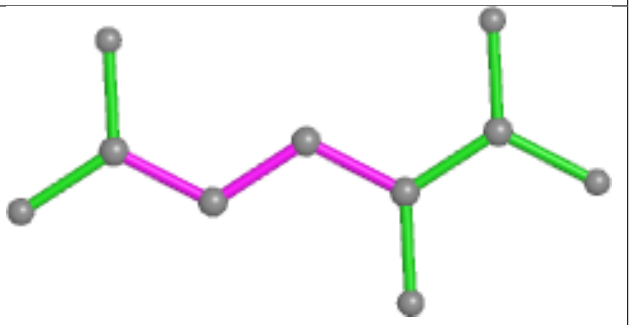
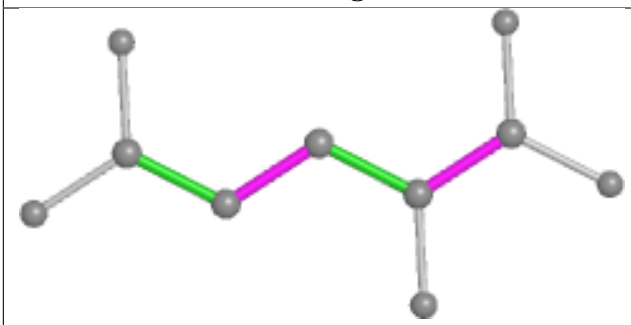
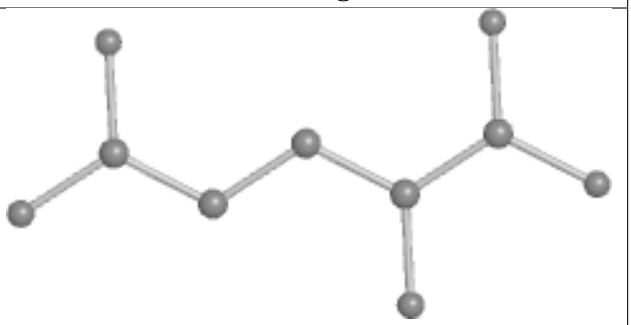
Mol	Chain	Res	Type	Atoms
2	F	301	GLN	CA-CB-CG-CD
2	D	301	GLN	CA-CB-CG-CD
2	E	301	GLN	CA-CB-CG-CD
2	F	301	GLN	OXT-C-CA-N
2	F	301	GLN	O-C-CA-N

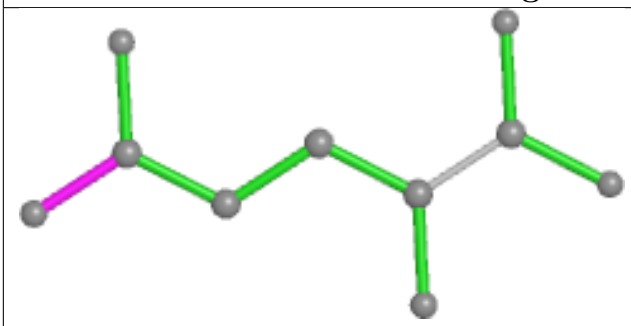
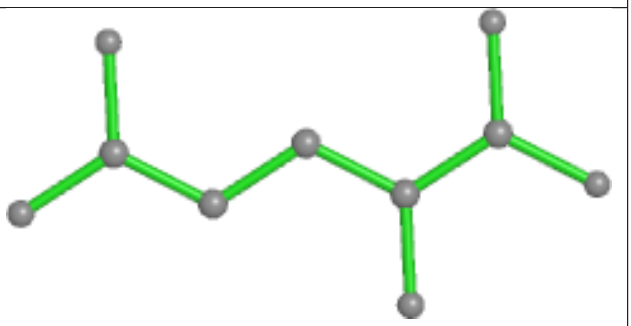
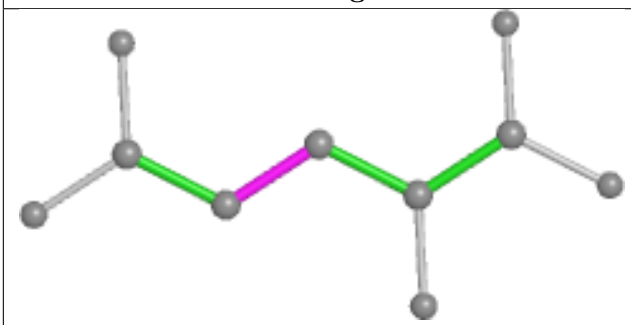
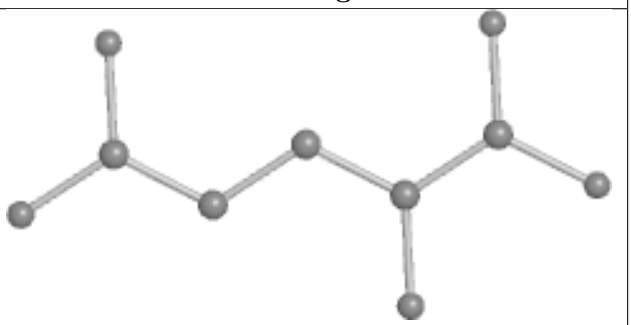
There are no ring outliers.

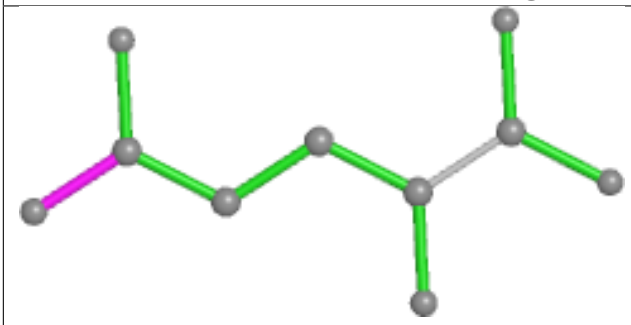
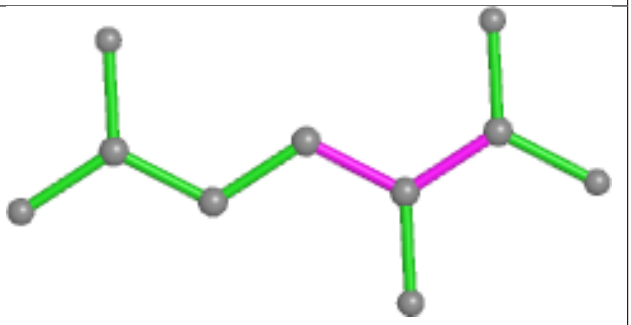
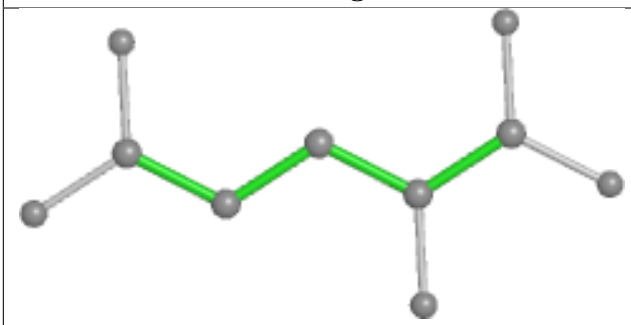
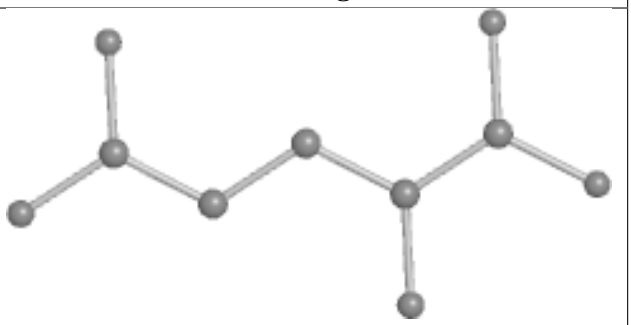
3 monomers are involved in 4 short contacts:

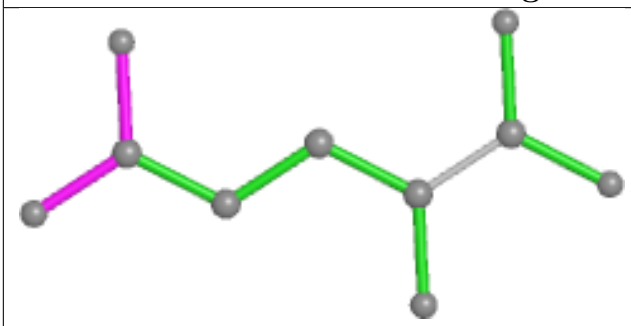
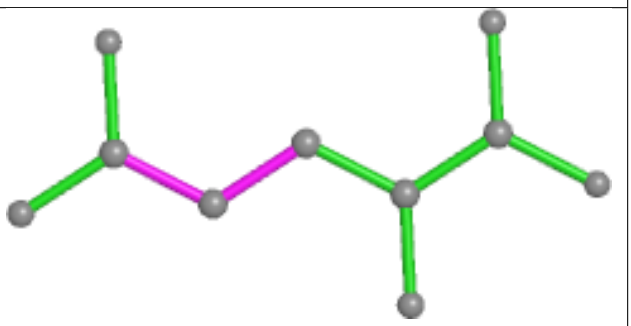
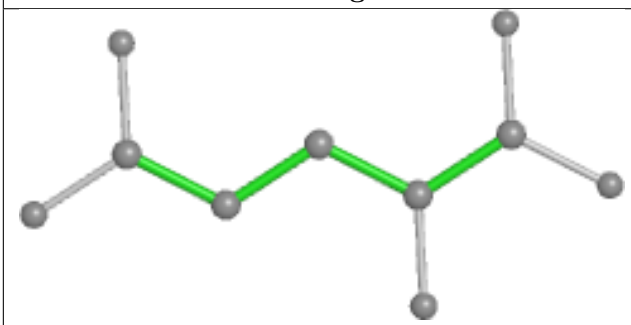
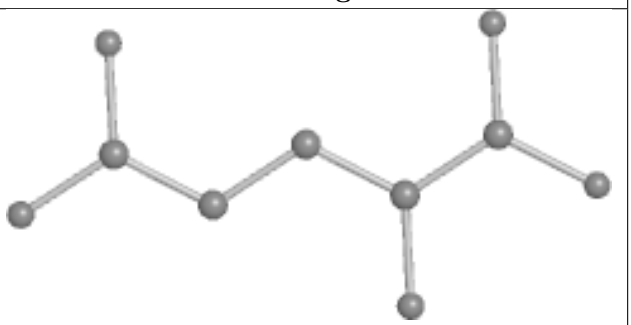
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	F	301	GLN	1	0
2	D	301	GLN	1	0
2	E	301	GLN	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

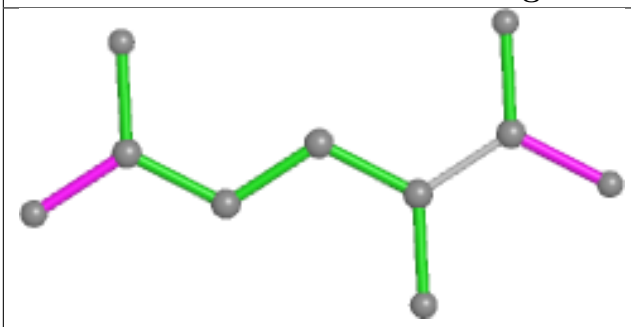
Ligand GLN F 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GLN D 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

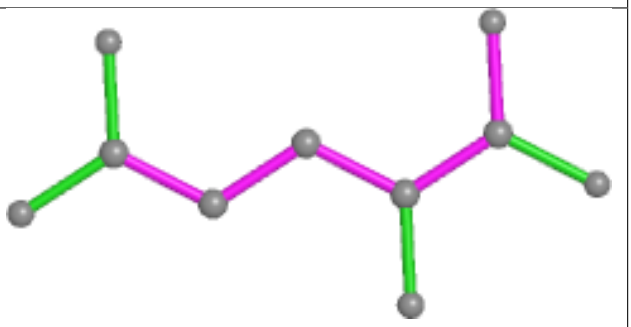
Ligand GLN C 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand GLN A 301	
 Bond lengths	 Bond angles
 Torsions	 Rings

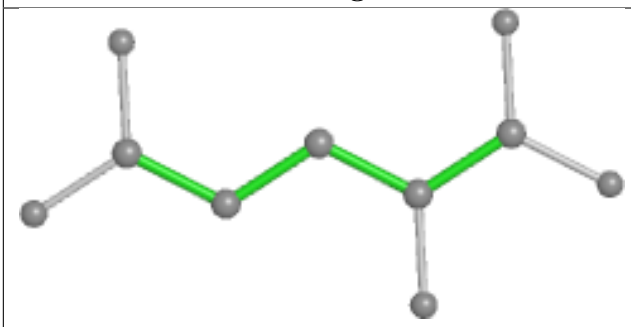
Ligand GLN B 301



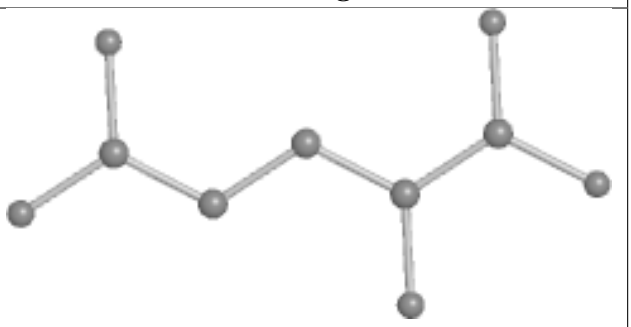
Bond lengths



Bond angles

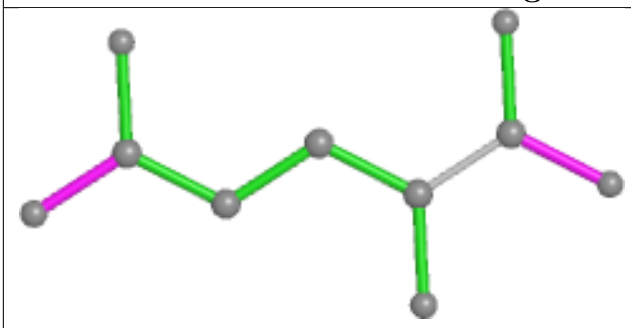


Torsions

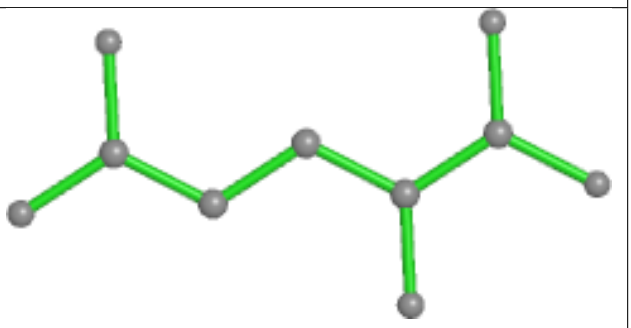


Rings

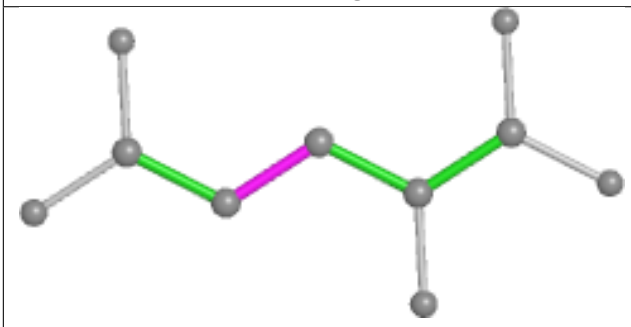
Ligand GLN E 301



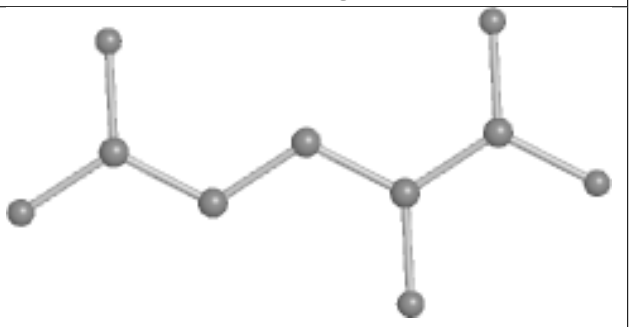
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} 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	219/230 (95%)	0.14	2 (0%) 84 83	19, 32, 51, 72	0
1	B	219/230 (95%)	0.23	1 (0%) 91 91	25, 41, 58, 73	0
1	C	219/230 (95%)	0.27	6 (2%) 54 54	22, 41, 64, 81	0
1	D	219/230 (95%)	0.91	31 (14%) 2 2	31, 55, 82, 92	0
1	E	219/230 (95%)	1.82	91 (41%) 0 0	29, 72, 96, 127	0
1	F	219/230 (95%)	0.46	10 (4%) 32 32	30, 50, 70, 82	0
All	All	1314/1380 (95%)	0.64	141 (10%) 6 5	19, 46, 83, 127	0

All (141) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	213	ILE	12.5
1	E	123	ALA	11.3
1	E	101	VAL	9.8
1	E	152	LEU	6.4
1	E	177	LEU	6.3
1	E	122	LYS	6.3
1	E	187	PRO	6.3
1	E	173	VAL	6.3
1	E	80	ASP	6.0
1	D	33	ALA	5.3
1	D	210	TYR	5.3
1	E	70	ASP	5.1
1	E	98	ILE	5.1
1	D	217	TRP	4.9
1	E	219	GLY	4.9
1	D	37	LYS	4.7
1	E	68	ILE	4.6
1	E	132	GLN	4.4
1	A	97	ASP	4.3

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	107	LYS	4.3
1	E	190	SER	4.2
1	E	113	SER	4.2
1	E	213	ILE	4.1
1	E	183	GLY	4.0
1	D	208	GLY	4.0
1	E	130	LEU	3.9
1	E	200	ALA	3.8
1	E	79	SER	3.7
1	E	89	VAL	3.7
1	E	82	TYR	3.7
1	E	124	ASN	3.7
1	E	192	GLU	3.6
1	E	209	THR	3.6
1	E	178	GLU	3.6
1	D	75	ALA	3.6
1	E	111	VAL	3.6
1	D	206	GLU	3.5
1	D	32	ILE	3.5
1	E	57	LYS	3.5
1	E	104	LEU	3.5
1	D	205	ARG	3.3
1	E	125	ILE	3.3
1	E	119	ASP	3.3
1	E	49	GLY	3.3
1	E	189	GLY	3.3
1	E	181	GLN	3.2
1	D	209	THR	3.2
1	E	50	ILE	3.2
1	E	144	GLY	3.2
1	E	108	VAL	3.2
1	E	69	THR	3.2
1	F	178	GLU	3.1
1	D	202	LYS	3.1
1	E	120	TYR	3.1
1	D	69	THR	3.1
1	E	174	GLY	3.1
1	E	176	SER	3.1
1	D	199	GLY	3.1
1	F	70	ASP	3.1
1	F	19	ASP	3.1
1	E	134	PRO	3.0

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	C	97	ASP	3.0
1	E	100	SER	3.0
1	E	215	LYS	3.0
1	D	28	LEU	3.0
1	E	216	LYS	3.0
1	E	109	VAL	2.9
1	E	195	ASP	2.9
1	C	219	GLY	2.8
1	F	122	LYS	2.8
1	E	191	ASP	2.8
1	D	19	ASP	2.8
1	C	167	ASN	2.8
1	E	117	SER	2.8
1	D	214	TYR	2.7
1	E	110	ALA	2.7
1	D	71	GLU	2.7
1	D	129	ASP	2.7
1	E	186	PHE	2.7
1	E	48	SER	2.6
1	E	205	ARG	2.6
1	A	98	ILE	2.6
1	E	74	LYS	2.6
1	E	129	ASP	2.6
1	E	175	ASP	2.6
1	F	20	LEU	2.6
1	E	75	ALA	2.5
1	F	192	GLU	2.5
1	E	55	GLN	2.5
1	E	197	VAL	2.5
1	E	182	TYR	2.5
1	E	218	PHE	2.5
1	C	98	ILE	2.4
1	E	148	ALA	2.4
1	F	2	LEU	2.4
1	F	38	LEU	2.4
1	E	114	GLY	2.4
1	D	122	LYS	2.4
1	C	166	GLY	2.4
1	E	97	ASP	2.4
1	E	179	ALA	2.4
1	D	102	LYS	2.4
1	E	66	ILE	2.4

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	E	83	TYR	2.4
1	E	133	PHE	2.4
1	E	139	ALA	2.3
1	D	188	LYS	2.3
1	E	193	LEU	2.3
1	B	97	ASP	2.3
1	E	199	GLY	2.3
1	E	95	ASN	2.3
1	D	104	LEU	2.3
1	D	131	ARG	2.3
1	E	88	LEU	2.2
1	D	38	LEU	2.2
1	E	64	ALA	2.2
1	E	37	LYS	2.2
1	F	215	LYS	2.2
1	E	115	THR	2.2
1	E	72	ARG	2.2
1	E	51	ILE	2.1
1	E	87	LEU	2.1
1	D	74	LYS	2.1
1	E	151	VAL	2.1
1	F	1	MET	2.1
1	D	177	LEU	2.1
1	D	35	GLU	2.1
1	E	102	LYS	2.1
1	E	81	GLY	2.1
1	E	33	ALA	2.1
1	E	76	ILE	2.1
1	E	77	ASP	2.1
1	E	34	LYS	2.1
1	E	54	LEU	2.0
1	D	81	GLY	2.0
1	E	210	TYR	2.0
1	D	80	ASP	2.0
1	D	39	ASP	2.0
1	E	31	ALA	2.0
1	E	201	LEU	2.0
1	C	108	VAL	2.0

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

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

6.3 Carbohydrates (i)

There are no monosaccharides in this entry.

6.4 Ligands (i)

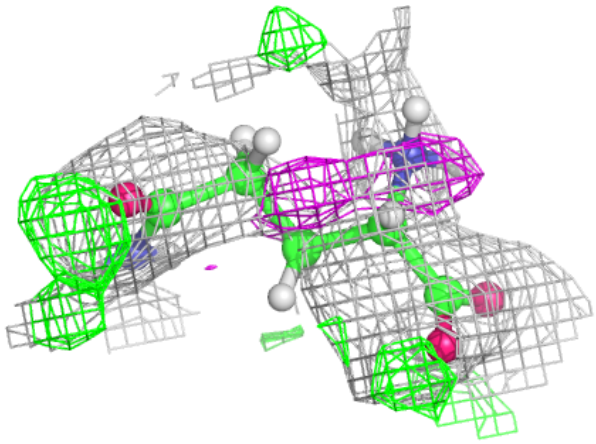
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9'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

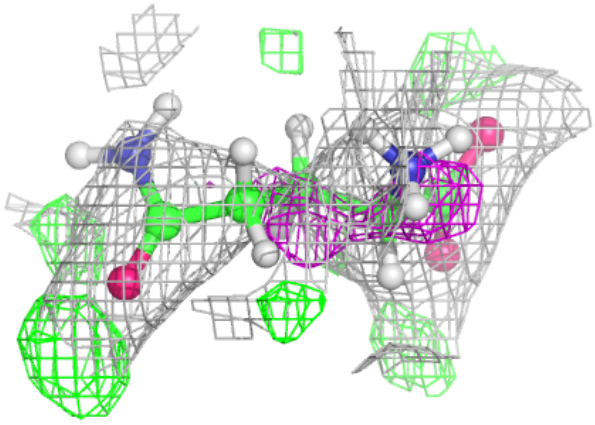
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å^2)	Q<0.9
2	GLN	E	301	10/10	0.70	0.25	37,51,61,61	0
2	GLN	F	301	10/10	0.86	0.17	26,37,46,46	0
2	GLN	D	301	10/10	0.92	0.15	28,36,40,40	0
2	GLN	B	301	10/10	0.95	0.19	21,28,36,36	0
2	GLN	C	301	10/10	0.97	0.18	22,27,31,33	0
2	GLN	A	301	10/10	0.98	0.20	20,24,29,29	0

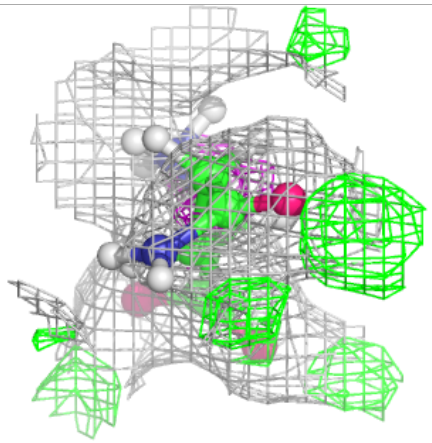
The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation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

Electron density around GLN 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)

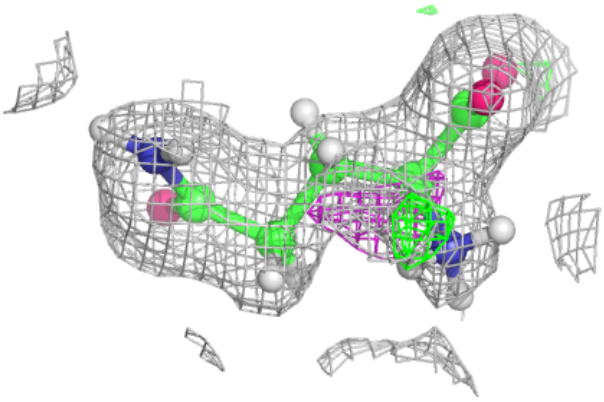


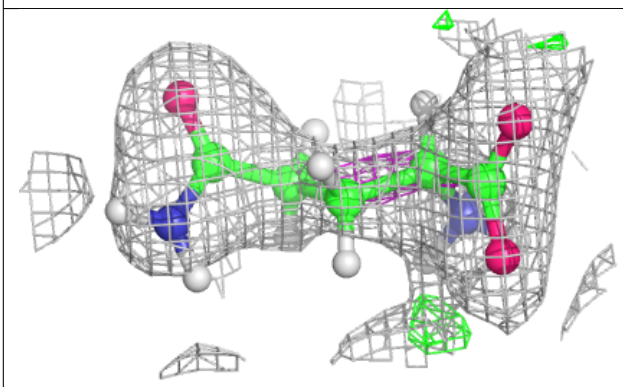


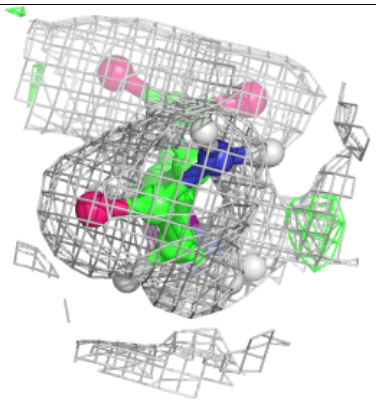


Electron density around GLN F 301:

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

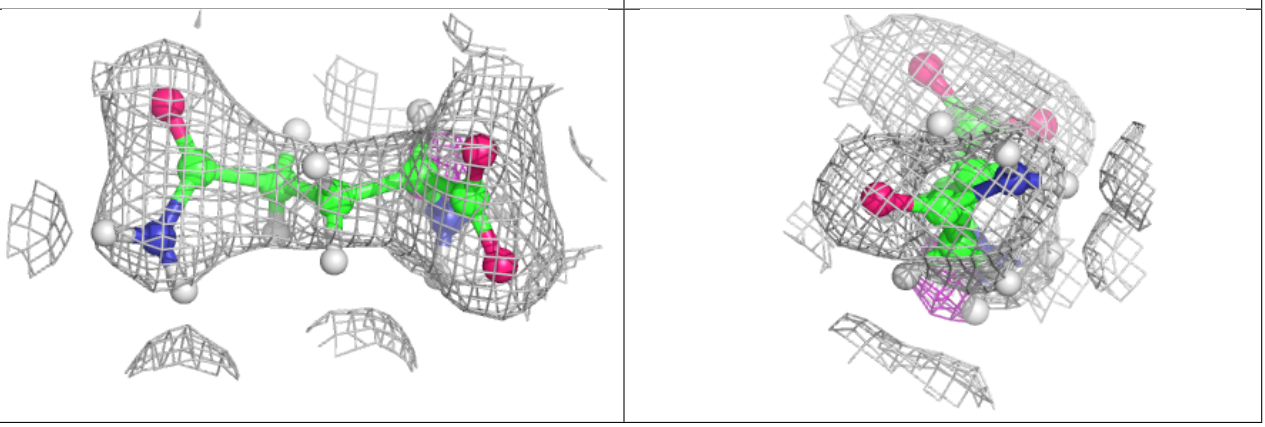






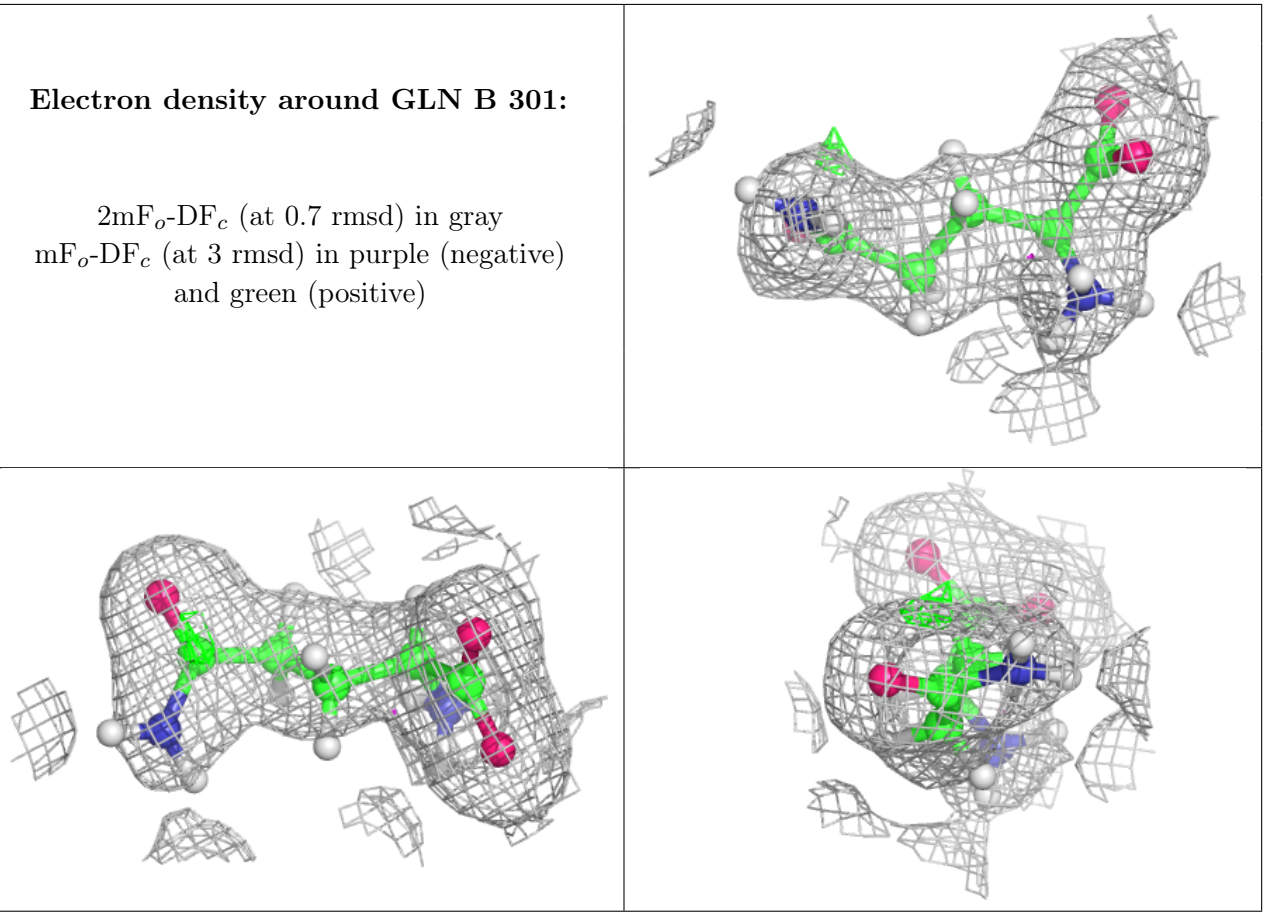
Electron density around GLN D 301:

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



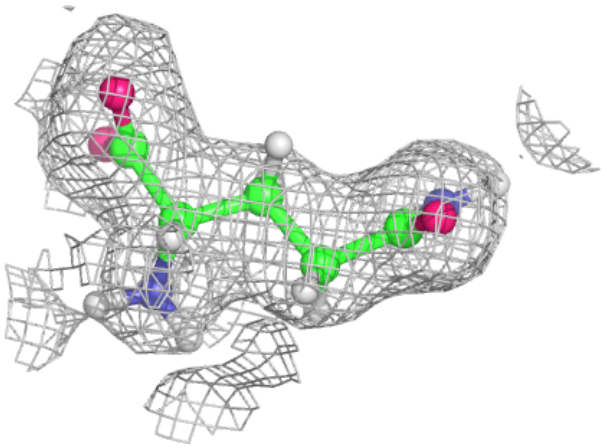
Electron density around GLN B 301:

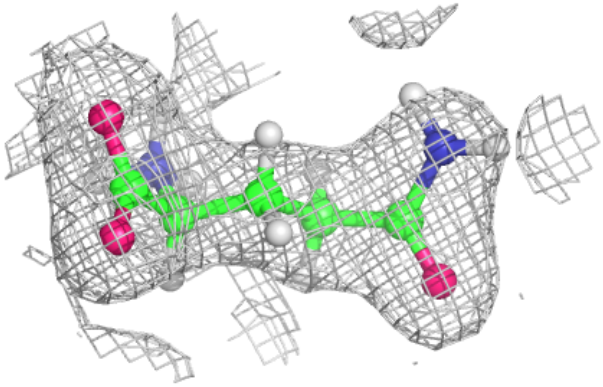
$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative) and green (positive)

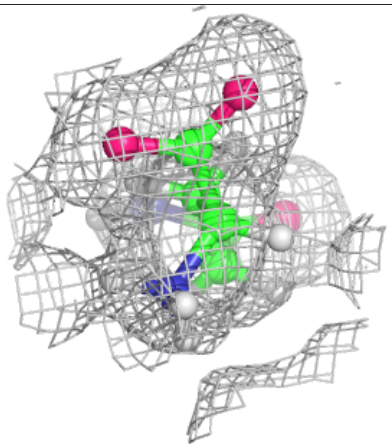


Electron density around GLN C 301:

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

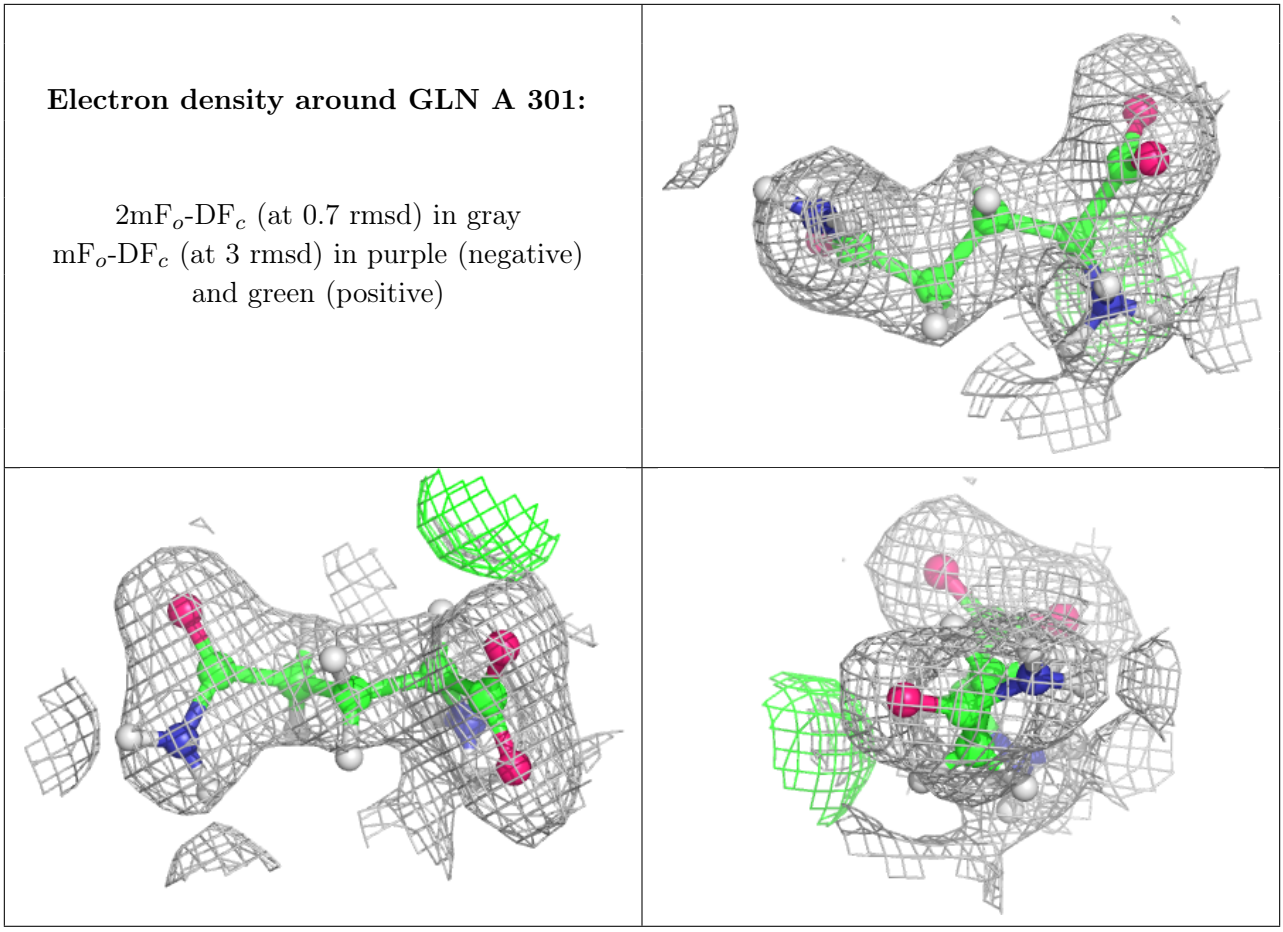






Electron density around GLN A 301:

$2mF_o$-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.