



# Full wwPDB X-ray Structure Validation Report ⓘ

Jan 26, 2022 – 08:07 AM EST

PDB ID : 7SBM  
Title : Human glutaminase C (Y466W) with L-Gln, open conformation  
Authors : Nguyen, T.-T.T.; Cerione, R.A.  
Deposited on : 2021-09-25  
Resolution : 2.80 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](mailto: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.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.26  
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) : 2.26

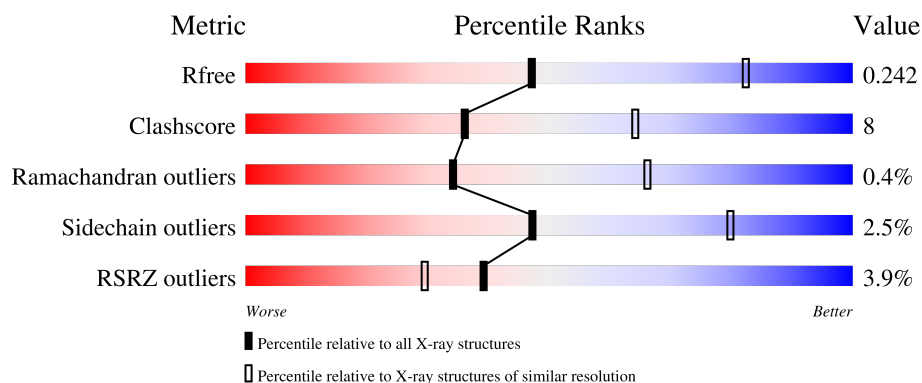
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 2.80 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	3140 (2.80-2.80)
Clashscore	141614	3569 (2.80-2.80)
Ramachandran outliers	138981	3498 (2.80-2.80)
Sidechain outliers	138945	3500 (2.80-2.80)
RSRZ outliers	127900	3078 (2.80-2.80)

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  $\geq 3$ , 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	539	<div> <div>4%</div> <div>58% 15% . 26%</div> </div>
1	B	539	<div> <div>3%</div> <div>61% 11% . 27%</div> </div>
1	C	539	<div> <div>2%</div> <div>60% 13% . 26%</div> </div>
1	D	539	<div> <div>3%</div> <div>60% 14% . 25%</div> </div>

## 2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 12563 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 Isoform 3 of Glutaminase kidney isoform, mitochondrial.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	400	Total	C	N	O	S	3	0	0
			3117	1988	525	576	28			
1	B	392	Total	C	N	O	S	2	0	0
			3060	1952	516	564	28			
1	C	399	Total	C	N	O	S	2	0	0
			3114	1986	524	576	28			
1	D	403	Total	C	N	O	S	2	0	0
			3143	2003	529	583	28			

There are 52 discrepancies between the modelled and reference sequences:

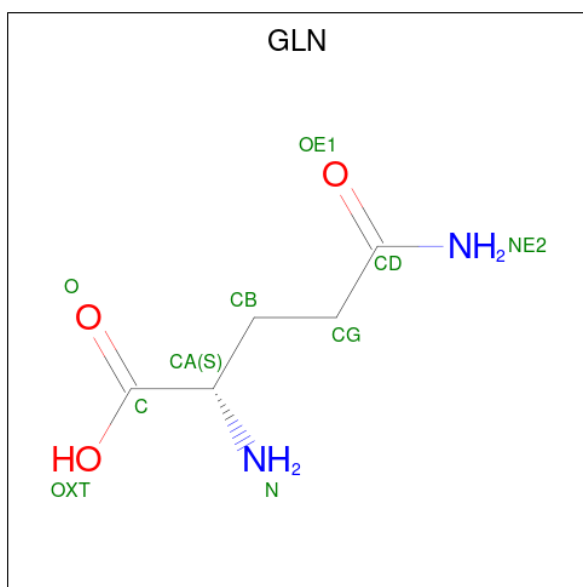
Chain	Residue	Modelled	Actual	Comment	Reference
A	60	MET	-	initiating methionine	UNP O94925
A	61	ARG	-	expression tag	UNP O94925
A	62	GLY	-	expression tag	UNP O94925
A	63	SER	-	expression tag	UNP O94925
A	64	HIS	-	expression tag	UNP O94925
A	65	HIS	-	expression tag	UNP O94925
A	66	HIS	-	expression tag	UNP O94925
A	67	HIS	-	expression tag	UNP O94925
A	68	HIS	-	expression tag	UNP O94925
A	69	HIS	-	expression tag	UNP O94925
A	70	GLY	-	expression tag	UNP O94925
A	71	SER	-	expression tag	UNP O94925
A	466	TRP	TYR	engineered mutation	UNP O94925
B	60	MET	-	initiating methionine	UNP O94925
B	61	ARG	-	expression tag	UNP O94925
B	62	GLY	-	expression tag	UNP O94925
B	63	SER	-	expression tag	UNP O94925
B	64	HIS	-	expression tag	UNP O94925
B	65	HIS	-	expression tag	UNP O94925
B	66	HIS	-	expression tag	UNP O94925
B	67	HIS	-	expression tag	UNP O94925

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Chain	Residue	Modelled	Actual	Comment	Reference
B	68	HIS	-	expression tag	UNP O94925
B	69	HIS	-	expression tag	UNP O94925
B	70	GLY	-	expression tag	UNP O94925
B	71	SER	-	expression tag	UNP O94925
B	466	TRP	TYR	engineered mutation	UNP O94925
C	60	MET	-	initiating methionine	UNP O94925
C	61	ARG	-	expression tag	UNP O94925
C	62	GLY	-	expression tag	UNP O94925
C	63	SER	-	expression tag	UNP O94925
C	64	HIS	-	expression tag	UNP O94925
C	65	HIS	-	expression tag	UNP O94925
C	66	HIS	-	expression tag	UNP O94925
C	67	HIS	-	expression tag	UNP O94925
C	68	HIS	-	expression tag	UNP O94925
C	69	HIS	-	expression tag	UNP O94925
C	70	GLY	-	expression tag	UNP O94925
C	71	SER	-	expression tag	UNP O94925
C	466	TRP	TYR	engineered mutation	UNP O94925
D	60	MET	-	initiating methionine	UNP O94925
D	61	ARG	-	expression tag	UNP O94925
D	62	GLY	-	expression tag	UNP O94925
D	63	SER	-	expression tag	UNP O94925
D	64	HIS	-	expression tag	UNP O94925
D	65	HIS	-	expression tag	UNP O94925
D	66	HIS	-	expression tag	UNP O94925
D	67	HIS	-	expression tag	UNP O94925
D	68	HIS	-	expression tag	UNP O94925
D	69	HIS	-	expression tag	UNP O94925
D	70	GLY	-	expression tag	UNP O94925
D	71	SER	-	expression tag	UNP O94925
D	466	TRP	TYR	engineered mutation	UNP O94925

- 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	N	O	0	0
			10	5	2	3		
2	B	1	Total	C	N	O	0	0
			10	5	2	3		
2	C	1	Total	C	N	O	0	0
			10	5	2	3		
2	D	1	Total	C	N	O	0	0
			10	5	2	3		

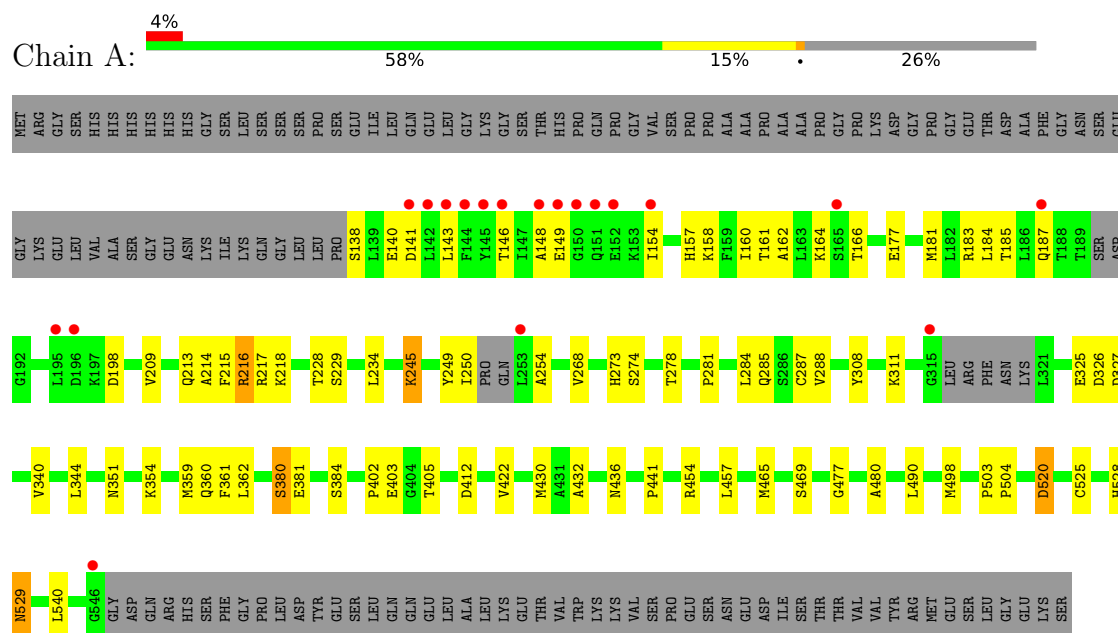
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	22	Total	O	0	0
			22	22		
3	B	28	Total	O	0	0
			28	28		
3	C	20	Total	O	0	0
			20	20		
3	D	19	Total	O	0	0
			19	19		

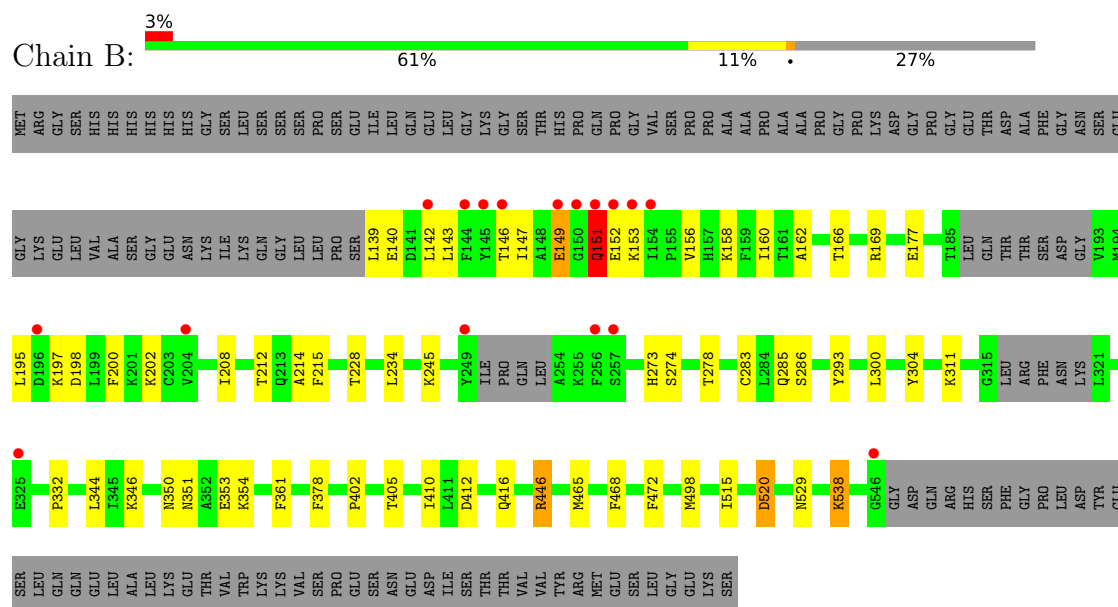
### 3 Residue-property plots [i](#)

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.

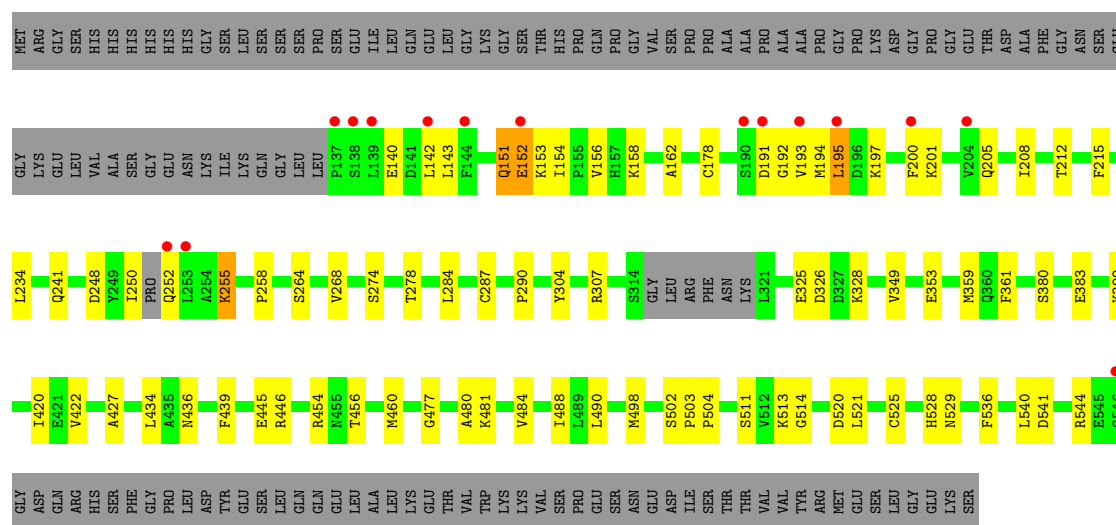
- Molecule 1: Isoform 3 of Glutaminase kidney isoform, mitochondrial



- Molecule 1: Isoform 3 of Glutaminase kidney isoform, mitochondrial



- Chain C:  2% 60% 13% 26%



## 4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	98.84Å 139.10Å 177.44Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	39.29 – 2.80 39.29 – 2.80	Depositor EDS
% Data completeness (in resolution range)	99.4 (39.29-2.80) 99.4 (39.29-2.80)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	2.87 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, $R_{free}$	0.200 , 0.243 0.200 , 0.242	Depositor DCC
$R_{free}$ test set	1993 reflections (3.28%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	34.5	Xtriage
Anisotropy	0.918	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.31 , 33.8	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.47$ , $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.95	EDS
Total number of atoms	12563	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	38.0	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 57.01 % 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 2.5200e-05. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical 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

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	0.51	0/3184	0.72	6/4294 (0.1%)
1	B	0.53	2/3127 (0.1%)	0.77	7/4216 (0.2%)
1	C	0.50	2/3181 (0.1%)	0.76	9/4289 (0.2%)
1	D	0.47	0/3212	0.69	4/4334 (0.1%)
All	All	0.50	4/12704 (0.0%)	0.73	26/17133 (0.2%)

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	1
All	All	0	3

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	283	CYS	CB-SG	-6.38	1.71	1.82
1	C	303	GLU	CB-CG	-6.13	1.40	1.52
1	C	304	TYR	CB-CG	5.30	1.59	1.51
1	B	169	ARG	CG-CD	5.09	1.64	1.51

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	245	LYS	CD-CE-NZ	-9.68	89.43	111.70
1	B	152	GLU	CA-CB-CG	9.65	134.63	113.40
1	C	326	ASP	CB-CG-OD2	-8.87	110.31	118.30
1	B	446	ARG	NE-CZ-NH1	8.17	124.39	120.30
1	C	544	ARG	CB-CG-CD	-8.09	90.56	111.60
1	B	446	ARG	NE-CZ-NH2	-8.01	116.30	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	544	ARG	NE-CZ-NH1	-7.85	116.38	120.30
1	B	169	ARG	CB-CG-CD	7.45	130.97	111.60
1	D	152	GLU	CA-CB-CG	-7.13	97.72	113.40
1	C	544	ARG	NE-CZ-NH2	7.03	123.81	120.30
1	D	142	LEU	CB-CG-CD2	-6.34	100.22	111.00
1	D	195	LEU	CA-CB-CG	6.22	129.62	115.30
1	A	403	GLU	CA-CB-CG	6.03	126.67	113.40
1	A	177	GLU	CA-CB-CG	-5.97	100.28	113.40
1	C	353	GLU	CA-CB-CG	5.91	126.39	113.40
1	C	240	LYS	CB-CG-CD	5.84	126.79	111.60
1	D	142	LEU	CB-CG-CD1	5.79	120.84	111.00
1	B	538	LYS	CD-CE-NZ	5.61	124.61	111.70
1	A	217	ARG	CG-CD-NE	5.56	123.47	111.80
1	A	327	ASP	C-N-CA	5.24	134.81	121.70
1	A	217	ARG	CA-CB-CG	5.22	124.89	113.40
1	B	152	GLU	N-CA-CB	-5.21	101.23	110.60
1	C	303	GLU	CB-CA-C	-5.19	100.01	110.40
1	A	403	GLU	CB-CG-CD	-5.17	100.25	114.20
1	C	303	GLU	CB-CG-CD	-5.04	100.58	114.20
1	C	326	ASP	CB-CG-OD1	5.01	122.81	118.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	149	GLU	Peptide
1	B	151	GLN	Peptide
1	D	151	GLN	Peptide

## 5.2 Too-close contacts ⓘ

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3117	0	3090	47	0
1	B	3060	0	3027	41	0
1	C	3114	0	3082	62	0
1	D	3143	0	3113	56	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
2	A	10	0	7	2	0
2	B	10	0	7	4	0
2	C	10	0	7	5	0
2	D	10	0	7	1	0
3	A	22	0	0	0	0
3	B	28	0	0	0	0
3	C	20	0	0	0	0
3	D	19	0	0	1	0
All	All	12563	0	12340	198	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 8.

All (198) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:SER:HB2	2:B:601:GLN:OE1	1.53	1.05
1:D:153:LYS:HB3	1:D:194:MET:HG2	1.44	0.95
1:C:189:THR:HG22	1:C:191:ASP:OD1	1.72	0.89
1:B:286:SER:CB	2:B:601:GLN:OE1	2.22	0.88
1:C:153:LYS:HB3	1:C:194:MET:HG2	1.56	0.86
1:D:250:ILE:HD12	1:D:252:GLN:HB2	1.62	0.82
1:B:228:THR:HG23	1:B:273:HIS:CE1	2.20	0.76
1:A:166:THR:HG21	1:A:214:ALA:HB1	1.66	0.76
1:D:153:LYS:HB3	1:D:194:MET:CG	2.16	0.75
1:A:209:VAL:O	1:A:213:GLN:HG3	1.87	0.74
1:C:198:ASP:HA	1:C:201:LYS:HB3	1.70	0.73
1:A:184:LEU:HG	1:C:281:PRO:HG3	1.71	0.73
1:C:274:SER:HB3	1:C:278:THR:HG21	1.70	0.71
1:B:285:GLN:HB3	2:B:601:GLN:HG2	1.73	0.71
1:B:162:ALA:HB1	1:B:215:PHE:HE1	1.58	0.68
1:B:350:ASN:ND2	1:B:353:GLU:OE1	2.26	0.68
1:B:140:GLU:HG3	1:B:208:ILE:HG12	1.76	0.68
1:B:234:LEU:HD22	1:B:520:ASP:HB3	1.77	0.67
1:C:228:THR:HG23	1:C:273:HIS:CE1	2.30	0.66
1:A:359:MET:HG3	1:C:188:THR:HG22	1.77	0.66
1:D:541:ASP:HB3	1:D:544:ARG:HG3	1.77	0.66
1:A:480:ALA:HB2	1:A:490:LEU:HD12	1.78	0.66
1:D:234:LEU:HD22	1:D:520:ASP:HB3	1.77	0.66
1:D:325:GLU:H	1:D:325:GLU:CD	1.99	0.66
1:A:162:ALA:HB1	1:A:215:PHE:HE1	1.59	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:465:MET:H	1:A:469:SER:HB3	1.60	0.65
1:C:285:GLN:HB3	2:C:601:GLN:HE21	1.61	0.65
1:A:362:LEU:HD22	1:A:430:MET:HE1	1.78	0.65
1:C:153:LYS:HB3	1:C:194:MET:CG	2.26	0.64
1:A:157:HIS:O	1:A:161:THR:HG23	1.97	0.64
1:A:274:SER:HB3	1:A:278:THR:HG21	1.79	0.63
1:B:402:PRO:O	1:B:405:THR:OG1	2.14	0.63
1:D:152:GLU:OE2	1:D:197:LYS:HB2	1.98	0.63
1:D:192:GLY:O	1:D:194:MET:N	2.32	0.62
1:B:274:SER:HB3	1:B:278:THR:HG21	1.80	0.62
1:D:484:VAL:N	2:D:601:GLN:OE1	2.31	0.62
1:A:234:LEU:HD22	1:A:520:ASP:HB3	1.81	0.62
1:C:140:GLU:HB2	1:C:201:LYS:HD2	1.82	0.61
1:A:228:THR:HG23	1:A:273:HIS:CE1	2.35	0.60
1:C:349:VAL:CG1	1:C:353:GLU:HB2	2.32	0.60
1:A:250:ILE:HB	1:A:380:SER:OG	2.02	0.60
1:D:156:VAL:HG12	1:D:195:LEU:HD13	1.83	0.60
1:D:498:MET:HE1	1:D:521:LEU:HD22	1.84	0.59
1:B:143:LEU:HD13	1:B:212:THR:HG22	1.83	0.59
1:C:484:VAL:H	2:C:601:GLN:HE22	1.51	0.59
1:C:362:LEU:HD23	1:C:365:MET:CE	2.34	0.58
1:C:234:LEU:HD22	1:C:520:ASP:HB3	1.85	0.58
1:C:484:VAL:H	2:C:601:GLN:NE2	2.01	0.57
1:D:152:GLU:O	1:D:153:LYS:HG3	2.03	0.57
1:C:536:PHE:CZ	1:C:544:ARG:NH2	2.73	0.57
1:D:153:LYS:HB3	1:D:194:MET:SD	2.45	0.57
1:C:191:ASP:O	1:C:193:VAL:N	2.39	0.56
1:D:274:SER:HB3	1:D:278:THR:HG21	1.87	0.56
1:D:326:ASP:HB3	1:D:328:LYS:HG3	1.87	0.56
1:A:187:GLN:HB3	1:C:280:VAL:HG22	1.86	0.56
1:C:153:LYS:HE2	1:C:194:MET:HG2	1.88	0.56
1:D:208:ILE:O	1:D:212:THR:HG23	2.06	0.56
1:D:439:PHE:CE2	1:D:446:ARG:HB2	2.41	0.55
1:D:456:THR:HG22	1:D:460:MET:HE2	1.89	0.55
1:A:268:VAL:HG12	1:A:436:ASN:HB2	1.87	0.55
1:C:541:ASP:O	1:C:544:ARG:HB2	2.07	0.55
1:D:252:GLN:HB3	1:D:380:SER:OG	2.06	0.54
1:B:143:LEU:HD23	1:B:200:PHE:HZ	1.72	0.54
1:D:140:GLU:OE2	1:D:140:GLU:N	2.30	0.54
1:C:156:VAL:HG12	1:C:195:LEU:HD13	1.89	0.54
1:D:153:LYS:CB	1:D:194:MET:HG2	2.30	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:216:ARG:HB3	1:A:218:LYS:HE2	1.90	0.53
1:A:249:TYR:CD1	1:A:250:ILE:HG23	2.43	0.53
1:D:304:TYR:HA	1:D:307:ARG:HD2	1.91	0.53
1:B:166:THR:HG21	1:B:214:ALA:HB1	1.91	0.53
1:A:181:MET:O	1:A:185:THR:HG23	2.10	0.52
1:A:381:GLU:OE2	2:A:601:GLN:N	2.43	0.52
1:C:142:LEU:HG	1:C:142:LEU:O	2.08	0.52
1:B:139:LEU:CD2	1:B:208:ILE:HG13	2.40	0.51
1:A:250:ILE:HG13	1:A:254:ALA:H	1.75	0.51
1:B:351:ASN:HA	1:B:354:LYS:HB2	1.91	0.51
1:C:217:ARG:HH22	1:C:223:ASP:HB2	1.74	0.51
1:C:217:ARG:NH2	1:C:223:ASP:HB2	2.25	0.51
1:A:529:ASN:OD1	1:D:529:ASN:OD1	2.28	0.51
1:D:477:GLY:O	1:D:529:ASN:HB2	2.11	0.51
1:A:402:PRO:HD2	1:A:405:THR:HG21	1.92	0.51
1:D:156:VAL:HG12	1:D:195:LEU:CD1	2.41	0.51
1:A:140:GLU:OE1	1:A:140:GLU:N	2.34	0.50
1:A:432:ALA:HB1	1:A:441:PRO:HG3	1.92	0.50
1:C:140:GLU:OE2	1:C:140:GLU:N	2.43	0.50
1:C:189:THR:HG22	1:C:191:ASP:CG	2.32	0.50
1:B:465:MET:HE2	1:B:515:ILE:HD11	1.93	0.50
1:C:303:GLU:OE2	1:C:307:ARG:NH1	2.44	0.50
1:B:300:LEU:HD13	1:B:304:TYR:CE1	2.47	0.50
1:C:192:GLY:O	1:C:194:MET:N	2.44	0.50
1:C:162:ALA:HB1	1:C:215:PHE:HE1	1.75	0.50
1:C:285:GLN:HB3	2:C:601:GLN:NE2	2.26	0.50
1:C:488:ILE:HD12	1:C:514:GLY:HA3	1.92	0.50
1:A:216:ARG:O	1:A:218:LYS:HG2	2.13	0.49
1:D:201:LYS:O	1:D:205:GLN:HB2	2.12	0.49
1:B:139:LEU:HD23	1:B:208:ILE:HG13	1.95	0.49
1:C:149:GLU:O	1:C:151:GLN:HG2	2.13	0.49
1:A:360:GLN:HE21	1:C:184:LEU:HD21	1.78	0.49
1:C:323:LEU:HG	1:C:394:TYR:HE2	1.76	0.49
1:C:325:GLU:H	1:C:325:GLU:CD	2.16	0.49
1:A:160:ILE:HG22	1:A:164:LYS:HD2	1.93	0.49
1:A:528:HIS:CD2	1:D:454:ARG:HD2	2.48	0.49
1:A:281:PRO:HA	1:A:422:VAL:O	2.13	0.48
1:D:268:VAL:HG12	1:D:436:ASN:HB2	1.95	0.48
1:D:456:THR:HG22	1:D:460:MET:CE	2.44	0.48
1:D:162:ALA:HB1	1:D:215:PHE:HE1	1.79	0.48
1:C:300:LEU:HD13	1:C:304:TYR:CE2	2.49	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:525:CYS:HA	1:A:540:LEU:O	2.13	0.47
1:B:149:GLU:HG2	1:B:151:GLN:HG2	1.97	0.47
1:C:153:LYS:HE2	1:C:194:MET:CG	2.45	0.47
1:D:290:PRO:HD3	1:D:481:LYS:HD3	1.97	0.47
1:A:245:LYS:N	1:A:245:LYS:HD2	2.30	0.47
1:C:435:ALA:HB2	1:C:491:VAL:HG13	1.95	0.47
1:C:506:ASP:HB3	1:C:512:VAL:HG22	1.98	0.46
1:D:258:PRO:HA	1:D:504:PRO:HD3	1.97	0.46
1:D:498:MET:CE	1:D:521:LEU:HD22	2.45	0.46
1:B:197:LYS:HB3	1:B:197:LYS:HE2	1.71	0.46
1:B:149:GLU:CG	1:B:151:GLN:HG2	2.46	0.46
1:B:498:MET:HB2	1:B:498:MET:HE2	1.84	0.46
1:B:142:LEU:O	1:B:146:THR:OG1	2.34	0.46
1:C:188:THR:O	1:C:189:THR:OG1	2.30	0.45
1:B:153:LYS:HB3	1:B:195:LEU:C	2.36	0.45
1:B:344:LEU:HD23	1:B:402:PRO:HG3	1.98	0.45
1:A:284:LEU:HD22	1:A:287:CYS:HB2	1.99	0.45
1:D:195:LEU:HD23	1:D:200:PHE:HD1	1.82	0.45
1:C:365:MET:HG3	1:C:447:VAL:HG11	1.98	0.45
1:C:247:ALA:HB2	1:C:484:VAL:HG22	1.99	0.45
1:D:248:ASP:O	1:D:255:LYS:NZ	2.44	0.45
1:D:359:MET:HE1	1:D:420:ILE:HG23	1.98	0.45
1:C:148:ALA:HB1	1:C:151:GLN:O	2.15	0.45
1:C:384:SER:O	1:C:384:SER:OG	2.28	0.45
1:C:381:GLU:OE2	2:C:601:GLN:N	2.50	0.44
1:C:286:SER:O	1:C:481:LYS:HE3	2.18	0.44
1:A:454:ARG:HD2	1:D:528:HIS:CD2	2.52	0.44
1:A:285:GLN:HB3	2:A:601:GLN:OE1	2.17	0.44
1:D:349:VAL:HG11	1:D:353:GLU:HB2	1.99	0.44
1:C:465:MET:HE2	1:C:515:ILE:HD11	2.00	0.44
1:A:148:ALA:HB2	1:A:154:ILE:HG12	1.99	0.44
1:C:249:TYR:OH	1:C:484:VAL:HG21	2.18	0.44
1:B:143:LEU:HD23	1:B:200:PHE:CZ	2.53	0.43
1:D:143:LEU:O	1:D:143:LEU:HG	2.18	0.43
1:C:349:VAL:HG13	1:C:353:GLU:HB2	2.00	0.43
1:B:346:LYS:O	1:B:354:LYS:HE2	2.18	0.43
1:D:197:LYS:HE3	1:D:197:LYS:HB3	1.70	0.43
1:B:162:ALA:HB1	1:B:215:PHE:CE1	2.46	0.43
1:D:536:PHE:HZ	1:D:544:ARG:HE	1.64	0.43
1:A:308:TYR:HB3	1:A:340:VAL:HG11	2.00	0.43
1:C:427:ALA:HB3	1:C:499:MET:HG2	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:GLY:O	1:A:529:ASN:HB2	2.18	0.43
1:B:149:GLU:HB2	1:B:151:GLN:HG2	2.01	0.43
1:D:503:PRO:N	1:D:504:PRO:HD2	2.34	0.43
1:A:503:PRO:N	1:A:504:PRO:HD2	2.34	0.42
1:C:143:LEU:HD23	1:C:200:PHE:HZ	1.84	0.42
1:C:477:GLY:O	1:C:529:ASN:HB2	2.19	0.42
1:D:513:LYS:HG3	3:D:714:HOH:O	2.19	0.42
1:B:410:ILE:HD13	1:B:410:ILE:HA	1.87	0.42
1:B:198:ASP:O	1:B:202:LYS:HB2	2.19	0.42
1:B:378:PHE:CE1	1:B:416:GLN:HG3	2.54	0.42
1:D:154:ILE:HG23	1:D:158:LYS:HE3	2.01	0.42
1:D:445:GLU:OE2	1:D:445:GLU:HA	2.19	0.42
1:A:325:GLU:N	1:A:325:GLU:OE1	2.53	0.42
1:C:143:LEU:HD23	1:C:200:PHE:CZ	2.54	0.42
1:D:349:VAL:CG1	1:D:353:GLU:HB2	2.49	0.42
1:C:303:GLU:OE2	1:C:303:GLU:O	2.38	0.42
1:C:362:LEU:HD23	1:C:365:MET:HE3	2.00	0.42
1:D:284:LEU:HD22	1:D:287:CYS:HB2	2.02	0.42
1:A:498:MET:HB2	1:A:498:MET:HE2	1.71	0.41
1:D:241:GLN:O	1:D:513:LYS:HE3	2.20	0.41
1:D:480:ALA:HB2	1:D:490:LEU:HD12	2.02	0.41
1:A:351:ASN:HA	1:A:354:LYS:HB2	2.02	0.41
1:B:286:SER:N	2:B:601:GLN:OE1	2.53	0.41
1:C:479:PRO:HD2	1:C:491:VAL:O	2.21	0.41
1:B:177:GLU:H	1:B:177:GLU:CD	2.24	0.41
1:C:457:LEU:HD23	1:C:460:MET:HE1	2.01	0.41
1:D:422:VAL:HG21	1:D:427:ALA:HB2	2.02	0.41
1:A:454:ARG:HD2	1:D:528:HIS:CG	2.55	0.41
1:A:457:LEU:HD23	1:A:457:LEU:HA	1.91	0.41
1:A:285:GLN:O	1:A:288:VAL:HG12	2.20	0.41
1:A:432:ALA:CB	1:A:441:PRO:HG3	2.50	0.41
1:B:139:LEU:HD23	1:B:208:ILE:CG1	2.51	0.41
1:B:143:LEU:O	1:B:147:ILE:HG12	2.21	0.41
1:C:459:LEU:HD23	1:C:459:LEU:HA	1.87	0.41
1:C:536:PHE:HZ	1:C:544:ARG:NH2	2.17	0.41
1:C:503:PRO:N	1:C:504:PRO:HD2	2.36	0.41
1:B:156:VAL:O	1:B:160:ILE:HG12	2.21	0.41
1:B:468:PHE:CD2	1:B:472:PHE:HB2	2.56	0.41
1:D:488:ILE:HD12	1:D:514:GLY:HA3	2.01	0.41
1:B:293:TYR:CD1	1:B:332:PRO:HG3	2.56	0.41
1:A:344:LEU:CD2	1:A:402:PRO:HG3	2.52	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:140:GLU:HG3	1:C:208:ILE:HG12	2.03	0.40
1:D:383:GLU:HA	1:D:383:GLU:OE1	2.21	0.40
1:B:153:LYS:HB3	1:B:195:LEU:O	2.21	0.40
1:D:502:SER:HB3	1:D:511:SER:OG	2.22	0.40
1:A:143:LEU:HA	1:A:146:THR:OG1	2.20	0.40
1:C:193:VAL:HG13	1:C:193:VAL:O	2.21	0.40
1:D:434:LEU:HD13	1:D:460:MET:HE1	2.03	0.40
1:D:525:CYS:HA	1:D:540:LEU:O	2.22	0.40
1:B:465:MET:CE	1:B:515:ILE:HD11	2.51	0.40

There are no symmetry-related clashes.

## 5.3 Torsion angles

### 5.3.1 Protein backbone

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	392/539 (73%)	381 (97%)	11 (3%)	0	100	100
1	B	384/539 (71%)	372 (97%)	11 (3%)	1 (0%)	41	72
1	C	390/539 (72%)	375 (96%)	12 (3%)	3 (1%)	19	49
1	D	397/539 (74%)	381 (96%)	13 (3%)	3 (1%)	19	49
All	All	1563/2156 (72%)	1509 (96%)	47 (3%)	7 (0%)	34	66

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	151	GLN
1	C	192	GLY
1	D	193	VAL
1	B	151	GLN
1	D	151	GLN
1	D	191	ASP

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Mol	Chain	Res	Type
1	C	193	VAL

### 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	345/462 (75%)	328 (95%)	17 (5%)	25	57
1	B	338/462 (73%)	330 (98%)	8 (2%)	49	81
1	C	345/462 (75%)	341 (99%)	4 (1%)	71	92
1	D	349/462 (76%)	344 (99%)	5 (1%)	67	90
All	All	1377/1848 (74%)	1343 (98%)	34 (2%)	47	80

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	138	SER
1	A	141	ASP
1	A	149	GLU
1	A	158	LYS
1	A	183	ARG
1	A	198	ASP
1	A	216	ARG
1	A	229	SER
1	A	245	LYS
1	A	311	LYS
1	A	326	ASP
1	A	361	PHE
1	A	380	SER
1	A	384	SER
1	A	412	ASP
1	A	520	ASP
1	A	529	ASN
1	B	158	LYS
1	B	311	LYS
1	B	361	PHE

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Mol	Chain	Res	Type
1	B	412	ASP
1	B	446	ARG
1	B	520	ASP
1	B	529	ASN
1	B	538	LYS
1	C	178	CYS
1	C	181	MET
1	C	361	PHE
1	C	520	ASP
1	D	178	CYS
1	D	255	LYS
1	D	264	SER
1	D	361	PHE
1	D	399	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (1) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	360	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The

Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
2	GLN	B	601	-	5,9,9	0.66	0	5,11,11	0.88	0
2	GLN	D	601	-	5,9,9	0.40	0	5,11,11	0.24	0
2	GLN	A	601	-	5,9,9	0.38	0	5,11,11	0.23	0
2	GLN	C	601	-	5,9,9	0.41	0	5,11,11	0.14	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	B	601	-	-	3/5/9/9	-
2	GLN	D	601	-	-	3/5/9/9	-
2	GLN	A	601	-	-	0/5/9/9	-
2	GLN	C	601	-	-	2/5/9/9	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (8) torsion outliers are listed below:

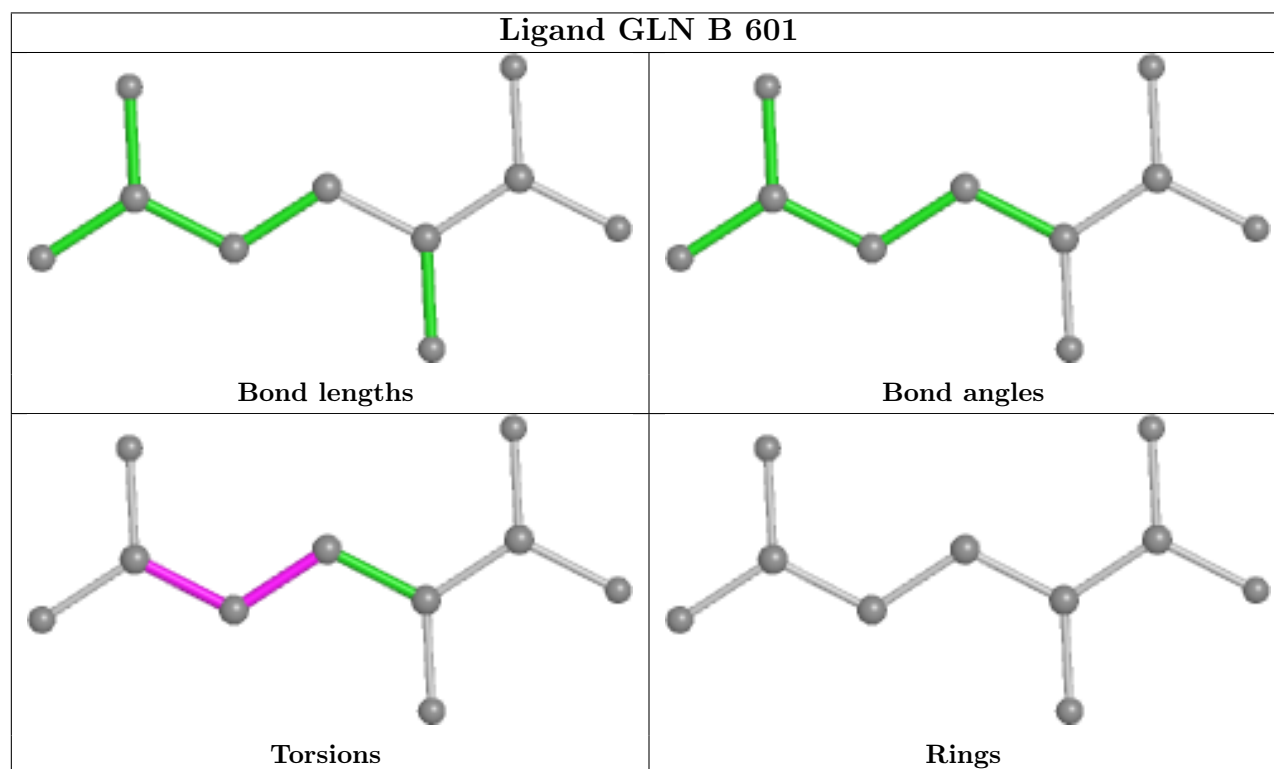
Mol	Chain	Res	Type	Atoms
2	B	601	GLN	OE1-CD-CG-CB
2	B	601	GLN	NE2-CD-CG-CB
2	D	601	GLN	NE2-CD-CG-CB
2	B	601	GLN	CA-CB-CG-CD
2	D	601	GLN	OE1-CD-CG-CB
2	C	601	GLN	NE2-CD-CG-CB
2	C	601	GLN	OE1-CD-CG-CB
2	D	601	GLN	N-CA-CB-CG

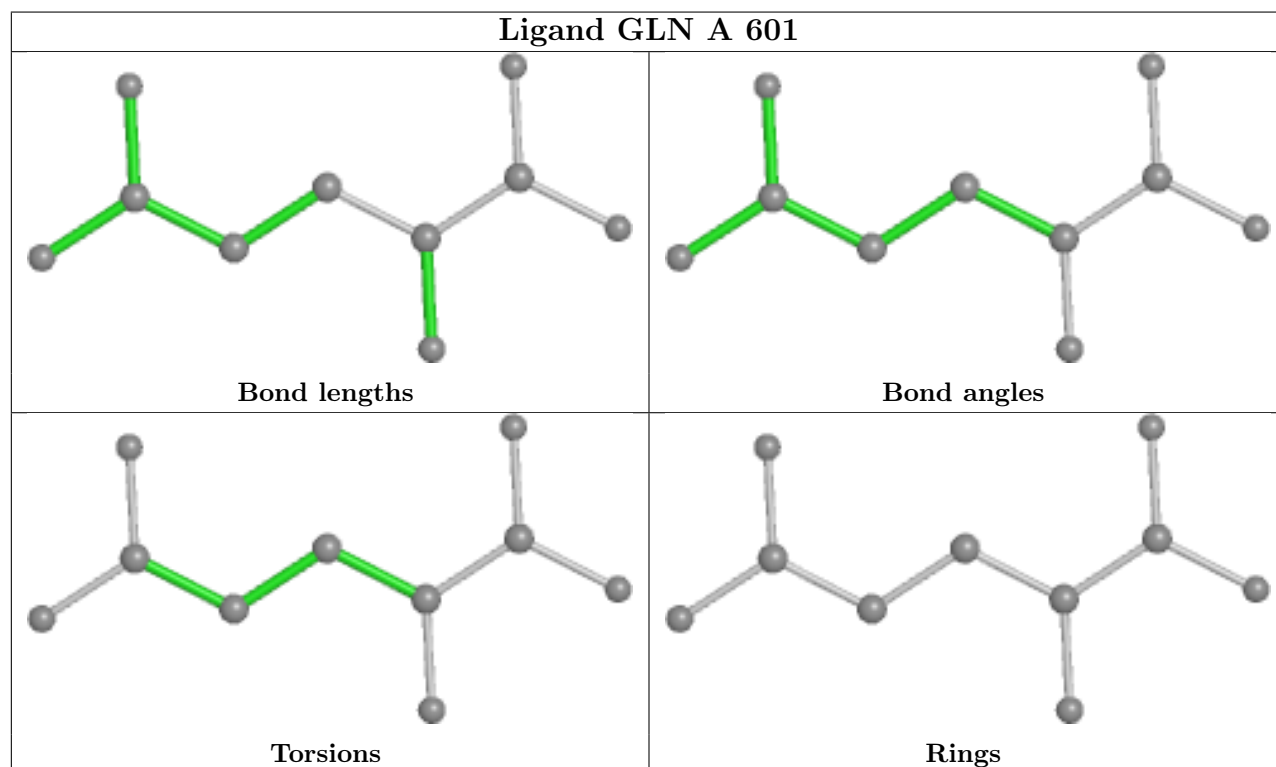
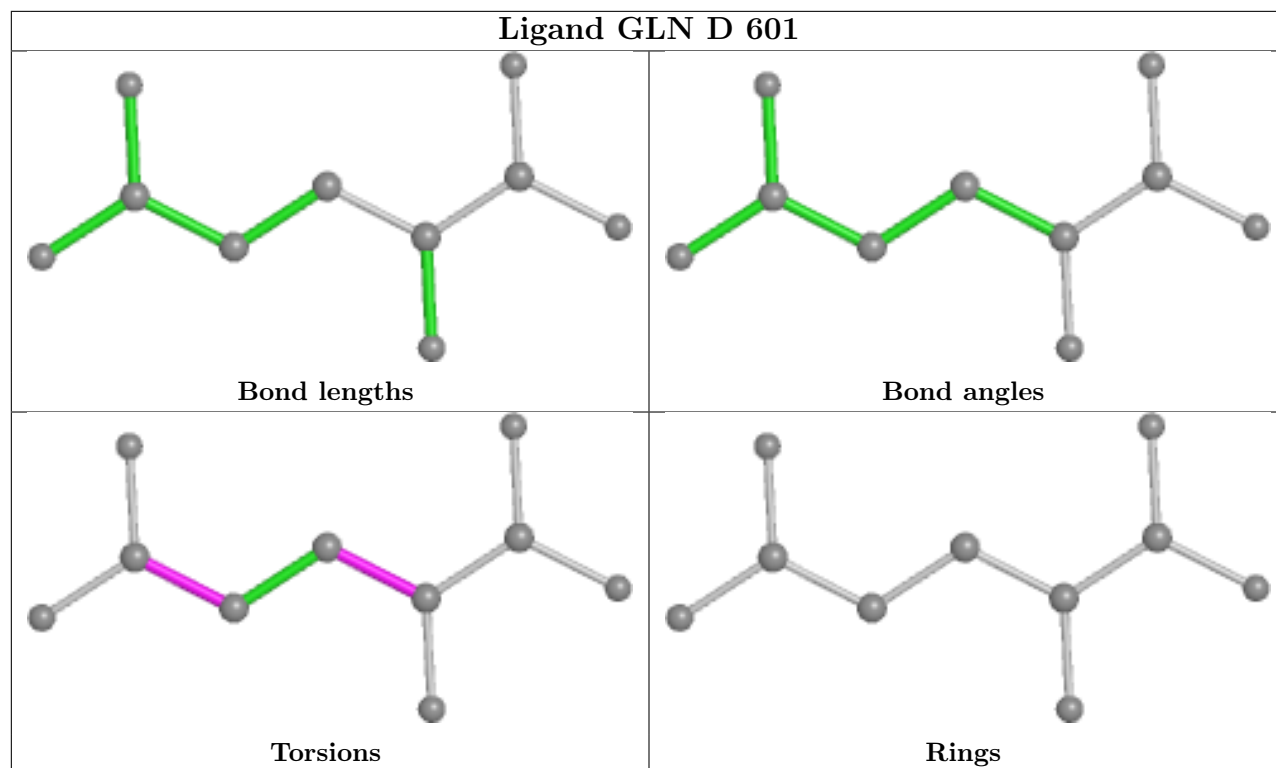
There are no ring outliers.

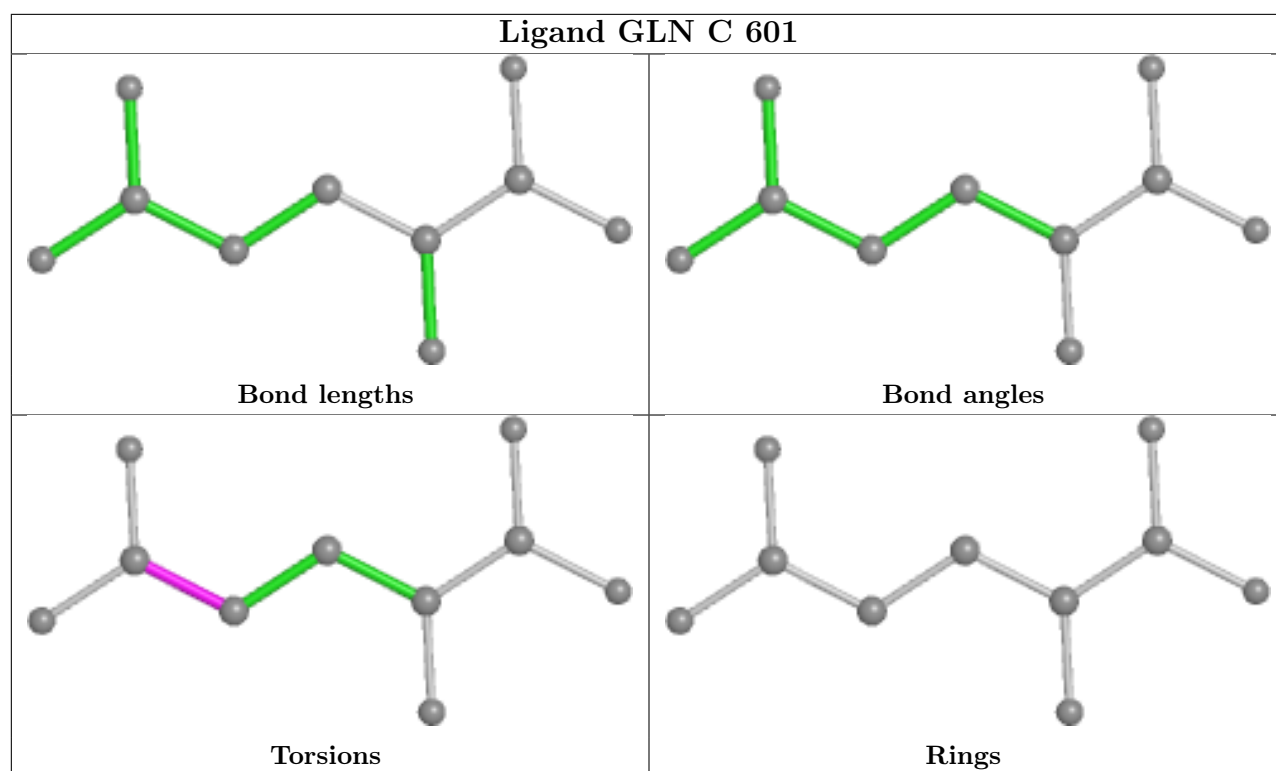
4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	GLN	4	0
2	D	601	GLN	1	0
2	A	601	GLN	2	0
2	C	601	GLN	5	0

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







## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

## 6 Fit of model and data

### 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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	400/539 (74%)	-0.05	19 (4%)	30 21	20, 31, 82, 124	2 (0%)
1	B	392/539 (72%)	-0.08	17 (4%)	35 25	19, 30, 78, 123	1 (0%)
1	C	399/539 (74%)	-0.17	11 (2%)	53 43	21, 32, 81, 110	1 (0%)
1	D	403/539 (74%)	-0.25	15 (3%)	41 31	18, 29, 78, 115	1 (0%)
All	All	1594/2156 (73%)	-0.14	62 (3%)	39 29	18, 31, 80, 124	5 (0%)

All (62) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	144	PHE	4.5
1	A	142	LEU	4.4
1	D	546	GLY	4.2
1	A	546	GLY	4.1
1	A	152	GLU	4.0
1	D	138	SER	4.0
1	A	150	GLY	4.0
1	D	191	ASP	3.9
1	A	315	GLY	3.8
1	C	150	GLY	3.7
1	B	149	GLU	3.7
1	D	204	VAL	3.6
1	B	145	TYR	3.6
1	A	144	PHE	3.6
1	A	148	ALA	3.5
1	B	256	PHE	3.4
1	B	152	GLU	3.4
1	B	257	SER	3.4
1	D	195	LEU	3.3
1	C	142	LEU	3.3
1	D	137	PRO	3.2

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Mol	Chain	Res	Type	RSRZ
1	D	190	SER	3.1
1	C	203	CYS	3.1
1	A	253	LEU	3.1
1	A	146	THR	3.1
1	C	204	VAL	3.1
1	D	200	PHE	2.9
1	D	142	LEU	2.9
1	D	193	VAL	2.8
1	A	149	GLU	2.8
1	A	145	TYR	2.8
1	D	152	GLU	2.8
1	B	546	GLY	2.7
1	C	191	ASP	2.6
1	A	143	LEU	2.5
1	A	165	SER	2.5
1	C	144	PHE	2.5
1	D	252	GLN	2.5
1	A	141	ASP	2.5
1	C	151	GLN	2.5
1	B	151	GLN	2.5
1	B	146	THR	2.5
1	B	142	LEU	2.5
1	D	253	LEU	2.4
1	B	153	LYS	2.3
1	B	204	VAL	2.3
1	D	139	LEU	2.3
1	C	152	GLU	2.3
1	A	196	ASP	2.2
1	A	187	GLN	2.2
1	B	249	TYR	2.2
1	C	321	LEU	2.2
1	A	195	LEU	2.1
1	B	325	GLU	2.1
1	B	196	ASP	2.1
1	A	151	GLN	2.1
1	B	150	GLY	2.1
1	C	193	VAL	2.1
1	B	144	PHE	2.1
1	C	256	PHE	2.0
1	B	154	ILE	2.0
1	A	154	ILE	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](#)

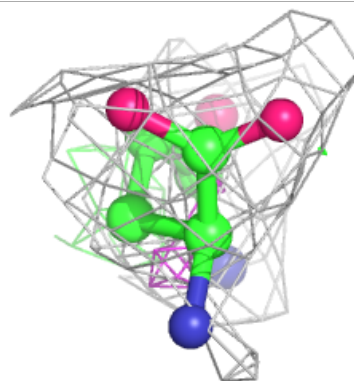
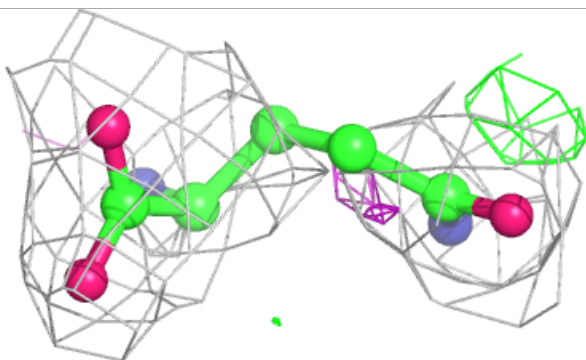
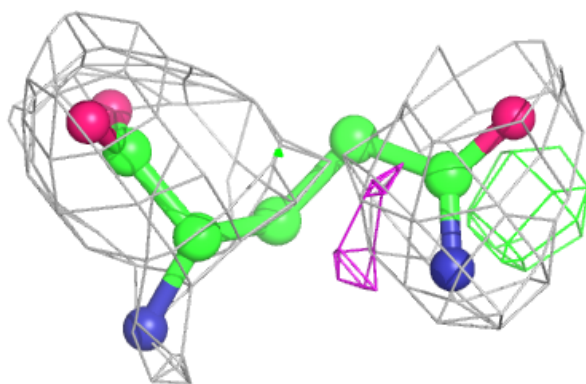
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 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	GLN	B	601	10/10	0.88	0.24	30,53,67,69	0
2	GLN	C	601	10/10	0.94	0.20	25,46,52,65	0
2	GLN	D	601	10/10	0.94	0.20	29,49,52,57	0
2	GLN	A	601	10/10	0.95	0.21	24,53,59,62	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.

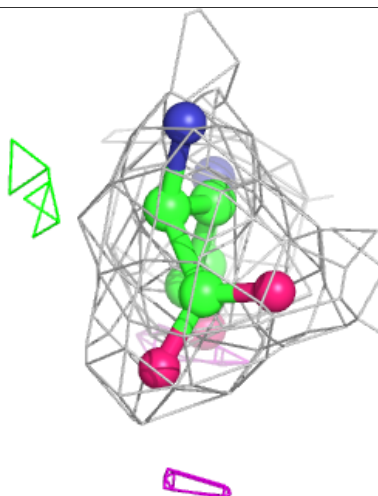
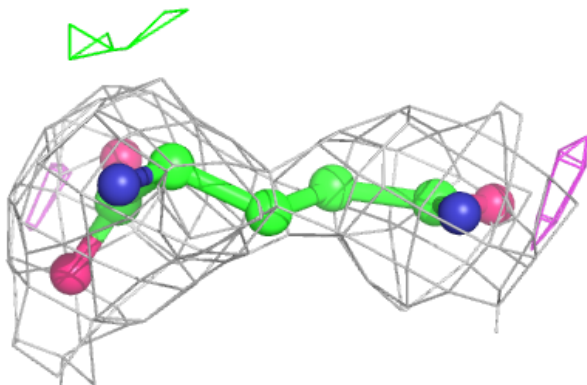
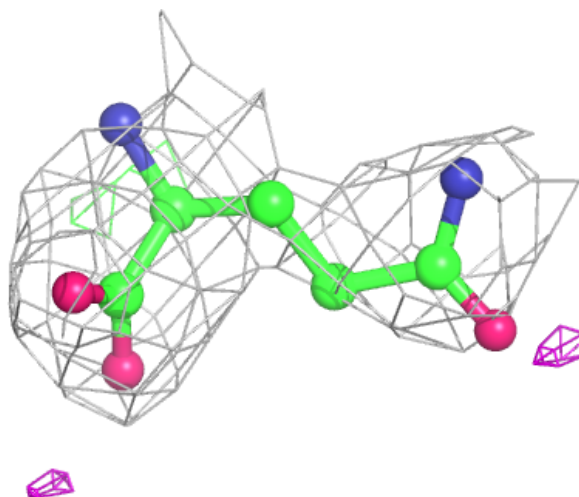
**Electron density around GLN B 601:**

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



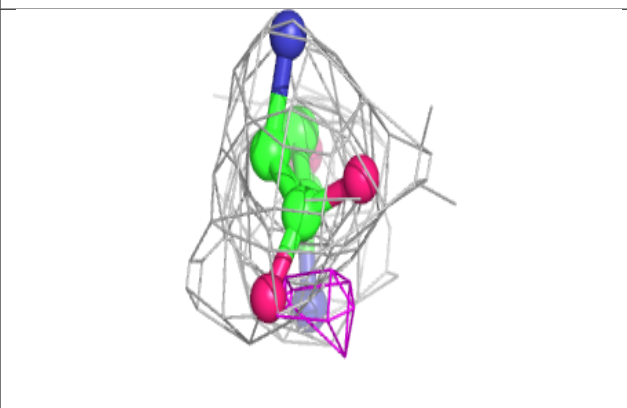
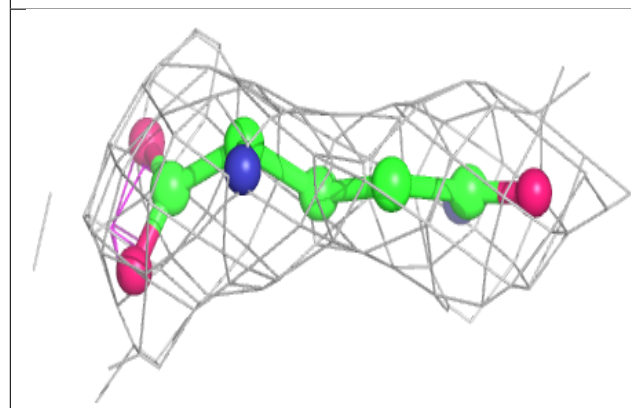
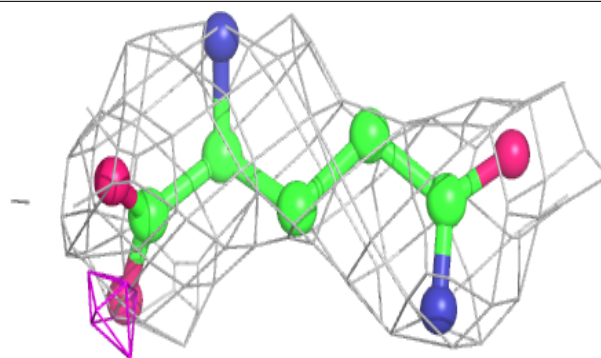
**Electron density around GLN C 601:**

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

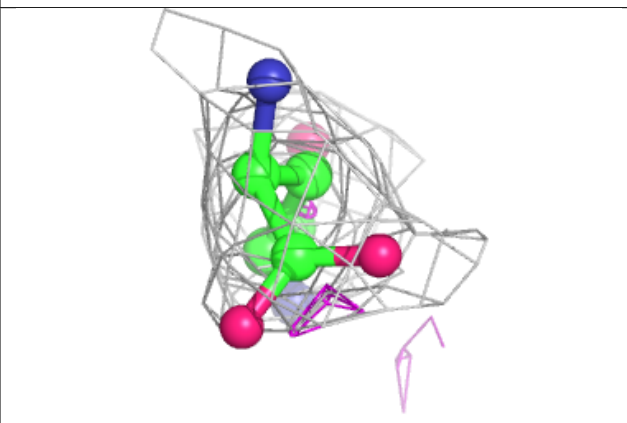
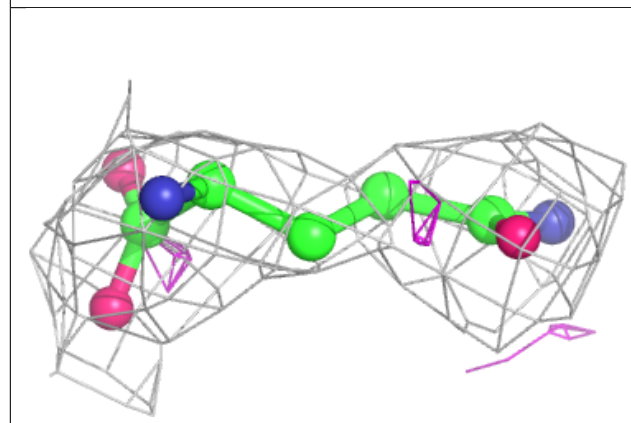
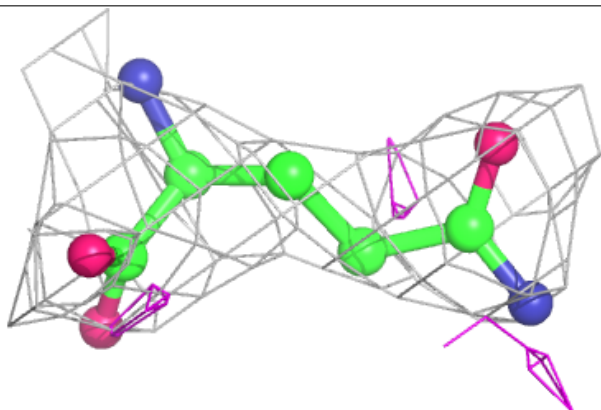


**Electron density around GLN D 601:**

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

**Electron density around GLN A 601:**

$2mF_o-DF_c$  (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.