



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:43 PM UTC

PDB ID : 7SBM / pdb_00007sbm
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.

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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

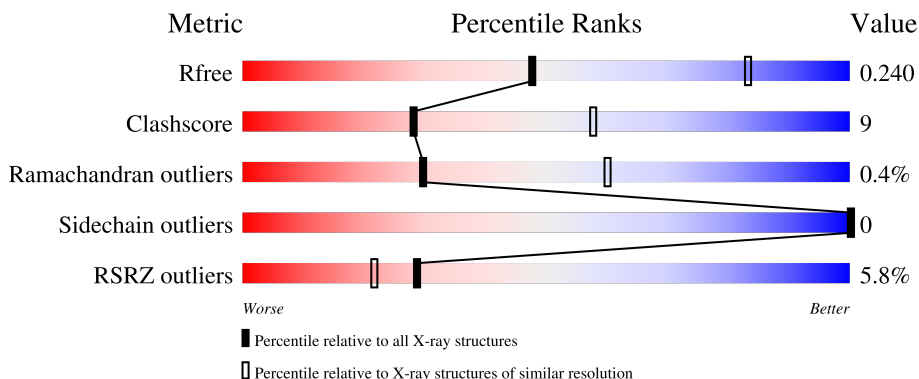
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.80 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}	180053	3866 (2.80-2.80)
Clashscore	190562	4276 (2.80-2.80)
Ramachandran outliers	187476	4196 (2.80-2.80)
Sidechain outliers	187428	4198 (2.80-2.80)
RSRZ outliers	180081	3869 (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 ≥ 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	 5% 60% 14% 26%
1	B	539	 4% 61% 11% 27%
1	C	539	 5% 59% 14% 26%
1	D	539	 4% 60% 14% 25%

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:

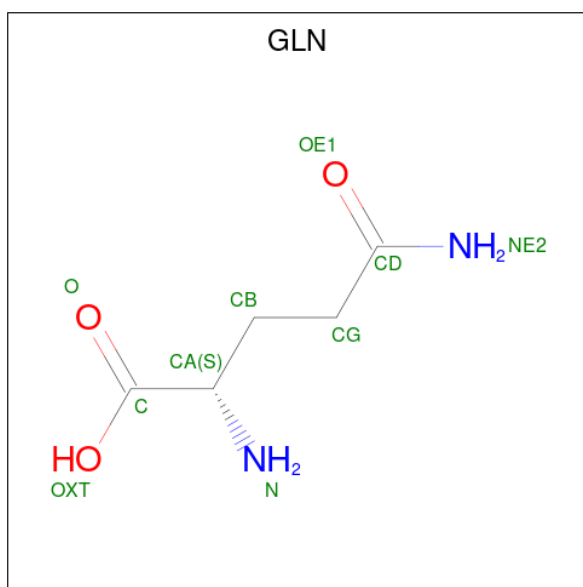
Chain	Residue	Modelled	Actual	Comment	Reference
A	60	MET	-	initiating methionine	UNP O94925
A	61	ARG	-	expression tag	UNP O94925
A	62	GLY	-	expression tag	UNP O94925
A	63	SER	-	expression tag	UNP O94925
A	64	HIS	-	expression tag	UNP O94925
A	65	HIS	-	expression tag	UNP O94925
A	66	HIS	-	expression tag	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 (CCD ID: 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		

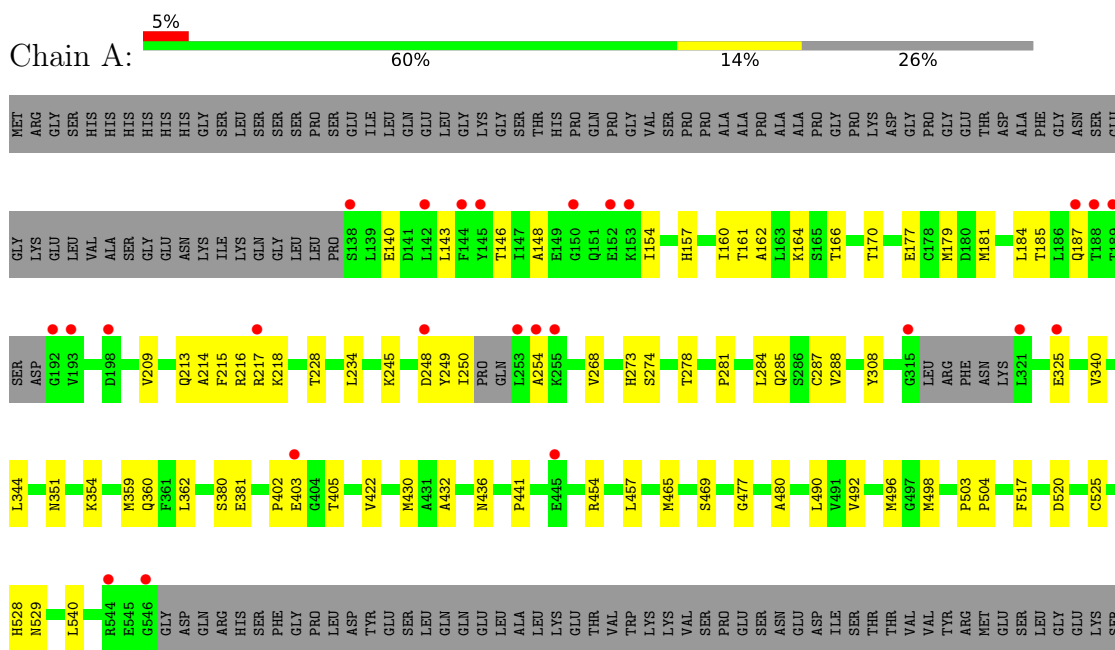
- Molecule 3 is water.

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		

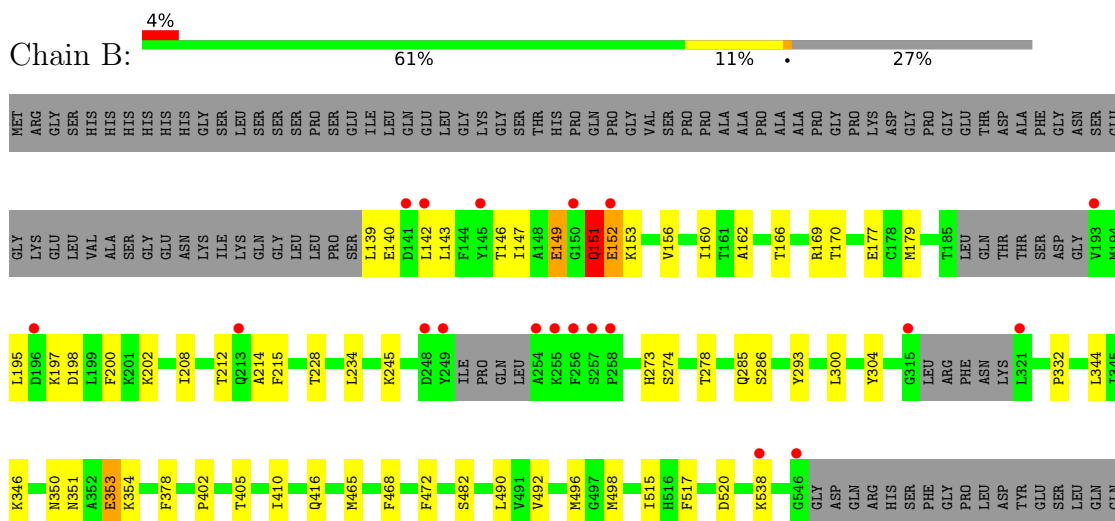
3 Residue-property plots

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



GLU
LEU
ALA
LEU
LYS
GLU
THR
VAL
THR
LYS
LYS
VAL
SER
PRO
GLU
GLU
ASN
GLU
ASP
ILE
SER
THR
THR
VAL
VAL
TYR
ARG
MET
GLU
SER
SER
LEU
GLY
LYS
SER

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

Chain C: 

MET
ARG
GLY
SER
HIS
HIS
HIS
HIS
GLY
ASN
SER
LEU
SER
SER
SER
PRO
GLU
SER
GLU
ILE
SER
LEU
Gln
GLN
GLU
LEU
VAL
GLY
LYS
GLY
SER
SER
PRO
PRO
ALA
ALA
PRO
GLY
PRO
LYS
ASP
GLY
PRO
GLY
THR
ASP
ALA
PHE
GLY
ASN
SER
GLU

GLY
LYS
GLU
VAL
SER
ALA
SER
GLY
ASN
LYS
ILE
LYS
Gln
GLY
SER
LEU
GLN
P137
SER
L139
L140
D141
L142
L143
F144
Y145
A148
E149
G150
Q151
E152
K153
V156
A162
L184
T188
T189
D191
G192
V193
L195
D198
L199
K201
V204
T208
F215
R216

R017
D223
F227
T228
L234
K240
A247
D248
Y249
I250
PRO
LEU
A254
K255
F256
S257
P258
V265
H273
S274
T278
K279
V280
P281
Q285
S286
L300
E303
Y304
R307
S314
GLY
LEU
PHE
ASN
LYS
L321
F322
L323
N324
E325
V349
E353

L362
M365
E381
S384
Y394
A427
L434
A435
V447
T456
L457
S458
M460
M465
G477
L478
P479
A480
K481
V484
I488
V491
M496
G497
M498
M499
P503
P504
L505
D506
V512
K513
G514
I515
D520
N529
F536
D541

R544
E545
G546
ASP
GLN
ARG
HIS
SER
PHE
GLY
PRO
LEU
ASP
TYR
GLU
SER
LEU
GLN
SER
LEU
GLN
THR
VAL
TRP
LYS
VAL
PRO
SER
ASN
GLU
ASP
ILE
SER
THR
VAL
VAL
TYR
ARG
MET
SER
LEU
GLY
LYS
SER

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

Chain D: 

MET
ARG
GLY
SER
HIS
HIS
HIS
HIS
GLY
ASN
SER
LEU
SER
SER
SER
PRO
SER
GLU
ILE
LEU
Gln
GLN
GLU
LEU
GLY
LYS
GLY
SER
THR
VAL
TRP
HIS
PRO
Gln
PRO
GLN
VAL
SER
SER
PRO
ALA
ALA
PRO
ALA
PRO
GLY
PRO
LYS
ASP
GLY
PRO
GLY
GLU
THR
ASP
PHE
GLY
ASN
SER
GLU

GLY
LYS
GLU
VAL
SER
GLY
ASN
LYS
ILE
LYS
Gln
GLY
LEU
P137
S138
L139
E140
D141
L142
L143
F144
Y145
E149
G150
Q151
E152
K153
I154
P155
H157
K158
A162
S190
D191
V193
M194
L195
D196
K197
F200
K201
Q205
L208
T212
F215

L234
Q241
A247
D248
Y249
I250
PRO
L253
L254
K255
F256
S257
P258
D259
V268
S274
T278
L284
C287
P290
Y304
R307
S314
GLY
ARG
PHE
ASN
LYS
E325
D326
K328
V349
E353
S380
E383
V422
A427

L434
A435
M436
F439
E445
R446
R454
N455
T456
L457
M460
G477
A480
K481
V484
L488
L489
L490
V491
M496
G497
M498
S502
P503
P504
S511
V512
K513
G514
D520
L521
C525
H528
N529
F536
L540
D541
R544
E545
G546
ASP

GLN
ARG
HIS
PHE
GLY
PRO
LEU
ASP
TYR
GLU
SER
LEU
Gln
GLN
GLU
LEU
ALA
LEU
LYS
THR
VAL
TRP
LYS
VAL
SER
PRO
GLU
SER
ASN
GLU
ASP
ILE
SER
THR
THR
VAL
TYR
ARG
MET
GLU
SER
LEU
GLY
GLY
LYS
SER

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	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) 99.5 (39.29-2.80)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.87 (at 2.81Å)	Xtriage
Refinement program	PHENIX 1.15.2_3472	Depositor
R, R_{free}	0.200 , 0.243 0.199 , 0.240	Depositor DCC
R_{free} test set	2000 reflections (3.27%)	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.918	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 40.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	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 ²)	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.*

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

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	0.43	0/3184	0.73	6/4294 (0.1%)
1	B	0.44	0/3127	0.76	7/4216 (0.2%)
1	C	0.43	0/3181	0.77	7/4289 (0.2%)
1	D	0.39	0/3212	0.70	2/4334 (0.0%)
All	All	0.42	0/12704	0.74	22/17133 (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	1
All	All	0	3

There are no bond length outliers.

All (22) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	152	GLU	CA-CB-CG	10.27	134.63	114.10
1	C	544	ARG	CB-CG-CD	-9.02	90.56	111.30
1	B	169	ARG	CB-CG-CD	8.55	130.97	111.30
1	D	152	GLU	CA-CB-CG	-8.19	97.72	114.10
1	A	403	GLU	CB-CG-CD	-7.27	100.25	112.60
1	C	303	GLU	CB-CG-CD	-7.07	100.58	112.60
1	B	245	LYS	CD-CE-NZ	-7.02	89.43	111.90
1	A	177	GLU	CA-CB-CG	-6.91	100.28	114.10
1	C	240	LYS	CB-CG-CD	6.74	126.79	111.30
1	A	403	GLU	CA-CB-CG	6.29	126.67	114.10
1	C	353	GLU	CA-CB-CG	6.14	126.39	114.10
1	D	152	GLU	CB-CA-C	-5.94	102.88	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	152	GLU	N-CA-CB	-5.48	101.23	110.49
1	A	217	ARG	CA-CB-CG	5.39	124.87	114.10
1	A	248	ASP	N-CA-CB	-5.33	102.82	110.65
1	A	217	ARG	CG-CD-NE	5.21	123.47	112.00
1	B	538	LYS	CA-CB-CG	5.14	124.39	114.10
1	C	544	ARG	NE-CZ-NH2	5.13	123.81	119.20
1	C	544	ARG	NE-CZ-NH1	-5.12	116.38	121.50
1	C	544	ARG	CA-CB-CG	5.11	124.31	114.10
1	B	245	LYS	CA-CB-CG	-5.06	103.99	114.10
1	B	353	GLU	N-CA-CB	-5.01	102.73	110.20

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	52	0
1	B	3060	0	3027	48	0
1	C	3114	0	3082	69	0
1	D	3143	0	3113	60	0
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	221	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 9.

All (221) 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:456:THR:HG22	1:D:460:MET:HE2	1.61	0.83
1:D:250:ILE:HD12	1:D:252:GLN:HB2	1.62	0.82
1:A:170:THR:HB	1:A:179:MET:HE2	1.64	0.79
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:D:325:GLU:CD	1:D:325:GLU:H	1.99	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:D:434:LEU:HD13	1:D:460:MET:HE1	1.75	0.68
1:B:498:MET:HE1	1:B:517:PHE:HE2	1.58	0.68
1:C:434:LEU:HD13	1:C:460:MET:HE1	1.75	0.67
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:A:162:ALA:HB1	1:A:215:PHE:HE1	1.59	0.66
1:A:465:MET:H	1:A:469:SER:HB3	1.60	0.65
1:A:498:MET:HE1	1:A:517:PHE:HE1	1.60	0.65
1:C:285:GLN:HB3	2:C:601:GLN:HE21	1.61	0.65
1:C:153:LYS:HB3	1:C:194:MET:CG	2.26	0.64
1:A:362:LEU:HD22	1:A:430:MET:HE1	1.79	0.64
1:A:157:HIS:O	1:A:161:THR:HG23	1.97	0.64
1:C:456:THR:HG22	1:C:460:MET:HE2	1.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:457:LEU:HD23	1:C:460:MET:HE3	1.81	0.61
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: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:B:170:THR:HB	1:B:179:MET:HE2	1.84	0.58
1:C:362:LEU:HD23	1:C:365:MET:CE	2.34	0.58
1:B:498:MET:HE1	1:B:517:PHE:CE2	2.37	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:A:268:VAL:HG12	1:A:436:ASN:HB2	1.87	0.55
1:C:189:THR:HG22	1:C:191:ASP:CG	2.32	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:325:GLU:CD	1:C:325:GLU:H	2.16	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
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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:498:MET:HE1	1:A:517:PHE:CE1	2.42	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:NH2	1:C:223:ASP:HB2	2.25	0.51
1:C:217:ARG:HH22	1:C:223:ASP:HB2	1.74	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:B:465:MET:HE2	1:B:515:ILE:HD11	1.93	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:D:498:MET:HE1	1:D:521:LEU:HD22	1.93	0.50
1:C:140:GLU:OE2	1:C:140:GLU:N	2.43	0.50
1:C:227:PHE:HZ	1:C:496:MET:HE1	1.76	0.50
1:C:303:GLU:OE2	1:C:307:ARG:NH1	2.44	0.50
1:B:153:LYS:HB3	1:B:195:LEU:C	2.36	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:C:496:MET:HE3	1:C:498:MET:HE3	1.94	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: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:B:492:VAL:HG21	1:B:496:MET:HE2	1.96	0.48
1:D:248:ASP:HA	1:D:255:LYS:HZ2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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
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:HD2	1:A:245:LYS:N	2.30	0.47
1:C:435:ALA:HB2	1:C:491:VAL:HG13	1.95	0.47
1:B:465:MET:HE1	1:B:482:SER:HB3	1.96	0.47
1:C:506:ASP:HB3	1:C:512:VAL:HG22	1.98	0.46
1:B:177:GLU:CD	1:B:177:GLU:H	2.24	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:HE2	1:B:197:LYS:HB3	1.71	0.46
1:B:149:GLU:CG	1:B:151:GLN:HG2	2.46	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:C:265:VAL:HG22	1:C:498:MET:HE2	1.97	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:194:MET:HE3	1:D:194:MET:HB2	1.90	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: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:C:194:MET:HE3	1:C:194:MET:HB2	1.91	0.44
1:D:349:VAL:HG11	1:D:353:GLU:HB2	1.99	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:A:492:VAL:HG21	1:A:496:MET:HE2	2.00	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:A:359:MET:HE3	1:A:359:MET:HB3	1.76	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:492:VAL:HG21	1:D:496:MET:HE2	2.01	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:150:GLY:O	1:C:151:GLN:C	2.62	0.43
1:A:529:ASN:HD22	1:A:529:ASN:C	2.25	0.43
1:C:427:ALA:HB3	1:C:499:MET:HG2	2.01	0.43
1:C:465:MET:HE2	1:C:515:ILE:HD11	2.01	0.43
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:D:325:GLU:CD	1:D:325:GLU:N	2.74	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:C:362:LEU:HD23	1:C:365:MET:HE1	2.00	0.42
1:D:154:ILE:HG23	1:D:158:LYS:HE3	2.01	0.42
1:D:247:ALA:O	1:D:255:LYS:NZ	2.51	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:B:152:GLU:CD	1:B:153:LYS:H	2.27	0.42
1:C:303:GLU:OE2	1:C:303:GLU:O	2.38	0.42
1:D:284:LEU:HD22	1:D:287:CYS:HB2	2.02	0.42
1:B:490:LEU:CD2	1:B:498:MET:HE2	2.50	0.42
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:151:GLN:O	1:B:152:GLU:C	2.63	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

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
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:457:LEU:HD23	1:D:460:MET:HE3	2.02	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
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:B:465:MET:CE	1:B:515:ILE:HD11	2.51	0.40
1:C:193:VAL:HG13	1:C:193:VAL:O	2.21	0.40
1:D:525:CYS:HA	1:D:540:LEU:O	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	392/539 (73%)	381 (97%)	11 (3%)	0	100	100
1	B	384/539 (71%)	372 (97%)	11 (3%)	1 (0%)	36	66
1	C	390/539 (72%)	375 (96%)	12 (3%)	3 (1%)	16	44
1	D	397/539 (74%)	381 (96%)	13 (3%)	3 (1%)	16	44
All	All	1563/2156 (72%)	1509 (96%)	47 (3%)	7 (0%)	30	60

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
1	C	193	VAL

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	345/462 (75%)	345 (100%)	0	100	100
1	B	338/462 (73%)	338 (100%)	0	100	100
1	C	345/462 (75%)	345 (100%)	0	100	100
1	D	349/462 (76%)	349 (100%)	0	100	100
All	All	1377/1848 (74%)	1377 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (14) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	213	GLN
1	A	330	HIS
1	A	360	GLN
1	A	436	ASN
1	A	455	ASN
1	A	529	ASN
1	B	516	HIS
1	C	347	GLN
1	C	375	ASN
1	C	379	GLN
1	D	151	GLN

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Mol	Chain	Res	Type
1	D	187	GLN
1	D	347	GLN
1	D	375	ASN

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 ⓘ

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	D	601	-	8,9,9	0.90	1 (12%)	8,11,11	0.83	1 (12%)
2	GLN	C	601	-	8,9,9	0.89	1 (12%)	8,11,11	1.05	1 (12%)
2	GLN	B	601	-	8,9,9	0.98	1 (12%)	8,11,11	0.97	0
2	GLN	A	601	-	8,9,9	0.88	1 (12%)	8,11,11	0.95	1 (12%)

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	D	601	-	-	3/9/9/9	-
2	GLN	C	601	-	-	2/9/9/9	-
2	GLN	B	601	-	-	7/9/9/9	-
2	GLN	A	601	-	-	2/9/9/9	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	C	601	GLN	OXT-C	-2.32	1.23	1.30
2	D	601	GLN	OXT-C	-2.26	1.23	1.30
2	B	601	GLN	OXT-C	-2.20	1.23	1.30
2	A	601	GLN	OXT-C	-2.10	1.23	1.30

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	601	GLN	OXT-C-O	-2.94	117.41	124.08
2	A	601	GLN	OXT-C-O	-2.61	118.15	124.08
2	D	601	GLN	OXT-C-O	-2.23	119.01	124.08

There are no chirality outliers.

All (14) torsion outliers are listed below:

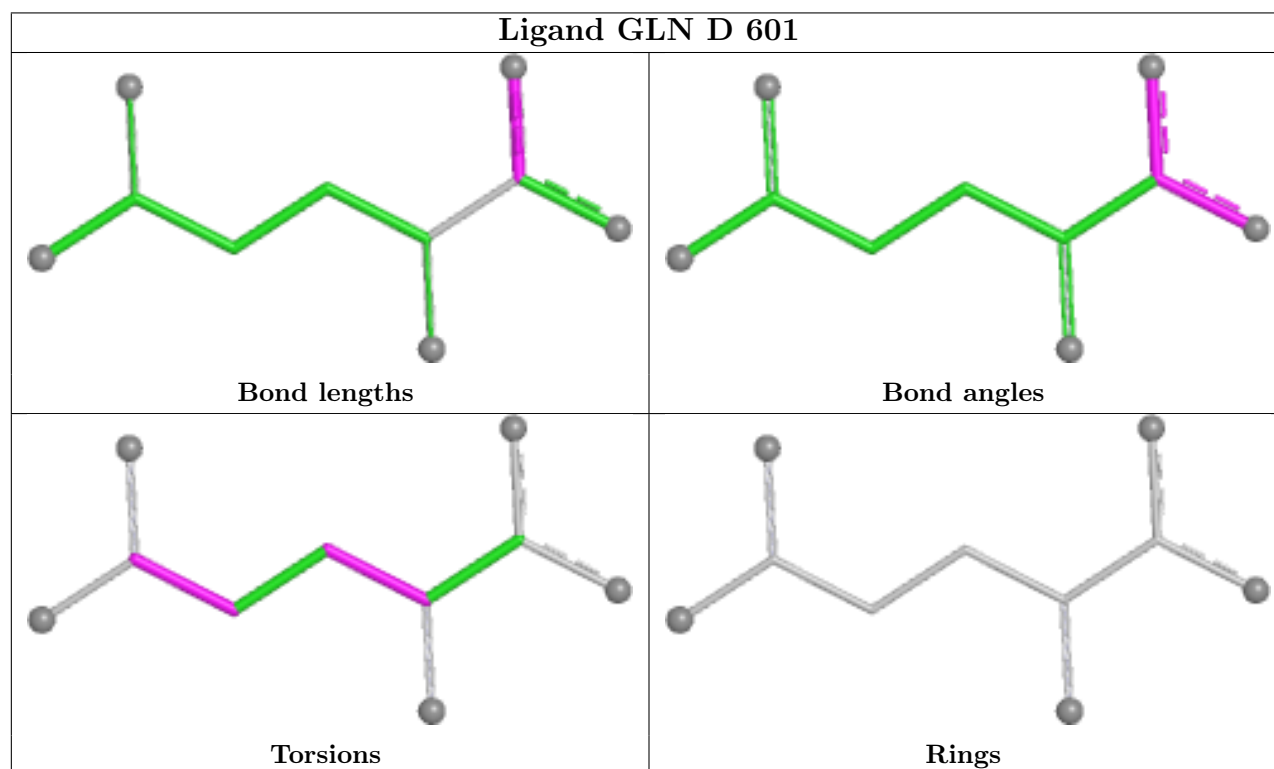
Mol	Chain	Res	Type	Atoms
2	B	601	GLN	O-C-CA-N
2	B	601	GLN	OXT-C-CA-N
2	B	601	GLN	OE1-CD-CG-CB
2	A	601	GLN	OXT-C-CA-N
2	B	601	GLN	NE2-CD-CG-CB
2	A	601	GLN	O-C-CA-N
2	D	601	GLN	NE2-CD-CG-CB
2	B	601	GLN	CA-CB-CG-CD
2	B	601	GLN	OXT-C-CA-CB
2	B	601	GLN	O-C-CA-CB
2	D	601	GLN	OE1-CD-CG-CB
2	C	601	GLN	NE2-CD-CG-CB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

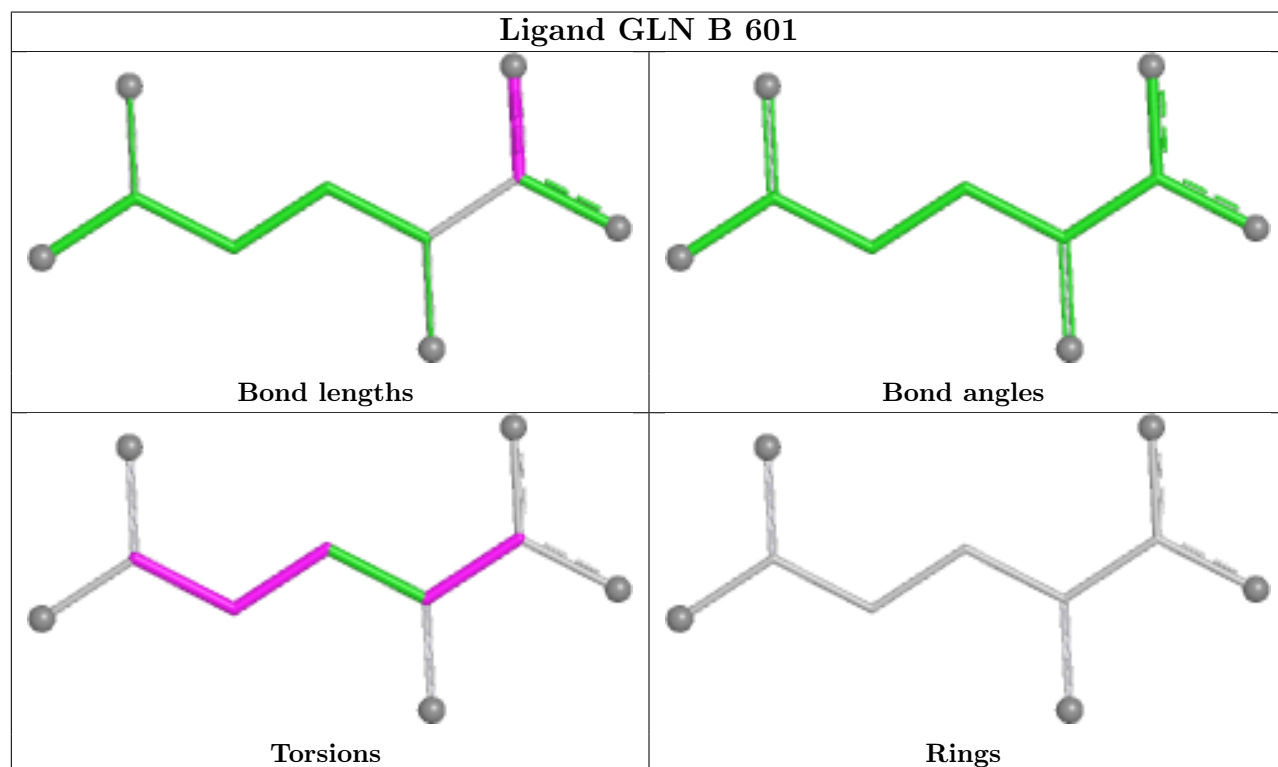
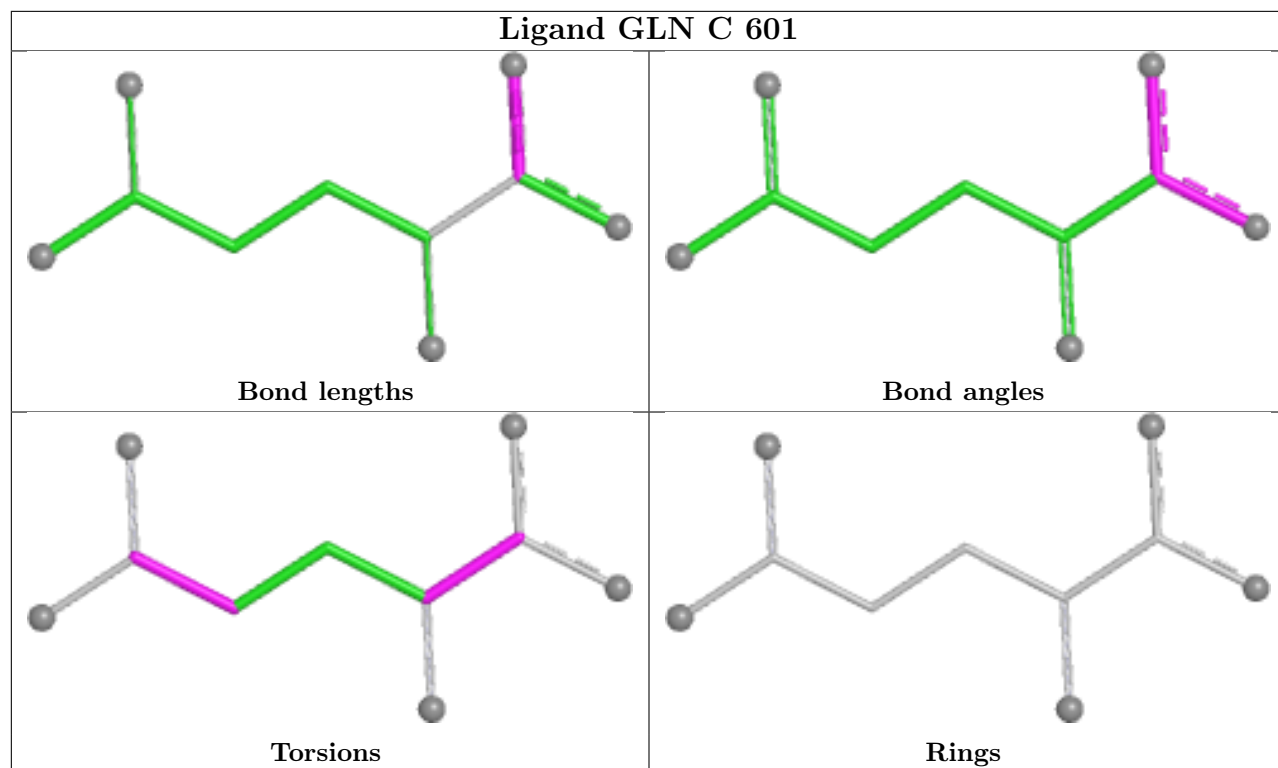
There are no ring outliers.

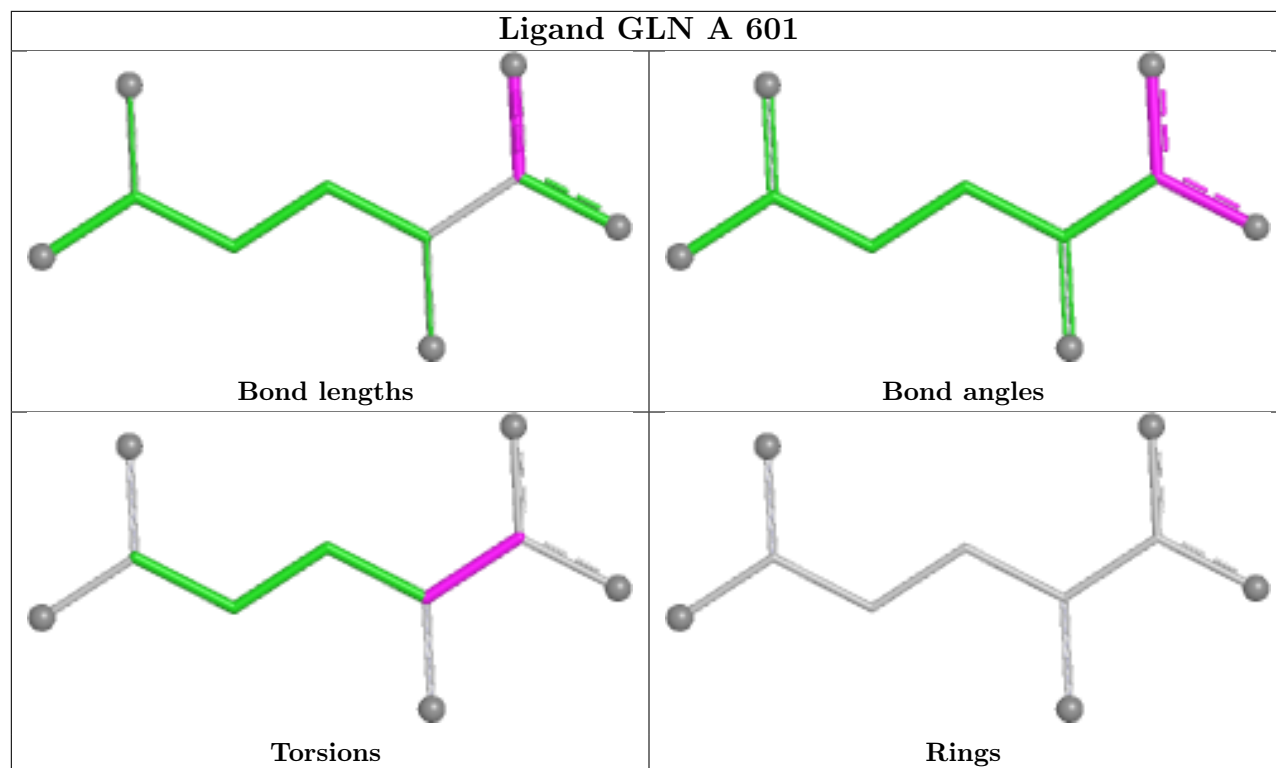
4 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	D	601	GLN	1	0
2	C	601	GLN	5	0
2	B	601	GLN	4	0
2	A	601	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 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, 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	400/539 (74%)	0.10	25 (6%)	26 19	20, 31, 82, 124	2 (0%)
1	B	392/539 (72%)	0.08	19 (4%)	35 28	19, 30, 78, 123	1 (0%)
1	C	399/539 (74%)	0.13	25 (6%)	26 19	21, 32, 81, 110	1 (0%)
1	D	403/539 (74%)	0.01	24 (5%)	27 21	18, 29, 78, 115	1 (0%)
All	All	1594/2156 (73%)	0.08	93 (5%)	29 22	18, 31, 80, 124	5 (0%)

All (93) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	315	GLY	7.1
1	B	254	ALA	6.4
1	A	253	LEU	5.9
1	B	249	TYR	5.7
1	A	189	THR	5.1
1	D	253	LEU	5.0
1	D	193	VAL	4.8
1	C	249	TYR	4.8
1	C	193	VAL	4.3
1	D	546	GLY	4.2
1	D	137	PRO	4.1
1	C	254	ALA	3.9
1	A	188	THR	3.8
1	D	144	PHE	3.8
1	D	190	SER	3.7
1	C	321	LEU	3.7
1	C	303	GLU	3.7
1	C	137	PRO	3.7
1	C	255	LYS	3.6
1	B	257	SER	3.6
1	B	256	PHE	3.5

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Mol	Chain	Res	Type	RSRZ
1	B	193	VAL	3.5
1	A	248	ASP	3.5
1	B	141	ASP	3.5
1	B	255	LYS	3.4
1	D	142	LEU	3.4
1	A	145	TYR	3.4
1	A	187	GLN	3.4
1	C	250	ILE	3.4
1	D	145	TYR	3.4
1	C	256	PHE	3.4
1	A	192	GLY	3.3
1	C	192	GLY	3.3
1	C	546	GLY	3.3
1	C	139	LEU	3.2
1	B	150	GLY	3.2
1	A	142	LEU	3.2
1	C	258	PRO	3.2
1	D	254	ALA	3.2
1	B	152	GLU	3.1
1	A	138	SER	3.0
1	D	138	SER	3.0
1	D	252	GLN	3.0
1	C	189	THR	2.9
1	D	321	LEU	2.9
1	D	152	GLU	2.9
1	C	142	LEU	2.9
1	A	254	ALA	2.8
1	B	546	GLY	2.8
1	B	321	LEU	2.8
1	B	258	PRO	2.7
1	C	257	SER	2.7
1	C	199	LEU	2.6
1	C	144	PHE	2.6
1	C	198	ASP	2.6
1	A	325	GLU	2.6
1	A	445	GLU	2.6
1	D	445	GLU	2.5
1	A	144	PHE	2.5
1	A	153	LYS	2.5
1	A	217	ARG	2.5
1	B	145	TYR	2.4
1	D	249	TYR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	321	LEU	2.4
1	A	255	LYS	2.4
1	A	152	GLU	2.4
1	C	152	GLU	2.3
1	B	142	LEU	2.3
1	D	256	PHE	2.3
1	B	248	ASP	2.3
1	D	191	ASP	2.3
1	A	544	ARG	2.3
1	C	204	VAL	2.3
1	B	315	GLY	2.3
1	A	198	ASP	2.2
1	D	259	ASP	2.2
1	A	193	VAL	2.2
1	A	150	GLY	2.2
1	D	545	GLU	2.2
1	B	196	ASP	2.2
1	D	255	LYS	2.1
1	A	546	GLY	2.1
1	A	403	GLU	2.1
1	C	141	ASP	2.1
1	C	322	PHE	2.1
1	B	213	GLN	2.1
1	D	200	PHE	2.1
1	C	150	GLY	2.1
1	D	250	ILE	2.1
1	B	538	LYS	2.0
1	D	139	LEU	2.0
1	D	149	GLU	2.0
1	C	145	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](#)

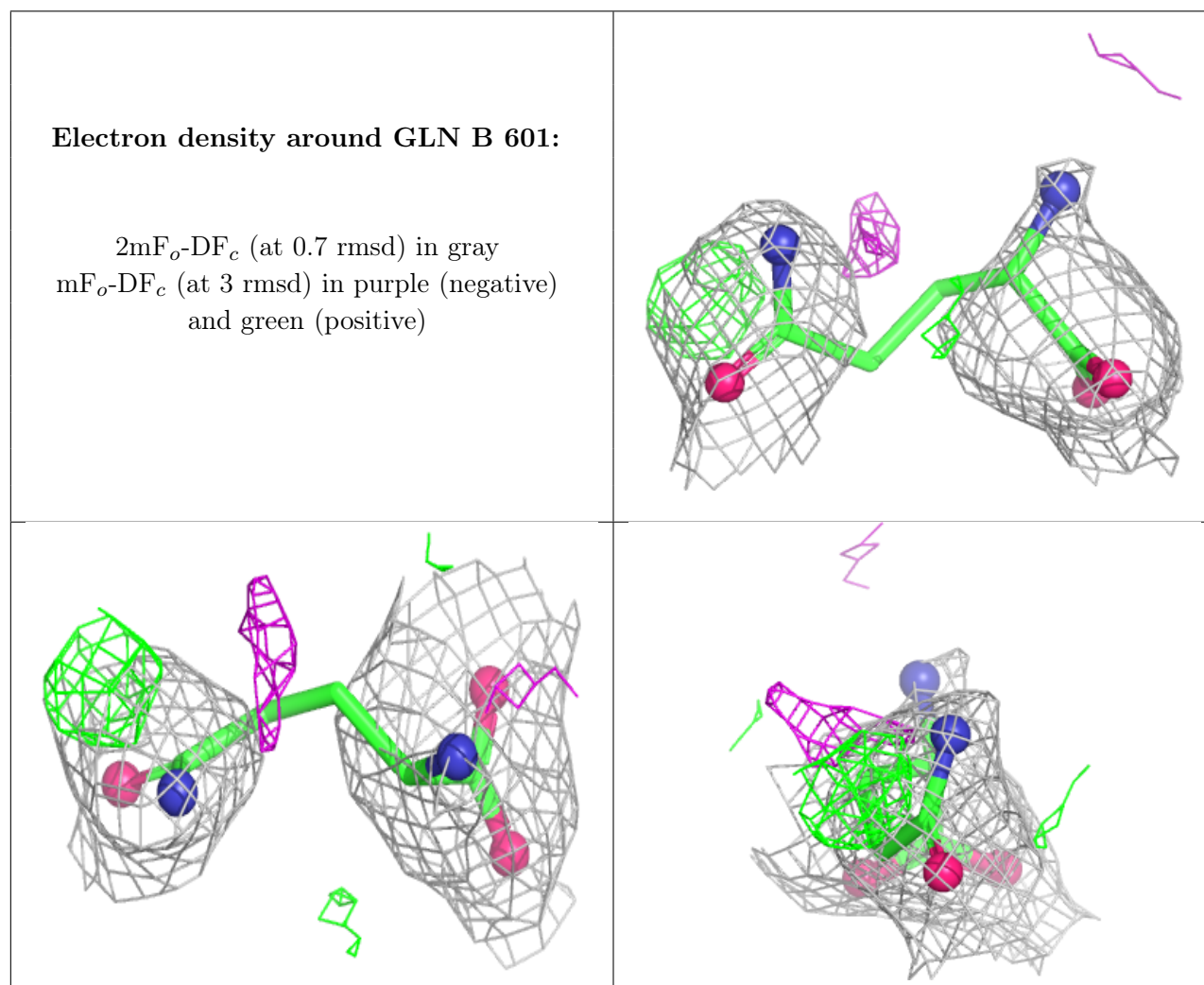
There are no oligosaccharides in this entry.

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.

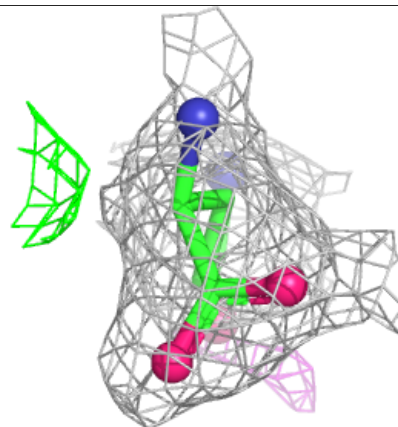
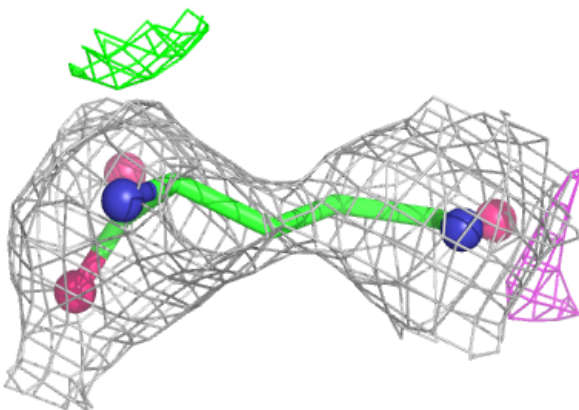
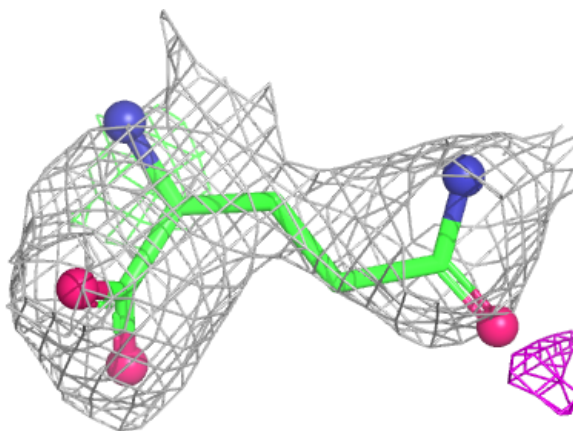
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
2	GLN	B	601	10/10	0.85	0.19	30,53,67,69	0
2	GLN	C	601	10/10	0.89	0.14	25,46,52,65	0
2	GLN	D	601	10/10	0.94	0.12	29,49,52,57	0
2	GLN	A	601	10/10	0.95	0.19	24,53,59,62	0

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.

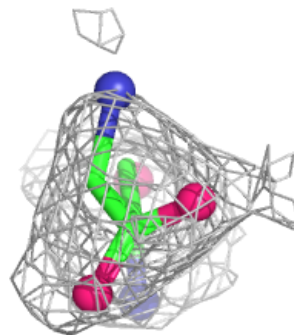
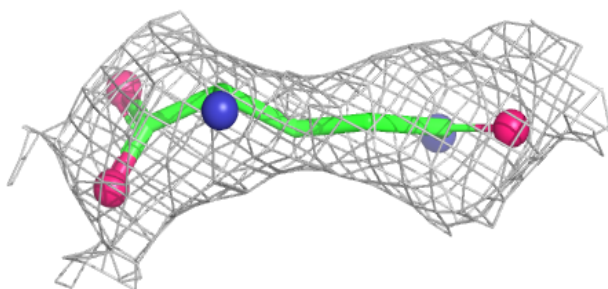
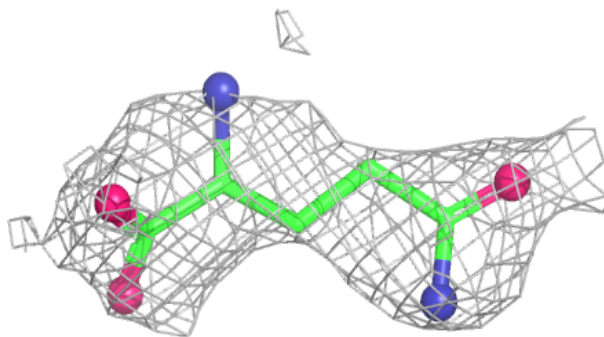


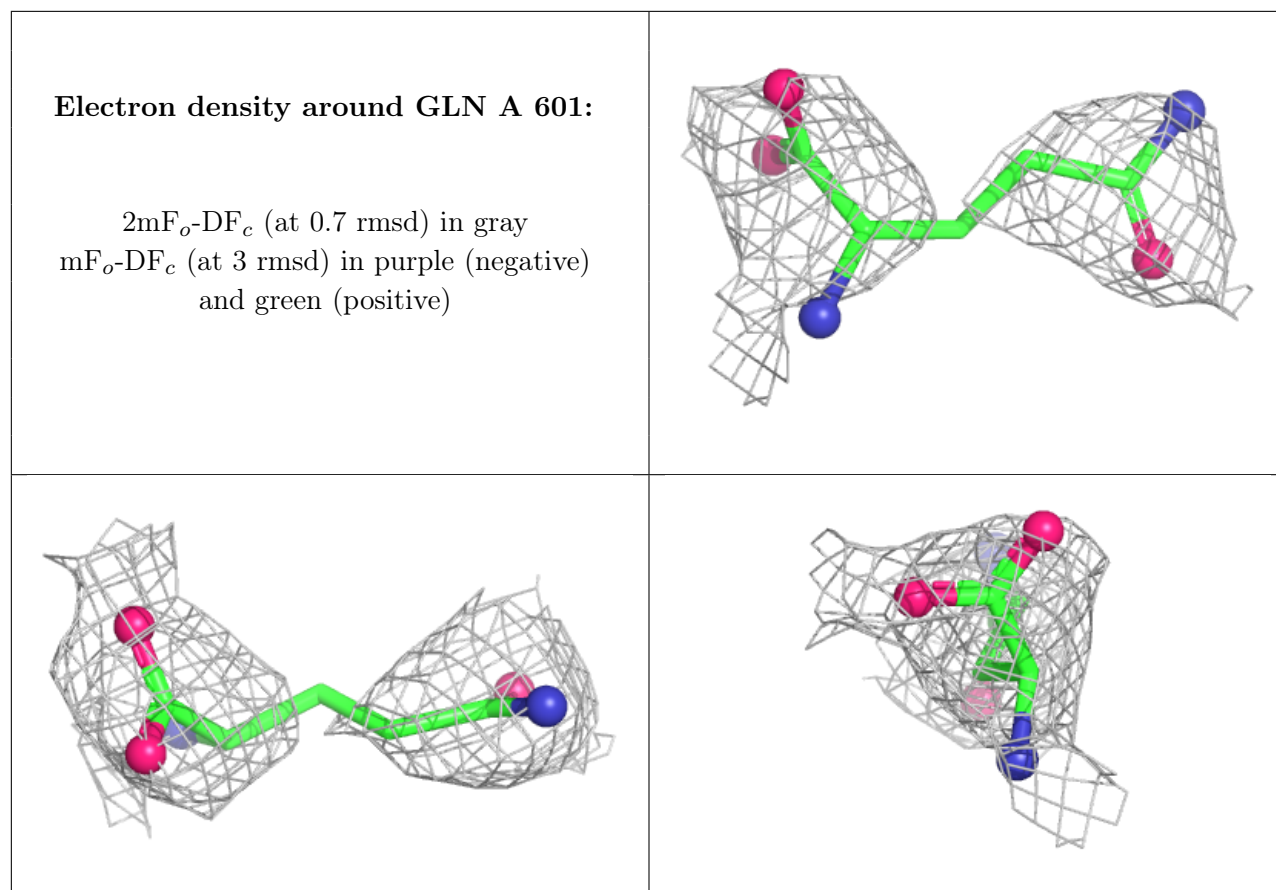
Electron density around GLN C 601:

$2mF_o-DF_c$ (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)





6.5 Other polymers [i](#)

There are no such residues in this entry.