



Full wwPDB X-ray Structure Validation Report ⓘ

Oct 16, 2025 – 02:55 pm BST

PDB ID : 9HYT / pdb_00009hyt
Title : Crystal structure of the GFRaL receptor in complex with an inhibitory cyclic peptide
Authors : Sandmark, J.; Ek, M.
Deposited on : 2025-01-10
Resolution : 1.90 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	1.8.4, CSD as541be (2020)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
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)	:	2.46

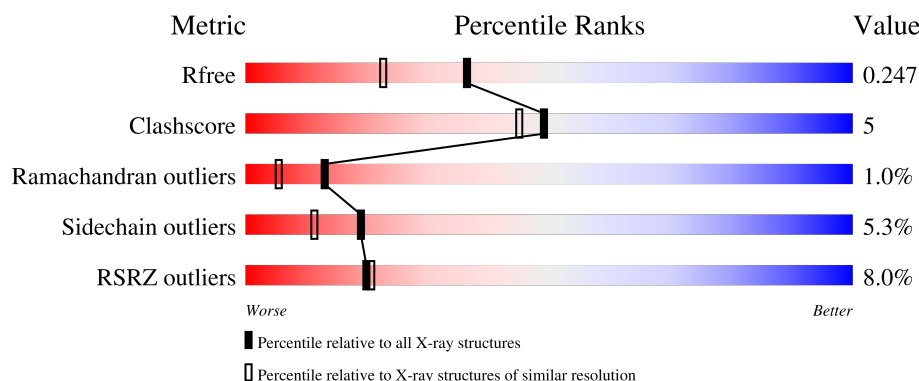
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.90 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}	164625	7293 (1.90-1.90)
Clashscore	180529	8090 (1.90-1.90)
Ramachandran outliers	177936	8022 (1.90-1.90)
Sidechain outliers	177891	8022 (1.90-1.90)
RSRZ outliers	164620	7292 (1.90-1.90)

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	245	<div> <div>7%</div> <div>67%</div> <div>12%</div> <div>•</div> <div>19%</div> </div>
1	B	245	<div> <div>8%</div> <div>66%</div> <div>12%</div> <div>•</div> <div>20%</div> </div>
1	C	245	<div> <div>6%</div> <div>69%</div> <div>9%</div> <div>•</div> <div>20%</div> </div>
2	D	17	<div> <div>76%</div> <div>24%</div> </div>
2	E	17	<div> <div>82%</div> <div>6%</div> <div>12%</div> </div>

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Mol	Chain	Length	Quality of chain
2	F	17	 94%6%

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 5382 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 GDNF family receptor alpha-like.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	199	Total	C	N	O	S	0	1	0
			1547	955	275	291	26			
1	B	195	Total	C	N	O	S	0	2	0
			1522	940	268	289	25			
1	C	196	Total	C	N	O	S	0	1	0
			1522	938	269	289	26			

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	107	HIS	-	expression tag	UNP Q6UXV0
A	108	HIS	-	expression tag	UNP Q6UXV0
A	109	HIS	-	expression tag	UNP Q6UXV0
A	110	HIS	-	expression tag	UNP Q6UXV0
A	111	HIS	-	expression tag	UNP Q6UXV0
A	112	HIS	-	expression tag	UNP Q6UXV0
A	113	GLY	-	expression tag	UNP Q6UXV0
A	114	GLY	-	expression tag	UNP Q6UXV0
B	107	HIS	-	expression tag	UNP Q6UXV0
B	108	HIS	-	expression tag	UNP Q6UXV0
B	109	HIS	-	expression tag	UNP Q6UXV0
B	110	HIS	-	expression tag	UNP Q6UXV0
B	111	HIS	-	expression tag	UNP Q6UXV0
B	112	HIS	-	expression tag	UNP Q6UXV0
B	113	GLY	-	expression tag	UNP Q6UXV0
B	114	GLY	-	expression tag	UNP Q6UXV0
C	107	HIS	-	expression tag	UNP Q6UXV0
C	108	HIS	-	expression tag	UNP Q6UXV0
C	109	HIS	-	expression tag	UNP Q6UXV0
C	110	HIS	-	expression tag	UNP Q6UXV0
C	111	HIS	-	expression tag	UNP Q6UXV0
C	112	HIS	-	expression tag	UNP Q6UXV0
C	113	GLY	-	expression tag	UNP Q6UXV0

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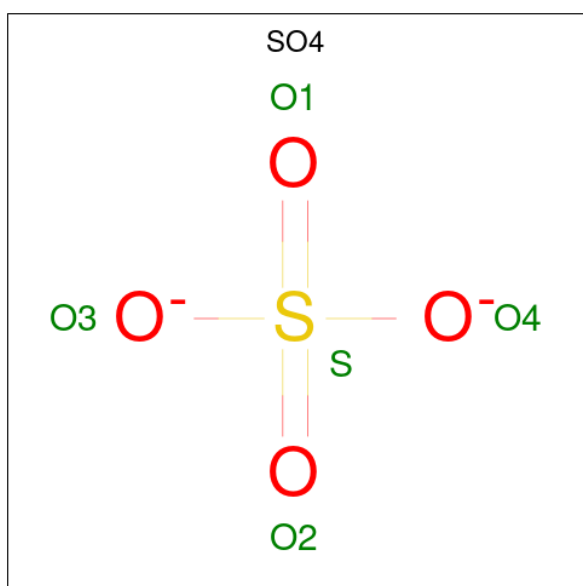
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Chain	Residue	Modelled	Actual	Comment	Reference
C	114	GLY	-	expression tag	UNP Q6UXV0

- Molecule 2 is a protein called Inhibitory cyclic peptide.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	D	17	Total 124	C 76	N 22	O 23	S 3	0	0	1
2	E	17	Total 124	C 76	N 22	O 23	S 3	0	0	1
2	F	17	Total 124	C 76	N 22	O 23	S 3	0	0	1

- Molecule 3 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



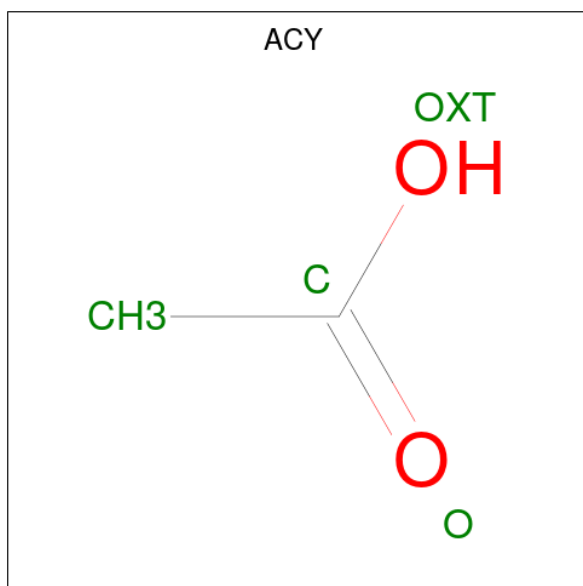
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	O	S	0	0
			5	4	1		
3	A	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	B	1	Total	O	S	0	0
			5	4	1		
3	C	1	Total	O	S	0	0
			5	4	1		

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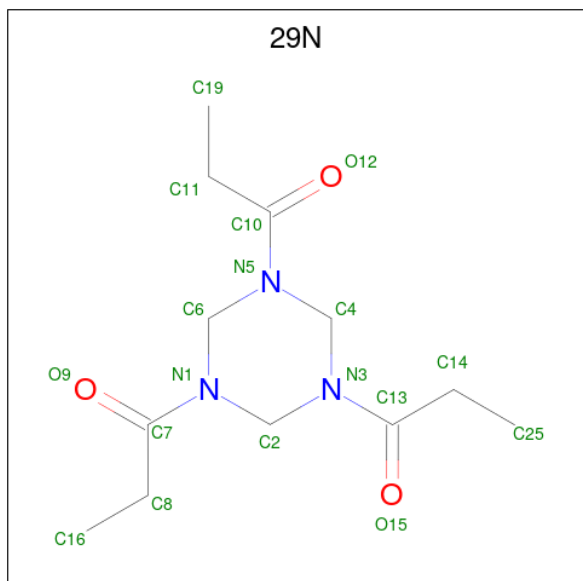
Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	C	1	Total	O	S	0	0
			5	4	1		

- Molecule 4 is ACETIC ACID (CCD ID: ACY) (formula: C₂H₄O₂).



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

- Molecule 5 is 1,1',1''-(1,3,5-triazinane-1,3,5-triyl)tripropan-1-one (CCD ID: 29N) (formula: C₁₂H₂₁N₃O₃) (labeled as "Ligand of Interest" by depositor).




Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
5	D	1	Total	C	N	O	0	0
			18	12	3	3		
5	E	1	Total	C	N	O	0	0
			18	12	3	3		
5	F	1	Total	C	N	O	0	0
			18	12	3	3		

- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	99	Total	O	0	0
			99	99		
6	B	107	Total	O	0	0
			107	107		
6	C	94	Total	O	0	0
			94	94		
6	D	9	Total	O	0	0
			9	9		
6	E	9	Total	O	0	0
			9	9		
6	F	8	Total	O	0	0
			8	8		


- Molecule 1: GDNF family receptor alpha-like

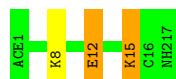


Chain D:  76% 24%



- Molecule 2: Inhibitory cyclic peptide

Chain E:  82% 6% 12%



- Molecule 2: Inhibitory cyclic peptide

Chain F:  94% 6%



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	59.54Å 148.18Å 198.05Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	99.00 – 1.90 99.00 – 1.92	Depositor EDS
% Data completeness (in resolution range)	55.7 (99.00-1.90) 57.0 (99.00-1.92)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.74 (at 1.91Å)	Xtriage
Refinement program	REFMAC 5.8.0352	Depositor
R, R_{free}	0.194 , 0.244 0.201 , 0.247	Depositor DCC
R_{free} test set	1952 reflections (2.88%)	wwPDB-VP
Wilson B-factor (Å ²)	29.1	Xtriage
Anisotropy	0.144	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 38.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	5382	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.74% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: 29N, NH2, ACE, ACY, SO4

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	0.63	1/1578 (0.1%)	1.01	0/2133
1	B	0.64	1/1555 (0.1%)	0.96	0/2106
1	C	0.64	0/1552	1.02	0/2099
2	D	1.04	0/122	1.53	1/161 (0.6%)
2	E	1.34	0/122	1.64	2/161 (1.2%)
2	F	1.24	0/122	1.47	0/161
All	All	0.70	2/5051 (0.0%)	1.04	3/6821 (0.0%)

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	A	0	6
1	B	0	2
1	C	0	3
All	All	0	11

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	312	HIS	CE1-NE2	5.72	1.38	1.32
1	A	206	HIS	CE1-NE2	5.68	1.38	1.32

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	12	GLU	N-CA-CB	5.58	118.32	110.12
2	D	4	ASP	CA-CB-CG	-5.24	107.36	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	E	15	LYS	O-C-N	-5.17	115.47	122.41

There are no chirality outliers.

All (11) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	160	ASN	Peptide
1	A	172[A]	ARG	Sidechain
1	A	172[B]	ARG	Sidechain
1	A	235	ARG	Sidechain
1	A	250	ARG	Sidechain
1	A	294	ARG	Sidechain
1	B	235	ARG	Sidechain
1	B	294	ARG	Sidechain
1	C	235	ARG	Sidechain
1	C	294	ARG	Sidechain
1	C	313	ARG	Sidechain

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	1547	0	1487	19	0
1	B	1522	0	1463	18	0
1	C	1522	0	1463	13	0
2	D	124	0	116	1	0
2	E	124	0	116	0	0
2	F	124	0	116	0	0
3	A	10	0	0	0	0
3	B	15	0	0	1	0
3	C	10	0	0	0	0
4	B	4	0	3	0	0
5	D	18	0	18	1	0
5	E	18	0	18	0	0
5	F	18	0	18	0	0
6	A	99	0	0	2	0
6	B	107	0	0	3	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
6	C	94	0	0	2	0
6	D	9	0	0	1	0
6	E	9	0	0	0	0
6	F	8	0	0	0	0
All	All	5382	0	4818	48	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 5.

All (48) 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:C:247:ARG:NH1	6:C:502:HOH:O	2.33	0.61
1:A:157:ALA:O	1:A:158:ASN:HB2	2.02	0.59
1:B:151:TYR:OH	1:B:205:LEU:O	2.20	0.58
1:B:221:LEU:HD12	1:B:296:ILE:HD11	1.86	0.58
1:A:160:ASN:HB3	1:A:161:PRO:HD2	1.86	0.57
1:A:221:LEU:HD12	1:A:296:ILE:HD11	1.85	0.57
1:A:157:ALA:HB2	1:B:297:THR:CG2	2.34	0.57
1:A:298:GLN:HB2	1:C:160:ASN:HD21	1.71	0.56
1:C:221:LEU:HD12	1:C:296:ILE:HD11	1.87	0.55
1:B:182:ILE:HA	1:B:185:MET:HE3	1.90	0.53
1:C:314:LYS:HE2	6:C:505:HOH:O	2.07	0.53
1:A:224:ILE:O	1:A:228:GLN:HG3	2.08	0.52
1:B:172:ARG:NH2	6:B:605:HOH:O	2.44	0.51
1:B:247:ARG:NH1	6:B:604:HOH:O	2.44	0.50
1:A:221:LEU:HD11	1:A:300:GLU:HB2	1.95	0.48
1:B:238:ARG:HD2	6:B:662:HOH:O	2.13	0.48
1:B:221:LEU:HD11	1:B:300:GLU:HB2	1.96	0.47
1:A:294:ARG:HD2	6:A:558:HOH:O	2.13	0.47
1:B:157:ALA:HA	1:B:161:PRO:O	2.14	0.47
1:A:193:GLN:O	1:B:165:LYS:NZ	2.41	0.47
1:C:231:GLU:O	1:C:235:ARG:HG3	2.15	0.47
1:A:231:GLU:O	1:A:235:ARG:HG3	2.15	0.46
1:C:182:ILE:HA	1:C:185:MET:HE3	1.96	0.46
1:B:238:ARG:NH2	3:B:502:SO4:O4	2.44	0.46
1:B:276:LYS:HE2	1:B:319:TYR:OH	2.17	0.44
1:A:151:TYR:CD1	1:A:151:TYR:C	2.95	0.44
1:C:303:LEU:HD11	1:C:307:PHE:CE2	2.52	0.43
1:A:297:THR:HG22	1:A:300:GLU:CG	2.48	0.43
1:C:157:ALA:HA	1:C:161:PRO:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ALA:CB	1:B:297:THR:HG22	2.48	0.43
1:C:157:ALA:O	1:C:158:ASN:HB2	2.18	0.43
1:C:221:LEU:HD11	1:C:300:GLU:HB2	2.00	0.43
1:C:151:TYR:CD1	1:C:151:TYR:C	2.96	0.42
1:B:132:LEU:O	1:B:136:GLU:HG2	2.20	0.42
1:C:294:ARG:O	1:C:295:THR:OG1	2.29	0.42
1:B:303:LEU:HD11	1:B:307:PHE:CE2	2.54	0.42
1:A:157:ALA:HA	1:A:161:PRO:O	2.19	0.42
1:B:219:THR:HA	1:B:292:THR:O	2.19	0.42
2:D:14:THR:O	2:D:15:LYS:HB2	2.20	0.42
1:A:247:ARG:NH1	1:A:251:LYS:HE3	2.34	0.42
1:A:253:HIS:CE1	6:A:508:HOH:O	2.74	0.41
1:B:231:GLU:O	1:B:235:ARG:HG3	2.21	0.41
1:A:239:THR:O	1:A:243:LYS:HG2	2.20	0.41
1:A:303:LEU:HD11	1:A:307:PHE:CE2	2.55	0.41
1:B:208:LYS:HD2	1:B:213:ASN:ND2	2.36	0.41
5:D:101:29N:H13	6:D:207:HOH:O	2.19	0.41
1:C:240:PHE:HA	1:C:278:ALA:HB1	2.03	0.41
1:A:219:THR:HA	1:A:292:THR:O	2.21	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	198/245 (81%)	192 (97%)	3 (2%)	3 (2%)	8	2
1	B	195/245 (80%)	189 (97%)	5 (3%)	1 (0%)	25	17
1	C	195/245 (80%)	190 (97%)	3 (2%)	2 (1%)	13	5
2	D	15/17 (88%)	15 (100%)	0	0	100	100
2	E	15/17 (88%)	15 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	F	15/17 (88%)	15 (100%)	0	0	100	100
All	All	633/786 (80%)	616 (97%)	11 (2%)	6 (1%)	13	7

All (6) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	158	ASN
1	B	158	ASN
1	C	158	ASN
1	A	162	CYS
1	C	162	CYS
1	A	160	ASN

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	177/217 (82%)	169 (96%)	8 (4%)	23	16
1	B	176/217 (81%)	167 (95%)	9 (5%)	20	12
1	C	176/217 (81%)	167 (95%)	9 (5%)	20	12
2	D	14/14 (100%)	13 (93%)	1 (7%)	12	5
2	E	14/14 (100%)	11 (79%)	3 (21%)	1	0
2	F	14/14 (100%)	13 (93%)	1 (7%)	12	5
All	All	571/693 (82%)	540 (95%)	31 (5%)	19	11

All (31) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	151	TYR
1	A	203	GLU
1	A	208	LYS
1	A	250	ARG
1	A	264	LYS

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Mol	Chain	Res	Type
1	A	268	THR
1	A	281	ASP
1	A	322	LEU
1	B	151	TYR
1	B	158	ASN
1	B	160	ASN
1	B	208	LYS
1	B	264	LYS
1	B	268	THR
1	B	281[A]	ASP
1	B	281[B]	ASP
1	B	322	LEU
1	C	151	TYR
1	C	160	ASN
1	C	208	LYS
1	C	246	GLN
1	C	268	THR
1	C	281	ASP
1	C	298	GLN
1	C	302	SER
1	C	314	LYS
2	D	8	LYS
2	E	8	LYS
2	E	12	GLU
2	E	15	LYS
2	F	15	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	160	ASN
1	A	184	GLN
1	A	193	GLN
1	A	308	GLN
1	B	241	GLN
1	B	253	HIS
1	B	257	ASN
1	B	290	GLN
1	B	312	HIS
1	C	290	GLN
1	C	308	GLN
2	E	13	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 ⓘ

11 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	$\# Z > 2$
5	29N	F	101	2	18,18,18	0.89	1 (5%)	24,24,24	1.98	5 (20%)
3	SO4	B	502	-	4,4,4	0.39	0	6,6,6	0.12	0
3	SO4	A	401	-	4,4,4	0.33	0	6,6,6	0.20	0
3	SO4	C	401	-	4,4,4	0.31	0	6,6,6	0.19	0
4	ACY	B	501	-	3,3,3	1.04	0	3,3,3	1.03	0
3	SO4	B	504	-	4,4,4	0.32	0	6,6,6	0.16	0
5	29N	D	101	2	18,18,18	0.77	0	24,24,24	2.23	6 (25%)
3	SO4	C	402	-	4,4,4	0.36	0	6,6,6	0.11	0
3	SO4	A	402	-	4,4,4	0.30	0	6,6,6	0.25	0
5	29N	E	101	2	18,18,18	0.82	0	24,24,24	1.89	7 (29%)
3	SO4	B	503	-	4,4,4	0.29	0	6,6,6	0.12	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
5	29N	D	101	2	-	1/18/30/30	0/0/1/1
5	29N	F	101	2	-	2/18/30/30	0/0/1/1
5	29N	E	101	2	-	4/18/30/30	0/0/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	F	101	29N	O15-C13	-2.02	1.18	1.23

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	D	101	29N	N3-C2-N1	-5.57	102.12	110.77
5	F	101	29N	C16-C8-C7	-5.24	103.03	112.72
5	D	101	29N	N5-C4-N3	-5.09	102.87	110.77
5	E	101	29N	N5-C4-N3	-5.04	102.95	110.77
5	F	101	29N	N5-C4-N3	-4.93	103.12	110.77
5	D	101	29N	C19-C11-C10	-4.65	104.13	112.72
5	E	101	29N	N3-C2-N1	-4.26	104.15	110.77
5	D	101	29N	C16-C8-C7	-3.77	105.74	112.72
5	F	101	29N	N3-C2-N1	-3.51	105.33	110.77
5	E	101	29N	C6-N1-C7	2.81	131.61	122.49
5	E	101	29N	O9-C7-C8	-2.59	115.89	121.42
5	D	101	29N	N5-C6-N1	-2.56	106.80	110.77
5	E	101	29N	C16-C8-C7	-2.36	108.36	112.72
5	F	101	29N	C14-C13-N3	2.17	121.45	117.95
5	F	101	29N	C6-N1-C7	2.12	129.38	122.49
5	D	101	29N	O12-C10-C11	-2.09	116.96	121.42
5	E	101	29N	N5-C6-N1	-2.05	107.59	110.77
5	E	101	29N	C6-N1-C2	-2.04	106.94	111.73

There are no chirality outliers.

All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
5	F	101	29N	N1-C7-C8-C16
5	F	101	29N	O9-C7-C8-C16
5	D	101	29N	N1-C7-C8-C16
5	E	101	29N	N1-C7-C8-C16
5	E	101	29N	O9-C7-C8-C16
5	E	101	29N	O12-C10-C11-C19
5	E	101	29N	N5-C10-C11-C19

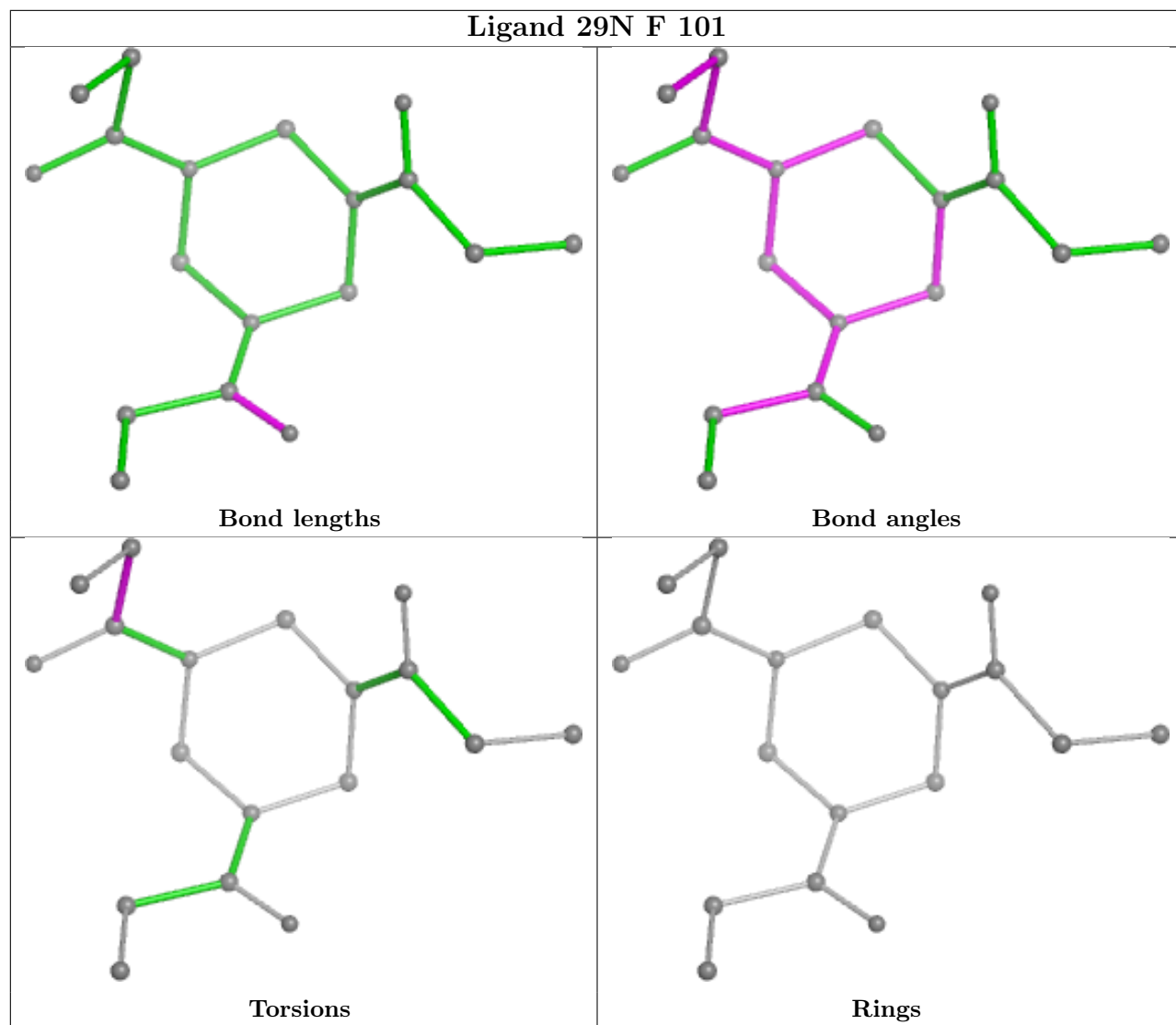
There are no ring outliers.

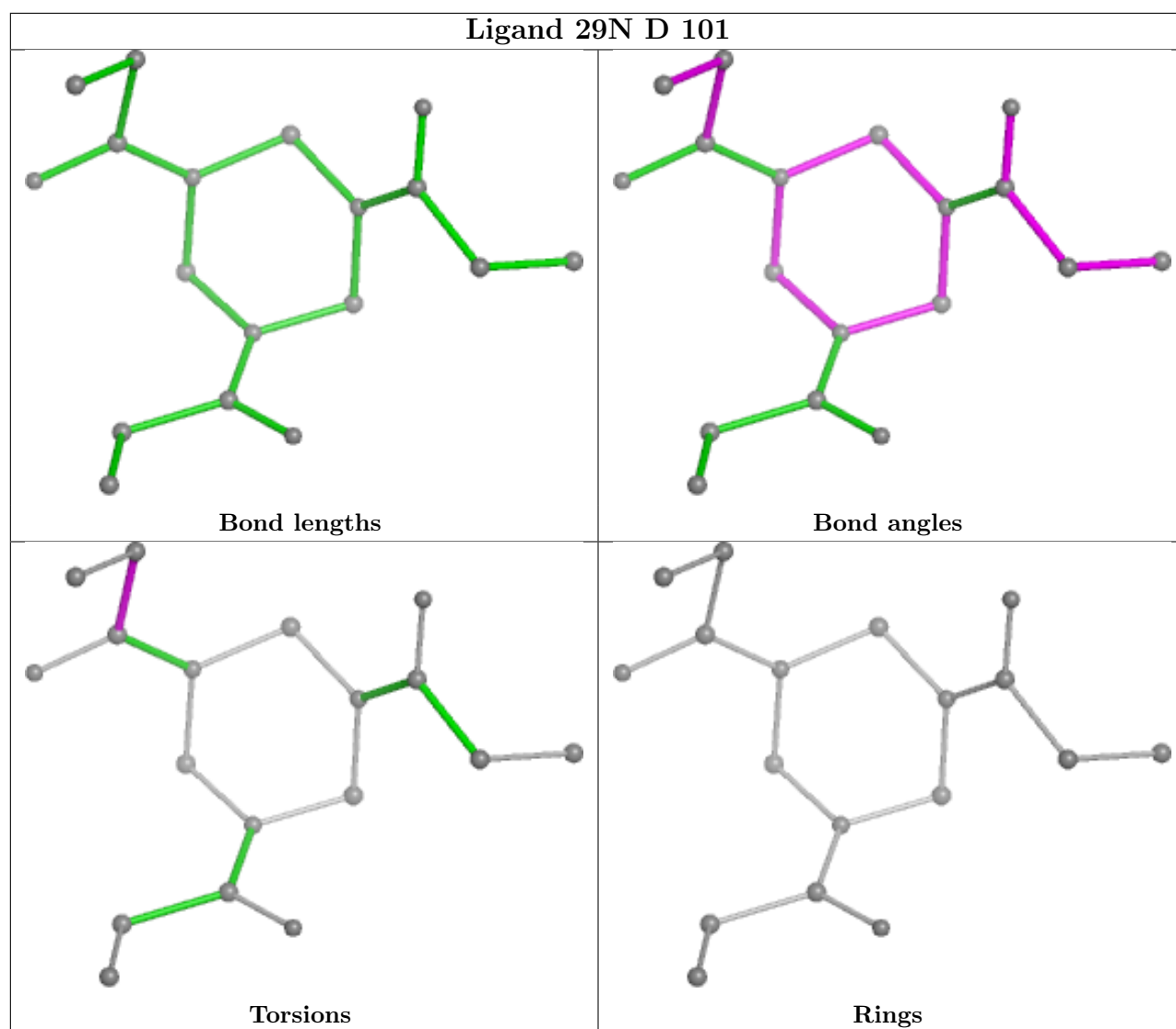
2 monomers are involved in 2 short contacts:

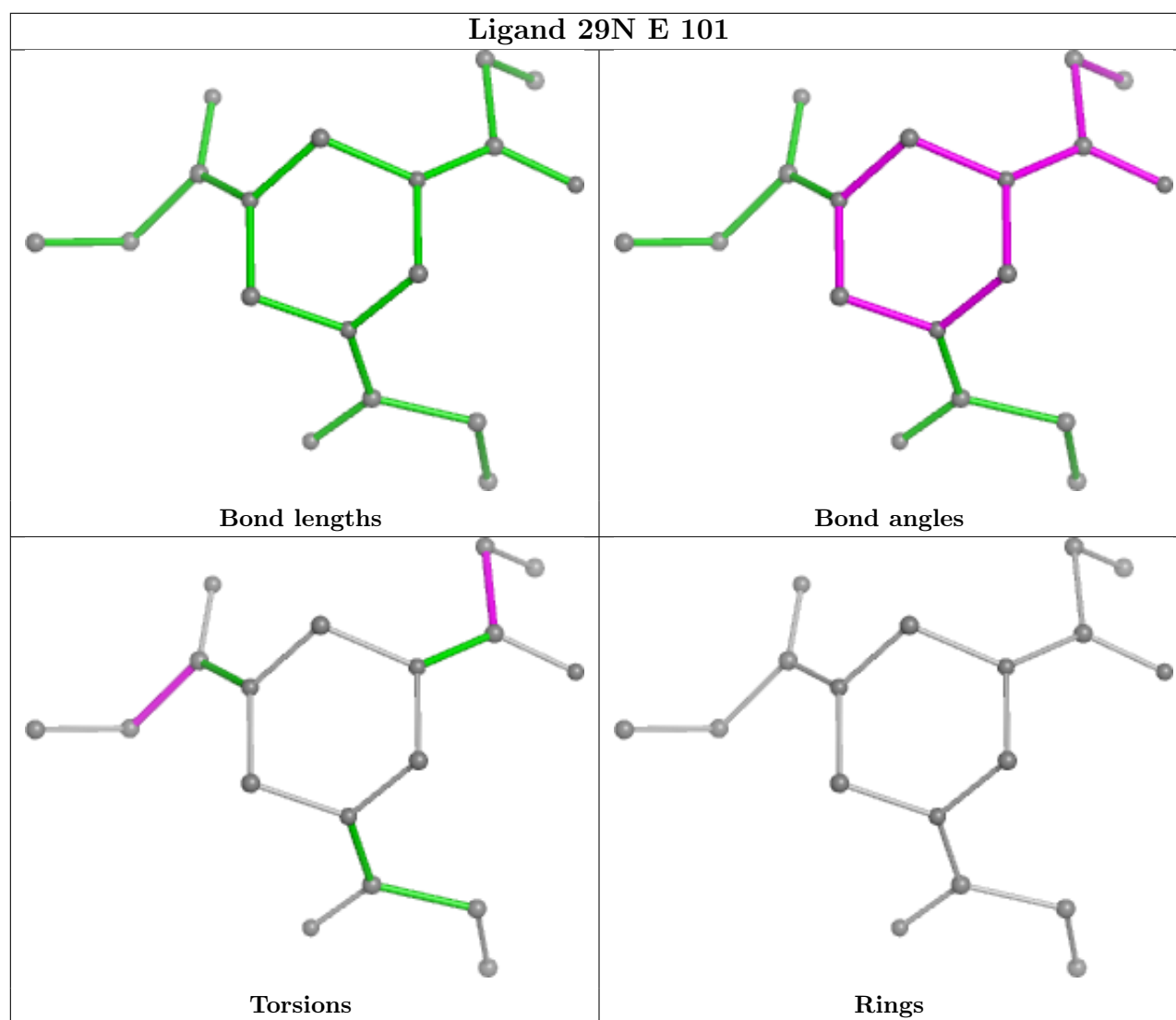
Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	502	SO4	1	0
5	D	101	29N	1	0

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

Ligand 29N F 101







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	199/245 (81%)	0.53	17 (8%)	18 19	18, 35, 65, 93	1 (0%)
1	B	195/245 (79%)	0.45	19 (9%)	15 15	21, 33, 64, 101	2 (1%)
1	C	196/245 (80%)	0.44	15 (7%)	21 22	16, 32, 74, 104	1 (0%)
2	D	15/17 (88%)	0.19	0	100 100	30, 37, 53, 54	0
2	E	15/17 (88%)	-0.07	0	100 100	28, 31, 49, 51	0
2	F	15/17 (88%)	-0.21	0	100 100	25, 30, 44, 51	0
All	All	635/786 (80%)	0.44	51 (8%)	20 21	16, 34, 65, 104	4 (0%)

All (51) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	319	TYR	6.9
1	B	323	SER	5.9
1	C	159	GLY	5.8
1	B	129	TRP	5.7
1	C	320	PRO	4.7
1	B	157	ALA	4.7
1	C	317	PHE	4.4
1	A	159	GLY	4.4
1	B	161	PRO	4.4
1	A	142	VAL	4.4
1	C	322	LEU	4.4
1	C	157	ALA	4.1
1	C	160	ASN	4.1
1	C	128	MET	4.0
1	B	322	LEU	3.9
1	C	129	TRP	3.9
1	C	161	PRO	3.8
1	A	160	ASN	3.7
1	A	157	ALA	3.7

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Mol	Chain	Res	Type	RSRZ
1	B	319	TYR	3.6
1	B	159	GLY	3.6
1	C	264	LYS	3.3
1	B	160	ASN	3.2
1	C	321	THR	3.2
1	C	127	GLY	3.0
1	A	124	GLY	2.9
1	A	125	PHE	2.9
1	B	158	ASN	2.9
1	B	271	GLY	2.9
1	A	161	PRO	2.7
1	B	162	CYS	2.7
1	A	143	VAL	2.6
1	C	265	GLN	2.6
1	A	158	ASN	2.6
1	B	321	THR	2.5
1	A	126	LYS	2.3
1	A	322	LEU	2.3
1	B	178[A]	ILE	2.3
1	A	181	ASN	2.2
1	A	264	LYS	2.2
1	B	264	LYS	2.2
1	B	320	PRO	2.2
1	B	147	GLN	2.2
1	A	268	THR	2.1
1	B	317	PHE	2.1
1	A	265	GLN	2.1
1	B	163	ASP	2.1
1	C	271	GLY	2.1
1	B	176	GLN	2.0
1	A	178	ILE	2.0
1	A	246	GLN	2.0

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

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

6.3 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

6.4 Ligands

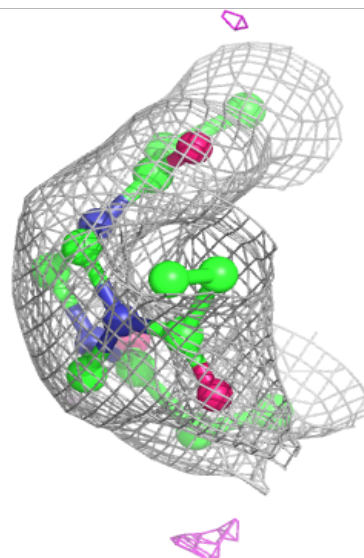
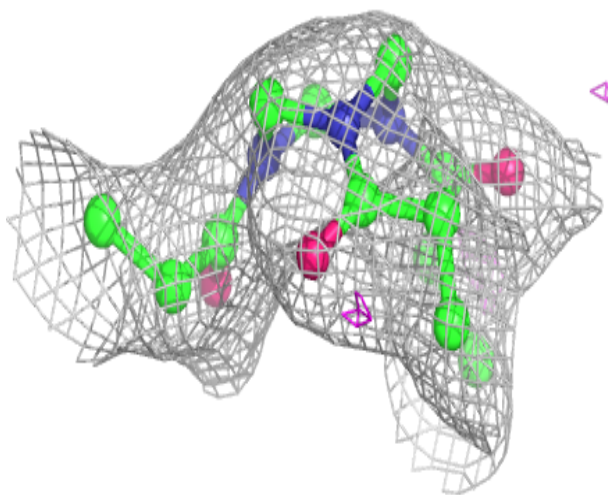
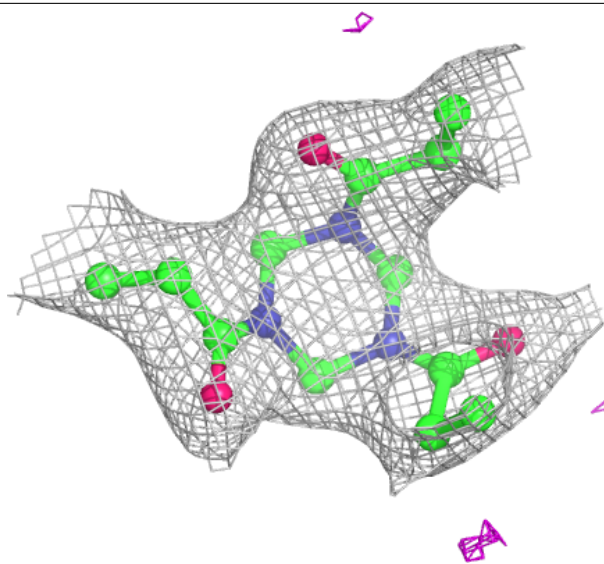
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	SO4	B	504	5/5	0.81	0.10	75,75,82,95	0
4	ACY	B	501	4/4	0.82	0.13	34,34,36,37	0
3	SO4	A	402	5/5	0.83	0.12	71,72,78,84	0
3	SO4	A	401	5/5	0.89	0.10	68,69,78,97	0
3	SO4	B	503	5/5	0.89	0.10	80,81,86,87	0
5	29N	D	101	18/18	0.92	0.09	31,34,37,38	0
3	SO4	C	401	5/5	0.94	0.07	55,55,62,64	0
3	SO4	C	402	5/5	0.94	0.08	73,75,81,84	0
5	29N	F	101	18/18	0.95	0.07	22,28,30,30	0
5	29N	E	101	18/18	0.96	0.06	25,29,31,33	0
3	SO4	B	502	5/5	0.97	0.06	43,46,49,56	0

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

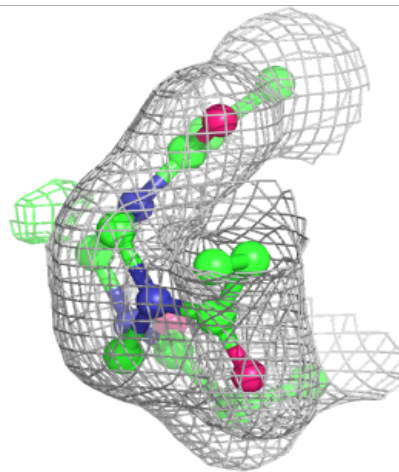
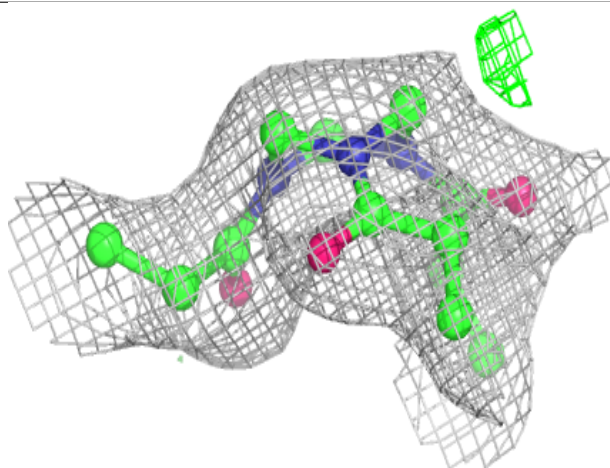
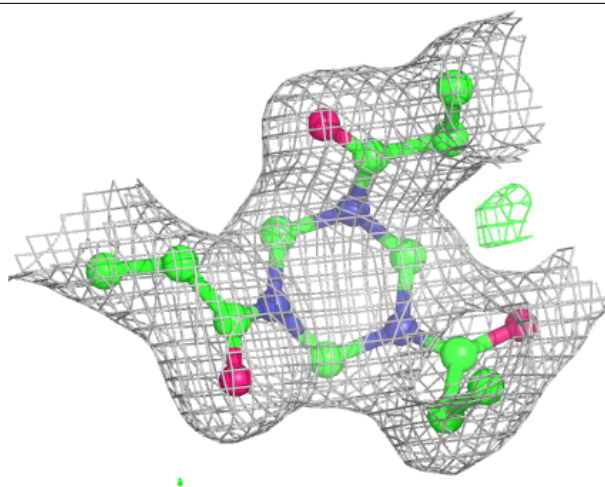
Electron density around 29N D 101:

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



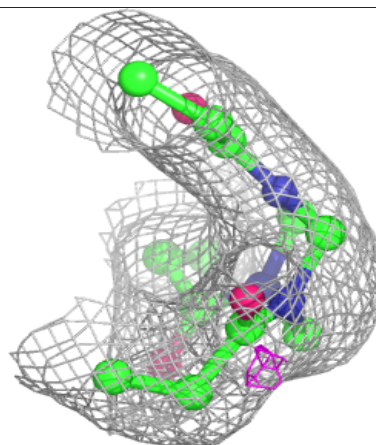
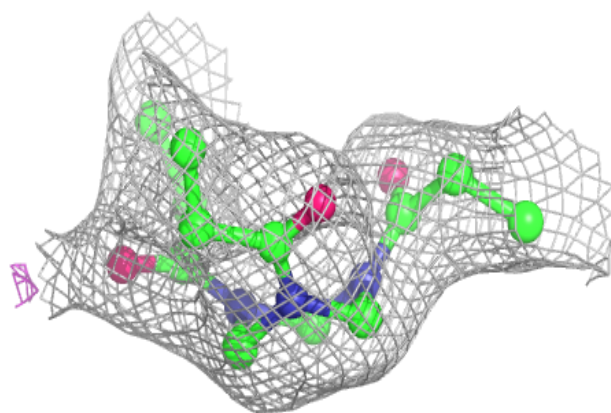
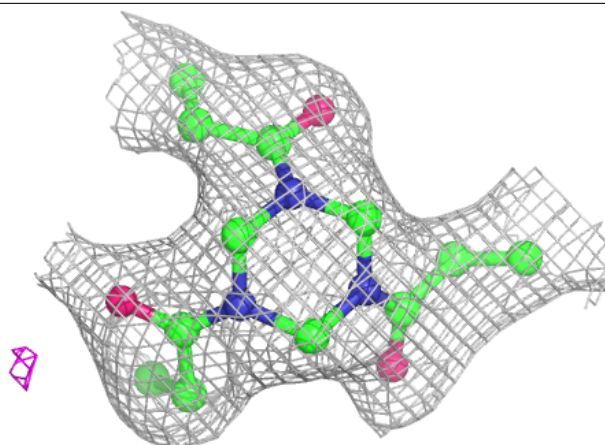
Electron density around 29N F 101:

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



Electron density around 29N E 101:

$2mF_o-DF_c$ (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.