



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:37 PM UTC

PDB ID : 3N7S / pdb_00003n7s
Title : Crystal structure of the ectodomain complex of the CGRP receptor, a Class-B GPCR, reveals the site of drug antagonism
Authors : Ter Haar, E.
Deposited on : 2010-05-27
Resolution : 2.10 Å(reported)

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

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

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

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

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

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

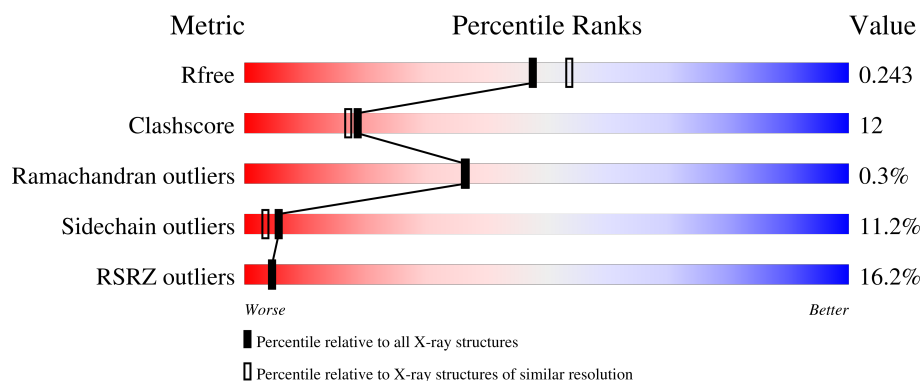
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.10 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



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

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

Mol	Chain	Length	Quality of chain
1	A	115	18% 69% 10% • 18%
1	B	115	15% 60% 17% 6% 17%
2	C	96	15% 68% 16% 10% • 5%
2	D	96	7% 71% 12% •• 12%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard

residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
4	3N7	B	1	-	X	X	-

2 Entry composition

There are 6 unique types of molecules in this entry. The entry contains 3116 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 Calcitonin gene-related peptide type 1 receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	94	Total	C	N	O	S	0	0	0
			740	460	128	143	9			
1	B	95	Total	C	N	O	S	0	0	0
			760	472	132	147	9			

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	19	GLY	-	expression tag	UNP Q16602
A	20	SER	-	expression tag	UNP Q16602
A	21	HIS	-	expression tag	UNP Q16602
A	22	MET	-	expression tag	UNP Q16602
B	19	GLY	-	expression tag	UNP Q16602
B	20	SER	-	expression tag	UNP Q16602
B	21	HIS	-	expression tag	UNP Q16602
B	22	MET	-	expression tag	UNP Q16602

- Molecule 2 is a protein called Receptor activity-modifying protein 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	C	91	Total	C	N	O	S	0	0	0
			725	458	129	130	8			
2	D	84	Total	C	N	O	S	0	0	0
			675	430	119	118	8			

There are 8 discrepancies between the modelled and reference sequences:

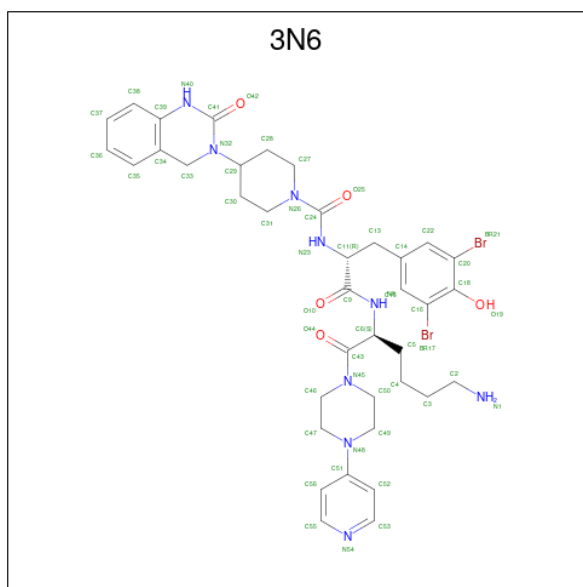
Chain	Residue	Modelled	Actual	Comment	Reference
C	22	GLY	-	expression tag	UNP O60894
C	23	SER	-	expression tag	UNP O60894
C	24	HIS	-	expression tag	UNP O60894
C	25	MET	-	expression tag	UNP O60894

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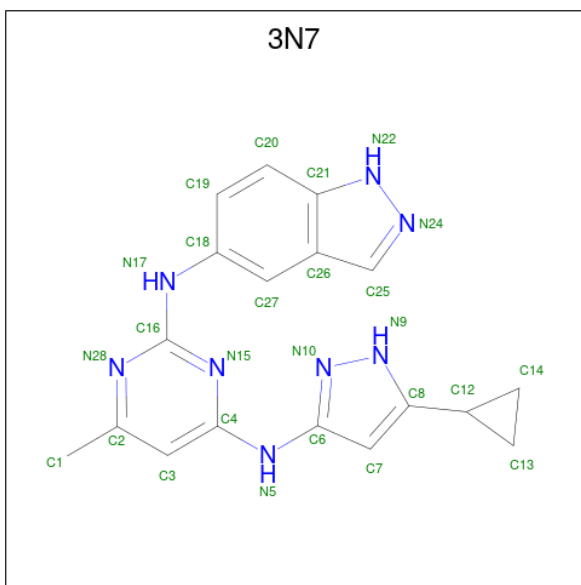
Chain	Residue	Modelled	Actual	Comment	Reference
D	22	GLY	-	expression tag	UNP O60894
D	23	SER	-	expression tag	UNP O60894
D	24	HIS	-	expression tag	UNP O60894
D	25	MET	-	expression tag	UNP O60894

- Molecule 3 is N-{(1S)-5-amino-1-[(4-pyridin-4-ylpiperazin-1-yl)carbonyl]pentyl}-3,5-dibrom o-Nalpa-α-{[4-(2-oxo-1,4-dihydroquinazolin-3 (2H)-yl)piperidin-1-yl]carbonyl}-D-tyrosinami de (CCD ID: 3N6) (formula: C₃₈H₄₇Br₂N₉O₅).



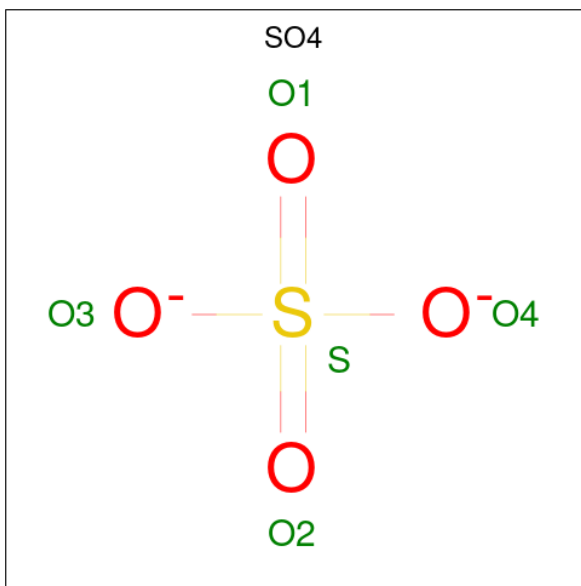
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
			Total	Br	C	N	O		
3	A	1	54	2	38	9	5	0	0

- Molecule 4 is N 4 -(5-cyclopropyl-1H-pyrazol-3-yl)-N 2 -1H-indazol-5-yl-6-methylpyrimidine -2,4-diamine (CCD ID: 3N7) (formula: C₁₈H₁₈N₈).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	N	0	0
			26	18	8		

- Molecule 5 is SULFATE ION (CCD ID: SO4) (formula: O₄S).



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

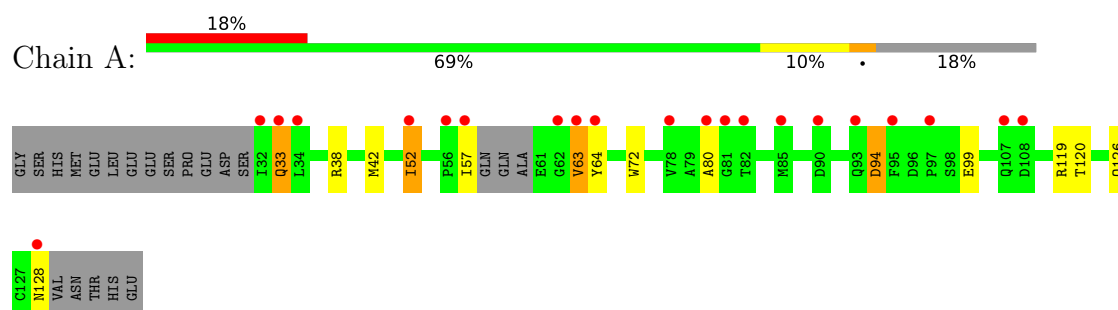
- Molecule 6 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
6	A	27	Total 27	O 27	0	0
6	B	41	Total 41	O 41	0	0
6	C	35	Total 35	O 35	0	0
6	D	28	Total 28	O 28	0	0

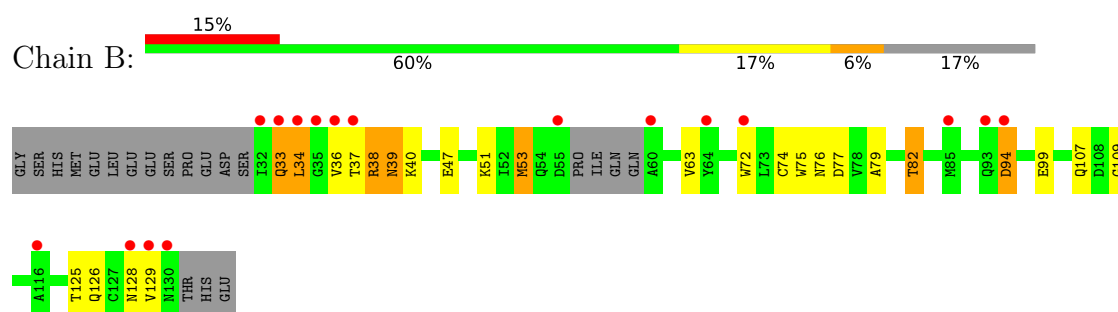
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

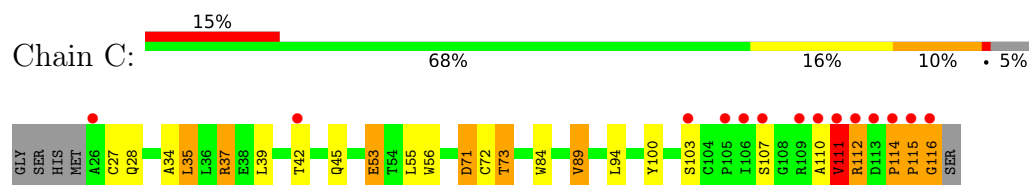
- Molecule 1: Calcitonin gene-related peptide type 1 receptor



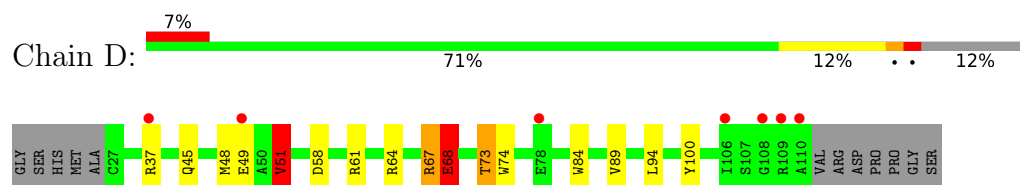
- Molecule 1: Calcitonin gene-related peptide type 1 receptor



- Molecule 2: Receptor activity-modifying protein 1



- Molecule 2: Receptor activity-modifying protein 1



4 Data and refinement statistics

Property	Value	Source
Space group	C 2 2 21	Depositor
Cell constants a, b, c, α , β , γ	73.31Å 119.13Å 137.16Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	46.17 – 2.10 46.17 – 2.10	Depositor EDS
% Data completeness (in resolution range)	(Not available) (46.17-2.10) 86.7 (46.17-2.10)	Depositor EDS
R_{merge}	0.07	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.36 (at 2.10Å)	Xtriage
Refinement program	BUSTER-TNT BUSTER 2.9.2, BUSTER 2.9.2	Depositor
R, R_{free}	0.208 , 0.226 0.218 , 0.243	Depositor DCC
R_{free} test set	1509 reflections (4.95%)	wwPDB-VP
Wilson B-factor (Å ²)	29.7	Xtriage
Anisotropy	0.648	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.37 , 53.5	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3116	wwPDB-VP
Average B, all atoms (Å ²)	42.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.32% 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: SO4, 3N7, 3N6

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	0.67	0/761	1.18	3/1036 (0.3%)
1	B	0.65	0/780	1.14	3/1058 (0.3%)
2	C	0.71	0/746	1.42	11/1012 (1.1%)
2	D	0.66	1/694 (0.1%)	1.15	1/941 (0.1%)
All	All	0.67	1/2981 (0.0%)	1.23	18/4047 (0.4%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	D	68	GLU	C-O	-5.62	1.17	1.24

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	115	PRO	CB-CA-C	11.95	126.73	111.56
2	C	110	ALA	N-CA-C	9.52	127.22	109.24
2	C	115	PRO	N-CA-C	-7.60	99.14	111.15
1	B	33	GLN	N-CA-C	-7.47	104.17	113.28
2	C	114	PRO	CA-C-N	6.85	126.89	119.90
2	C	114	PRO	C-N-CA	6.85	126.89	119.90
1	A	63	VAL	N-CA-C	6.79	123.47	109.34
2	C	89	VAL	N-CA-CB	6.76	119.74	110.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	C	111	VAL	N-CA-C	6.74	123.36	109.34
2	C	114	PRO	O-C-N	6.36	128.97	121.46
2	C	116	GLY	N-CA-C	-6.16	95.43	113.30
2	D	51	VAL	N-CA-CB	5.57	118.94	110.58
2	C	72	CYS	CA-C-N	5.49	127.63	120.28
2	C	72	CYS	C-N-CA	5.49	127.63	120.28
1	B	37	THR	N-CA-C	5.47	116.94	110.97
1	B	125	THR	N-CA-C	5.30	117.06	111.28
1	A	64	TYR	N-CA-CB	-5.21	102.94	110.70
1	A	120	THR	N-CA-C	-5.14	102.30	109.96

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	128	ASN	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	740	0	629	14	0
1	B	760	0	667	23	0
2	C	725	0	663	17	0
2	D	675	0	621	18	0
3	A	54	0	46	3	0
4	B	26	0	18	15	0
5	C	5	0	0	0	0
6	A	27	0	0	0	0
6	B	41	0	0	4	0
6	C	35	0	0	3	0
6	D	28	0	0	2	0
All	All	3116	0	2644	67	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 12.

All (67) 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)
2:D:37:ARG:NH2	6:D:205:HOH:O	1.90	1.03
4:B:1:3N7:H25	6:B:216:HOH:O	1.63	0.98
1:B:76:ASN:H	4:B:1:3N7:H27	1.37	0.89
1:B:79:ALA:O	1:B:82:THR:HG23	1.76	0.85
2:C:111:VAL:HG12	2:C:112:ARG:N	1.92	0.84
2:C:73:THR:CG2	2:C:84:TRP:HE1	1.90	0.83
2:C:94:LEU:HB3	6:C:230:HOH:O	1.80	0.82
2:D:73:THR:CG2	2:D:84:TRP:HE1	1.93	0.82
1:B:38:ARG:NH2	2:C:71:ASP:OD2	2.16	0.78
2:C:111:VAL:HG12	2:C:112:ARG:H	1.47	0.78
1:B:75:TRP:HA	4:B:1:3N7:H27	1.66	0.77
1:A:99:GLU:HG2	1:A:126:GLN:O	1.85	0.75
1:A:52:ILE:HG22	2:D:94:LEU:HD21	1.67	0.75
2:C:73:THR:HG23	2:C:84:TRP:HE1	1.53	0.72
2:C:111:VAL:CG1	2:C:112:ARG:N	2.54	0.70
1:B:76:ASN:N	4:B:1:3N7:H27	2.05	0.70
4:B:1:3N7:H14	6:B:208:HOH:O	1.95	0.67
2:C:37:ARG:NH2	6:C:209:HOH:O	2.29	0.65
2:D:73:THR:HG23	2:D:84:TRP:HE1	1.62	0.63
1:B:51:LYS:HD2	4:B:1:3N7:H1B	1.81	0.62
1:A:119:ARG:HH12	2:C:35:LEU:HD13	1.66	0.61
2:D:64:ARG:O	2:D:68:GLU:HG2	2.00	0.61
1:B:76:ASN:H	4:B:1:3N7:C27	2.11	0.60
2:D:58:ASP:OD2	2:D:61:ARG:HG2	2.04	0.58
2:D:73:THR:HG22	2:D:84:TRP:HE1	1.69	0.57
1:B:47:GLU:HG2	4:B:1:3N7:H1	1.86	0.57
4:B:1:3N7:N15	4:B:1:3N7:H19	2.20	0.57
2:D:45:GLN:HG2	2:D:100:TYR:OH	2.05	0.57
2:C:111:VAL:HG12	2:C:112:ARG:HG2	1.87	0.56
1:B:39:ASN:ND2	6:B:218:HOH:O	2.40	0.55
1:A:63:VAL:O	1:A:80:ALA:HB2	2.08	0.54
1:A:42:MET:HG3	2:D:67:ARG:HB2	1.90	0.54
1:A:38:ARG:CZ	2:D:67:ARG:HG3	2.38	0.54
1:B:72:TRP:NE1	6:B:238:HOH:O	2.16	0.52
1:B:36:VAL:O	1:B:40:LYS:HG3	2.09	0.51
1:A:119:ARG:HD2	2:C:34:ALA:HB1	1.91	0.51
2:D:48:MET:HA	2:D:51:VAL:HG13	1.94	0.49
2:C:53:GLU:HA	2:C:56:TRP:CD2	2.47	0.49
1:B:33:GLN:O	1:B:38:ARG:HB2	2.14	0.48
2:D:64:ARG:O	2:D:68:GLU:CG	2.61	0.47
1:B:47:GLU:OE2	4:B:1:3N7:H3	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:72:TRP:CZ3	3:A:1:3N6:H33A	2.50	0.47
2:C:114:PRO:HA	2:C:115:PRO:HD2	1.64	0.47
1:B:36:VAL:CG1	1:B:40:LYS:HE3	2.45	0.46
2:C:111:VAL:CG1	2:C:112:ARG:HG2	2.46	0.46
1:B:74:CYS:HB3	4:B:1:3N7:N28	2.32	0.45
3:A:1:3N6:H2A	2:D:74:TRP:CE2	2.52	0.45
1:B:99:GLU:HG3	1:B:126:GLN:O	2.16	0.45
1:B:34:LEU:CD1	1:B:38:ARG:NH1	2.79	0.45
2:D:67:ARG:NH2	6:D:209:HOH:O	2.48	0.44
1:A:33:GLN:HG2	1:A:33:GLN:O	2.17	0.44
1:A:38:ARG:NH2	2:D:67:ARG:HG2	2.33	0.44
1:A:52:ILE:CG2	2:D:94:LEU:HD21	2.42	0.43
2:C:45:GLN:HG2	2:C:100:TYR:OH	2.18	0.43
1:A:94:ASP:OD1	1:A:94:ASP:N	2.50	0.43
1:B:51:LYS:HD2	4:B:1:3N7:C1	2.46	0.43
1:A:38:ARG:NE	2:D:67:ARG:HG3	2.34	0.43
2:C:103:SER:HB2	6:C:226:HOH:O	2.18	0.42
1:B:94:ASP:OD1	1:B:94:ASP:N	2.46	0.42
3:A:1:3N6:H2A	2:D:74:TRP:CD1	2.54	0.42
1:B:63:VAL:HG12	1:B:109:GLY:HA3	2.01	0.42
1:A:52:ILE:HD13	1:A:52:ILE:HG21	1.63	0.41
1:B:53:MET:HE3	1:B:53:MET:HB3	1.84	0.41
1:B:75:TRP:HA	4:B:1:3N7:C27	2.45	0.41
4:B:1:3N7:C3	4:B:1:3N7:C7	2.95	0.41
2:C:115:PRO:HA	2:C:116:GLY:HA2	1.83	0.41
1:B:75:TRP:CA	4:B:1:3N7:H27	2.42	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	90/115 (78%)	86 (96%)	4 (4%)	0	100	100
1	B	91/115 (79%)	86 (94%)	4 (4%)	1 (1%)	11	8
2	C	89/96 (93%)	85 (96%)	4 (4%)	0	100	100
2	D	82/96 (85%)	80 (98%)	2 (2%)	0	100	100
All	All	352/422 (83%)	337 (96%)	14 (4%)	1 (0%)	36	36

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	129	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	75/104 (72%)	70 (93%)	5 (7%)	15	12
1	B	80/104 (77%)	72 (90%)	8 (10%)	7	5
2	C	73/79 (92%)	59 (81%)	14 (19%)	1	1
2	D	67/79 (85%)	61 (91%)	6 (9%)	9	6
All	All	295/366 (81%)	262 (89%)	33 (11%)	6	3

All (33) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	52	ILE
1	A	57	ILE
1	A	94	ASP
1	A	128	ASN
1	B	34	LEU
1	B	38	ARG
1	B	39	ASN
1	B	53	MET
1	B	77	ASP

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Mol	Chain	Res	Type
1	B	82	THR
1	B	94	ASP
1	B	107	GLN
2	C	27	CYS
2	C	28	GLN
2	C	35	LEU
2	C	37	ARG
2	C	39	LEU
2	C	42	THR
2	C	53	GLU
2	C	55	LEU
2	C	71	ASP
2	C	73	THR
2	C	89	VAL
2	C	107	SER
2	C	111	VAL
2	C	112	ARG
2	D	49	GLU
2	D	51	VAL
2	D	67	ARG
2	D	68	GLU
2	D	73	THR
2	D	89	VAL

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	33	GLN
1	A	45	GLN
1	A	66	ASN
1	A	86	GLN
1	A	128	ASN
1	B	66	ASN
1	B	86	GLN
2	C	45	GLN
2	D	45	GLN

5.3.3 RNA ⓘ

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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 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	$\# Z > 2$
4	3N7	B	1	-	30,30,30	3.47	16 (53%)	36,43,43	6.15	20 (55%)
3	3N6	A	1	-	59,59,59	0.80	1 (1%)	79,82,82	1.38	14 (17%)
5	SO4	C	1	-	4,4,4	0.42	0	6,6,6	0.23	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
4	3N7	B	1	-	-	4/12/14/14	0/5/5/5
3	3N6	A	1	-	-	4/41/73/73	0/6/6/6

All (17) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1	3N7	C26-C25	-10.96	1.29	1.42
4	B	1	3N7	C25-N24	-7.43	1.27	1.32
4	B	1	3N7	C27-C26	-5.09	1.32	1.40
4	B	1	3N7	C7-C8	-5.01	1.29	1.37
4	B	1	3N7	C3-C4	4.98	1.52	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	1	3N7	C4-N5	3.88	1.49	1.40
4	B	1	3N7	N9-N10	3.64	1.44	1.36
4	B	1	3N7	C6-N5	3.21	1.42	1.37
4	B	1	3N7	C6-N10	3.19	1.37	1.33
4	B	1	3N7	C8-N9	3.04	1.38	1.34
4	B	1	3N7	C19-C18	2.76	1.43	1.39
4	B	1	3N7	C21-N22	-2.67	1.31	1.36
4	B	1	3N7	N22-N24	-2.52	1.34	1.36
3	A	1	3N6	C39-C34	2.29	1.43	1.40
4	B	1	3N7	C18-N17	2.18	1.45	1.40
4	B	1	3N7	C20-C21	-2.13	1.36	1.39
4	B	1	3N7	C3-C2	-2.04	1.35	1.38

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	1	3N7	C21-N22-N24	-17.41	102.99	111.52
4	B	1	3N7	C25-N24-N22	15.50	114.11	106.02
4	B	1	3N7	C8-C7-C6	14.58	114.98	104.78
4	B	1	3N7	C12-C8-N9	12.77	142.11	122.62
4	B	1	3N7	C12-C8-C7	-9.83	115.24	131.09
4	B	1	3N7	C7-C6-N10	-8.21	106.28	112.14
4	B	1	3N7	C26-C25-N24	-5.98	107.33	111.68
4	B	1	3N7	N5-C6-N10	5.82	131.11	117.81
4	B	1	3N7	C1-C2-N28	5.31	124.58	116.56
4	B	1	3N7	C3-C4-N15	-5.05	112.88	123.35
4	B	1	3N7	C3-C2-N28	-4.95	114.61	121.50
4	B	1	3N7	C7-C8-N9	-4.24	102.65	106.19
4	B	1	3N7	C19-C18-C27	-4.21	114.56	119.66
4	B	1	3N7	C27-C26-C21	4.17	121.71	119.13
3	A	1	3N6	N40-C41-N32	4.10	123.23	116.66
4	B	1	3N7	C16-N28-C2	3.79	123.34	115.98
4	B	1	3N7	C20-C19-C18	3.66	124.51	120.30
3	A	1	3N6	O42-C41-N32	-3.13	119.34	123.10
4	B	1	3N7	N28-C16-N15	-3.10	121.17	126.26
3	A	1	3N6	C34-C33-N32	2.93	116.65	111.94
3	A	1	3N6	C35-C34-C39	2.75	120.95	118.32
3	A	1	3N6	C55-N54-C53	2.72	123.07	116.86
3	A	1	3N6	C47-N48-C51	-2.68	110.81	118.11
4	B	1	3N7	C27-C26-C25	-2.61	131.65	135.46
3	A	1	3N6	C50-N45-C46	2.59	117.97	112.68
3	A	1	3N6	O42-C41-N40	-2.58	117.42	121.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	1	3N6	BR17-C16-C18	2.56	121.67	118.80
3	A	1	3N6	C31-N26-C27	2.52	117.83	112.68
4	B	1	3N7	C3-C4-N5	2.51	129.27	122.53
3	A	1	3N6	C49-N48-C51	-2.47	111.38	118.11
4	B	1	3N7	C26-C27-C18	2.36	121.57	119.00
3	A	1	3N6	C20-C18-C16	2.28	119.64	116.67
3	A	1	3N6	C15-C16-C18	-2.27	119.48	121.92
3	A	1	3N6	C52-C53-N54	-2.23	119.80	123.60

There are no chirality outliers.

All (8) torsion outliers are listed below:

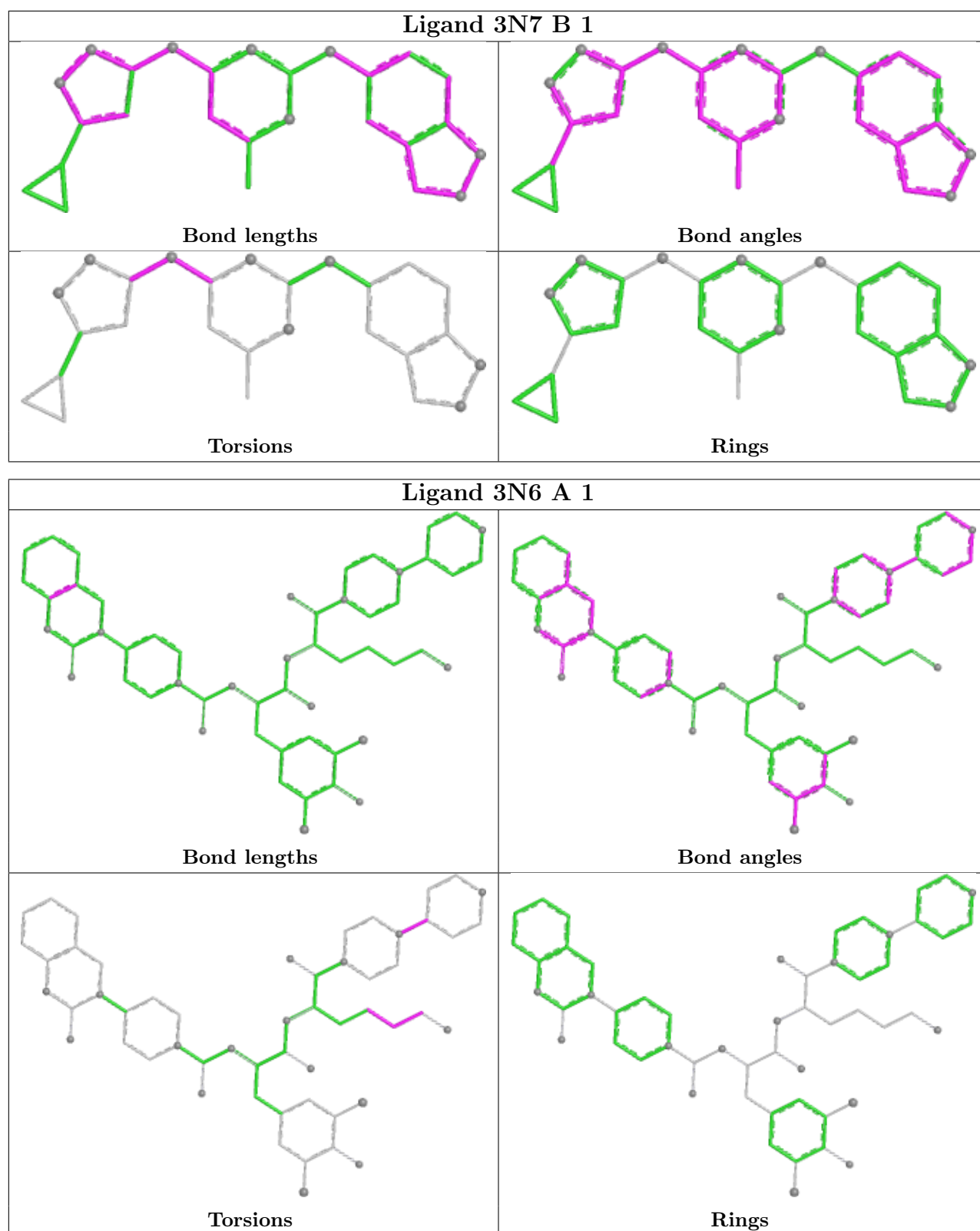
Mol	Chain	Res	Type	Atoms
4	B	1	3N7	N15-C4-N5-C6
4	B	1	3N7	C7-C6-N5-C4
4	B	1	3N7	N10-C6-N5-C4
3	A	1	3N6	C2-C3-C4-C5
4	B	1	3N7	C3-C4-N5-C6
3	A	1	3N6	C52-C51-N48-C47
3	A	1	3N6	N1-C2-C3-C4
3	A	1	3N6	C56-C51-N48-C47

There are no ring outliers.

2 monomers are involved in 18 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	B	1	3N7	15	0
3	A	1	3N6	3	0

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



5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	94/115 (81%)	1.13	21 (22%) 2 2	28, 51, 78, 95	0
1	B	95/115 (82%)	0.93	17 (17%) 3 4	19, 39, 74, 87	0
2	C	91/96 (94%)	0.98	14 (15%) 5 5	20, 33, 68, 78	0
2	D	84/96 (87%)	0.71	7 (8%) 17 18	27, 37, 61, 72	0
All	All	364/422 (86%)	0.94	59 (16%) 4 4	19, 39, 72, 95	0

All (59) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	C	115	PRO	9.1
2	C	110	ALA	7.5
2	D	110	ALA	7.3
2	C	116	GLY	6.9
2	C	111	VAL	6.9
1	B	32	ILE	6.8
2	C	106	ILE	6.0
1	A	57	ILE	5.7
1	B	35	GLY	5.7
1	B	130	ASN	5.6
2	C	109	ARG	5.5
1	B	129	VAL	5.2
2	C	114	PRO	4.7
1	B	34	LEU	4.4
1	A	63	VAL	4.4
1	A	34	LEU	4.4
1	A	128	ASN	4.4
2	C	26	ALA	3.9
2	D	109	ARG	3.8
2	C	103	SER	3.7
1	A	32	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	64	TYR	3.6
1	A	78	VAL	3.6
1	B	60	ALA	3.6
1	B	94	ASP	3.4
1	A	85	MET	3.3
1	B	55	ASP	3.3
1	B	72	TRP	3.1
1	A	107	GLN	3.0
2	D	78	GLU	2.9
1	B	36	VAL	2.9
2	D	108	GLY	2.9
2	C	105	PRO	2.8
2	D	49	GLU	2.8
2	D	37	ARG	2.8
1	B	85	MET	2.8
1	A	52	ILE	2.8
1	B	93	GLN	2.7
2	C	113	ASP	2.7
1	A	33	GLN	2.6
1	A	62	GLY	2.6
1	A	93	GLN	2.6
1	A	82	THR	2.6
1	A	56	PRO	2.6
2	D	106	ILE	2.5
2	C	112	ARG	2.5
1	B	128	ASN	2.4
1	A	80	ALA	2.3
1	B	116	ALA	2.3
1	A	95	PHE	2.3
2	C	107	SER	2.2
1	A	90	ASP	2.2
1	B	37	THR	2.2
1	B	64	TYR	2.1
1	A	81	GLY	2.1
1	A	108	ASP	2.1
1	A	97	PRO	2.1
1	B	33	GLN	2.0
2	C	42	THR	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 [i](#)

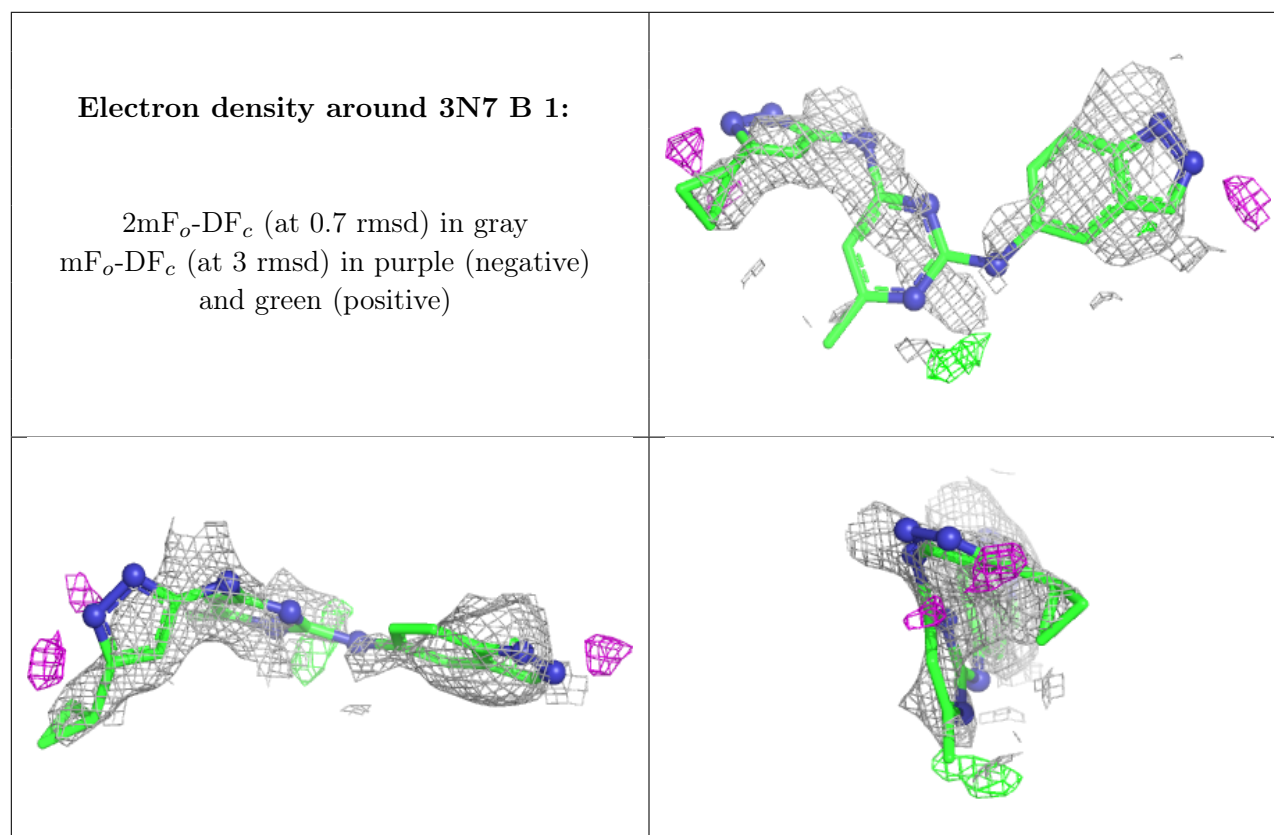
There are no oligosaccharides in this entry.

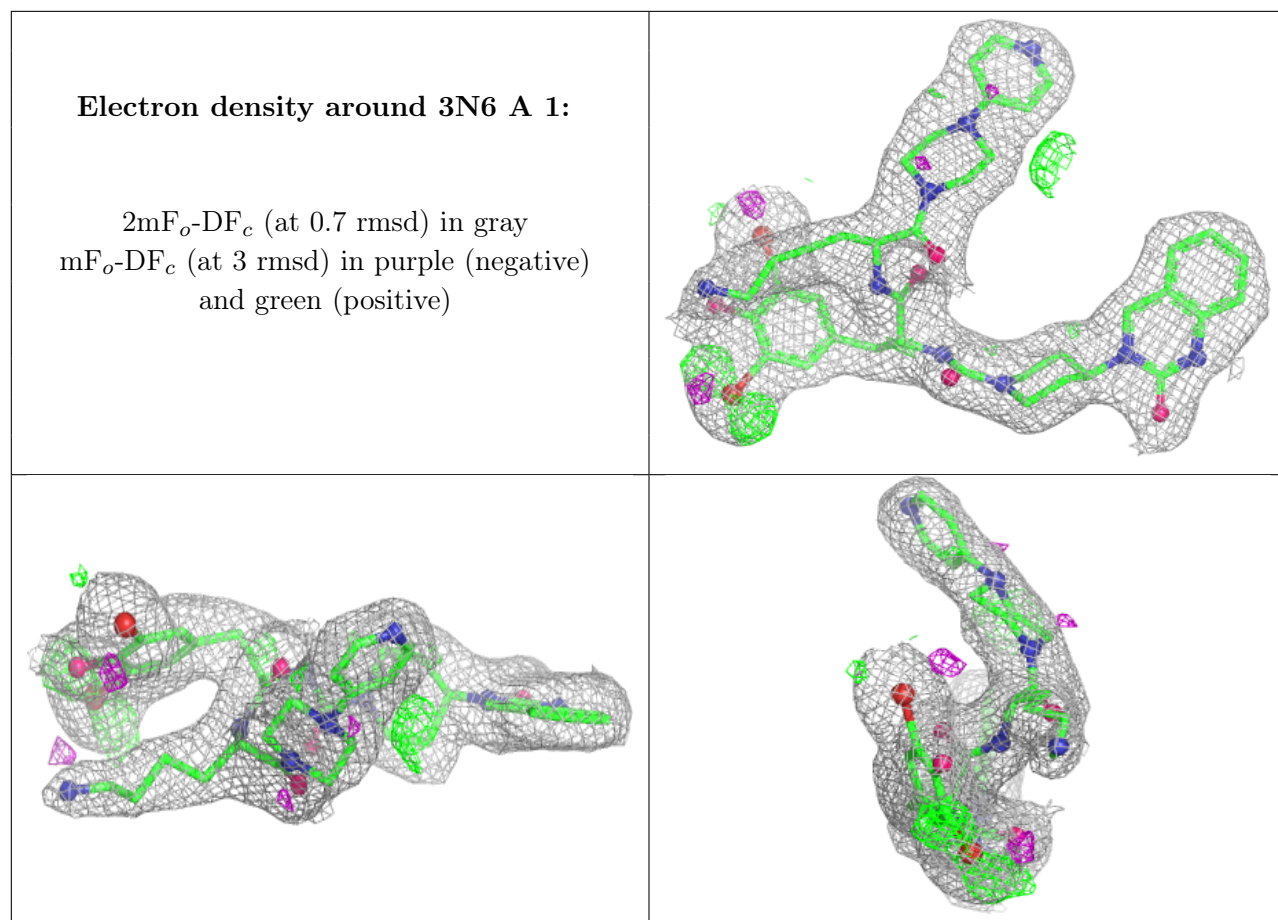
6.4 Ligands [i](#)

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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
5	SO4	C	1	5/5	0.79	0.22	78,82,83,84	0
4	3N7	B	1	26/26	0.82	0.25	108,110,111,111	0
3	3N6	A	1	54/54	0.96	0.10	26,34,47,48	2

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.





6.5 Other polymers ⓘ

There are no such residues in this entry.