



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 07:32 AM UTC

PDB ID : 3UYK / pdb_00003uyk
Title : Spinosyn Rhamnosyltransferase SpnG complexed with spinosyn aglycone
Authors : Isiorho, E.A.; Liu, H.-W.; Keatinge-Clay, A.T.
Deposited on : 2011-12-06
Resolution : 1.70 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

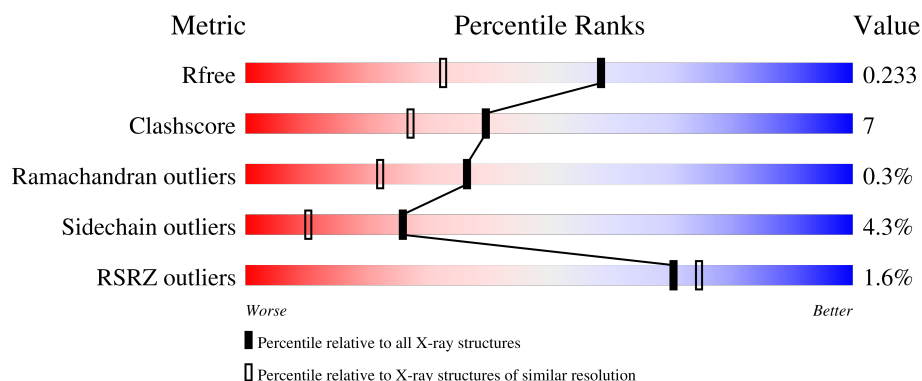
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.70 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	5551 (1.70-1.70)
Clashscore	190562	5924 (1.70-1.70)
Ramachandran outliers	187476	5846 (1.70-1.70)
Sidechain outliers	187428	5846 (1.70-1.70)
RSRZ outliers	180081	5554 (1.70-1.70)

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	387	2% 76% 17% • •
1	B	387	2% 77% 17% • 5%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6079 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 NDP-rhamnosyltransferase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	373	Total	C	N	O	S	0	0	0
			2780	1763	491	511	15			
1	B	369	Total	C	N	O	S	0	0	0
			2747	1744	482	506	15			

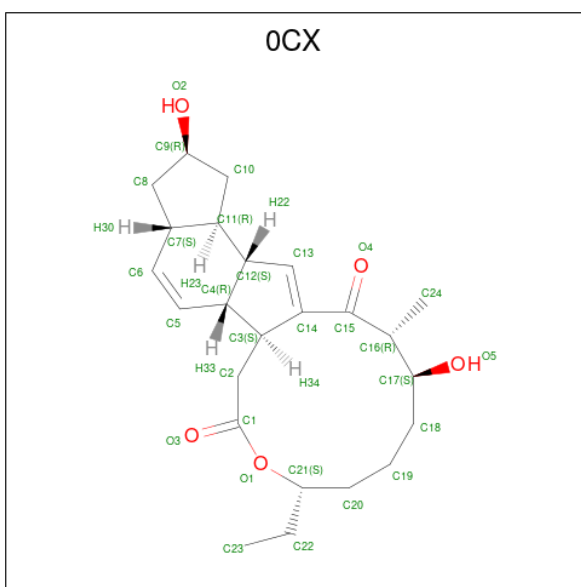
There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	0	HIS	-	expression tag	UNP Q9ALM8
A	360	ALA	SER	SEE REMARK 999	UNP Q9ALM8
B	0	HIS	-	expression tag	UNP Q9ALM8
B	360	ALA	SER	SEE REMARK 999	UNP Q9ALM8

- Molecule 2 is MAGNESIUM ION (CCD ID: MG) (formula: Mg).

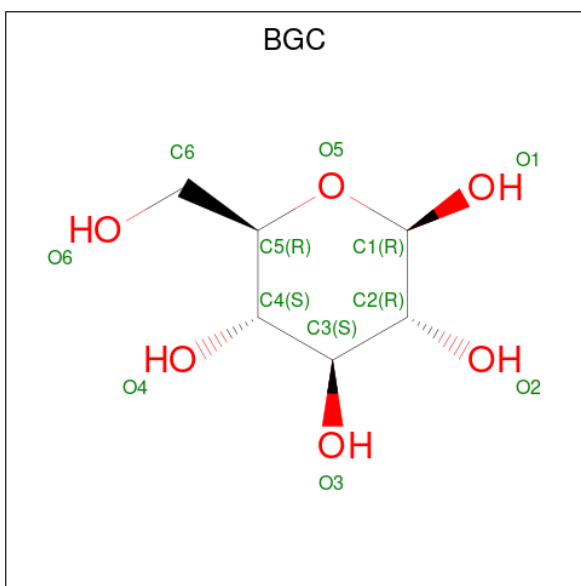
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	1	Total	Mg	0	0
			1	1		

- Molecule 3 is (2R,3aS,5aR,5bS,9S,13S,14R,16aS,16bR)-9-ethyl-2,13-dihydroxy-14-methyl-2,3,3a,5a,5b,6,9,10,11,12,13,14,16a,16b-tetradecahydro-1H-as-indaceno[3,2-d]oxacyclododecine-7,15-dione (CCD ID: OCX) (formula: C₂₄H₃₄O₅).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	B	1	Total	C	O	0	0
			29	24	5		

- Molecule 4 is beta-D-glucopyranose (CCD ID: BGC) (formula: $C_6H_{12}O_6$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	B	1	Total	C	O	0	0
			12	6	6		

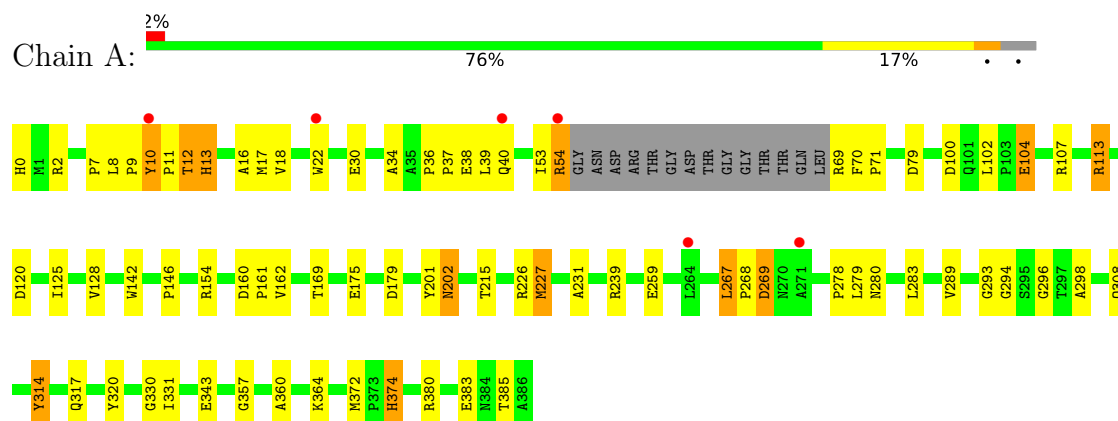
- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	259	Total 259	O 259	0	0
5	B	251	Total 251	O 251	0	0

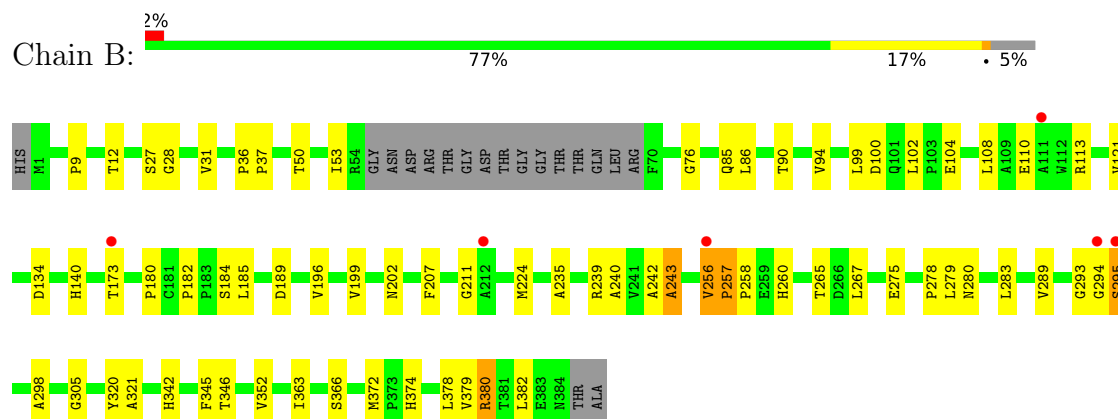
3 Residue-property plots

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: NDP-rhamnosyltransferase



• Molecule 1: NDP-rhamnosyltransferase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	54.02Å 57.08Å 68.10Å 81.98° 74.10° 86.07°	Depositor
Resolution (Å)	29.83 – 1.70 29.83 – 1.70	Depositor EDS
% Data completeness (in resolution range)	96.9 (29.83-1.70) 96.9 (29.83-1.70)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.23 (at 1.71Å)	Xtriage
Refinement program	REFMAC version: 5.5.0072	Depositor
R, R_{free}	0.189 , 0.234 0.188 , 0.233	Depositor DCC
R_{free} test set	4101 reflections (4.99%)	wwPDB-VP
Wilson B-factor (Å ²)	18.4	Xtriage
Anisotropy	0.010	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 35.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	6079	wwPDB-VP
Average B, all atoms (Å ²)	21.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.68% 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: MG, BGC, OCX

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	1.57	19/2850 (0.7%)	1.35	18/3911 (0.5%)
1	B	1.55	17/2816 (0.6%)	1.44	29/3865 (0.8%)
All	All	1.56	36/5666 (0.6%)	1.40	47/7776 (0.6%)

All (36) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	199	VAL	N-CA	-7.55	1.39	1.46
1	B	76	GLY	C-O	7.53	1.32	1.24
1	B	257	PRO	CA-C	7.07	1.55	1.51
1	B	295	SER	CA-C	6.53	1.61	1.52
1	B	235	ALA	N-CA	6.43	1.52	1.46
1	A	142	TRP	CD2-CE2	6.15	1.51	1.41
1	A	374	HIS	ND1-CE1	6.07	1.38	1.32
1	A	364	LYS	N-CA	6.03	1.53	1.46
1	A	13	HIS	CG-CD2	6.00	1.42	1.35
1	A	13	HIS	ND1-CE1	5.96	1.38	1.32
1	A	360	ALA	N-CA	5.80	1.53	1.46
1	B	374	HIS	ND1-CE1	5.72	1.38	1.32
1	A	18	VAL	CA-CB	5.72	1.57	1.53
1	A	102	LEU	CA-C	5.66	1.59	1.52
1	A	34	ALA	N-CA	5.62	1.53	1.46
1	A	120	ASP	CA-C	5.57	1.59	1.52
1	B	100	ASP	N-CA	5.48	1.52	1.46
1	A	314	TYR	C-O	5.43	1.30	1.23
1	B	374	HIS	CG-CD2	5.40	1.41	1.35
1	A	331	ILE	N-CA	5.37	1.52	1.46
1	B	321	ALA	N-CA	5.33	1.52	1.46
1	A	239	ARG	CD-NE	5.30	1.53	1.46
1	B	239	ARG	N-CA	5.29	1.52	1.46
1	B	256	VAL	CA-CB	5.24	1.60	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	162	VAL	N-CA	-5.24	1.40	1.46
1	A	16	ALA	N-CA	-5.23	1.39	1.46
1	B	242	ALA	N-CA	5.20	1.52	1.46
1	A	179	ASP	C-N	5.19	1.38	1.33
1	A	201	TYR	CA-C	-5.17	1.46	1.52
1	B	85	GLN	CA-C	5.16	1.59	1.52
1	B	86	LEU	N-CA	5.16	1.52	1.46
1	B	243	ALA	N-CA	5.11	1.52	1.46
1	B	352	VAL	C-O	5.10	1.30	1.24
1	A	330	GLY	C-O	5.07	1.30	1.24
1	B	31	VAL	N-CA	5.07	1.52	1.46
1	A	296	GLY	C-O	5.06	1.29	1.23

All (47) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	267	LEU	CA-C-N	8.21	130.10	119.84
1	A	267	LEU	C-N-CA	8.21	130.10	119.84
1	B	256	VAL	CA-C-N	7.94	125.45	119.66
1	B	256	VAL	C-N-CA	7.94	125.45	119.66
1	B	102	LEU	CA-C-N	-7.26	111.49	119.19
1	B	102	LEU	C-N-CA	-7.26	111.49	119.19
1	B	199	VAL	CA-C-N	-6.97	112.58	119.76
1	B	199	VAL	C-N-CA	-6.97	112.58	119.76
1	B	372	MET	CG-SD-CE	-6.96	85.58	100.90
1	B	207	PHE	CA-C-N	-6.85	112.88	120.14
1	B	207	PHE	C-N-CA	-6.85	112.88	120.14
1	A	12	THR	N-CA-C	6.73	118.61	111.28
1	B	173	THR	CA-C-N	-6.72	113.73	120.31
1	B	173	THR	C-N-CA	-6.72	113.73	120.31
1	B	121	VAL	CG1-CB-CG2	-6.60	96.28	110.80
1	A	364	LYS	CD-CE-NZ	-6.48	91.17	111.90
1	B	295	SER	N-CA-C	6.34	124.30	110.80
1	B	189	ASP	N-CA-C	6.29	120.66	112.92
1	B	257	PRO	CA-C-O	-6.09	116.52	120.90
1	B	239	ARG	N-CA-C	-6.07	104.74	111.36
1	B	257	PRO	O-C-N	6.05	124.09	121.31
1	B	293	GLY	N-CA-C	6.04	119.06	112.29
1	B	265	THR	N-CA-C	5.98	119.84	112.54
1	B	257	PRO	CB-CA-C	-5.94	105.81	111.39
1	B	108	LEU	N-CA-C	5.92	117.40	111.07
1	A	22	TRP	CB-CA-C	-5.90	100.99	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	128	VAL	N-CA-C	-5.84	104.81	110.42
1	A	357	GLY	N-CA-C	-5.78	107.17	114.16
1	A	17	MET	CA-C-N	-5.77	116.60	120.24
1	A	17	MET	C-N-CA	-5.77	116.60	120.24
1	A	231	ALA	N-CA-C	5.77	117.37	111.14
1	A	100	ASP	N-CA-C	5.67	117.46	111.28
1	B	211	GLY	CA-C-N	5.67	130.27	120.58
1	B	211	GLY	C-N-CA	5.67	130.27	120.58
1	A	10	TYR	CB-CA-C	-5.57	102.89	109.47
1	A	293	GLY	N-CA-C	-5.32	107.68	115.72
1	B	104	GLU	N-CA-C	5.31	116.75	111.07
1	B	224	MET	N-CA-C	-5.12	106.12	112.93
1	B	50	THR	N-CA-C	5.08	117.88	109.85
1	A	317	GLN	N-CA-C	5.07	117.54	111.71
1	B	366	SER	N-CA-C	-5.07	105.02	111.11
1	B	267	LEU	CA-C-N	-5.07	115.01	120.03
1	B	267	LEU	C-N-CA	-5.07	115.01	120.03
1	A	380	ARG	N-CA-C	5.04	117.16	111.11
1	A	372	MET	CA-C-N	-5.02	114.78	119.85
1	A	372	MET	C-N-CA	-5.02	114.78	119.85
1	A	383	GLU	N-CA-C	-5.01	105.82	111.28

There are no chirality outliers.

There are no planarity outliers.

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	2780	0	2774	36	0
1	B	2747	0	2742	39	0
2	A	1	0	0	0	0
3	B	29	0	34	5	0
4	B	12	0	12	0	0
5	A	259	0	0	7	0
5	B	251	0	0	4	0
All	All	6079	0	5562	74	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 7.

All (74) 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:A:175:GLU:HG2	1:A:385:THR:HG23	1.15	1.08
1:A:113:ARG:HD2	5:A:599:HOH:O	1.61	1.01
1:A:175:GLU:HG2	1:A:385:THR:CG2	1.89	1.01
1:B:196:VAL:HB	1:B:378:LEU:HD11	1.43	0.99
1:B:202:ASN:ND2	1:B:280:ASN:OD1	1.95	0.99
1:B:196:VAL:HB	1:B:378:LEU:CD1	2.00	0.91
1:A:202:ASN:OD1	1:A:280:ASN:OD1	1.88	0.91
1:A:107:ARG:HD3	5:A:485:HOH:O	1.77	0.84
1:B:196:VAL:CG2	1:B:378:LEU:HD12	2.10	0.82
1:A:175:GLU:CG	1:A:385:THR:HG23	2.07	0.80
1:B:90:THR:HG23	3:B:387:OCX:H34	1.68	0.76
1:A:53:ILE:O	1:A:54:ARG:HB2	1.86	0.75
1:B:94:VAL:CG2	3:B:387:OCX:H36	2.18	0.73
1:A:9:PRO:HB3	1:A:36:PRO:HG2	1.71	0.72
1:B:258:PRO:HA	1:B:275:GLU:OE2	1.91	0.70
1:B:256:VAL:HB	1:B:257:PRO:HD2	1.73	0.70
1:B:257:PRO:C	1:B:275:GLU:OE2	2.34	0.70
1:B:258:PRO:N	1:B:275:GLU:OE2	2.25	0.70
1:B:258:PRO:CA	1:B:275:GLU:OE2	2.42	0.68
1:A:259:GLU:OE1	1:A:259:GLU:N	2.28	0.66
1:B:294:GLY:O	1:B:298:ALA:HB3	1.97	0.65
1:B:380:ARG:HB3	5:B:414:HOH:O	1.96	0.64
1:A:79:ASP:HB2	5:A:653:HOH:O	1.98	0.62
1:B:342:HIS:O	1:B:346:THR:HG23	2.02	0.60
1:B:256:VAL:HB	1:B:257:PRO:CD	2.33	0.58
1:B:140:HIS:HE1	5:B:524:HOH:O	1.87	0.57
1:B:294:GLY:HA3	5:B:598:HOH:O	2.05	0.56
1:A:283:LEU:HD11	1:A:289:VAL:HG22	1.89	0.55
1:B:94:VAL:HG23	3:B:387:OCX:H36	1.89	0.54
1:B:196:VAL:CB	1:B:378:LEU:CD1	2.80	0.54
1:A:374:HIS:CE1	1:B:28:GLY:HA3	2.43	0.53
1:A:0:HIS:CE1	1:A:30:GLU:HG3	2.44	0.52
1:A:154:ARG:NH2	5:A:550:HOH:O	2.41	0.52
1:B:37:PRO:HD3	1:B:53:ILE:O	2.09	0.52
1:A:0:HIS:HE1	1:A:30:GLU:OE1	1.91	0.52
1:A:7:PRO:HG2	1:A:39:LEU:CD1	2.40	0.52
1:B:196:VAL:HG23	1:B:378:LEU:HD12	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:257:PRO:HG2	1:B:260:HIS:ND1	2.25	0.51
1:B:196:VAL:HB	1:B:378:LEU:HD12	1.91	0.51
1:A:294:GLY:N	5:A:415:HOH:O	2.44	0.51
1:A:104:GLU:HG3	1:A:107:ARG:NH2	2.26	0.51
1:A:215:THR:HG21	5:A:666:HOH:O	2.12	0.50
1:A:2:ARG:NH2	1:A:2:ARG:HG2	2.27	0.50
1:B:196:VAL:CB	1:B:378:LEU:HD12	2.41	0.49
1:B:110:GLU:OE2	1:B:113:ARG:NH1	2.45	0.49
1:A:343:GLU:HG2	5:A:536:HOH:O	2.13	0.49
1:B:12:THR:HG22	5:B:570:HOH:O	2.12	0.49
1:A:36:PRO:HA	1:A:53:ILE:O	2.13	0.49
1:A:226:ARG:NE	1:A:259:GLU:OE2	2.43	0.48
1:B:196:VAL:HG21	1:B:378:LEU:HD12	1.91	0.48
1:B:243:ALA:HA	1:B:346:THR:HG22	1.95	0.48
1:A:227:MET:HE3	1:A:227:MET:HA	1.97	0.47
1:A:54:ARG:N	1:A:104:GLU:OE2	2.40	0.47
1:B:180:PRO:HA	1:B:196:VAL:O	2.15	0.47
1:B:240:ALA:HA	1:B:345:PHE:CZ	2.50	0.46
1:A:160:ASP:N	1:A:161:PRO:CD	2.79	0.45
1:B:305:GLY:HA3	1:B:363:ILE:HD13	1.98	0.45
1:B:94:VAL:HG23	3:B:387:OCX:C2	2.47	0.44
1:B:27:SER:OG	1:B:379:VAL:HG11	2.17	0.44
1:A:298:ALA:HB1	1:A:320:TYR:CZ	2.52	0.44
1:A:70:PHE:HA	1:A:71:PRO:C	2.41	0.43
1:B:9:PRO:HB3	1:B:36:PRO:HG2	2.01	0.43
1:A:54:ARG:HD3	1:A:54:ARG:HA	1.60	0.43
1:A:267:LEU:HD12	1:A:267:LEU:HA	1.91	0.43
1:A:38:GLU:OE2	1:A:38:GLU:N	2.44	0.42
1:B:283:LEU:HD11	1:B:289:VAL:HG22	2.00	0.42
1:A:8:LEU:HD12	1:A:13:HIS:CE1	2.54	0.42
1:A:269:ASP:OD1	1:A:269:ASP:N	2.52	0.42
1:B:298:ALA:HB1	1:B:320:TYR:CZ	2.55	0.42
1:B:182:PRO:HG2	1:B:185:LEU:HD12	2.02	0.41
1:B:94:VAL:CG2	3:B:387:OCX:C2	2.93	0.41
1:A:283:LEU:HD11	1:A:289:VAL:CG2	2.51	0.41
1:A:37:PRO:HD3	1:A:54:ARG:HB2	2.02	0.40
1:A:113:ARG:HH11	1:A:113:ARG:HG2	1.87	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	369/387 (95%)	359 (97%)	9 (2%)	1 (0%)	36	22
1	B	365/387 (94%)	356 (98%)	8 (2%)	1 (0%)	36	22
All	All	734/774 (95%)	715 (97%)	17 (2%)	2 (0%)	36	22

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	295	SER
1	A	146	PRO

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	290/300 (97%)	272 (94%)	18 (6%)	16	5
1	B	287/300 (96%)	280 (98%)	7 (2%)	43	26
All	All	577/600 (96%)	552 (96%)	25 (4%)	26	10

All (25) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	10	TYR
1	A	11	PRO
1	A	12	THR
1	A	40	GLN

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Mol	Chain	Res	Type
1	A	54	ARG
1	A	69	ARG
1	A	104	GLU
1	A	113	ARG
1	A	125	ILE
1	A	169	THR
1	A	202	ASN
1	A	227	MET
1	A	268	PRO
1	A	269	ASP
1	A	278	PRO
1	A	279	LEU
1	A	308	GLN
1	A	314	TYR
1	B	99	LEU
1	B	134	ASP
1	B	184	SER
1	B	278	PRO
1	B	279	LEU
1	B	380	ARG
1	B	382	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (16) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	0	HIS
1	A	25	GLN
1	A	166	HIS
1	A	197	GLN
1	A	344	GLN
1	A	374	HIS
1	B	25	GLN
1	B	89	GLN
1	B	140	HIS
1	B	166	HIS
1	B	202	ASN
1	B	280	ASN
1	B	308	GLN
1	B	313	GLN
1	B	337	GLN
1	B	339	GLN

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 ⓘ

Of 3 ligands modelled in this entry, 1 is monoatomic - leaving 2 for Mogul analysis.

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
3	OCX	B	387	-	31,32,32	1.54	6 (19%)	31,47,47	1.99	8 (25%)
4	BGC	B	388	-	12,12,12	0.99	1 (8%)	17,17,17	1.50	4 (23%)

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
3	OCX	B	387	-	-	2/28/65/65	0/3/4/4
4	BGC	B	388	-	-	2/2/22/22	0/1/1/1

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	387	OCX	C13-C14	4.80	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	387	OCX	C16-C15	-3.32	1.48	1.52
3	B	387	OCX	C10-C9	3.23	1.58	1.52
3	B	387	OCX	C12-C13	2.67	1.53	1.50
3	B	387	OCX	C3-C14	-2.57	1.47	1.51
4	B	388	BGC	O5-C1	2.28	1.48	1.42
3	B	387	OCX	O1-C1	2.25	1.40	1.34

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	387	OCX	O1-C1-C2	4.44	119.38	111.43
3	B	387	OCX	C8-C9-C10	4.03	108.91	103.81
3	B	387	OCX	C12-C4-C5	3.68	118.41	113.35
3	B	387	OCX	C3-C2-C1	-3.47	107.38	113.25
3	B	387	OCX	O5-C17-C16	-3.46	101.21	109.44
3	B	387	OCX	C18-C17-C16	3.45	117.87	113.25
4	B	388	BGC	O5-C5-C4	3.11	115.30	109.70
3	B	387	OCX	O1-C1-O3	-3.09	116.47	123.70
4	B	388	BGC	C4-C3-C2	-2.88	105.78	110.83
4	B	388	BGC	O5-C1-C2	2.72	115.08	110.30
3	B	387	OCX	C21-O1-C1	-2.09	112.79	117.80
4	B	388	BGC	C1-C2-C3	2.03	114.49	110.36

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	387	OCX	O5-C17-C18-C19
4	B	388	BGC	C4-C5-C6-O6
4	B	388	BGC	O5-C5-C6-O6
3	B	387	OCX	C16-C17-C18-C19

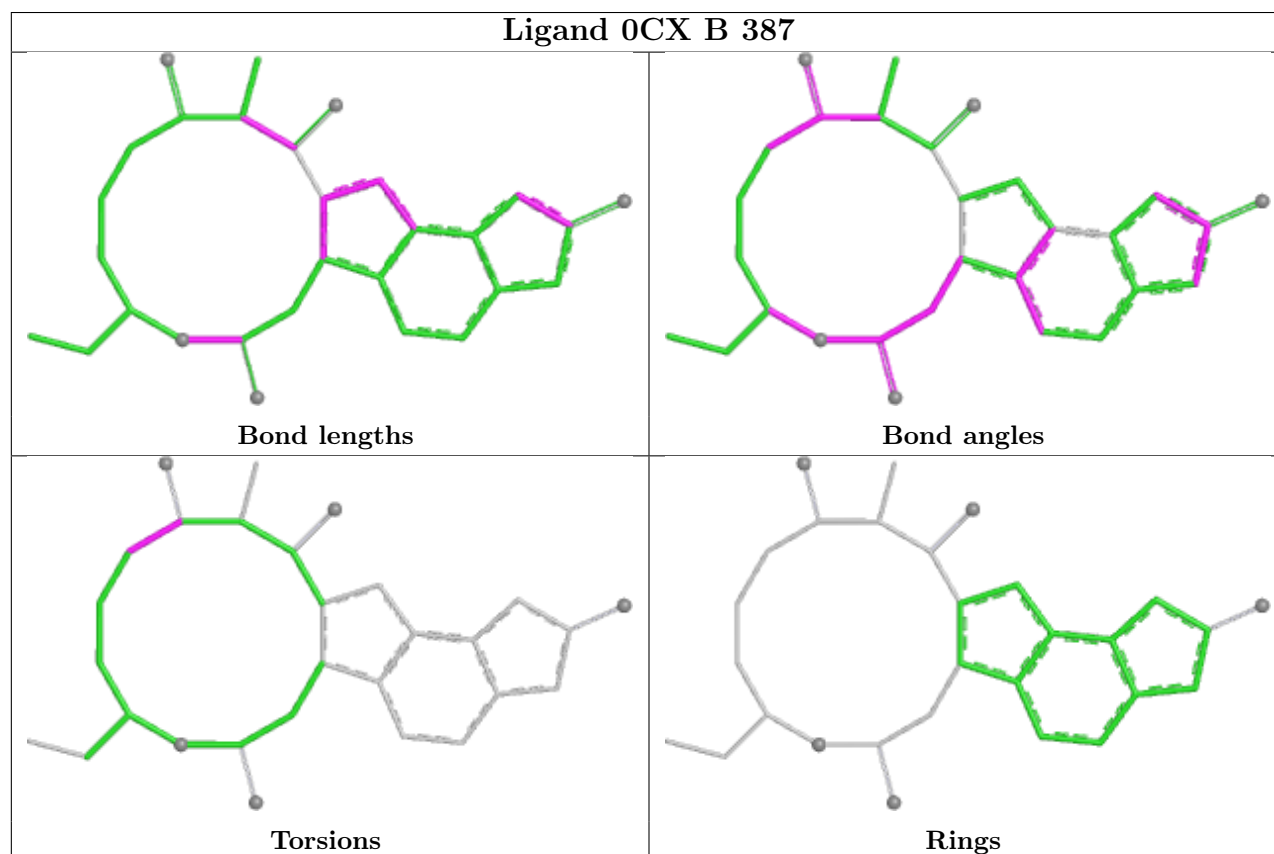
There are no ring outliers.

1 monomer is involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	387	OCX	5	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will

also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data [i](#)

6.1 Protein, DNA and RNA chains [i](#)

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	373/387 (96%)	-0.01	6 (1%) 70 75	9, 18, 36, 61	0
1	B	369/387 (95%)	-0.02	6 (1%) 70 75	10, 19, 31, 55	0
All	All	742/774 (95%)	-0.02	12 (1%) 70 75	9, 19, 34, 61	0

All (12) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	294	GLY	7.1
1	A	10	TYR	4.3
1	A	54	ARG	4.2
1	B	295	SER	2.7
1	B	111	ALA	2.4
1	B	256	VAL	2.3
1	B	173	THR	2.3
1	A	40	GLN	2.2
1	A	264	LEU	2.1
1	A	22	TRP	2.1
1	B	212	ALA	2.0
1	A	271	ALA	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](#)

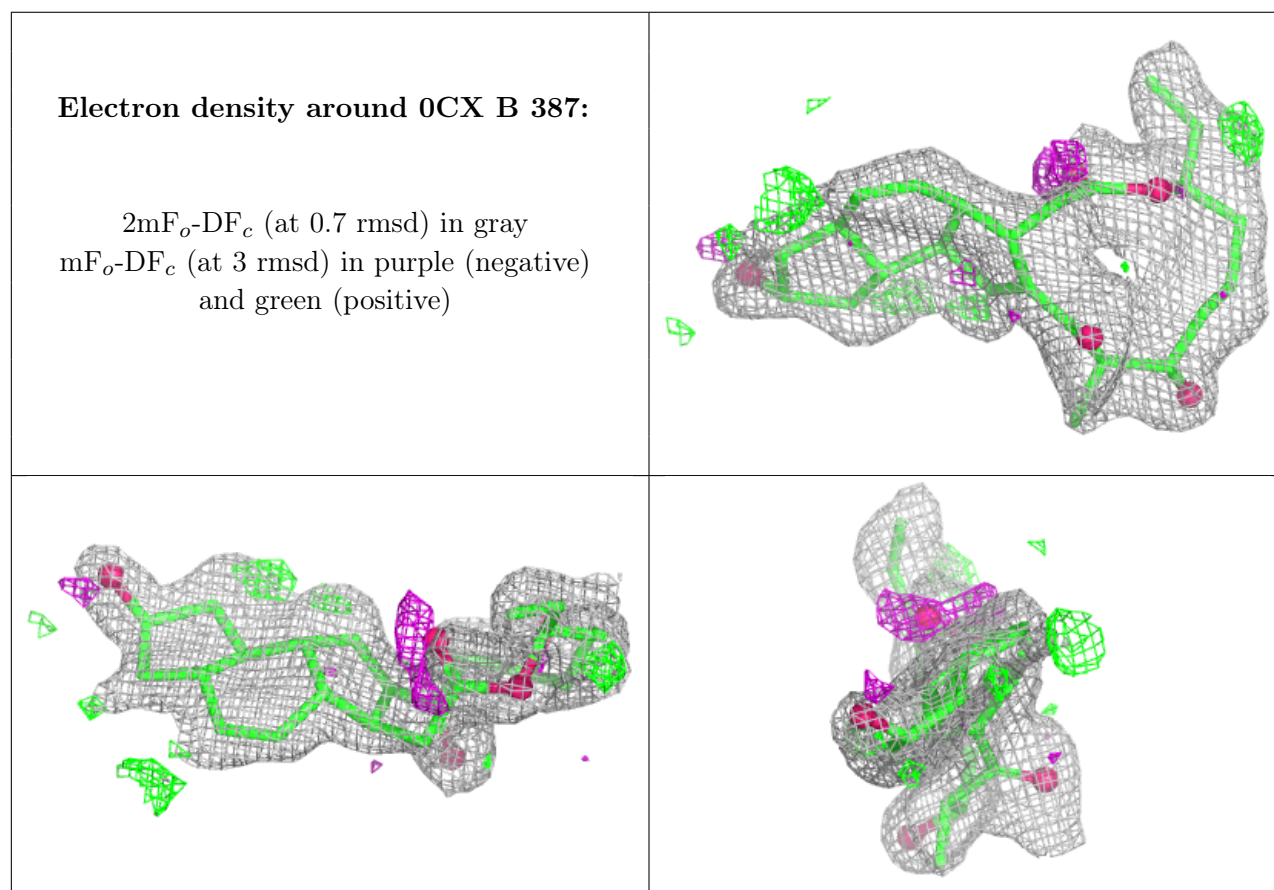
There are no oligosaccharides in this entry.

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($\text{\AA}^2$)	Q<0.9
3	OCX	B	387	29/29	0.74	0.15	31,36,39,43	0
4	BGC	B	388	12/12	0.93	0.11	16,24,41,57	0
2	MG	A	387	1/1	0.99	0.02	11,11,11,11	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.



6.5 Other polymers [i](#)

There are no such residues in this entry.