



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 08:26 AM UTC

PDB ID : 7CXA / pdb_00007cxa
Title : Structure of human Galectin-3 CRD in complex with TD-139 belonging to P31 space group.
Authors : Kumar, A.
Deposited on : 2020-09-01
Resolution : 1.97 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

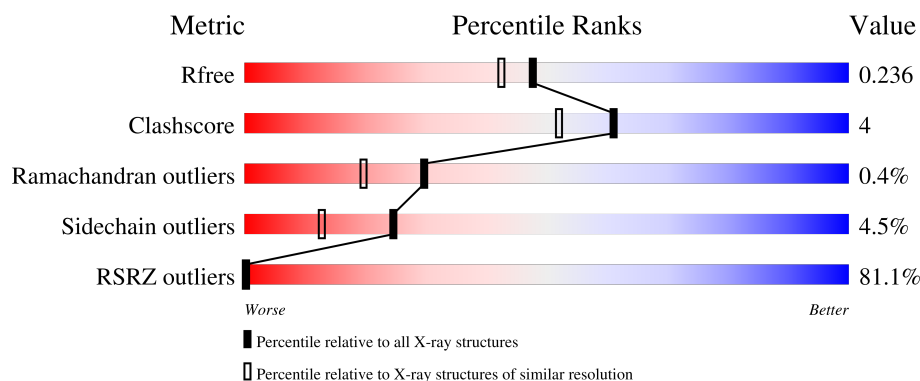
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.97 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	165	68% 73% 10% • 17%
1	B	165	67% 71% 12% • 16%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 2390 atoms, of which 60 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 Galectin-3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	137	Total	C	N	O	S	0	0	0
			1065	682	189	191	3			
1	B	138	Total	C	N	O	S	0	0	0
			1069	688	187	191	3			

There are 44 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	86	MET	-	expression tag	UNP P17931
A	87	GLY	-	expression tag	UNP P17931
A	88	SER	-	expression tag	UNP P17931
A	89	SER	-	expression tag	UNP P17931
A	90	HIS	-	expression tag	UNP P17931
A	91	HIS	-	expression tag	UNP P17931
A	92	HIS	-	expression tag	UNP P17931
A	93	HIS	-	expression tag	UNP P17931
A	94	HIS	-	expression tag	UNP P17931
A	95	HIS	-	expression tag	UNP P17931
A	96	SER	-	expression tag	UNP P17931
A	97	SER	-	expression tag	UNP P17931
A	98	GLY	-	expression tag	UNP P17931
A	99	GLU	-	expression tag	UNP P17931
A	100	THR	-	expression tag	UNP P17931
A	101	VAL	-	expression tag	UNP P17931
A	102	ARG	-	expression tag	UNP P17931
A	103	PHE	-	expression tag	UNP P17931
A	104	GLN	-	expression tag	UNP P17931
A	105	GLY	-	expression tag	UNP P17931
A	106	HIS	-	expression tag	UNP P17931
A	107	MET	-	expression tag	UNP P17931
B	86	MET	-	expression tag	UNP P17931
B	87	GLY	-	expression tag	UNP P17931
B	88	SER	-	expression tag	UNP P17931

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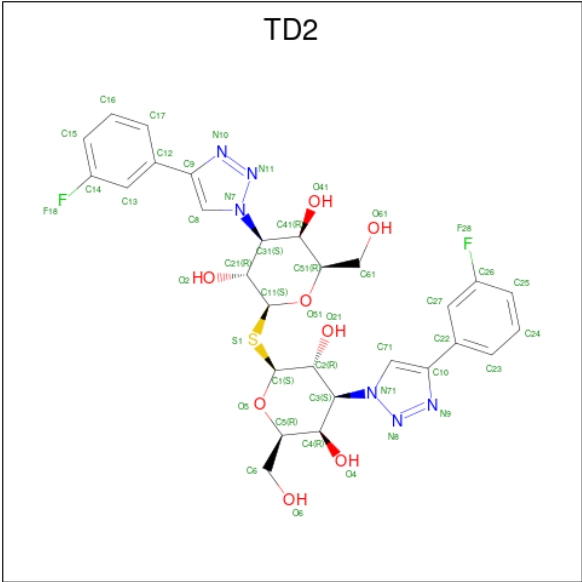
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Chain	Residue	Modelled	Actual	Comment	Reference
B	89	SER	-	expression tag	UNP P17931
B	90	HIS	-	expression tag	UNP P17931
B	91	HIS	-	expression tag	UNP P17931
B	92	HIS	-	expression tag	UNP P17931
B	93	HIS	-	expression tag	UNP P17931
B	94	HIS	-	expression tag	UNP P17931
B	95	HIS	-	expression tag	UNP P17931
B	96	SER	-	expression tag	UNP P17931
B	97	SER	-	expression tag	UNP P17931
B	98	GLY	-	expression tag	UNP P17931
B	99	GLU	-	expression tag	UNP P17931
B	100	THR	-	expression tag	UNP P17931
B	101	VAL	-	expression tag	UNP P17931
B	102	ARG	-	expression tag	UNP P17931
B	103	PHE	-	expression tag	UNP P17931
B	104	GLN	-	expression tag	UNP P17931
B	105	GLY	-	expression tag	UNP P17931
B	106	HIS	-	expression tag	UNP P17931
B	107	MET	-	expression tag	UNP P17931

- Molecule 2 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Cl 1 1	0	0
2	B	1	Total Cl 1 1	0	0

- Molecule 3 is 3-deoxy-3-[4-(3-fluorophenyl)-1H-1,2,3-triazol-1-yl]-beta-D-galactopyranosyl 3-deoxy-3-[4-(3-fluorophenyl)-1H-1,2,3-triazol-1-yl]-1-thio-beta-D-galactopyranoside (CCD ID: TD2) (formula: C₂₈H₃₀F₂N₆O₈S) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms							ZeroOcc	AltConf
			Total	C	F	H	N	O	S		
3	A	1	75	28	2	30	6	8	1	0	0
3	B	1	75	28	2	30	6	8	1	0	0

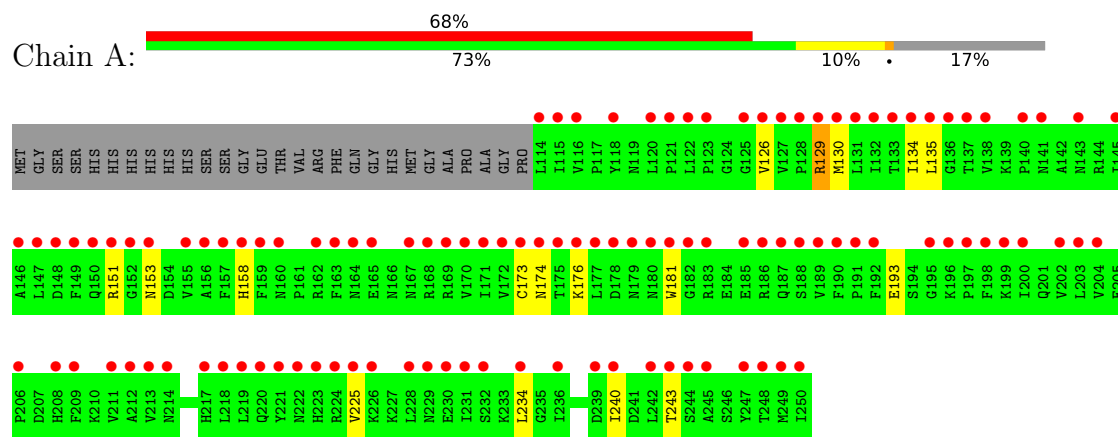
- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	49	Total	O	0	0
			49	49		
4	B	55	Total	O	0	0
			55	55		

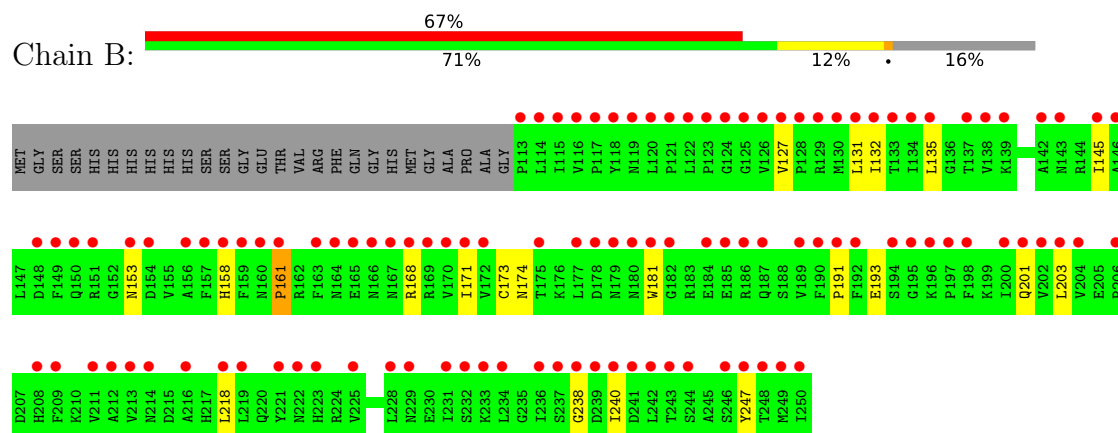
3 Residue-property plots

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: Galectin-3



• Molecule 1: Galectin-3



4 Data and refinement statistics

Property	Value	Source
Space group	P 31	Depositor
Cell constants a, b, c, α , β , γ	40.84Å 40.84Å 152.63Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	32.09 – 1.97 32.09 – 1.97	Depositor EDS
% Data completeness (in resolution range)	99.6 (32.09-1.97) 99.6 (32.09-1.97)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.90 (at 1.97Å)	Xtriage
Refinement program	REFMAC 5.8.0258	Depositor
R, R_{free}	0.202 , 0.235 0.202 , 0.236	Depositor DCC
R_{free} test set	1119 reflections (5.54%)	wwPDB-VP
Wilson B-factor (Å ²)	49.1	Xtriage
Anisotropy	0.483	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 50.0	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.097 for -h,-k,l 0.144 for h,-h-k,-l 0.360 for -k,-h,-l	Xtriage
Reported twinning fraction	0.035 for H, K, L 0.322 for K, H, -L 0.606 for -h,-k,l 0.038 for -K, -H, -L	Depositor
Outliers	0 of 20131 reflections	Xtriage
F_o, F_c correlation	0.74	EDS
Total number of atoms	2390	wwPDB-VP
Average B, all atoms (Å ²)	64.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.36% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: TD2, CL

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	0/1090	1.01	0/1483
1	B	0.62	0/1095	1.04	1/1491 (0.1%)
All	All	0.63	0/2185	1.03	1/2974 (0.0%)

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	161	PRO	CB-CA-C	-5.34	104.99	111.46

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts [i](#)

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	1065	0	1030	7	0
1	B	1069	0	1026	12	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	45	30	0	0	0
3	B	45	30	0	0	0
4	A	49	0	0	1	0
4	B	55	0	0	4	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
All	All	2330	60	2056	18	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 4.

All (18) 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:203:LEU:HB2	4:B:437:HOH:O	1.74	0.87
1:A:129:ARG:NH1	4:A:401:HOH:O	2.17	0.78
1:A:243:THR:HG23	1:B:193:GLU:HG3	1.87	0.56
1:B:171:ILE:HD13	1:B:218:LEU:HD21	1.87	0.56
1:B:168:ARG:NH1	4:B:401:HOH:O	2.40	0.54
1:A:151:ARG:HD2	1:A:225:VAL:HG11	1.93	0.51
1:B:132:ILE:HD13	1:B:247:TYR:HB2	1.92	0.51
1:B:131:LEU:HD12	4:B:437:HOH:O	2.13	0.48
1:B:171:ILE:CD1	1:B:218:LEU:HD21	2.44	0.48
1:A:174:ASN:ND2	1:A:181:TRP:HB3	2.29	0.47
1:B:174:ASN:ND2	1:B:181:TRP:HB3	2.29	0.47
1:A:126:VAL:HG12	1:A:130:MET:HE1	1.97	0.46
1:A:134:ILE:HD11	1:A:234:LEU:HD21	2.00	0.43
1:B:238:GLY:HA2	4:B:428:HOH:O	2.19	0.42
1:B:145:ILE:O	1:B:161:PRO:HD2	2.20	0.42
1:B:158:HIS:O	1:B:173:CYS:HA	2.20	0.42
1:A:158:HIS:O	1:A:173:CYS:HA	2.21	0.41
1:B:191:PRO:HG3	1:B:218:LEU:HD13	2.02	0.41

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	135/165 (82%)	132 (98%)	2 (2%)	1 (1%)	18	9
1	B	136/165 (82%)	133 (98%)	3 (2%)	0	100	100
All	All	271/330 (82%)	265 (98%)	5 (2%)	1 (0%)	30	20

All (1) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	129	ARG

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	111/144 (77%)	106 (96%)	5 (4%)	24	13
1	B	109/144 (76%)	104 (95%)	5 (5%)	24	12
All	All	220/288 (76%)	210 (96%)	10 (4%)	24	13

All (10) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	135	LEU
1	A	153	ASN
1	A	176	LYS
1	A	193	GLU
1	A	240	ILE
1	B	127	VAL
1	B	135	LEU
1	B	153	ASN
1	B	201	GLN
1	B	240	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (6) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	119	ASN
1	A	220	GLN
1	A	222	ASN
1	B	119	ASN
1	B	201	GLN
1	B	220	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 4 ligands modelled in this entry, 2 are 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	TD2	B	302	-	48,50,50	1.99	18 (37%)	60,73,73	1.47	8 (13%)
3	TD2	A	302	-	48,50,50	2.25	19 (39%)	60,73,73	1.33	4 (6%)

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	TD2	B	302	-	-	3/24/64/64	0/6/6/6
3	TD2	A	302	-	-	4/24/64/64	0/6/6/6

All (37) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	A	302	TD2	C71-N71	5.09	1.43	1.34
3	B	302	TD2	N7-N11	4.83	1.41	1.35
3	B	302	TD2	C8-N7	4.77	1.42	1.34
3	A	302	TD2	N71-N8	4.47	1.40	1.35
3	A	302	TD2	C8-N7	4.28	1.41	1.34
3	A	302	TD2	C41-C31	4.20	1.60	1.53
3	A	302	TD2	C4-C3	3.80	1.59	1.53
3	A	302	TD2	C10-N9	3.58	1.43	1.36
3	B	302	TD2	C4-C3	3.52	1.59	1.53
3	A	302	TD2	C15-C14	3.43	1.43	1.37
3	A	302	TD2	C27-C26	3.19	1.43	1.37
3	B	302	TD2	C4-C5	3.12	1.59	1.53
3	A	302	TD2	C23-C22	3.09	1.44	1.39
3	B	302	TD2	C21-C31	3.09	1.58	1.53
3	B	302	TD2	C12-C9	-3.08	1.43	1.47
3	B	302	TD2	C15-C14	3.03	1.43	1.37
3	B	302	TD2	C2-C3	2.88	1.58	1.53
3	B	302	TD2	N71-N8	2.80	1.38	1.35
3	A	302	TD2	C27-C22	2.78	1.43	1.39
3	B	302	TD2	C10-N9	2.77	1.42	1.36
3	A	302	TD2	C22-C10	-2.75	1.43	1.47
3	A	302	TD2	C25-C26	2.70	1.42	1.37
3	A	302	TD2	C1-S1	2.67	1.86	1.80
3	B	302	TD2	C8-C9	2.67	1.41	1.37
3	B	302	TD2	C41-C51	2.64	1.58	1.53
3	A	302	TD2	C2-C3	2.57	1.57	1.53
3	B	302	TD2	C25-C26	2.56	1.42	1.37
3	B	302	TD2	C71-C10	2.42	1.41	1.37
3	A	302	TD2	C71-C10	2.36	1.41	1.37
3	A	302	TD2	C4-C5	2.33	1.58	1.53
3	A	302	TD2	O4-C4	-2.13	1.37	1.43
3	B	302	TD2	C13-C12	2.11	1.42	1.39
3	A	302	TD2	C9-N10	2.07	1.40	1.36
3	A	302	TD2	N7-N11	2.05	1.37	1.35
3	B	302	TD2	O51-C11	-2.03	1.39	1.42
3	B	302	TD2	C11-S1	2.03	1.85	1.80
3	B	302	TD2	O41-C41	2.00	1.47	1.43

All (12) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	302	TD2	C51-C41-C31	-5.94	103.83	110.58
3	B	302	TD2	C51-C41-C31	-4.51	105.45	110.58
3	B	302	TD2	C5-C4-C3	-4.45	105.52	110.58
3	B	302	TD2	N71-N8-N9	2.73	109.39	107.09
3	B	302	TD2	O5-C1-C2	-2.66	106.64	110.32
3	A	302	TD2	C9-N10-N11	2.65	112.08	109.23
3	A	302	TD2	O5-C5-C6	-2.57	100.07	106.44
3	A	302	TD2	O4-C4-C3	-2.51	102.64	109.14
3	B	302	TD2	O6-C6-C5	-2.49	102.87	111.33
3	B	302	TD2	C1-O5-C5	-2.44	108.19	112.56
3	B	302	TD2	C8-N7-N11	-2.36	108.41	110.63
3	B	302	TD2	C9-N10-N11	2.00	111.38	109.23

There are no chirality outliers.

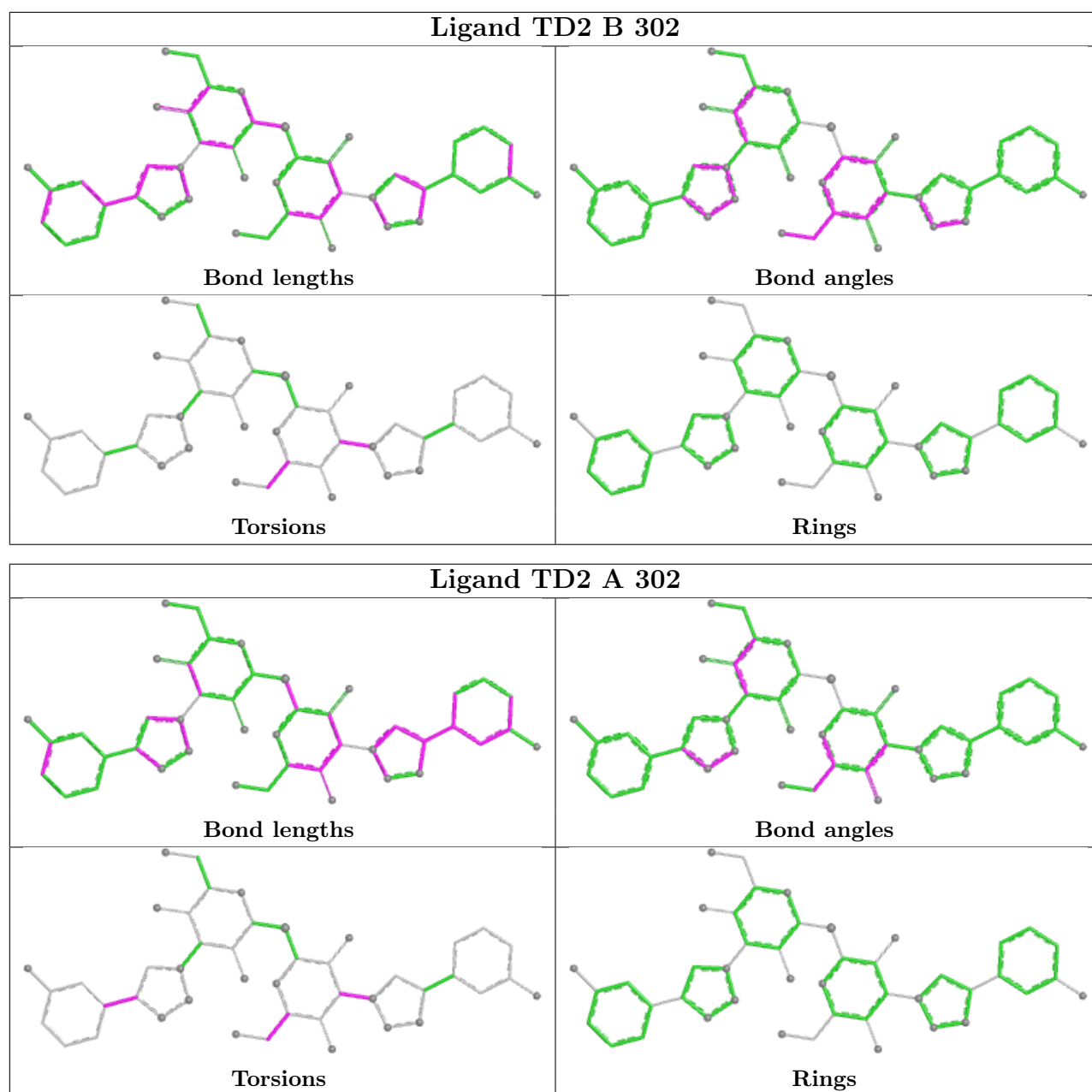
All (7) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	302	TD2	O5-C5-C6-O6
3	A	302	TD2	O5-C5-C6-O6
3	A	302	TD2	C2-C3-N71-N8
3	B	302	TD2	C2-C3-N71-N8
3	A	302	TD2	C2-C3-N71-C71
3	B	302	TD2	C2-C3-N71-C71
3	A	302	TD2	C13-C12-C9-N10

There are no ring outliers.

No monomer is involved in short contacts.

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	137/165 (83%)	3.12	112 (81%) 0 0	17, 63, 88, 107	2 (1%)
1	B	138/165 (83%)	3.12	111 (80%) 0 0	26, 63, 82, 96	1 (0%)
All	All	275/330 (83%)	3.12	223 (81%) 0 0	17, 63, 85, 107	3 (1%)

All (223) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	181	TRP	8.7
1	B	204	VAL	8.5
1	A	225	VAL	6.9
1	A	171	ILE	6.8
1	A	130	MET	6.6
1	B	236	ILE	6.2
1	B	171	ILE	6.1
1	A	134	ILE	6.1
1	B	116	VAL	6.1
1	A	175	THR	6.0
1	A	122	LEU	5.8
1	B	175	THR	5.8
1	B	221	TYR	5.7
1	B	243	THR	5.6
1	B	237	SER	5.4
1	A	131	LEU	5.4
1	A	219	LEU	5.4
1	B	134	ILE	5.3
1	B	166	ASN	5.2
1	B	117	PRO	5.2
1	B	203	LEU	5.2
1	B	250	ILE	5.2
1	B	159	PHE	5.0
1	A	189	VAL	5.0

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Mol	Chain	Res	Type	RSRZ
1	A	250	ILE	5.0
1	B	122	LEU	5.0
1	B	120	LEU	4.8
1	A	211	VAL	4.8
1	A	157	PHE	4.8
1	A	143	ASN	4.8
1	B	135	LEU	4.7
1	A	138	VAL	4.7
1	B	202	VAL	4.6
1	A	245	ALA	4.5
1	A	232	SER	4.4
1	B	131	LEU	4.4
1	A	247	TYR	4.3
1	B	213	VAL	4.3
1	A	229	ASN	4.3
1	B	127	VAL	4.2
1	B	145	ILE	4.2
1	A	116	VAL	4.2
1	A	208	HIS	4.2
1	A	159	PHE	4.2
1	B	198	PHE	4.2
1	A	172	VAL	4.2
1	A	244	SER	4.2
1	A	221	TYR	4.2
1	A	242	LEU	4.2
1	A	163	PHE	4.1
1	B	240	ILE	4.1
1	B	194	SER	4.1
1	A	182	GLY	4.1
1	A	199	LYS	4.1
1	A	145	ILE	4.0
1	B	123	PRO	4.0
1	B	191	PRO	4.0
1	B	118	TYR	4.0
1	B	185	GLU	4.0
1	A	114	LEU	4.0
1	B	197	PRO	4.0
1	B	124	GLY	4.0
1	B	143	ASN	4.0
1	B	189	VAL	4.0
1	A	140	PRO	3.9
1	A	212	ALA	3.9

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Mol	Chain	Res	Type	RSRZ
1	B	232	SER	3.9
1	A	206	PRO	3.9
1	A	146	ALA	3.9
1	B	137	THR	3.9
1	A	170	VAL	3.9
1	A	231	ILE	3.9
1	B	115	ILE	3.8
1	B	121	PRO	3.7
1	A	222	ASN	3.7
1	B	157	PHE	3.7
1	A	147	LEU	3.7
1	B	242	LEU	3.7
1	A	213	VAL	3.7
1	A	127	VAL	3.6
1	B	247	TYR	3.6
1	A	135	LEU	3.6
1	B	156	ALA	3.5
1	B	181	TRP	3.5
1	B	133	THR	3.5
1	B	119	ASN	3.5
1	B	154	ASP	3.5
1	A	218	LEU	3.5
1	A	132	ILE	3.4
1	B	138	VAL	3.4
1	B	229	ASN	3.4
1	A	118	TYR	3.4
1	A	155	VAL	3.4
1	A	123	PRO	3.4
1	A	243	THR	3.4
1	A	217	HIS	3.4
1	A	148	ASP	3.3
1	B	212	ALA	3.3
1	B	214	ASN	3.3
1	B	234	LEU	3.3
1	B	178	ASP	3.3
1	B	132	ILE	3.3
1	B	146	ALA	3.3
1	A	248	THR	3.3
1	B	148	ASP	3.2
1	B	239	ASP	3.2
1	A	169	ARG	3.2
1	B	195	GLY	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	115	ILE	3.2
1	A	137	THR	3.2
1	A	196	LYS	3.2
1	B	209	PHE	3.2
1	B	216	ALA	3.2
1	A	128	PRO	3.2
1	A	153	ASN	3.2
1	B	153	ASN	3.2
1	A	177	LEU	3.2
1	A	195	GLY	3.1
1	B	160	ASN	3.1
1	A	133	THR	3.1
1	A	126	VAL	3.1
1	B	177	LEU	3.1
1	B	241	ASP	3.1
1	B	128	PRO	3.1
1	B	161	PRO	3.1
1	A	239	ASP	3.1
1	B	130	MET	3.1
1	B	244	SER	3.1
1	A	156	ALA	3.1
1	B	180	ASN	3.0
1	B	246	SER	3.0
1	B	248	THR	3.0
1	B	179	ASN	3.0
1	B	219	LEU	3.0
1	B	249	MET	3.0
1	B	228	LEU	2.9
1	B	233	LYS	2.9
1	A	198	PHE	2.9
1	A	249	MET	2.9
1	A	174	ASN	2.9
1	A	179	ASN	2.9
1	A	223	HIS	2.9
1	B	196	LYS	2.9
1	A	186	ARG	2.9
1	B	211	VAL	2.9
1	A	180	ASN	2.9
1	B	150	GLN	2.9
1	B	139	LYS	2.9
1	B	114	LEU	2.9
1	B	184	GLU	2.9

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Mol	Chain	Res	Type	RSRZ
1	A	228	LEU	2.9
1	B	218	LEU	2.9
1	B	172	VAL	2.8
1	B	163	PHE	2.8
1	B	167	ASN	2.8
1	B	208	HIS	2.8
1	A	226	LYS	2.8
1	A	185	GLU	2.8
1	A	160	ASN	2.8
1	B	187	GLN	2.8
1	B	170	VAL	2.8
1	A	190	PHE	2.7
1	A	152	GLY	2.7
1	A	203	LEU	2.7
1	A	167	ASN	2.7
1	A	192	PHE	2.7
1	B	200	ILE	2.7
1	B	168	ARG	2.7
1	A	125	GLY	2.7
1	B	169	ARG	2.6
1	B	164	ASN	2.6
1	A	202	VAL	2.6
1	A	168	ARG	2.6
1	A	141	ASN	2.6
1	B	192	PHE	2.6
1	B	186	ARG	2.6
1	A	178	ASP	2.6
1	B	206	PRO	2.6
1	A	129	ARG	2.6
1	B	129	ARG	2.6
1	A	149	PHE	2.5
1	B	231	ILE	2.5
1	A	162	ARG	2.5
1	A	224	ARG	2.5
1	A	187	GLN	2.5
1	A	176	LYS	2.5
1	A	164	ASN	2.5
1	B	165	GLU	2.5
1	A	236	ILE	2.4
1	B	201	GLN	2.4
1	B	223	HIS	2.4
1	B	225	VAL	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	220	GLN	2.4
1	B	149	PHE	2.4
1	B	142	ALA	2.4
1	A	209	PHE	2.3
1	B	158	HIS	2.3
1	B	222	ASN	2.3
1	A	136	GLY	2.3
1	B	125	GLY	2.3
1	A	234	LEU	2.3
1	A	240	ILE	2.2
1	A	150	GLN	2.2
1	A	173	CYS	2.2
1	A	121	PRO	2.2
1	A	191	PRO	2.2
1	B	113	PRO	2.2
1	B	190	PHE	2.2
1	A	200	ILE	2.2
1	A	214	ASN	2.2
1	A	183	ARG	2.2
1	A	230	GLU	2.2
1	A	188	SER	2.2
1	A	120	LEU	2.2
1	A	158	HIS	2.1
1	B	126	VAL	2.1
1	A	151	ARG	2.1
1	A	197	PRO	2.1
1	A	204	VAL	2.1
1	A	165	GLU	2.0
1	B	151	ARG	2.0
1	B	182	GLY	2.0
1	B	238	GLY	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](#)

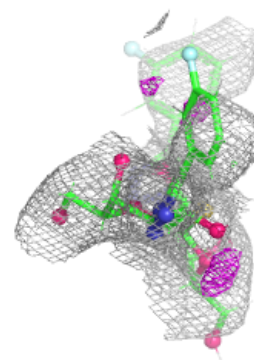
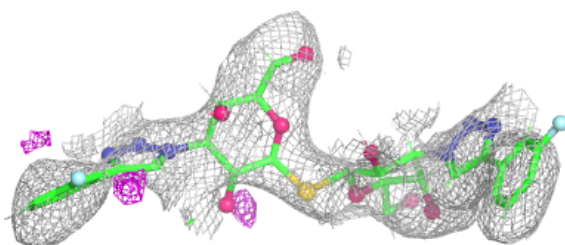
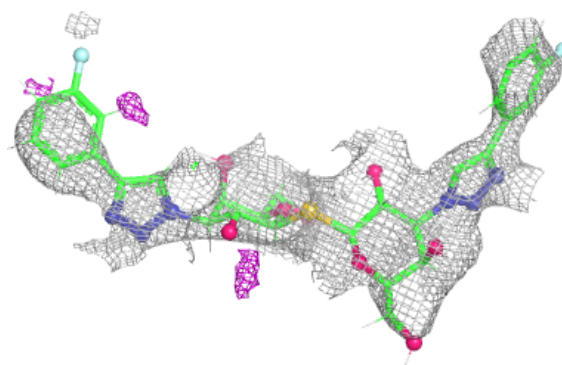
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists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

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å ²)	Q<0.9
3	TD2	A	302	45/45	0.60	0.17	52,65,78,101	0
2	CL	B	301	1/1	0.61	0.18	90,90,90,90	0
3	TD2	B	302	45/45	0.61	0.15	48,62,74,78	0
2	CL	A	301	1/1	0.75	0.14	71,71,71,71	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.

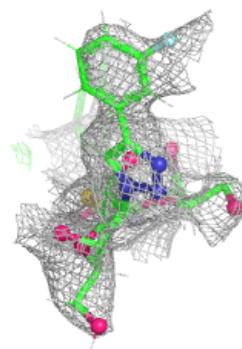
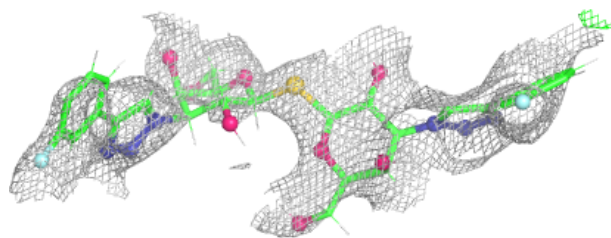
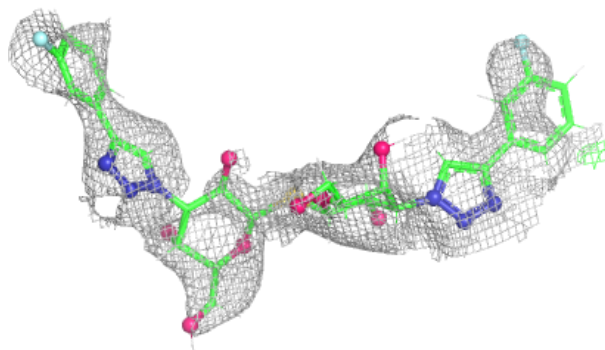
Electron density around TD2 A 302:

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 TD2 B 302:

$2mF_o-DF_c$ (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.