



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:16 PM UTC

PDB ID : 3C10 / pdb_00003c10
Title : Crystal structure of catalytic domain of human histone deacetylase HDAC7 in complex with Trichostatin A (TSA)
Authors : Min, J.; Schuetz, A.; Loppnau, P.; Weigelt, J.; Sundstrom, M.; Arrowsmith, C.H.; Edwards, A.M.; Bochkarev, A.; Plotnikov, A.N.; Structural Genomics Consortium (SGC)
Deposited on : 2008-01-21
Resolution : 2.00 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](#) ①) 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

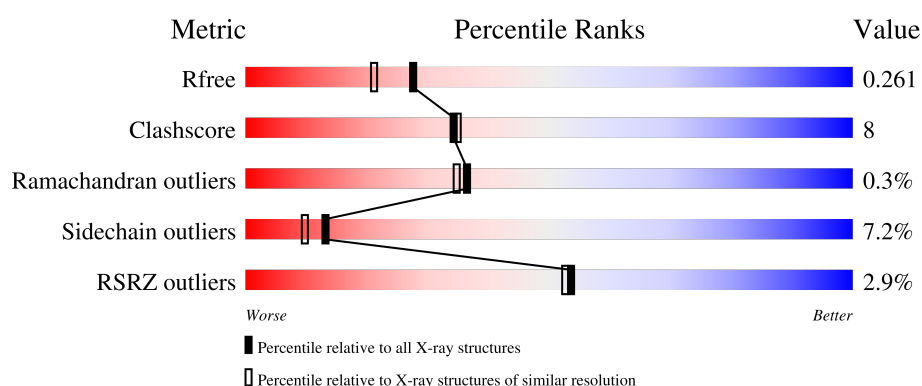
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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	10052 (2.00-2.00)
Clashscore	190562	11152 (2.00-2.00)
Ramachandran outliers	187476	11031 (2.00-2.00)
Sidechain outliers	187428	11029 (2.00-2.00)
RSRZ outliers	180081	10067 (2.00-2.00)

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	423	3% 74% 14% • 9%
1	B	423	3% 66% 19% • 13%
1	C	423	% 67% 15% • 15%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 8961 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 Histone deacetylase 7a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	383	Total	C	N	O	S	0	0	0
			2902	1819	524	540	19			
1	B	368	Total	C	N	O	S	0	0	0
			2794	1751	506	518	19			
1	C	359	Total	C	N	O	S	0	0	0
			2728	1706	494	510	18			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	481	GLY	-	expression tag	UNP Q8WUI4
B	481	GLY	-	expression tag	UNP Q8WUI4
C	481	GLY	-	expression tag	UNP Q8WUI4

- Molecule 2 is ZINC ION (CCD ID: ZN) (formula: Zn).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Zn	0	0
			2	2		
2	B	2	Total	Zn	0	0
			2	2		
2	C	2	Total	Zn	0	0
			2	2		

- Molecule 3 is POTASSIUM ION (CCD ID: K) (formula: K).

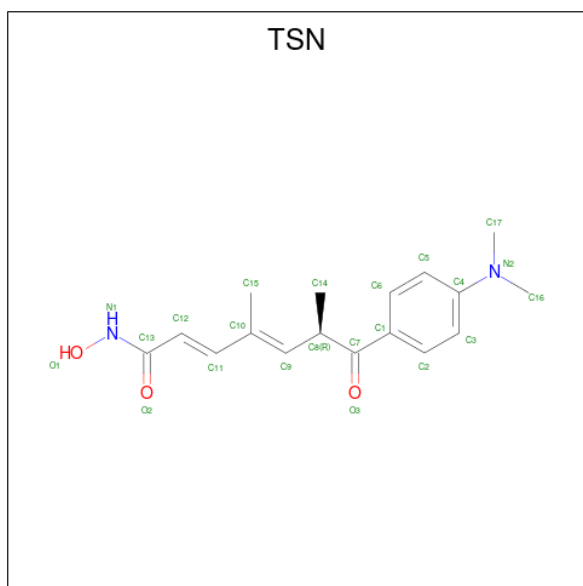
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	2	Total	K	0	0
			2	2		
3	B	2	Total	K	0	0
			2	2		

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Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
3	C	2	Total K 2 2	0	0

- Molecule 4 is TRICHOSTATIN A (CCD ID: TSN) (formula: $C_{17}H_{22}N_2O_3$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C N O 22 17 2 3	0	0
4	B	1	Total C N O 22 17 2 3	0	0
4	C	1	Total C N O 22 17 2 3	0	0

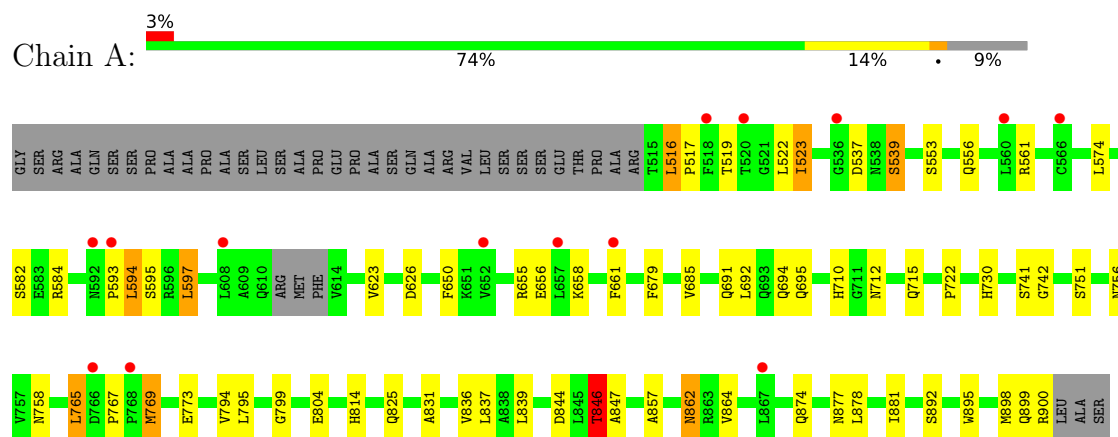
- Molecule 5 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	170	Total O 170 170	0	0
5	B	159	Total O 159 159	0	0
5	C	130	Total O 130 130	0	0

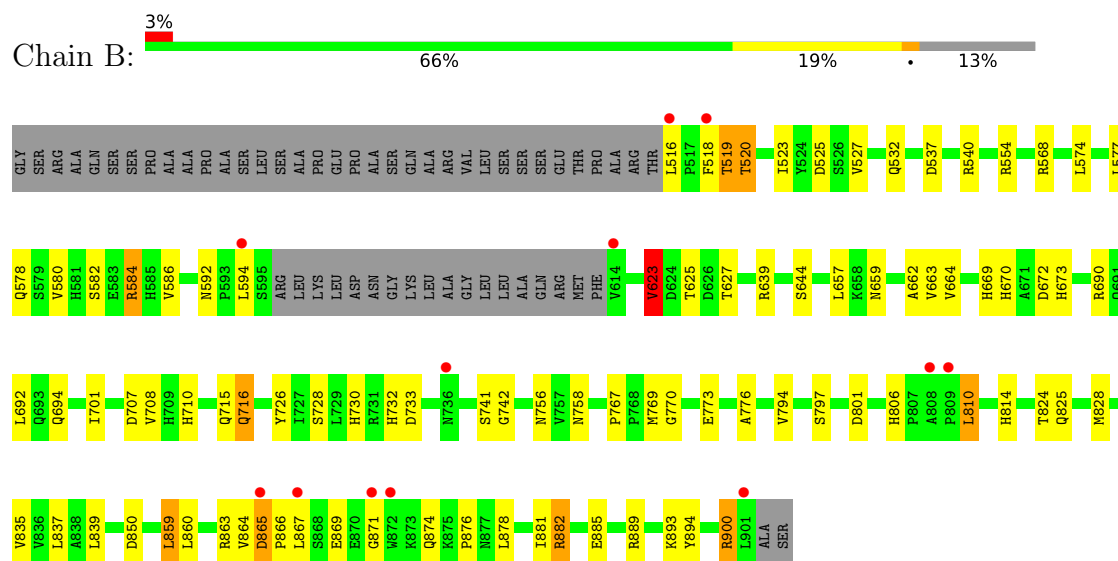
3 Residue-property plots [i](#)

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: Histone deacetylase 7a



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4 Data and refinement statistics

Property	Value	Source
Space group	P 32	Depositor
Cell constants a, b, c, α , β , γ	81.83Å 81.83Å 148.97Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	35.42 – 2.00 35.42 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.5 (35.42-2.00) 97.5 (35.42-2.00)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.10 (at 2.00Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.201 , 0.263 0.199 , 0.261	Depositor DCC
R_{free} test set	3651 reflections (4.85%)	wwPDB-VP
Wilson B-factor (Å ²)	34.8	Xtriage
Anisotropy	0.013	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.34 , 39.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	0.006 for -h,-k,l 0.035 for h,-h-k,-l 0.019 for -k,-h,-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	8961	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.00% 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: TSN, K, ZN

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	1.07	5/2970 (0.2%)	1.09	3/4029 (0.1%)
1	B	1.07	5/2862 (0.2%)	1.16	13/3883 (0.3%)
1	C	0.91	0/2794	1.05	5/3791 (0.1%)
All	All	1.02	10/8626 (0.1%)	1.10	21/11703 (0.2%)

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	C	0	1

All (10) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	663	VAL	CA-CB	7.53	1.64	1.53
1	A	846	THR	CA-CB	6.81	1.64	1.53
1	A	794	VAL	C-O	-5.84	1.17	1.24
1	B	580	VAL	CA-CB	5.78	1.62	1.54
1	A	685	VAL	CA-CB	5.64	1.60	1.54
1	A	831	ALA	CA-CB	5.64	1.62	1.53
1	B	776	ALA	CA-CB	-5.41	1.44	1.53
1	A	712	ASN	C-O	-5.36	1.18	1.24
1	B	664	VAL	CA-CB	5.13	1.61	1.54
1	B	662	ALA	CA-CB	5.12	1.60	1.53

All (21) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	809	PRO	N-CA-C	-8.86	99.69	114.75
1	B	806	HIS	CA-C-N	-6.30	113.79	120.03
1	B	806	HIS	C-N-CA	-6.30	113.79	120.03
1	B	865	ASP	CA-C-N	-6.28	113.82	120.03
1	B	865	ASP	C-N-CA	-6.28	113.82	120.03
1	C	806	HIS	CA-C-N	6.24	126.20	120.03
1	C	806	HIS	C-N-CA	6.24	126.20	120.03
1	B	707	ASP	N-CA-C	-6.17	101.81	110.50
1	B	537	ASP	N-CA-C	6.10	118.23	108.41
1	A	799	GLY	N-CA-C	-6.00	104.55	112.82
1	B	669	HIS	N-CA-C	5.96	119.81	112.54
1	B	623	VAL	N-CA-C	-5.86	105.37	111.58
1	B	801	ASP	N-CA-C	5.55	119.79	113.19
1	B	519	THR	CB-CA-C	-5.44	100.84	114.11
1	B	540	ARG	N-CA-C	-5.34	106.93	113.50
1	A	516	LEU	CA-C-N	5.28	125.74	120.14
1	A	516	LEU	C-N-CA	5.28	125.74	120.14
1	C	865	ASP	CA-C-N	5.10	124.71	119.56
1	C	865	ASP	C-N-CA	5.10	124.71	119.56
1	B	767	PRO	CA-C-N	5.01	125.24	119.83
1	B	767	PRO	C-N-CA	5.01	125.24	119.83

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	C	808	ALA	Peptide

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	2902	0	2803	38	0
1	B	2794	0	2688	45	0
1	C	2728	0	2617	43	0
2	A	2	0	0	0	0
2	B	2	0	0	0	0
2	C	2	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
3	A	2	0	0	0	0
3	B	2	0	0	0	0
3	C	2	0	0	1	0
4	A	22	0	21	0	0
4	B	22	0	21	2	0
4	C	22	0	21	1	0
5	A	170	0	0	4	0
5	B	159	0	0	7	0
5	C	130	0	0	2	0
All	All	8961	0	8171	126	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 8.

All (126) 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:769:MET:HE1	5:B:1023:HOH:O	1.68	0.94
1:B:672:ASP:HB2	1:B:716:GLN:NE2	1.83	0.92
1:B:825:GLN:HE22	1:B:864:VAL:H	1.19	0.90
1:B:672:ASP:HB2	1:B:716:GLN:HE21	1.33	0.89
1:C:807:PRO:O	1:C:808:ALA:C	2.21	0.83
1:C:833:GLY:O	5:C:938:HOH:O	1.95	0.83
1:C:892:SER:O	1:C:899:GLN:HG3	1.79	0.82
1:A:519:THR:O	1:A:658:LYS:N	2.16	0.76
1:B:733:ASP:OD1	5:B:1035:HOH:O	2.04	0.76
1:B:670:HIS:HE2	4:B:301:TSN:HN1	1.33	0.76
1:A:804:GLU:OE1	1:A:814:HIS:HD2	1.69	0.76
1:C:592:ASN:HB2	1:C:593:PRO:HA	1.68	0.75
1:B:520:THR:HB	1:B:659:ASN:OD1	1.88	0.73
1:C:715:GLN:HE22	1:C:758:ASN:HD21	1.33	0.73
1:B:673:HIS:H	1:B:716:GLN:HE22	1.36	0.71
1:A:825:GLN:HE22	1:A:864:VAL:H	1.38	0.70
1:B:525:ASP:OD2	1:B:527:VAL:HG23	1.92	0.70
1:B:769:MET:CE	5:B:1023:HOH:O	2.29	0.69
1:B:554:ARG:NH2	1:B:850:ASP:OD1	2.23	0.69
1:A:715:GLN:HE22	1:A:758:ASN:HD21	1.43	0.67
1:B:825:GLN:NE2	1:B:864:VAL:H	1.92	0.67
1:C:654:SER:O	1:C:655:ARG:HB2	1.94	0.66
1:C:888:ILE:HA	1:C:898:MET:HE3	1.80	0.63
1:A:722:PRO:HD3	1:A:751:SER:HB3	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:900:ARG:NE	5:A:270:HOH:O	2.32	0.62
1:C:825:GLN:HE22	1:C:864:VAL:H	1.49	0.60
3:C:202:K:K	5:C:906:HOH:O	2.11	0.60
1:A:710:HIS:HD2	1:A:741:SER:OG	1.85	0.59
1:B:876:PRO:HG2	1:B:881:ILE:HD11	1.83	0.59
1:C:580:VAL:O	1:C:673:HIS:HD2	1.85	0.59
1:A:825:GLN:NE2	1:A:864:VAL:H	2.01	0.59
1:B:715:GLN:HE22	1:B:758:ASN:HD21	1.48	0.58
1:A:556:GLN:HB2	1:A:561:ARG:CZ	2.34	0.58
1:B:584:ARG:HD3	1:B:584:ARG:H	1.68	0.57
1:C:710:HIS:HD2	1:C:741:SER:OG	1.87	0.57
1:C:623:VAL:HG22	1:C:627:THR:HB	1.86	0.57
1:C:825:GLN:NE2	1:C:864:VAL:H	2.02	0.57
1:A:804:GLU:OE1	1:A:814:HIS:CD2	2.55	0.57
1:C:810:LEU:HG	4:C:301:TSN:H21	1.88	0.56
1:A:650:PHE:HE1	1:A:691:GLN:HB3	1.71	0.56
1:A:517:PRO:HG2	1:C:587:LEU:HD11	1.87	0.56
1:C:616:LEU:HB2	1:C:620:GLY:O	2.06	0.55
1:A:857:ALA:O	1:A:862:ASN:HB3	2.07	0.54
1:A:523:ILE:HG22	1:A:523:ILE:O	2.07	0.54
1:C:715:GLN:NE2	1:C:758:ASN:HD21	2.05	0.54
1:A:626:ASP:HB3	1:A:679:PHE:CE1	2.43	0.54
1:B:810:LEU:HD12	5:B:1038:HOH:O	2.07	0.53
1:C:689:CYS:O	1:C:693:GLN:HG3	2.09	0.53
1:C:795:LEU:HD23	1:C:836:VAL:HB	1.91	0.52
1:A:650:PHE:CE1	1:A:691:GLN:HB3	2.46	0.51
1:B:670:HIS:CD2	4:B:301:TSN:HN1	2.29	0.51
1:C:540:ARG:HE	1:C:618:CYS:HB3	1.76	0.50
1:C:523:ILE:HG13	1:C:648:LEU:HD22	1.92	0.50
1:C:592:ASN:CB	1:C:593:PRO:HA	2.38	0.50
1:B:582:SER:HB3	1:B:673:HIS:CE1	2.48	0.49
1:C:712:ASN:HD22	1:C:712:ASN:H	1.58	0.49
1:B:715:GLN:NE2	1:B:758:ASN:HD21	2.08	0.49
1:C:796:VAL:HB	1:C:837:LEU:HD22	1.94	0.49
1:B:710:HIS:HD2	1:B:741:SER:OG	1.95	0.48
1:B:520:THR:HG23	1:B:860:LEU:HD23	1.94	0.48
1:A:844:ASP:HB3	1:A:847:ALA:HB3	1.94	0.48
1:B:523:ILE:HG21	1:B:644:SER:HB3	1.95	0.48
1:B:885:GLU:CD	1:B:900:ARG:HH22	2.22	0.48
1:B:690:ARG:O	1:B:694:GLN:HG3	2.13	0.48
1:B:824:THR:O	1:B:828:MET:HG3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:650:PHE:HE2	1:A:695:GLN:HG2	1.79	0.47
1:B:710:HIS:CE1	1:B:715:GLN:NE2	2.83	0.47
1:C:525:ASP:OD2	1:C:527:VAL:HG23	2.15	0.47
1:B:578:GLN:HG3	1:B:586:VAL:HG21	1.97	0.47
1:C:766:ASP:HA	1:C:767:PRO:C	2.39	0.47
1:C:649:ALA:HA	1:C:836:VAL:HG21	1.96	0.47
1:B:871:GLY:HA2	1:B:874:GLN:HG2	1.96	0.46
1:C:726:TYR:CZ	1:C:728:SER:HB2	2.49	0.46
1:C:655:ARG:N	1:C:655:ARG:HD3	2.31	0.46
1:C:769:MET:HB2	1:C:813:TYR:CD2	2.51	0.46
1:C:892:SER:O	1:C:899:GLN:CG	2.58	0.46
1:A:595:SER:HB3	1:A:597:LEU:HB2	1.97	0.46
1:A:522:LEU:HD23	1:A:661:PHE:HB3	1.98	0.46
1:C:556:GLN:HB2	1:C:561:ARG:NH1	2.30	0.46
1:B:794:VAL:HB	1:B:835:VAL:HG22	1.98	0.46
1:C:658:LYS:HD3	1:C:659:ASN:ND2	2.31	0.46
1:A:556:GLN:HB2	1:A:561:ARG:NE	2.30	0.45
1:A:795:LEU:HD23	1:A:836:VAL:HB	1.98	0.45
1:A:846:THR:HG23	5:A:468:HOH:O	2.16	0.45
1:C:592:ASN:CB	1:C:593:PRO:CA	2.94	0.45
1:A:553:SER:HA	1:A:561:ARG:HH11	1.82	0.45
1:B:863:ARG:HD2	5:B:1060:HOH:O	2.16	0.45
1:B:867:LEU:C	1:B:869:GLU:H	2.23	0.45
1:C:626:ASP:HB3	1:C:679:PHE:CE1	2.52	0.45
1:A:730:HIS:HE1	1:A:742:GLY:O	2.01	0.44
1:A:895:TRP:O	1:A:899:GLN:HG3	2.17	0.44
1:A:769:MET:SD	1:A:773:GLU:HG2	2.58	0.44
1:C:586:VAL:O	1:C:590:GLY:HA3	2.16	0.44
1:A:892:SER:O	1:A:899:GLN:HG2	2.17	0.44
1:C:738:PHE:HA	1:C:739:PRO:HA	1.76	0.44
1:A:862:ASN:OD1	1:A:862:ASN:C	2.61	0.44
1:C:678:GLY:O	1:C:679:PHE:HB2	2.18	0.44
1:C:822:TYR:O	1:C:826:GLN:HG3	2.18	0.44
1:C:710:HIS:CE1	1:C:715:GLN:NE2	2.86	0.43
1:B:866:PRO:O	1:B:867:LEU:CB	2.67	0.43
1:A:582:SER:OG	1:A:584:ARG:HD3	2.19	0.43
1:A:900:ARG:NH2	5:A:270:HOH:O	2.50	0.43
1:B:623:VAL:HG22	1:B:627:THR:HB	2.01	0.43
1:B:728:SER:OG	1:B:730:HIS:HD2	2.01	0.43
1:A:593:PRO:HA	1:A:594:LEU:HA	1.72	0.43
1:B:577:LEU:HD11	1:B:639:ARG:HG2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:726:TYR:HD2	1:B:756:ASN:ND2	2.17	0.42
1:B:592:ASN:HD22	1:B:594:LEU:H	1.66	0.42
1:B:732:HIS:O	1:B:733:ASP:C	2.62	0.42
1:C:767:PRO:HG2	1:C:877:ASN:HB2	2.01	0.42
1:A:756:ASN:ND2	5:A:34:HOH:O	2.44	0.42
1:B:814:HIS:CD2	5:B:971:HOH:O	2.72	0.42
1:B:824:THR:CG2	1:B:859:LEU:HD13	2.49	0.42
1:A:877:ASN:O	1:A:881:ILE:HG13	2.19	0.42
1:B:730:HIS:HE1	1:B:742:GLY:O	2.02	0.42
1:A:898:MET:HA	1:A:898:MET:HE2	2.02	0.42
1:A:710:HIS:CE1	1:A:715:GLN:NE2	2.88	0.42
1:B:878:LEU:O	1:B:882:ARG:HG2	2.20	0.41
1:A:537:ASP:OD1	1:A:539:SER:HB3	2.20	0.41
1:C:824:THR:CG2	1:C:859:LEU:HD13	2.50	0.41
1:A:765:LEU:O	1:A:767:PRO:O	2.37	0.41
1:B:893:LYS:HD3	1:B:894:TYR:CZ	2.56	0.41
1:B:769:MET:SD	1:B:773:GLU:HG2	2.60	0.41
1:C:697:LYS:HD2	1:C:697:LYS:HA	1.81	0.41
1:C:822:TYR:HD1	1:C:864:VAL:HB	1.86	0.41
1:B:770:GLY:HA3	5:B:1015:HOH:O	2.21	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	379/423 (90%)	365 (96%)	14 (4%)	0	100	100
1	B	364/423 (86%)	351 (96%)	12 (3%)	1 (0%)	36	35
1	C	355/423 (84%)	339 (96%)	14 (4%)	2 (1%)	21	17
All	All	1098/1269 (86%)	1055 (96%)	40 (4%)	3 (0%)	36	35

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	808	ALA
1	C	592	ASN
1	B	518	PHE

5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	304/336 (90%)	285 (94%)	19 (6%)	16	13
1	B	293/336 (87%)	270 (92%)	23 (8%)	11	8
1	C	286/336 (85%)	264 (92%)	22 (8%)	12	8
All	All	883/1008 (88%)	819 (93%)	64 (7%)	13	10

All (64) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	516	LEU
1	A	523	ILE
1	A	539	SER
1	A	574	LEU
1	A	594	LEU
1	A	597	LEU
1	A	623	VAL
1	A	655	ARG
1	A	656	GLU
1	A	692	LEU
1	A	694	GLN
1	A	765	LEU
1	A	769	MET
1	A	837	LEU
1	A	839	LEU
1	A	846	THR
1	A	862	ASN
1	A	874	GLN

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Mol	Chain	Res	Type
1	A	878	LEU
1	B	516	LEU
1	B	519	THR
1	B	520	THR
1	B	532	GLN
1	B	568	ARG
1	B	574	LEU
1	B	584	ARG
1	B	623	VAL
1	B	625	THR
1	B	657	LEU
1	B	692	LEU
1	B	701	ILE
1	B	708	VAL
1	B	716	GLN
1	B	797	SER
1	B	810	LEU
1	B	837	LEU
1	B	839	LEU
1	B	859	LEU
1	B	865	ASP
1	B	882	ARG
1	B	889	ARG
1	B	900	ARG
1	C	523	ILE
1	C	534	SER
1	C	554	ARG
1	C	574	LEU
1	C	616	LEU
1	C	623	VAL
1	C	627	THR
1	C	628	ILE
1	C	655	ARG
1	C	657	LEU
1	C	674	SER
1	C	692	LEU
1	C	694	GLN
1	C	697	LYS
1	C	712	ASN
1	C	765	LEU
1	C	810	LEU
1	C	837	LEU

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Mol	Chain	Res	Type
1	C	839	LEU
1	C	859	LEU
1	C	878	LEU
1	C	899	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (44) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	532	GLN
1	A	578	GLN
1	A	636	ASN
1	A	673	HIS
1	A	710	HIS
1	A	712	ASN
1	A	715	GLN
1	A	716	GLN
1	A	730	HIS
1	A	736	ASN
1	A	756	ASN
1	A	814	HIS
1	A	825	GLN
1	A	879	ASN
1	B	532	GLN
1	B	578	GLN
1	B	592	ASN
1	B	673	HIS
1	B	710	HIS
1	B	712	ASN
1	B	715	GLN
1	B	716	GLN
1	B	730	HIS
1	B	732	HIS
1	B	756	ASN
1	B	825	GLN
1	B	826	GLN
1	B	879	ASN
1	B	899	GLN
1	C	592	ASN
1	C	673	HIS
1	C	693	GLN
1	C	710	HIS
1	C	712	ASN

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Mol	Chain	Res	Type
1	C	715	GLN
1	C	716	GLN
1	C	730	HIS
1	C	736	ASN
1	C	756	ASN
1	C	825	GLN
1	C	826	GLN
1	C	874	GLN
1	C	891	HIS
1	C	899	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 15 ligands modelled in this entry, 12 are monoatomic - leaving 3 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	$\# Z > 2$
4	TSN	C	301	2	21,22,22	0.99	2 (9%)	27,29,29	1.28	5 (18%)
4	TSN	B	301	2	21,22,22	0.92	1 (4%)	27,29,29	1.75	4 (14%)
4	TSN	A	301	2	21,22,22	1.01	0	27,29,29	1.48	6 (22%)

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	TSN	C	301	2	-	10/23/23/23	0/1/1/1
4	TSN	B	301	2	-	9/23/23/23	0/1/1/1
4	TSN	A	301	2	-	9/23/23/23	0/1/1/1

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	301	TSN	C8-C7	-2.99	1.49	1.53
4	B	301	TSN	C1-C7	2.34	1.52	1.49
4	C	301	TSN	C4-N2	2.16	1.42	1.37

All (15) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	B	301	TSN	C1-C7-C8	6.50	125.13	119.27
4	A	301	TSN	C12-C13-N1	3.72	120.97	114.41
4	A	301	TSN	C1-C7-C8	3.63	122.55	119.27
4	B	301	TSN	O3-C7-C1	-3.28	116.62	120.70
4	C	301	TSN	C14-C8-C9	2.88	113.49	110.73
4	B	301	TSN	C14-C8-C9	-2.72	108.13	110.73
4	C	301	TSN	O2-C13-C12	-2.33	117.57	122.95
4	C	301	TSN	C12-C11-C10	-2.31	122.82	126.23
4	C	301	TSN	C12-C13-N1	2.30	118.47	114.41
4	A	301	TSN	O3-C7-C8	-2.29	117.69	119.81
4	A	301	TSN	C14-C8-C9	2.25	112.89	110.73
4	B	301	TSN	C12-C11-C10	-2.23	122.94	126.23
4	A	301	TSN	O2-C13-N1	-2.16	119.10	122.87
4	A	301	TSN	C15-C10-C11	2.12	121.33	118.09
4	C	301	TSN	C15-C10-C11	2.04	121.21	118.09

There are no chirality outliers.

All (28) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
4	A	301	TSN	O2-C13-N1-O1
4	A	301	TSN	C12-C13-N1-O1
4	C	301	TSN	O2-C13-N1-O1

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Mol	Chain	Res	Type	Atoms
4	C	301	TSN	C12-C13-N1-O1
4	C	301	TSN	C9-C10-C11-C12
4	A	301	TSN	C5-C4-N2-C17
4	A	301	TSN	C3-C4-N2-C16
4	A	301	TSN	C3-C4-N2-C17
4	A	301	TSN	C5-C4-N2-C16
4	B	301	TSN	C5-C4-N2-C17
4	B	301	TSN	C3-C4-N2-C16
4	B	301	TSN	C5-C4-N2-C16
4	B	301	TSN	C3-C4-N2-C17
4	C	301	TSN	C15-C10-C11-C12
4	B	301	TSN	C11-C12-C13-O2
4	C	301	TSN	C2-C1-C7-O3
4	C	301	TSN	C6-C1-C7-O3
4	C	301	TSN	C2-C1-C7-C8
4	C	301	TSN	C6-C1-C7-C8
4	B	301	TSN	C11-C12-C13-N1
4	A	301	TSN	C7-C8-C9-C10
4	B	301	TSN	C7-C8-C9-C10
4	C	301	TSN	C7-C8-C9-C10
4	A	301	TSN	C11-C12-C13-N1
4	B	301	TSN	O3-C7-C8-C14
4	C	301	TSN	O3-C7-C8-C14
4	A	301	TSN	C1-C7-C8-C14
4	B	301	TSN	C1-C7-C8-C14

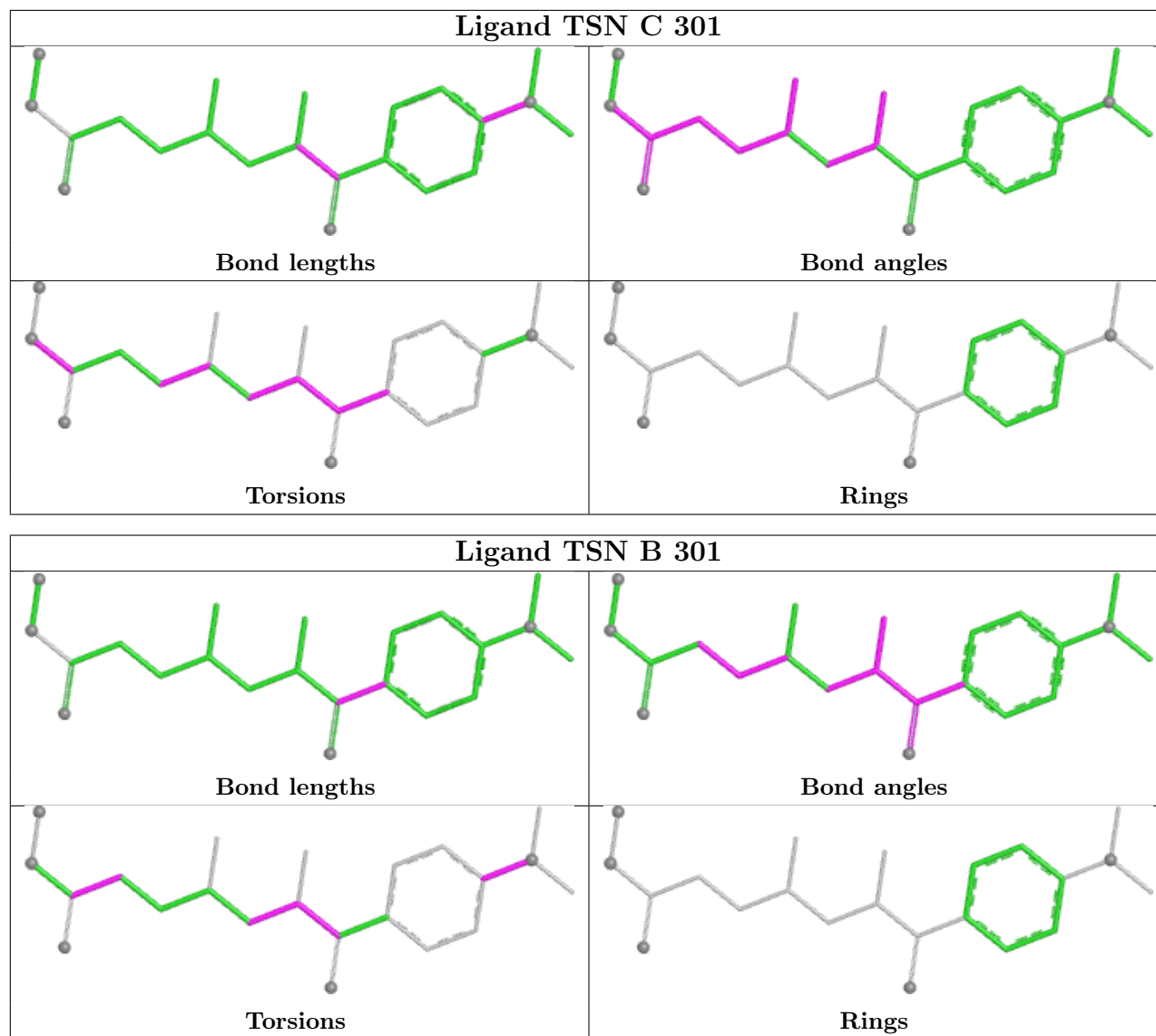
There are no ring outliers.

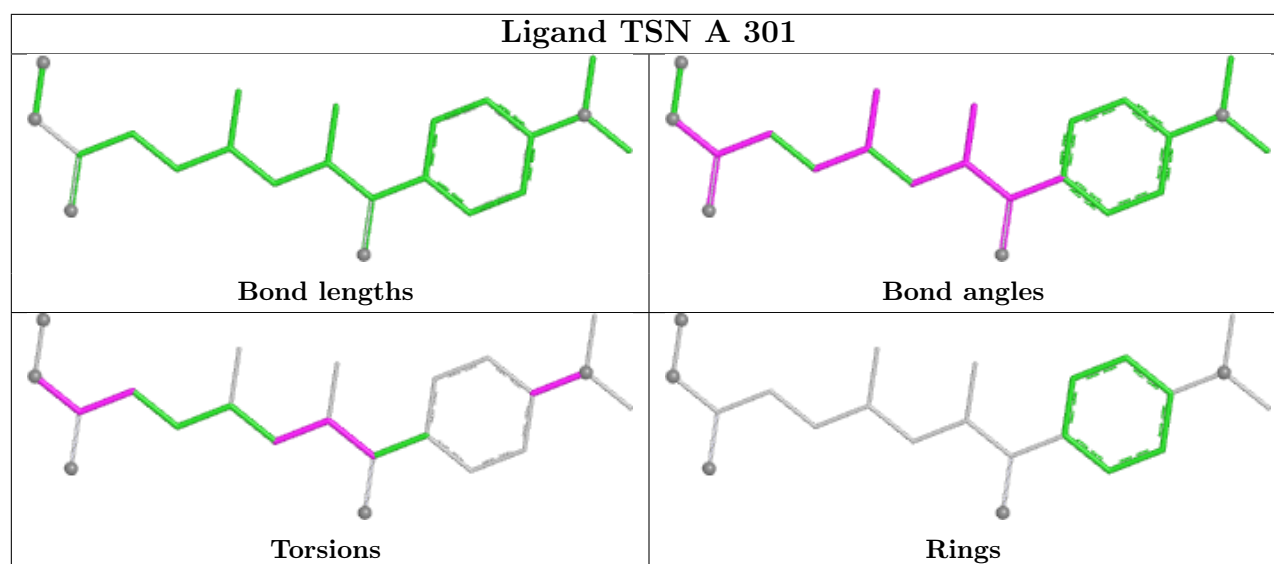
2 monomers are involved in 3 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	C	301	TSN	1	0
4	B	301	TSN	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and

any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.





5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	383/423 (90%)	0.14	14 (3%) 45 44	19, 33, 52, 59	0
1	B	368/423 (86%)	0.08	12 (3%) 49 48	21, 32, 52, 60	0
1	C	359/423 (84%)	0.31	6 (1%) 69 68	25, 40, 57, 66	0
All	All	1110/1269 (87%)	0.18	32 (2%) 53 52	19, 35, 54, 66	0

All (32) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	867	LEU	5.0
1	B	808	ALA	4.3
1	B	614	VAL	3.4
1	A	520	THR	3.1
1	C	524	TYR	3.1
1	A	593	PRO	2.8
1	A	768	PRO	2.7
1	A	518	PHE	2.7
1	A	536	GLY	2.7
1	A	657	LEU	2.6
1	A	592	ASN	2.6
1	B	865	ASP	2.4
1	A	608	LEU	2.4
1	B	809	PRO	2.3
1	B	872	TRP	2.3
1	B	871	GLY	2.3
1	B	901	LEU	2.3
1	A	661	PHE	2.3
1	A	652	VAL	2.3
1	B	518	PHE	2.2
1	A	766	ASP	2.2
1	A	560	LEU	2.2
1	C	536	GLY	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	594	LEU	2.2
1	C	519	THR	2.2
1	A	566	CYS	2.1
1	A	867	LEU	2.1
1	B	516	LEU	2.1
1	B	736	ASN	2.1
1	C	867	LEU	2.1
1	C	864	VAL	2.1
1	C	620	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
4	TSN	C	301	22/22	0.81	0.15	45,62,71,71	0
4	TSN	B	301	22/22	0.84	0.16	43,61,71,73	0
4	TSN	A	301	22/22	0.84	0.14	34,62,70,71	0
3	K	C	202	1/1	0.95	0.12	40,40,40,40	0
3	K	B	201	1/1	0.97	0.13	30,30,30,30	0
2	ZN	B	101	1/1	0.98	0.05	34,34,34,34	0
3	K	A	202	1/1	0.98	0.08	36,36,36,36	0
2	ZN	A	102	1/1	0.98	0.03	39,39,39,39	0
3	K	B	202	1/1	0.98	0.15	32,32,32,32	0
3	K	C	201	1/1	0.99	0.11	33,33,33,33	0
3	K	A	201	1/1	0.99	0.07	28,28,28,28	0
2	ZN	B	102	1/1	0.99	0.03	42,42,42,42	0
2	ZN	C	101	1/1	0.99	0.05	35,35,35,35	0
2	ZN	C	102	1/1	0.99	0.03	47,47,47,47	0

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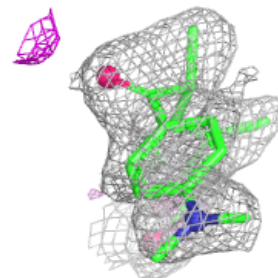
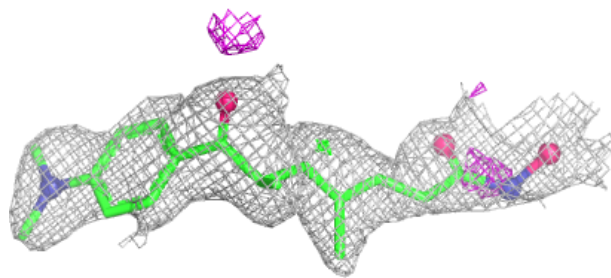
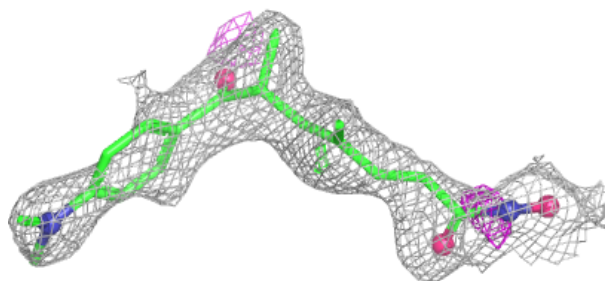
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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	A	101	1/1	1.00	0.01	29,29,29,29	0

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.

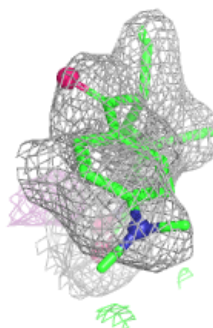
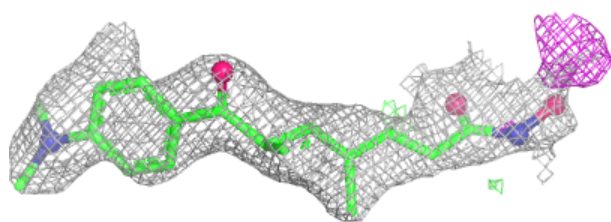
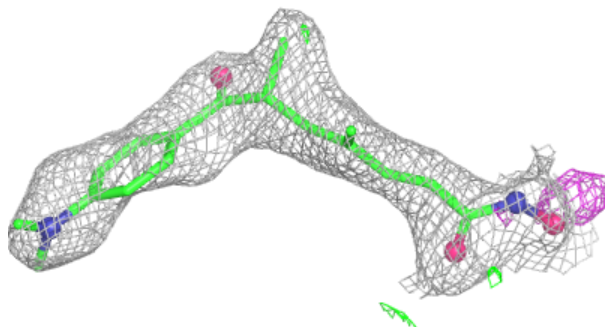
Electron density around TSN C 301:

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

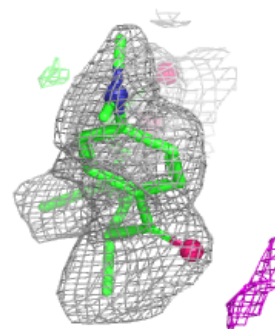
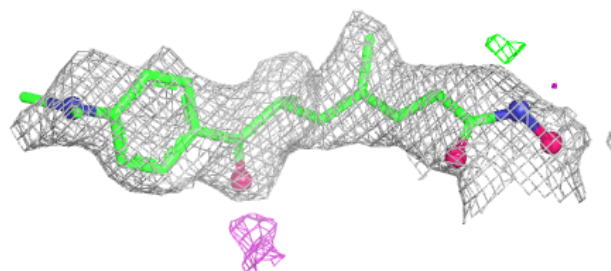
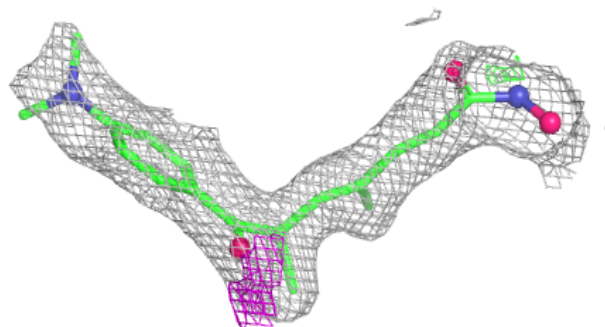


Electron density around TSN B 301:

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

**Electron density around TSN A 301:**

$2mF_o-DF_c$ (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.