



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 07:48 PM UTC

PDB ID : 1G7G / pdb_00001g7g
Title : HUMAN PTP1B CATALYTIC DOMAIN COMPLEXES WITH PNU179326
Authors : Bleasdale, J.E.; Ogg, D.; Larsen, S.D.
Deposited on : 2000-11-10
Resolution : 2.20 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

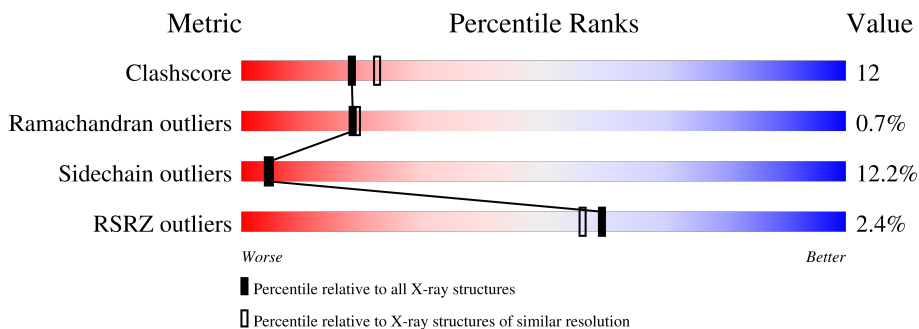
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.20 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))
Clashscore	190562	6851 (2.20-2.20)
Ramachandran outliers	187476	6768 (2.20-2.20)
Sidechain outliers	187428	6769 (2.20-2.20)
RSRZ outliers	180081	6166 (2.20-2.20)

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	298	

2 Entry composition [i](#)

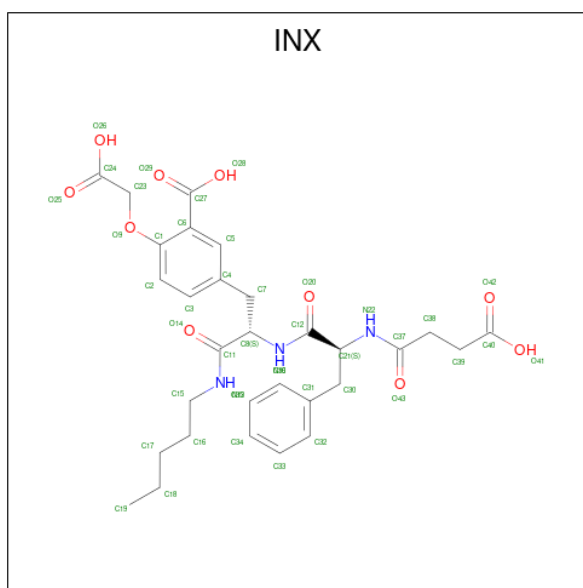
There are 3 unique types of molecules in this entry. The entry contains 2579 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 PROTEIN-TYROSINE PHOSPHATASE, NON-RECEPTOR TYPE 1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
			Total	C	N	O	S			
1	A	297	2427	1535	418	458	16	0	0	0

- Molecule 2 is 2-(CARBOXYMETHOXY)-5-[(2S)-2-({(2S)-2-[(3-CARBOXYPROPANOYL)AMINO]-3-PHENYLPROPANOYL}AMINO)-3-OXO-3-(PENTYLAMINO)PROPYL]BENZOIC ACID (CCD ID: INX) (formula: C₃₀H₃₇N₃O₁₀).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	43	30	3	10	0	0

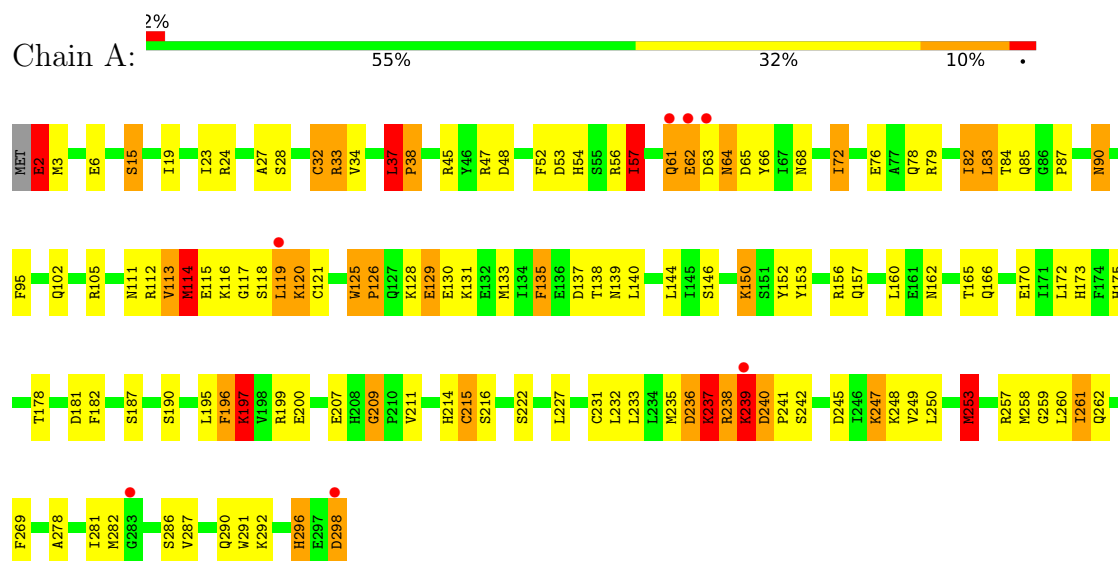
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	109	Total	O	0	0
			109	109		

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: PROTEIN-TYROSINE PHOSPHATASE, NON-RECEPTOR TYPE 1



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	52.92Å 82.44Å 88.65Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	50.00 – 2.20 50.00 – 2.20	Depositor EDS
% Data completeness (in resolution range)	(Not available) (50.00-2.20) 87.5 (50.00-2.20)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.17 (at 2.01Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.193 , 0.262 0.192 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	wwPDB-VP
Wilson B-factor (Å ²)	22.0	Xtriage
Anisotropy	1.003	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 56.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	2579	wwPDB-VP
Average B, all atoms (Å ²)	38.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.15% 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: INX

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	1.24	5/2482 (0.2%)	2.10	91/3344 (2.7%)

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	53	ASP	CA-CB	7.51	1.65	1.53
1	A	240	ASP	N-CA	-6.02	1.37	1.46
1	A	6	GLU	N-CA	5.95	1.53	1.46
1	A	28	SER	N-CA	-5.58	1.39	1.46
1	A	135	PHE	N-CA	5.01	1.53	1.46

All (91) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	239	LYS	CA-C-N	13.38	154.45	121.80
1	A	239	LYS	C-N-CA	13.38	154.45	121.80
1	A	296	HIS	CA-CB-CG	13.03	126.83	113.80
1	A	129	GLU	CA-CB-CG	10.92	135.94	114.10
1	A	129	GLU	CB-CG-CD	10.80	130.96	112.60
1	A	240	ASP	N-CA-CB	10.02	128.21	110.37
1	A	112	ARG	CD-NE-CZ	9.27	137.37	124.40
1	A	114	MET	CA-C-O	-8.53	111.49	120.70
1	A	238	ARG	CD-NE-CZ	8.52	136.33	124.40
1	A	162	ASN	CA-C-O	-8.40	111.11	120.60
1	A	61	GLN	CA-CB-CG	8.35	130.80	114.10
1	A	15	SER	N-CA-C	8.30	122.18	112.72
1	A	196	PHE	CA-CB-CG	-8.18	105.62	113.80
1	A	61	GLN	CB-CG-CD	7.79	125.85	112.60
1	A	82	ILE	N-CA-CB	7.67	121.13	111.46
1	A	32	CYS	CA-CB-SG	7.63	131.94	114.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	62	GLU	CA-C-N	7.26	130.24	120.65
1	A	62	GLU	C-N-CA	7.26	130.24	120.65
1	A	52	PHE	CA-C-O	-7.20	113.92	121.55
1	A	27	ALA	CA-C-N	7.11	131.48	120.75
1	A	27	ALA	C-N-CA	7.11	131.48	120.75
1	A	175	HIS	N-CA-C	6.95	120.19	108.02
1	A	269	PHE	CA-CB-CG	-6.88	106.92	113.80
1	A	209	GLY	N-CA-C	-6.76	103.89	112.00
1	A	126	PRO	CA-C-N	6.71	132.88	121.14
1	A	126	PRO	C-N-CA	6.71	132.88	121.14
1	A	24	ARG	NE-CZ-NH1	-6.70	114.80	121.50
1	A	125	TRP	O-C-N	6.64	126.73	121.55
1	A	236	ASP	CA-C-N	-6.62	111.74	122.26
1	A	236	ASP	C-N-CA	-6.62	111.74	122.26
1	A	259	GLY	N-CA-C	6.60	124.81	115.30
1	A	121	CYS	N-CA-CB	-6.47	100.95	111.24
1	A	135	PHE	CA-CB-CG	-6.43	107.37	113.80
1	A	156	ARG	NE-CZ-NH2	6.29	124.86	119.20
1	A	32	CYS	O-C-N	-6.13	113.68	121.83
1	A	173	HIS	CA-C-O	-6.09	113.78	120.30
1	A	247	LYS	CA-C-O	6.08	127.00	120.55
1	A	146	SER	CA-C-O	-6.05	114.44	121.10
1	A	137	ASP	CA-C-O	-6.05	113.26	120.10
1	A	66	TYR	N-CA-C	6.04	119.37	109.76
1	A	33	ARG	CD-NE-CZ	6.02	132.83	124.40
1	A	215	CYS	N-CA-C	-5.97	98.07	110.80
1	A	72	ILE	CB-CG1-CD1	5.96	126.31	113.80
1	A	187	SER	CB-CA-C	-5.88	101.97	110.03
1	A	237	LYS	CB-CA-C	5.88	119.43	109.55
1	A	6	GLU	CA-C-O	5.85	126.97	120.82
1	A	298	ASP	CA-CB-CG	5.84	118.44	112.60
1	A	257	ARG	NE-CZ-NH1	-5.78	115.72	121.50
1	A	233	LEU	N-CA-C	-5.76	105.08	111.36
1	A	199	ARG	CD-NE-CZ	5.75	132.45	124.40
1	A	125	TRP	CA-C-O	-5.70	115.00	120.64
1	A	160	LEU	CA-C-O	5.68	126.57	120.32
1	A	32	CYS	CA-C-O	5.64	129.17	121.89
1	A	150	LYS	N-CA-CB	5.64	119.17	110.60
1	A	79	ARG	CD-NE-CZ	5.58	132.22	124.40
1	A	173	HIS	CA-CB-CG	5.57	119.37	113.80
1	A	227	LEU	CA-C-N	-5.54	112.42	120.29
1	A	227	LEU	C-N-CA	-5.54	112.42	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	231	CYS	CA-C-N	5.52	128.13	120.29
1	A	231	CYS	C-N-CA	5.52	128.13	120.29
1	A	32	CYS	CA-C-N	5.52	127.94	120.65
1	A	32	CYS	C-N-CA	5.52	127.94	120.65
1	A	56	ARG	N-CA-CB	5.51	118.13	110.04
1	A	126	PRO	O-C-N	-5.49	116.82	123.03
1	A	215	CYS	CA-C-O	-5.49	112.66	120.51
1	A	52	PHE	O-C-N	5.48	129.55	122.81
1	A	65	ASP	N-CA-C	5.39	119.57	113.15
1	A	199	ARG	NE-CZ-NH2	5.38	124.04	119.20
1	A	57	ILE	CA-C-O	5.36	126.77	120.71
1	A	38	PRO	O-C-N	-5.35	116.09	122.24
1	A	61	GLN	CB-CA-C	5.32	118.42	109.48
1	A	172	LEU	CA-C-N	-5.31	115.51	123.00
1	A	172	LEU	C-N-CA	-5.31	115.51	123.00
1	A	253	MET	CG-SD-CE	-5.30	89.25	100.90
1	A	48	ASP	CA-C-N	-5.29	114.90	122.84
1	A	48	ASP	C-N-CA	-5.29	114.90	122.84
1	A	37	LEU	O-C-N	-5.28	117.05	121.38
1	A	113	VAL	N-CA-CB	-5.22	103.94	110.47
1	A	68	ASN	OD1-CG-ND2	5.21	127.81	122.60
1	A	33	ARG	CA-C-O	-5.20	115.54	121.00
1	A	245	ASP	CA-C-N	5.16	127.80	120.53
1	A	245	ASP	C-N-CA	5.16	127.80	120.53
1	A	139	ASN	CA-CB-CG	-5.11	107.49	112.60
1	A	121	CYS	CA-C-O	-5.09	115.05	120.75
1	A	64	ASN	CA-CB-CG	-5.06	107.54	112.60
1	A	138	THR	CA-C-O	5.06	125.15	119.18
1	A	2	GLU	CB-CG-CD	5.06	121.19	112.60
1	A	248	LYS	O-C-N	-5.03	116.42	122.15
1	A	57	ILE	N-CA-CB	5.02	116.19	110.72
1	A	197	LYS	CA-C-N	-5.00	114.26	120.56
1	A	197	LYS	C-N-CA	-5.00	114.26	120.56

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	2427	0	2380	59	0
2	A	43	0	34	2	0
3	A	109	0	0	2	0
All	All	2579	0	2414	59	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 (59) 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:90:ASN:H	1:A:90:ASN:HD22	1.10	0.96
1:A:236:ASP:HB2	1:A:281:ILE:HD12	1.50	0.94
1:A:45:ARG:H	1:A:85:GLN:HE22	1.12	0.94
1:A:2:GLU:HG2	1:A:242:SER:HB2	1.58	0.86
1:A:57:ILE:HD11	1:A:82:ILE:HG12	1.57	0.85
1:A:90:ASN:H	1:A:90:ASN:ND2	1.79	0.81
1:A:240:ASP:N	1:A:241:PRO:HD3	2.01	0.76
1:A:130:GLU:HG2	1:A:131:LYS:HE2	1.70	0.74
1:A:45:ARG:H	1:A:85:GLN:NE2	1.87	0.72
1:A:54:HIS:ND1	3:A:798:HOH:O	2.23	0.71
1:A:90:ASN:HD22	1:A:90:ASN:N	1.88	0.67
1:A:197:LYS:HB2	1:A:197:LYS:HZ3	1.60	0.66
1:A:286:SER:O	1:A:290:GLN:HG3	1.99	0.62
1:A:157:GLN:NE2	1:A:170:GLU:OE1	2.33	0.62
1:A:34:VAL:HA	1:A:37:LEU:HD22	1.81	0.60
1:A:133:MET:HE2	1:A:135:PHE:CZ	2.38	0.59
1:A:150:LYS:HG3	1:A:153:TYR:CZ	2.38	0.58
1:A:57:ILE:CD1	1:A:82:ILE:HG12	2.33	0.58
1:A:197:LYS:HB2	1:A:197:LYS:NZ	2.18	0.58
1:A:197:LYS:HZ3	1:A:197:LYS:CB	2.13	0.56
1:A:115:GLU:O	1:A:116:LYS:HB2	2.06	0.56
1:A:240:ASP:N	1:A:241:PRO:CD	2.69	0.56
1:A:128:LYS:HD3	1:A:131:LYS:HE3	1.88	0.55
1:A:196:PHE:O	1:A:200:GLU:HG3	2.07	0.55
1:A:90:ASN:ND2	1:A:90:ASN:N	2.50	0.55
1:A:235:MET:HE1	1:A:278:ALA:HB2	1.90	0.54
1:A:87:PRO:HG3	1:A:95:PHE:CD2	2.44	0.53
1:A:102:GLN:O	1:A:209:GLY:HA3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:3:MET:HE1	1:A:235:MET:SD	2.50	0.51
1:A:239:LYS:HA	1:A:239:LYS:HE2	1.93	0.51
1:A:152:TYR:HB2	1:A:178:THR:OG1	2.11	0.50
1:A:165:THR:O	1:A:166:GLN:HB2	2.12	0.50
1:A:120:LYS:HB3	1:A:216:SER:HB2	1.94	0.50
1:A:253:MET:HB2	1:A:260:LEU:HD12	1.94	0.49
1:A:61:GLN:HG3	1:A:63:ASP:HB3	1.95	0.49
1:A:84:THR:O	1:A:214:HIS:HB2	2.13	0.49
1:A:83:LEU:HD13	1:A:222:SER:HB3	1.94	0.49
1:A:250:LEU:HD22	1:A:261:ILE:HD12	1.95	0.48
1:A:47:ARG:NE	2:A:600:INX:O41	2.47	0.47
1:A:125:TRP:HB2	1:A:126:PRO:HD2	1.96	0.47
1:A:111:ASN:HD22	1:A:215:CYS:HA	1.79	0.47
1:A:126:PRO:HG2	1:A:144:LEU:HB2	1.97	0.46
1:A:116:LYS:O	1:A:118:SER:N	2.49	0.45
1:A:23:ILE:HD11	1:A:247:LYS:HG2	1.99	0.45
1:A:181:ASP:O	1:A:182:PHE:HB2	2.17	0.44
1:A:61:GLN:HG3	1:A:64:ASN:H	1.83	0.43
1:A:111:ASN:ND2	1:A:215:CYS:HA	2.34	0.43
1:A:262:GLN:HG3	2:A:600:INX:HC2	2.00	0.43
1:A:119:LEU:HD22	1:A:119:LEU:HA	1.79	0.42
1:A:287:VAL:HG22	1:A:291:TRP:CE2	2.54	0.42
1:A:114:MET:HG2	1:A:119:LEU:CD2	2.50	0.42
1:A:76:GLU:O	1:A:237:LYS:HE2	2.19	0.42
1:A:249:VAL:O	1:A:253:MET:HG3	2.20	0.42
1:A:211:VAL:HG12	3:A:731:HOH:O	2.19	0.41
1:A:239:LYS:C	1:A:241:PRO:HD3	2.45	0.41
1:A:239:LYS:HE2	1:A:239:LYS:CA	2.50	0.41
1:A:260:LEU:O	1:A:261:ILE:HB	2.20	0.41
1:A:37:LEU:O	1:A:38:PRO:C	2.64	0.41
1:A:111:ASN:HD21	1:A:214:HIS:CE1	2.38	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	295/298 (99%)	280 (95%)	13 (4%)	2 (1%)	18	19

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	261	ILE
1	A	117	GLY

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	270/271 (100%)	237 (88%)	33 (12%)	5	4

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

Mol	Chain	Res	Type
1	A	2	GLU
1	A	15	SER
1	A	19	ILE
1	A	32	CYS
1	A	33	ARG
1	A	37	LEU
1	A	57	ILE
1	A	62	GLU
1	A	72	ILE
1	A	78	GLN
1	A	83	LEU
1	A	90	ASN
1	A	105	ARG
1	A	113	VAL
1	A	114	MET
1	A	119	LEU
1	A	120	LYS

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Mol	Chain	Res	Type
1	A	129	GLU
1	A	140	LEU
1	A	190	SER
1	A	195	LEU
1	A	197	LYS
1	A	207	GLU
1	A	232	LEU
1	A	237	LYS
1	A	238	ARG
1	A	239	LYS
1	A	253	MET
1	A	258	MET
1	A	282	MET
1	A	292	LYS
1	A	296	HIS
1	A	298	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (3) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	85	GLN
1	A	90	ASN
1	A	111	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry ⓘ

1 ligand is 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	$\# Z > 2$
2	INX	A	600	-	44,44,44	1.97	15 (34%)	57,57,57	2.06	18 (31%)

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
2	INX	A	600	-	-	10/44/44/44	0/2/2/2

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	600	INX	O42-C40	4.60	1.37	1.22
2	A	600	INX	O28-C27	-3.73	1.19	1.30
2	A	600	INX	C6-C1	3.73	1.47	1.40
2	A	600	INX	C35-C36	3.59	1.45	1.38
2	A	600	INX	O26-C24	-3.24	1.20	1.30
2	A	600	INX	C32-C31	3.18	1.45	1.38
2	A	600	INX	C33-C32	2.80	1.43	1.38
2	A	600	INX	O25-C24	2.76	1.31	1.22
2	A	600	INX	C3-C4	2.59	1.44	1.38
2	A	600	INX	O41-C40	-2.55	1.22	1.30
2	A	600	INX	O29-C27	2.36	1.29	1.22
2	A	600	INX	C35-C34	2.24	1.43	1.38
2	A	600	INX	C39-C40	2.15	1.55	1.50
2	A	600	INX	C3-C2	2.11	1.42	1.38
2	A	600	INX	C2-C1	2.08	1.43	1.39

All (18) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	INX	C23-O9-C1	5.48	129.03	117.60
2	A	600	INX	O41-C40-C39	3.95	126.47	114.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	600	INX	C15-N13-C11	3.86	129.47	122.55
2	A	600	INX	O9-C1-C2	-3.65	115.98	123.95
2	A	600	INX	O9-C1-C6	3.65	124.99	116.97
2	A	600	INX	C36-C31-C32	3.63	123.63	118.23
2	A	600	INX	O29-C27-C6	-3.55	113.50	121.97
2	A	600	INX	O28-C27-C6	3.35	124.79	115.28
2	A	600	INX	O42-C40-C39	-3.32	112.55	123.09
2	A	600	INX	O25-C24-C23	-3.28	108.34	121.99
2	A	600	INX	C31-C30-C21	-3.02	105.31	113.36
2	A	600	INX	O14-C11-N13	2.90	129.12	122.98
2	A	600	INX	C8-C11-N13	-2.73	110.67	116.54
2	A	600	INX	C35-C36-C31	-2.64	116.90	120.61
2	A	600	INX	O26-C24-C23	2.49	125.39	113.66
2	A	600	INX	C8-N10-C12	-2.45	116.37	121.65
2	A	600	INX	C38-C37-N22	2.20	119.74	115.86
2	A	600	INX	O20-C12-C21	-2.11	116.06	120.48

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	600	INX	O29-C27-C6-C1
2	A	600	INX	C37-C38-C39-C40
2	A	600	INX	C15-C16-C17-C18
2	A	600	INX	O28-C27-C6-C1
2	A	600	INX	C2-C1-O9-C23
2	A	600	INX	C16-C17-C18-C19
2	A	600	INX	C6-C1-O9-C23
2	A	600	INX	O29-C27-C6-C5
2	A	600	INX	O28-C27-C6-C5
2	A	600	INX	N13-C15-C16-C17

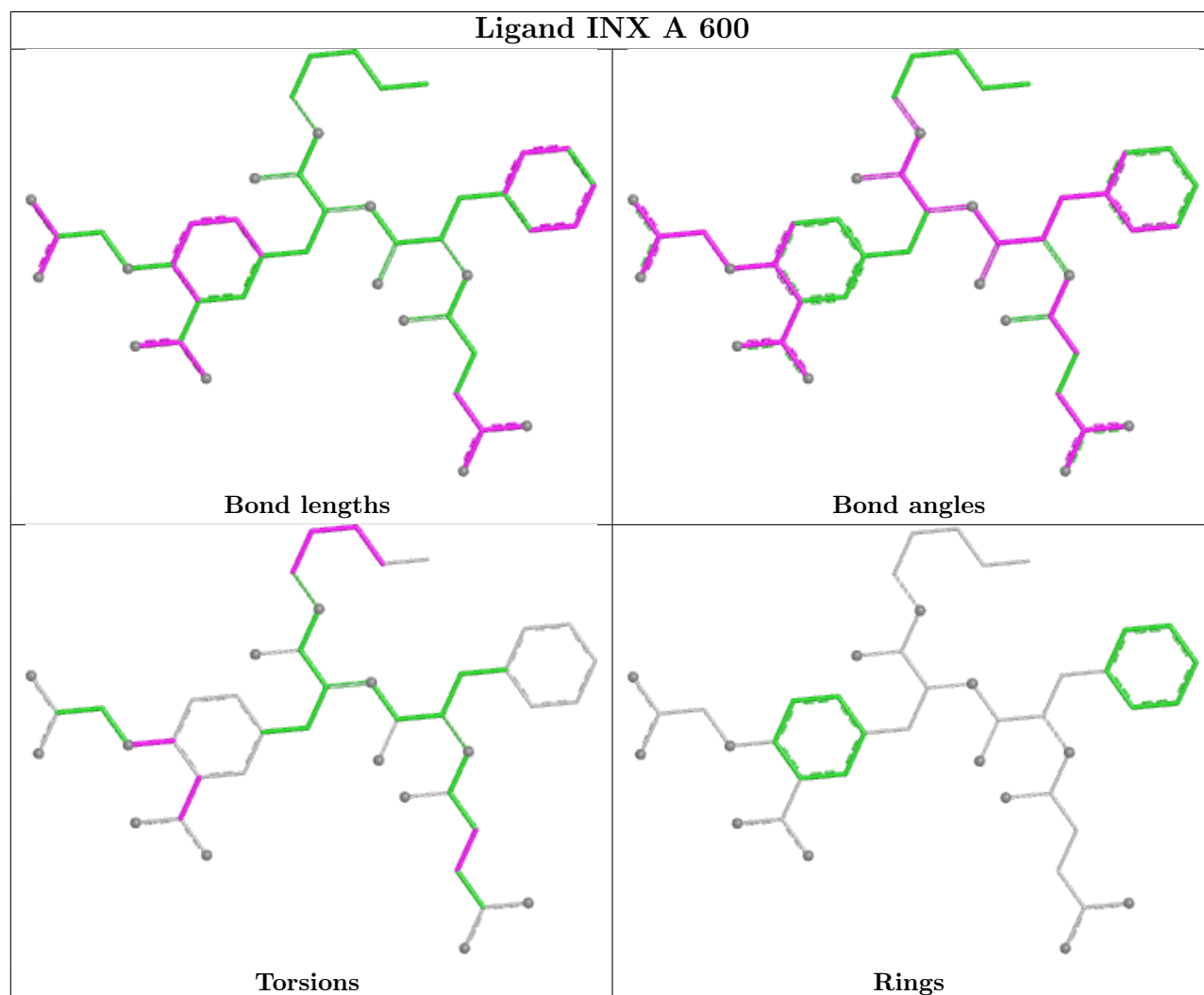
There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	600	INX	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 [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	297/298 (99%)	-0.04	7 (2%) 59 56	23, 34, 60, 91	0

All (7) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	239	LYS	4.1
1	A	298	ASP	2.4
1	A	63	ASP	2.3
1	A	119	LEU	2.3
1	A	62	GLU	2.3
1	A	61	GLN	2.1
1	A	283	GLY	2.1

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](#)

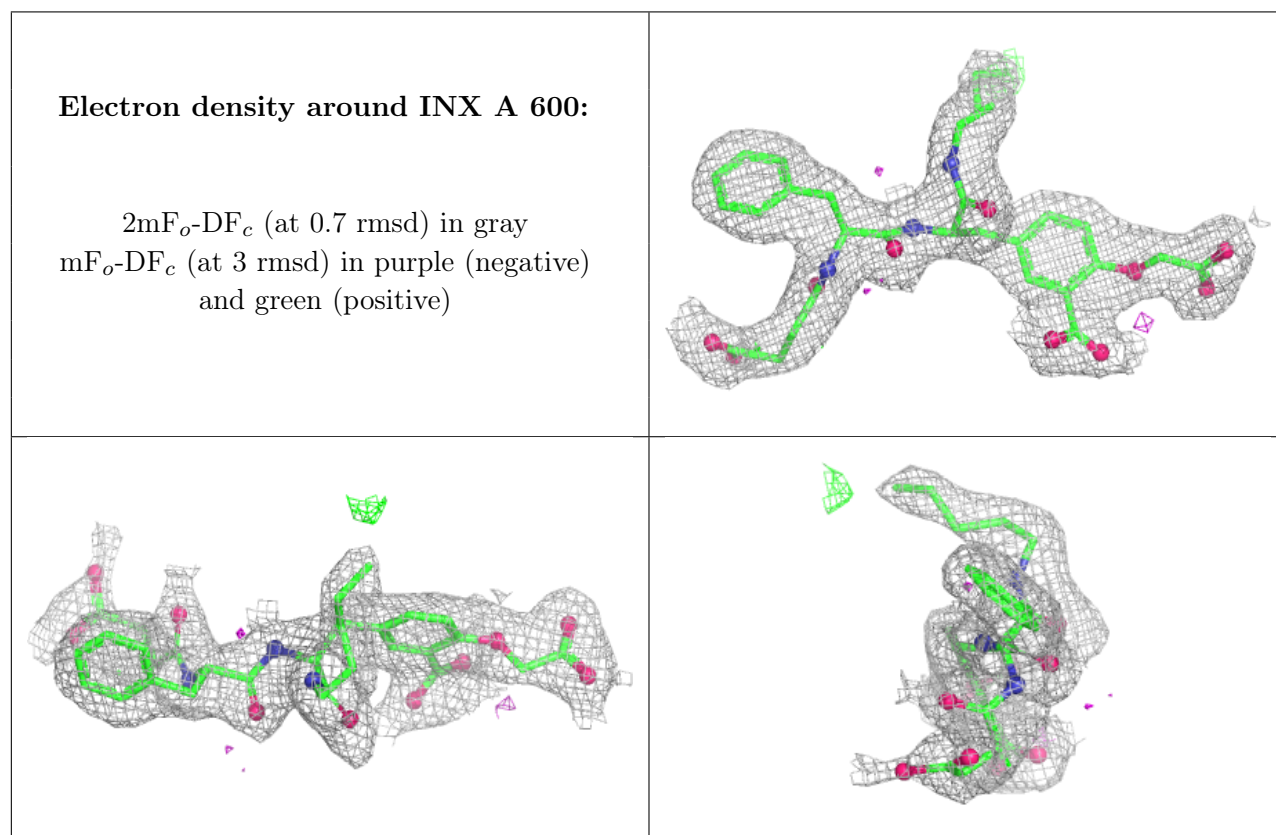
There are no oligosaccharides in this entry.

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
2	INX	A	600	43/43	0.94	0.10	30,40,62,73	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.