



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 08:19 AM UTC

PDB ID : 3CSO / pdb_00003cso
Title : HCV Polymerase in complex with a 1,5 Benzodiazepine inhibitor
Authors : Nyanguile, O.
Deposited on : 2008-04-10
Resolution : 2.71 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

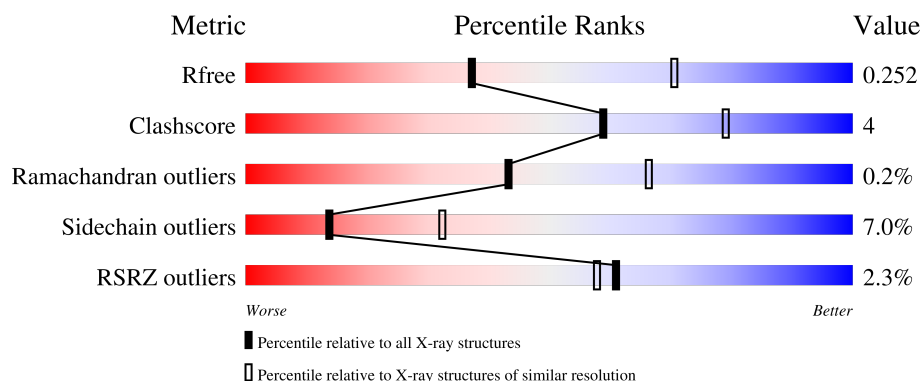
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.71 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	4348 (2.74-2.70)
Clashscore	190562	4665 (2.74-2.70)
Ramachandran outliers	187476	4584 (2.74-2.70)
Sidechain outliers	187428	4585 (2.74-2.70)
RSRZ outliers	180081	4348 (2.74-2.70)

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	581	2% 82% 13% ..
1	B	581	3% 81% 14% ..

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 9041 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.

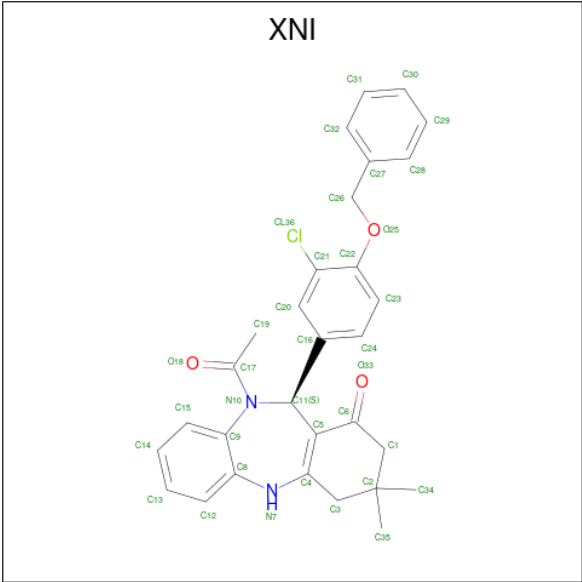
- Molecule 1 is a protein called RNA-directed RNA polymerase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	561	Total	C	N	O	S	0	0	0
			4371	2752	772	815	32			
1	B	560	Total	C	N	O	S	0	2	0
			4376	2754	775	815	32			

There are 22 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-2	MET	-	expression tag	UNP O92972
A	-1	ALA	-	expression tag	UNP O92972
A	0	SER	-	expression tag	UNP O92972
A	571	LEU	-	expression tag	UNP O92972
A	572	GLU	-	expression tag	UNP O92972
A	573	HIS	-	expression tag	UNP O92972
A	574	HIS	-	expression tag	UNP O92972
A	575	HIS	-	expression tag	UNP O92972
A	576	HIS	-	expression tag	UNP O92972
A	577	HIS	-	expression tag	UNP O92972
A	578	HIS	-	expression tag	UNP O92972
B	-2	MET	-	expression tag	UNP O92972
B	-1	ALA	-	expression tag	UNP O92972
B	0	SER	-	expression tag	UNP O92972
B	571	LEU	-	expression tag	UNP O92972
B	572	GLU	-	expression tag	UNP O92972
B	573	HIS	-	expression tag	UNP O92972
B	574	HIS	-	expression tag	UNP O92972
B	575	HIS	-	expression tag	UNP O92972
B	576	HIS	-	expression tag	UNP O92972
B	577	HIS	-	expression tag	UNP O92972
B	578	HIS	-	expression tag	UNP O92972

- Molecule 2 is (11S)-10-acetyl-11-[4-(benzyloxy)-3-chlorophenyl]-3,3-dimethyl-2,3,4,5,10,11-hexahydro-1H-dibenzo[b,e][1,4]diazepin-1-one (CCD ID: XNI) (formula: C₃₀H₂₉ClN₂O₃).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total 36	C 30	Cl 1	N 2	O 3	0	0
2	B	1	Total 36	C 30	Cl 1	N 2	O 3	0	0

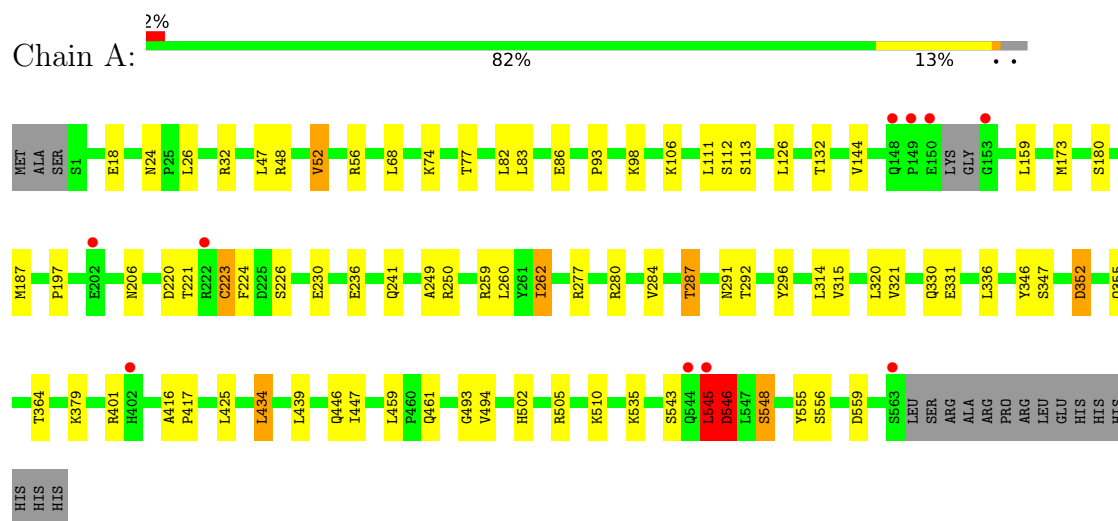
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	130	Total	O	0	0
			130	130		
3	B	92	Total	O	0	0
			92	92		

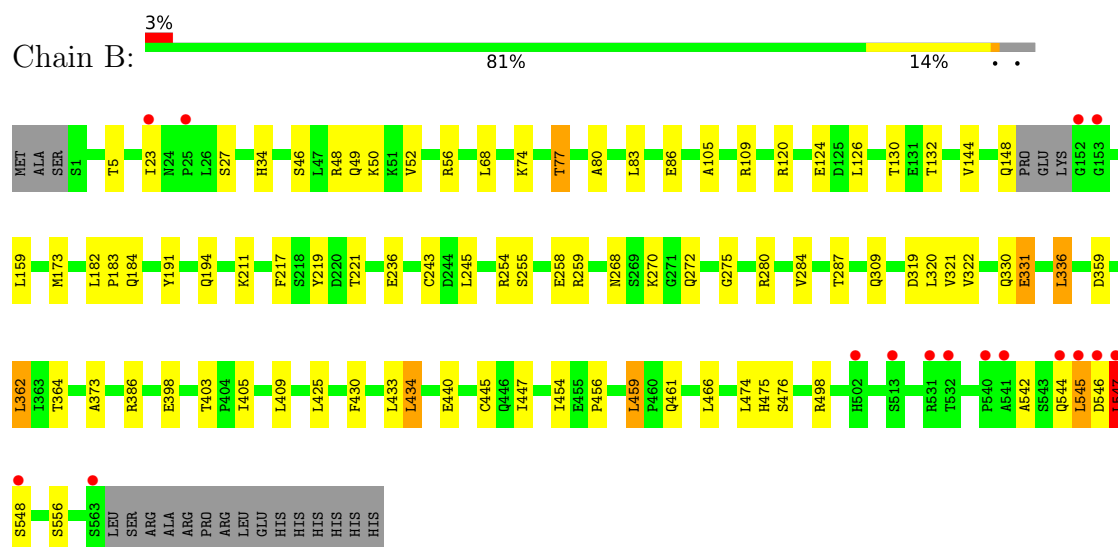
3 Residue-property plots [i](#)

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: RNA-directed RNA polymerase



• Molecule 1: RNA-directed RNA polymerase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	105.96Å 108.22Å 133.30Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	83.05 – 2.71 83.05 – 2.71	Depositor EDS
% Data completeness (in resolution range)	99.9 (83.05-2.71) 99.9 (83.05-2.71)	Depositor EDS
R_{merge}	0.16	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.84 (at 2.69Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.180 , 0.239 0.197 , 0.252	Depositor DCC
R_{free} test set	2114 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å ²)	33.4	Xtriage
Anisotropy	0.517	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 41.8	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	0.040 for k,h,-l	Xtriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	9041	wwPDB-VP
Average B, all atoms (Å ²)	34.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.13% 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: XNI

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	0.66	0/4466	0.85	4/6061 (0.1%)
1	B	0.62	0/4473	0.83	0/6068
All	All	0.64	0/8939	0.84	4/12129 (0.0%)

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	A	0	1
1	B	0	1
All	All	0	2

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	545	LEU	N-CA-C	5.37	118.38	110.59
1	A	546	ASP	N-CA-C	5.21	117.01	108.52
1	A	494	VAL	CA-C-N	-5.02	115.21	120.38
1	A	494	VAL	C-N-CA	-5.02	115.21	120.38

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	545	LEU	Peptide
1	B	548	SER	Peptide

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	4371	0	4380	37	0
1	B	4376	0	4388	41	0
2	A	36	0	29	1	0
2	B	36	0	29	0	0
3	A	130	0	0	4	0
3	B	92	0	0	4	0
All	All	9041	0	8826	77	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 (77) 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:476:SER:N	3:B:593:HOH:O	1.92	1.02
1:B:268:ASN:HD21	1:B:272:GLN:HE21	1.19	0.85
1:A:132:THR:O	1:A:259:ARG:HD2	1.78	0.84
1:A:236:GLU:OE1	1:A:280:ARG:NH2	2.23	0.72
1:B:268:ASN:HD21	1:B:272:GLN:NE2	1.91	0.66
1:A:74:LYS:O	1:A:77:THR:HB	2.02	0.60
1:B:191:TYR:O	1:B:194:GLN:HG2	2.03	0.58
1:B:284:VAL:O	1:B:287:THR:HG22	2.04	0.58
1:B:403:THR:HG22	3:B:609:HOH:O	2.02	0.58
1:A:82:LEU:HD11	1:A:249:ALA:HB2	1.85	0.58
1:A:284:VAL:O	1:A:287:THR:HG22	2.05	0.56
1:A:352:ASP:OD2	1:A:352:ASP:N	2.36	0.56
1:B:398:GLU:HG2	1:B:403:THR:HG21	1.88	0.56
1:B:236:GLU:CD	1:B:280:ARG:HH22	2.14	0.56
1:B:132:THR:O	1:B:259:ARG:HD2	2.06	0.55
1:A:545:LEU:HB3	3:A:631:HOH:O	2.06	0.55
1:A:505:ARG:NE	3:A:601:HOH:O	2.40	0.54
1:A:546:ASP:OD1	1:A:548:SER:OG	2.26	0.54
1:A:280:ARG:HD2	1:A:291:ASN:OD1	2.08	0.53
1:B:184:GLN:HG2	3:B:589:HOH:O	2.09	0.53
1:B:255:SER:O	1:B:259:ARG:HG3	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:82:LEU:CD1	1:A:249:ALA:HB2	2.39	0.52
1:B:83:LEU:HB2	1:B:173:MET:HA	1.91	0.52
1:A:187:MET:HE1	1:A:292:THR:HG22	1.93	0.51
1:B:219:TYR:HB3	1:B:320:LEU:HD23	1.93	0.51
1:A:83:LEU:HB2	1:A:173:MET:HA	1.92	0.51
1:B:405:ILE:HD12	1:B:445:CYS:HA	1.92	0.50
1:B:445:CYS:SG	1:B:454:ILE:HD12	2.52	0.50
1:B:120:ARG:O	1:B:124:GLU:HG2	2.12	0.49
1:B:74:LYS:O	1:B:77:THR:HG22	2.12	0.49
1:B:219:TYR:HE1	1:B:221:THR:HG22	1.77	0.49
1:B:80:ALA:HB3	1:B:245:LEU:HD23	1.95	0.49
1:B:182:LEU:HD12	1:B:243:CYS:SG	2.54	0.48
1:A:32:ARG:HD3	1:A:493:GLY:O	2.13	0.48
1:A:220:ASP:OD2	1:A:220:ASP:C	2.55	0.48
1:B:359:ASP:HB3	1:B:362:LEU:HD22	1.96	0.48
1:A:180:SER:HB3	1:A:555:TYR:OH	2.15	0.47
1:B:544:GLN:O	1:B:545:LEU:C	2.57	0.47
1:A:187:MET:HE3	1:A:296:TYR:CD2	2.50	0.47
1:A:18:GLU:HG2	1:A:401:ARG:HH12	1.79	0.47
1:A:314:LEU:HB3	1:A:321:VAL:HG13	1.97	0.46
1:B:544:GLN:O	1:B:546:ASP:N	2.48	0.46
1:A:230:GLU:HB3	1:A:262:ILE:HD11	1.98	0.46
1:B:546:ASP:O	1:B:547:LEU:C	2.59	0.46
1:A:260:LEU:O	1:A:277:ARG:NH2	2.49	0.46
1:B:5:THR:O	1:B:275:GLY:HA3	2.16	0.45
1:B:48:ARG:HG2	1:B:159:LEU:HG	1.97	0.45
1:A:52:VAL:HG22	1:A:226:SER:OG	2.16	0.45
1:A:197:PRO:HG3	2:A:579:XNI:H30	1.99	0.44
1:B:217:PHE:CD1	1:B:336:LEU:HD11	2.52	0.44
1:B:409:LEU:HD11	1:B:459:LEU:HD21	1.99	0.44
1:B:254:ARG:NH2	1:B:258:GLU:HG2	2.32	0.44
1:A:24:ASN:HD22	1:A:26:LEU:H	1.63	0.44
1:B:182:LEU:N	1:B:183:PRO:CD	2.81	0.44
1:A:416:ALA:N	1:A:417:PRO:CD	2.81	0.43
1:A:223:CYS:O	1:A:224:PHE:C	2.61	0.43
1:B:105:ALA:O	1:B:109:ARG:HG3	2.19	0.43
1:A:230:GLU:HG2	1:A:262:ILE:HG12	2.01	0.43
1:B:430:PHE:O	1:B:434:LEU:HB2	2.19	0.43
1:A:446:GLN:C	1:A:447:ILE:HD12	2.43	0.42
1:B:542:ALA:O	1:B:546:ASP:OD2	2.37	0.42
1:A:206:ASN:HD21	1:B:498:ARG:NE	2.17	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:86:GLU:HG2	1:A:111:LEU:HD11	2.00	0.42
1:B:447:ILE:HD12	1:B:447:ILE:N	2.35	0.42
1:A:505:ARG:NH1	3:A:581:HOH:O	2.52	0.42
1:A:434:LEU:HD21	1:A:510:LYS:HB3	2.01	0.42
1:B:475:HIS:N	3:B:593:HOH:O	2.41	0.42
1:B:46:SER:HA	1:B:49:GLN:NE2	2.35	0.41
1:A:502:HIS:CD2	3:A:652:HOH:O	2.73	0.41
1:A:241:GLN:OE1	1:A:250:ARG:HG3	2.21	0.41
1:B:331:GLU:H	1:B:331:GLU:CD	2.27	0.41
1:B:268:ASN:ND2	1:B:272:GLN:HE21	1.99	0.41
1:A:48:ARG:HG2	1:A:159:LEU:HG	2.03	0.41
1:B:456:PRO:O	1:B:459:LEU:HD23	2.20	0.41
1:A:346:TYR:O	1:A:347:SER:HB3	2.21	0.40
1:B:373:ALA:HB3	1:B:474:LEU:HD13	2.02	0.40
1:A:93:PRO:HD3	1:A:559:ASP: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	557/581 (96%)	543 (98%)	14 (2%)	0	100	100
1	B	558/581 (96%)	540 (97%)	16 (3%)	2 (0%)	30	52
All	All	1115/1162 (96%)	1083 (97%)	30 (3%)	2 (0%)	43	66

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	545	LEU
1	B	547	LEU

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	478/495 (97%)	445 (93%)	33 (7%)	14	33
1	B	478/495 (97%)	444 (93%)	34 (7%)	13	32
All	All	956/990 (97%)	889 (93%)	67 (7%)	14	32

All (67) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	47	LEU
1	A	52	VAL
1	A	56	ARG
1	A	68	LEU
1	A	98	LYS
1	A	106	LYS
1	A	112	SER
1	A	113	SER
1	A	126	LEU
1	A	144	VAL
1	A	221	THR
1	A	223	CYS
1	A	262	ILE
1	A	287	THR
1	A	315	VAL
1	A	320	LEU
1	A	330	GLN
1	A	331	GLU
1	A	336	LEU
1	A	352	ASP
1	A	355	GLN
1	A	364	THR
1	A	379	LYS
1	A	425	LEU
1	A	434	LEU
1	A	439	LEU
1	A	459	LEU

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Mol	Chain	Res	Type
1	A	461	GLN
1	A	535	LYS
1	A	543	SER
1	A	546	ASP
1	A	548	SER
1	A	556	SER
1	B	23	ILE
1	B	27	SER
1	B	34	HIS
1	B	50	LYS
1	B	52	VAL
1	B	56	ARG
1	B	68	LEU
1	B	77	THR
1	B	86	GLU
1	B	126	LEU
1	B	130	THR
1	B	144	VAL
1	B	148	GLN
1	B	211	LYS
1	B	270	LYS
1	B	309	GLN
1	B	319	ASP
1	B	321	VAL
1	B	322	VAL
1	B	330	GLN
1	B	331	GLU
1	B	336	LEU
1	B	362	LEU
1	B	364	THR
1	B	386	ARG
1	B	425	LEU
1	B	433	LEU
1	B	434	LEU
1	B	440	GLU
1	B	459	LEU
1	B	461	GLN
1	B	466	LEU
1	B	547	LEU
1	B	556	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (20) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	24	ASN
1	A	28	ASN
1	A	34	HIS
1	A	35	ASN
1	A	49	GLN
1	A	206	ASN
1	A	273	ASN
1	A	461	GLN
1	A	483	ASN
1	A	544	GLN
1	A	562	HIS
1	B	35	ASN
1	B	49	GLN
1	B	206	ASN
1	B	272	GLN
1	B	273	ASN
1	B	330	GLN
1	B	438	GLN
1	B	446	GLN
1	B	483	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 ⓘ

2 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
2	XNI	B	579	-	39,40,40	0.91	4 (10%)	57,59,59	1.37	11 (19%)
2	XNI	A	579	-	39,40,40	0.94	2 (5%)	57,59,59	1.43	8 (14%)

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	XNI	B	579	-	-	1/13/47/47	0/4/5/5
2	XNI	A	579	-	-	0/13/47/47	0/4/5/5

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	579	XNI	C4-N7	2.48	1.40	1.35
2	B	579	XNI	C17-N10	2.43	1.41	1.37
2	B	579	XNI	C3-C4	2.40	1.53	1.50
2	A	579	XNI	C4-N7	2.39	1.39	1.35
2	A	579	XNI	C8-C9	-2.33	1.38	1.40
2	B	579	XNI	C16-C11	2.31	1.55	1.52

All (19) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	579	XNI	C5-C4-N7	4.20	129.57	126.58
2	B	579	XNI	C2-C3-C4	4.08	117.86	113.40
2	A	579	XNI	C5-C11-N10	-3.67	104.94	111.27
2	A	579	XNI	C2-C3-C4	3.62	117.36	113.40
2	B	579	XNI	O33-C6-C5	-3.55	117.68	121.32
2	A	579	XNI	C3-C4-N7	-2.92	109.79	112.00
2	B	579	XNI	C26-O25-C22	2.83	123.37	117.76
2	A	579	XNI	C1-C6-C5	2.61	122.08	118.27
2	A	579	XNI	C19-C17-N10	2.61	121.46	117.87
2	B	579	XNI	C24-C16-C11	2.59	124.48	120.69
2	B	579	XNI	C3-C4-C5	-2.56	120.42	123.46
2	B	579	XNI	C19-C17-N10	2.47	121.28	117.87
2	A	579	XNI	C3-C4-C5	-2.45	120.55	123.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	A	579	XNI	O25-C22-C21	2.45	119.30	116.39
2	B	579	XNI	C9-N10-C11	-2.26	115.39	119.02
2	B	579	XNI	C8-C9-N10	-2.23	117.92	119.37
2	B	579	XNI	C20-C16-C11	-2.21	116.42	119.81
2	B	579	XNI	C5-C11-N10	-2.14	107.59	111.27
2	B	579	XNI	C1-C6-C5	2.05	121.27	118.27

There are no chirality outliers.

All (1) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	579	XNI	C27-C26-O25-C22

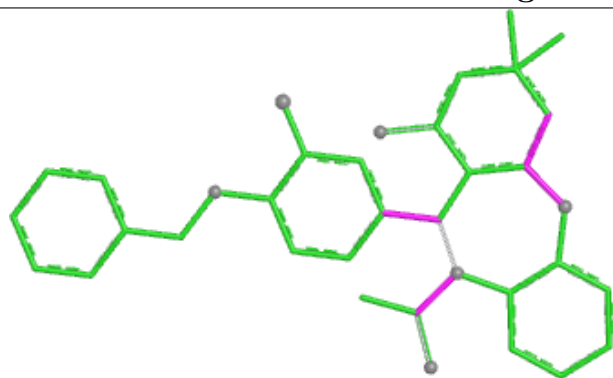
There are no ring outliers.

1 monomer is involved in 1 short contact:

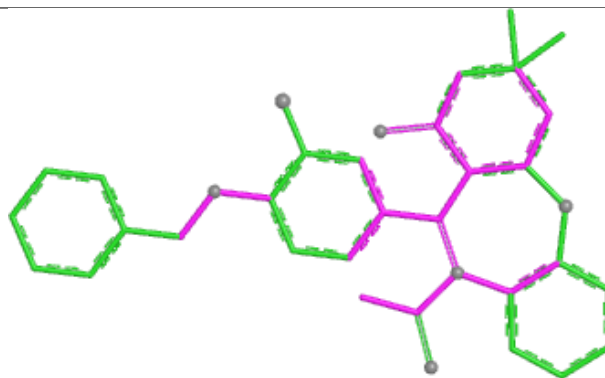
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	579	XNI	1	0

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.

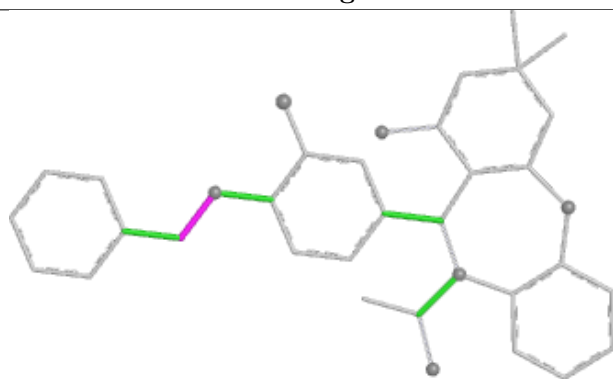
Ligand XNI B 579



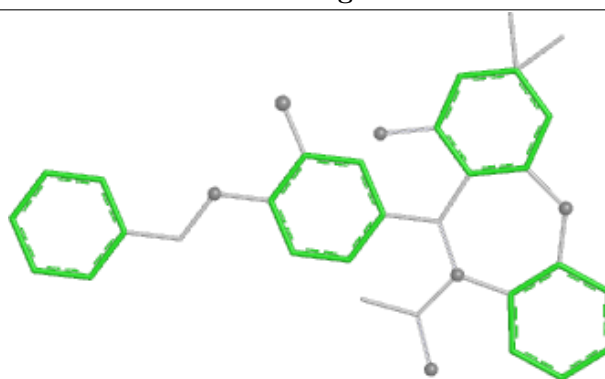
Bond lengths



Bond angles

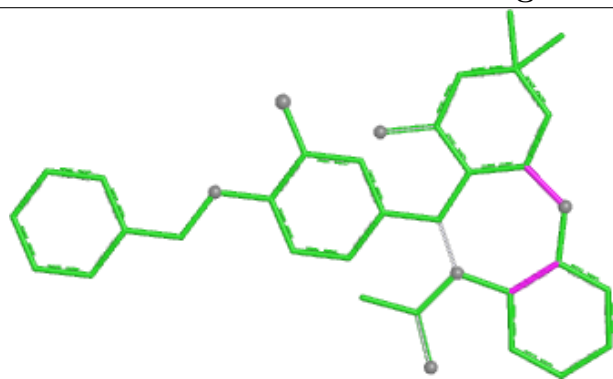


Torsions

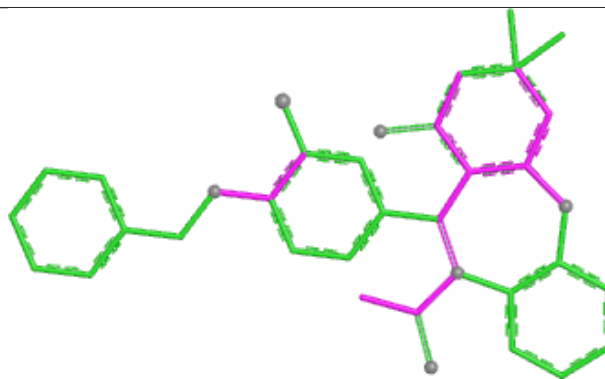


Rings

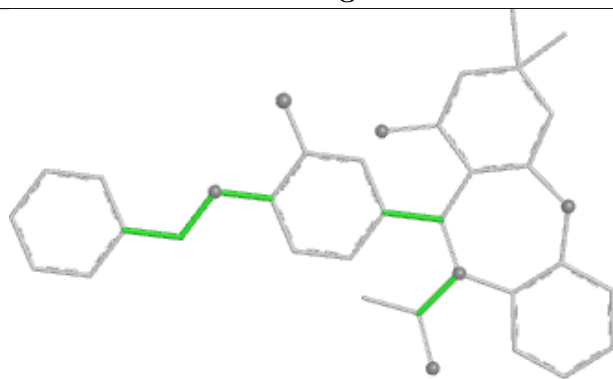
Ligand XNI A 579



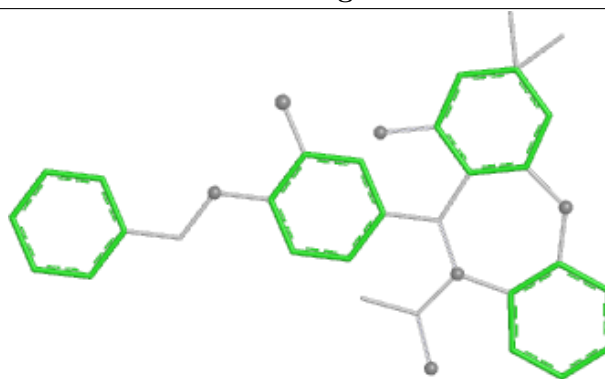
Bond lengths



Bond angles



Torsions



Rings

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	561/581 (96%)	-0.01	10 (1%) 67 65	20, 33, 48, 80	0
1	B	560/581 (96%)	0.21	16 (2%) 53 50	18, 32, 49, 70	2 (0%)
All	All	1121/1162 (96%)	0.10	26 (2%) 61 58	18, 33, 49, 80	2 (0%)

All (26) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	545	LEU	5.5
1	B	547	LEU	4.8
1	A	545	LEU	4.3
1	B	25	PRO	3.6
1	B	563	SER	3.5
1	B	546	ASP	3.4
1	B	532	THR	3.3
1	A	153	GLY	3.0
1	B	152	GLY	3.0
1	B	541	ALA	2.9
1	A	563	SER	2.8
1	B	531	ARG	2.7
1	A	148	GLN	2.6
1	B	513	SER	2.6
1	B	548	SER	2.5
1	A	150	GLU	2.5
1	A	544	GLN	2.4
1	B	153	GLY	2.4
1	A	222	ARG	2.4
1	A	202	GLU	2.3
1	B	544	GLN	2.3
1	B	23	ILE	2.3
1	B	502	HIS	2.2
1	A	149	PRO	2.2

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Mol	Chain	Res	Type	RSRZ
1	B	540	PRO	2.1
1	A	402	HIS	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](#)

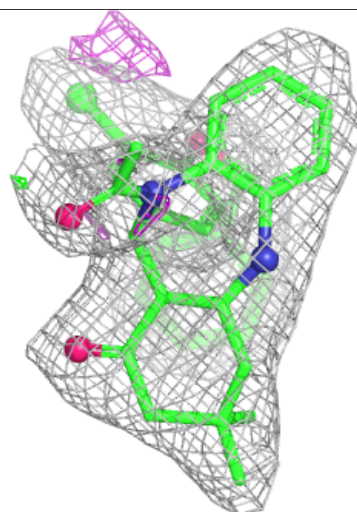
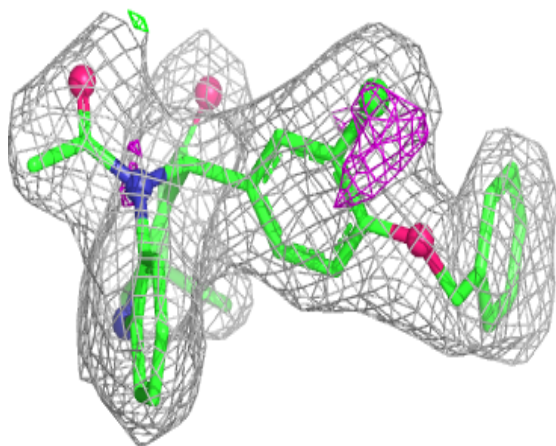
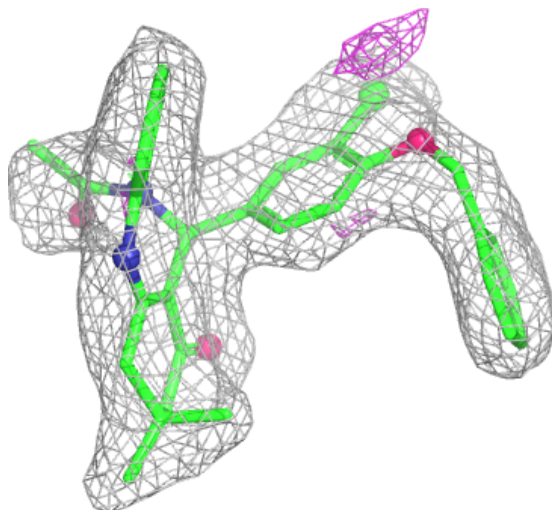
In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q < 0.9' lists 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
2	XNI	A	579	36/36	0.95	0.09	28,33,42,45	0
2	XNI	B	579	36/36	0.95	0.10	34,40,47,57	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.

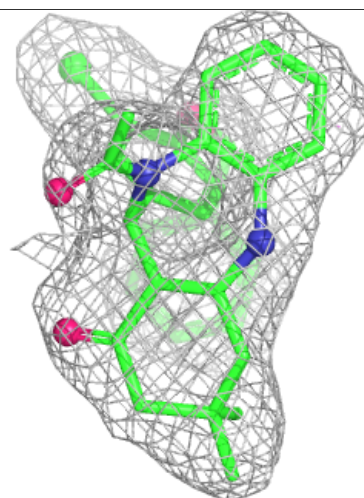
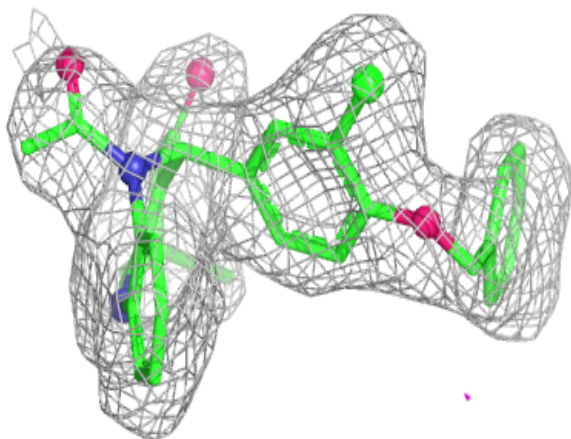
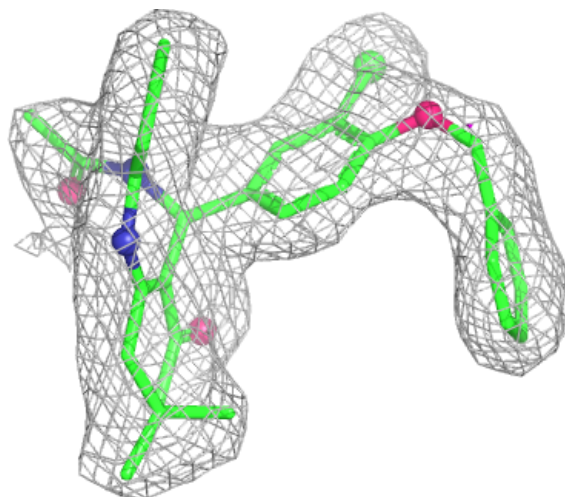
Electron density around XNI A 579:

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



Electron density around XNI B 579:

$2mF_o-DF_c$ (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.