



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 5, 2026 – 03:26 PM UTC

PDB ID : 3AI8 / pdb_00003ai8
Title : Cathepsin B in complex with the nitroxoline
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Deposited on : 2010-05-11
Resolution : 2.11 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
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

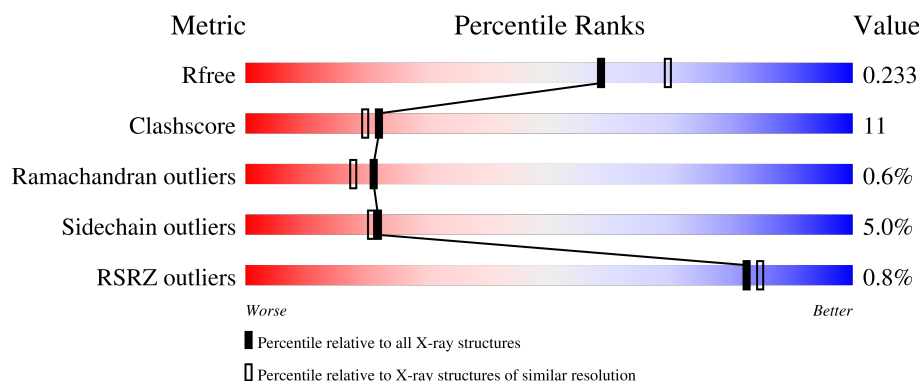
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

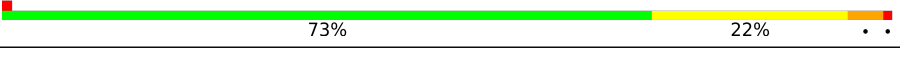
The reported resolution of this entry is 2.11 Å.

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	8290 (2.14-2.10)
Clashscore	190562	8817 (2.14-2.10)
Ramachandran outliers	187476	8738 (2.14-2.10)
Sidechain outliers	187428	8739 (2.14-2.10)
RSRZ outliers	180081	8294 (2.14-2.10)

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	256	 69% 29% ..
1	B	256	 73% 22% . .

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	HNQ	A	255	-	-	X	-
2	HNQ	B	255	-	X	X	-

2 Entry composition [i](#)

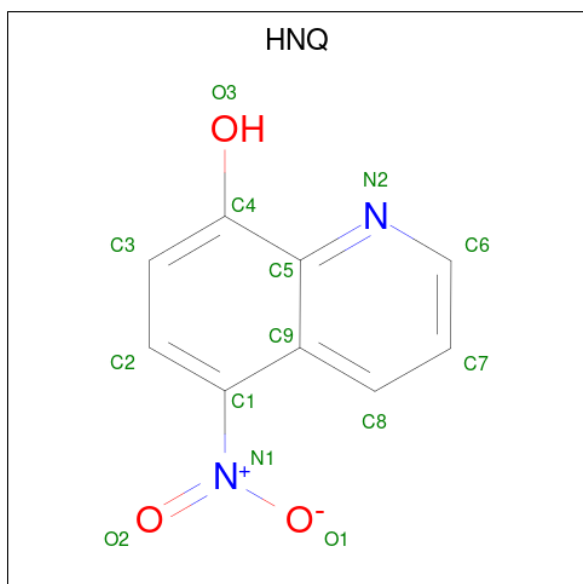
There are 3 unique types of molecules in this entry. The entry contains 4250 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Cathepsin B.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	B	256	Total	C	N	O	S	6	0	0
			1969	1234	337	380	18			
1	A	256	Total	C	N	O	S	11	0	0
			1969	1234	337	380	18			

- Molecule 2 is 5-nitroquinolin-8-ol (CCD ID: HNQ) (formula: $C_9H_6N_2O_3$).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	B	1	Total	C	N	O	0	0
			14	9	2	3		
2	A	1	Total	C	N	O	0	0
			14	9	2	3		

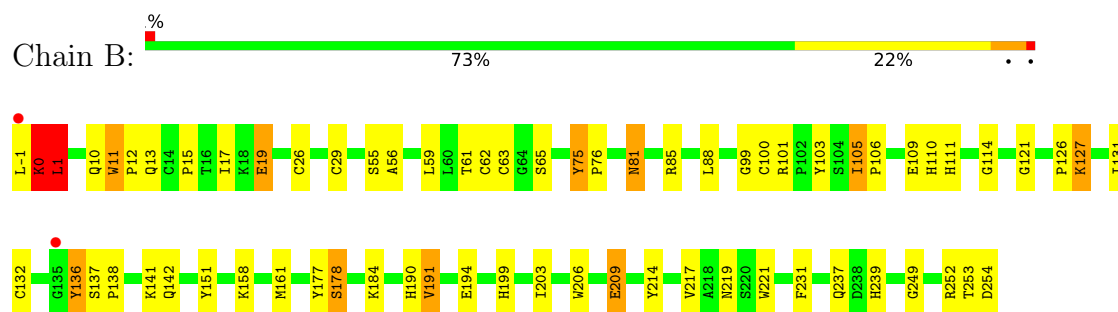
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	132	Total 132	O 132	0	0
3	A	152	Total 152	O 152	0	0

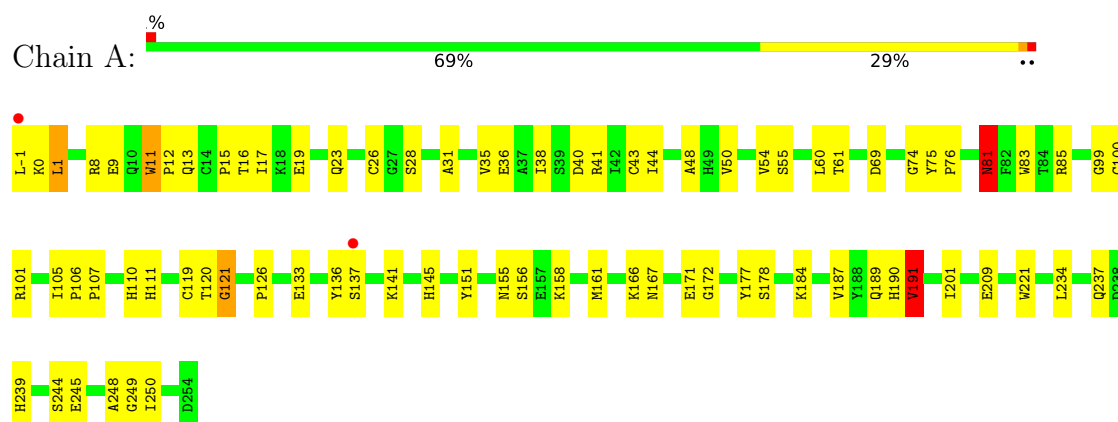
3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Cathepsin B



• Molecule 1: Cathepsin B



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	153.68Å 29.98Å 119.20Å 90.00° 126.25° 90.00°	Depositor
Resolution (Å)	29.10 – 2.11 29.10 – 2.11	Depositor EDS
% Data completeness (in resolution range)	86.2 (29.10-2.11) 86.5 (29.10-2.11)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	7.48 (at 2.10Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.183 , 0.244 0.183 , 0.233	Depositor DCC
R_{free} test set	1135 reflections (5.04%)	wwPDB-VP
Wilson B-factor (Å ²)	23.7	Xtriage
Anisotropy	0.137	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.38 , 57.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.45$, $\langle L^2 \rangle = 0.28$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	4250	wwPDB-VP
Average B, all atoms (Å ²)	22.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.44% 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: HNQ

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	1.20	6/2028 (0.3%)	1.35	20/2755 (0.7%)
1	B	1.09	1/2028 (0.0%)	1.31	21/2755 (0.8%)
All	All	1.15	7/4056 (0.2%)	1.33	41/5510 (0.7%)

All (7) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	248	ALA	CA-CB	7.03	1.62	1.54
1	A	81	ASN	C-O	-6.34	1.16	1.24
1	A	107	PRO	CA-C	6.12	1.60	1.52
1	B	203	ILE	CA-CB	5.95	1.61	1.54
1	A	36	GLU	C-O	5.29	1.30	1.24
1	A	83	TRP	C-O	-5.08	1.18	1.24
1	A	74	GLY	C-O	5.04	1.28	1.23

All (41) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	137	SER	CA-C-N	-15.91	104.72	120.31
1	A	137	SER	C-N-CA	-15.91	104.72	120.31
1	B	0	LYS	N-CA-C	-12.61	90.76	108.54
1	A	1	LEU	N-CA-C	7.86	119.62	109.64
1	B	106	PRO	N-CA-C	7.79	117.95	110.47
1	B	19	GLU	N-CA-C	7.63	122.13	109.46
1	B	55	SER	N-CA-C	7.57	120.40	108.67
1	B	11	TRP	CA-C-N	7.33	127.03	119.56
1	B	11	TRP	C-N-CA	7.33	127.03	119.56
1	B	136	TYR	N-CA-C	-6.82	97.41	108.52
1	A	136	TYR	N-CA-C	-6.76	98.68	109.76
1	B	137	SER	CA-C-N	-6.68	113.06	120.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	137	SER	C-N-CA	-6.68	113.06	120.14
1	A	250	ILE	CA-C-N	6.35	126.32	119.78
1	A	250	ILE	C-N-CA	6.35	126.32	119.78
1	A	167	ASN	N-CA-C	6.12	121.50	113.30
1	A	69	ASP	N-CA-C	6.09	120.01	111.30
1	A	177	TYR	N-CA-C	-6.05	100.76	110.14
1	B	253	THR	CB-CA-C	-5.89	100.14	109.80
1	A	191	VAL	CB-CA-C	-5.86	105.17	110.91
1	A	171	GLU	N-CA-C	-5.69	101.01	110.17
1	B	178	SER	N-CA-C	5.67	118.23	111.71
1	B	100	CYS	N-CA-C	5.61	117.20	111.14
1	B	101	ARG	CA-C-N	5.60	125.55	119.78
1	B	101	ARG	C-N-CA	5.60	125.55	119.78
1	B	105	ILE	CB-CA-C	5.50	116.36	110.53
1	A	50	VAL	CB-CA-C	-5.49	104.20	110.73
1	B	137	SER	N-CA-C	5.41	119.61	112.35
1	A	106	PRO	N-CA-C	5.30	117.17	110.70
1	B	56	ALA	N-CA-C	-5.29	105.51	111.28
1	A	172	GLY	N-CA-C	-5.28	103.25	111.12
1	B	177	TYR	N-CA-C	-5.25	102.00	110.14
1	B	191	VAL	N-CA-C	5.22	116.50	112.12
1	A	55	SER	N-CA-C	5.18	117.21	109.59
1	A	178	SER	N-CA-C	5.18	117.67	111.71
1	A	100	CYS	N-CA-C	5.16	116.59	110.97
1	A	105	ILE	CB-CA-C	5.11	116.65	110.78
1	B	1	LEU	CA-C-N	5.09	125.07	120.03
1	B	1	LEU	C-N-CA	5.09	125.07	120.03
1	A	11	TRP	CA-C-N	5.01	124.67	119.56
1	A	11	TRP	C-N-CA	5.01	124.67	119.56

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1969	0	1821	46	0
1	B	1969	0	1821	40	1
2	A	14	0	5	6	0
2	B	14	0	6	6	0
3	A	152	0	0	4	0
3	B	132	0	0	4	0
All	All	4250	0	3653	81	1

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 11.

All (81) 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:221:TRP:CZ2	2:A:255:HNQ:H2	2.06	0.90
1:B:221:TRP:CZ2	2:B:255:HNQ:H2	2.13	0.84
1:B:127:LYS:HD3	1:B:127:LYS:H	1.44	0.82
1:A:158:LYS:HA	1:A:161:MET:HE2	1.65	0.77
1:B:142:GLN:HE21	1:A:191:VAL:HG13	1.49	0.76
1:A:190:HIS:H	1:A:239:HIS:HE1	1.32	0.75
1:B:190:HIS:H	1:B:239:HIS:CE1	2.04	0.75
1:A:184:LYS:HE3	3:A:287:HOH:O	1.87	0.74
1:A:190:HIS:H	1:A:239:HIS:CE1	2.06	0.73
1:B:190:HIS:H	1:B:239:HIS:HE1	1.38	0.70
1:B:26:CYS:N	2:B:255:HNQ:H6	2.09	0.68
1:A:110:HIS:ND1	2:A:255:HNQ:O1	2.31	0.64
1:A:11:TRP:CD2	1:A:44:ILE:HG12	2.36	0.61
1:B:29:CYS:HB3	1:B:199:HIS:CE1	2.35	0.61
1:B:111:HIS:NE2	2:B:255:HNQ:O2	2.34	0.60
1:B:132:CYS:O	1:A:237:GLN:HG3	2.02	0.59
1:A:26:CYS:N	2:A:255:HNQ:H6	2.20	0.57
1:B:142:GLN:NE2	1:A:191:VAL:HG13	2.20	0.56
1:A:1:LEU:HD12	1:A:161:MET:HE3	1.87	0.55
1:B:151:TYR:CE2	1:B:249:GLY:HA2	2.41	0.55
1:A:151:TYR:CE2	1:A:249:GLY:HA2	2.42	0.55
1:A:11:TRP:CG	1:A:44:ILE:HG12	2.42	0.54
1:A:81:ASN:HD22	1:A:81:ASN:C	2.15	0.54
1:A:221:TRP:CZ2	2:A:255:HNQ:C2	2.87	0.54
1:A:187:VAL:O	1:A:189:GLN:HG3	2.08	0.53
1:B:110:HIS:ND1	2:B:255:HNQ:O1	2.41	0.53
1:B:26:CYS:H	2:B:255:HNQ:H6	1.74	0.52
1:B:221:TRP:CZ2	2:B:255:HNQ:C2	2.89	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:252:ARG:HG3	1:B:254:ASP:OD2	2.09	0.52
1:A:1:LEU:CD1	1:A:161:MET:HE3	2.39	0.52
1:A:23:GLN:NE2	2:A:255:HNQ:O3	2.43	0.52
1:B:0:LYS:HE3	1:B:0:LYS:HA	1.93	0.51
1:B:15:PRO:HD2	3:B:295:HOH:O	2.09	0.51
1:B:131:ILE:HD12	1:A:234:LEU:HD22	1.92	0.50
1:B:127:LYS:HD3	1:B:127:LYS:N	2.20	0.50
1:B:1:LEU:HD13	1:B:161:MET:HE2	1.94	0.49
1:A:23:GLN:NE2	2:A:255:HNQ:C4	2.76	0.49
1:A:15:PRO:O	1:A:19:GLU:HG3	2.13	0.49
1:B:161:MET:HE3	1:B:206:TRP:CE2	2.48	0.48
1:B:103:TYR:CE1	1:B:105:ILE:HB	2.49	0.48
1:B:219:ASN:HB3	3:B:271:HOH:O	2.14	0.48
1:A:110:HIS:O	1:A:111:HIS:HB2	2.14	0.47
1:B:99:GLY:HA2	1:B:136:TYR:CE2	2.49	0.47
1:B:132:CYS:H	1:A:237:GLN:NE2	2.13	0.47
1:A:81:ASN:ND2	1:A:85:ARG:HD3	2.30	0.47
1:B:10:GLN:HG3	1:B:11:TRP:CE2	2.50	0.47
1:A:110:HIS:NE2	1:A:119:CYS:SG	2.89	0.46
1:B:65:SER:HB2	3:B:298:HOH:O	2.14	0.46
1:B:75:TYR:HA	1:B:76:PRO:HD3	1.87	0.46
1:B:136:TYR:CE1	1:B:138:PRO:HG2	2.50	0.46
1:B:-1:LEU:HG	1:B:-1:LEU:O	2.16	0.45
1:B:109:GLU:OE1	1:B:114:GLY:HA3	2.16	0.45
1:A:16:THR:HA	1:A:19:GLU:HG3	1.98	0.45
1:A:75:TYR:HA	1:A:76:PRO:HD3	1.82	0.45
1:A:110:HIS:CD2	1:A:119:CYS:SG	3.10	0.45
1:A:9:GLU:O	1:A:12:PRO:HD3	2.16	0.44
1:A:43:CYS:SG	1:A:48:ALA:HA	2.57	0.44
1:B:59:LEU:HB2	1:B:88:LEU:CD2	2.48	0.44
1:A:38:ILE:HG22	1:A:54:VAL:HG21	1.99	0.44
1:A:145:HIS:HB3	3:A:297:HOH:O	2.17	0.43
1:A:31:ALA:O	1:A:35:VAL:HG22	2.18	0.43
1:A:99:GLY:O	1:A:133:GLU:OE2	2.37	0.43
1:A:61:THR:HG22	1:A:126:PRO:O	2.19	0.42
1:B:12:PRO:HB2	3:B:274:HOH:O	2.18	0.42
1:A:28:SER:HB3	1:A:60:LEU:HD13	2.01	0.42
1:A:201:ILE:HD12	1:A:201:ILE:C	2.45	0.42
1:A:41:ARG:HD3	1:A:249:GLY:O	2.19	0.42
1:A:8:ARG:HG2	1:A:17:ILE:HG22	2.02	0.41
1:A:155:ASN:ND2	1:A:244:SER:OG	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:120:THR:O	1:A:121:GLY:O	2.39	0.41
1:B:61:THR:HG21	1:B:126:PRO:HB2	2.02	0.41
1:A:13:GLN:HB2	3:A:275:HOH:O	2.21	0.41
1:B:13:GLN:O	1:B:15:PRO:HD3	2.21	0.41
1:A:101:ARG:HG2	3:A:306:HOH:O	2.19	0.41
1:B:62:CYS:O	1:B:63:CYS:C	2.61	0.41
1:B:209:GLU:HG2	1:B:214:TYR:CE2	2.55	0.41
1:B:217:VAL:HG11	1:B:231:PHE:CZ	2.56	0.41
1:A:23:GLN:HG3	1:A:26:CYS:O	2.20	0.41
1:A:17:ILE:HG12	1:A:40:ASP:CG	2.46	0.40
1:B:81:ASN:C	1:B:81:ASN:HD22	2.30	0.40
1:B:184:LYS:HD3	1:B:184:LYS:HA	1.86	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:19:GLU:OE2	1:B:85:ARG:NH2[1_545]	2.19	0.01

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	254/256 (99%)	243 (96%)	10 (4%)	1 (0%)	30	28
1	B	254/256 (99%)	244 (96%)	8 (3%)	2 (1%)	16	12
All	All	508/512 (99%)	487 (96%)	18 (4%)	3 (1%)	21	18

All (3) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	121	GLY

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Mol	Chain	Res	Type
1	B	1	LEU
1	A	121	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	211/211 (100%)	202 (96%)	9 (4%)	26	26
1	B	211/211 (100%)	199 (94%)	12 (6%)	18	16
All	All	422/422 (100%)	401 (95%)	21 (5%)	22	21

All (21) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	0	LYS
1	B	17	ILE
1	B	75	TYR
1	B	81	ASN
1	B	127	LYS
1	B	141	LYS
1	B	158	LYS
1	B	178	SER
1	B	191	VAL
1	B	194	GLU
1	B	209	GLU
1	B	237	GLN
1	A	-1	LEU
1	A	0	LYS
1	A	81	ASN
1	A	141	LYS
1	A	156	SER
1	A	166	LYS
1	A	191	VAL
1	A	209	GLU
1	A	245	GLU

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

Mol	Chain	Res	Type
1	B	10	GLN
1	B	23	GLN
1	B	49	HIS
1	B	81	ASN
1	B	113	ASN
1	B	142	GLN
1	B	190	HIS
1	B	239	HIS
1	A	23	GLN
1	A	81	ASN
1	A	113	ASN
1	A	155	ASN
1	A	167	ASN
1	A	190	HIS
1	A	237	GLN
1	A	239	HIS

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](#)

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	HNQ	A	255	-	15,15,15	6.80	11 (73%)	18,21,21	1.22	1 (5%)
2	HNQ	B	255	-	15,15,15	5.51	12 (80%)	18,21,21	1.48	3 (16%)

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	HNQ	A	255	-	-	2/2/4/4	0/2/2/2
2	HNQ	B	255	-	-	2/2/4/4	0/2/2/2

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	255	HNQ	O2-N1	-19.37	0.89	1.22
2	B	255	HNQ	O2-N1	-13.62	0.99	1.22
2	B	255	HNQ	C2-C1	-8.12	1.23	1.37
2	B	255	HNQ	C1-N1	-7.88	1.31	1.45
2	A	255	HNQ	C2-C1	-7.66	1.24	1.37
2	A	255	HNQ	C4-C5	-7.25	1.32	1.42
2	A	255	HNQ	C1-N1	-6.21	1.34	1.45
2	A	255	HNQ	C7-C8	-6.18	1.24	1.36
2	B	255	HNQ	C4-C5	-5.95	1.34	1.42
2	A	255	HNQ	C5-N2	-5.55	1.29	1.37
2	A	255	HNQ	O1-N1	-5.54	0.98	1.35
2	B	255	HNQ	C7-C8	-5.49	1.25	1.36
2	B	255	HNQ	C9-C5	-4.62	1.30	1.42
2	A	255	HNQ	C8-C9	-4.25	1.33	1.42
2	A	255	HNQ	C3-C4	-4.14	1.29	1.37
2	A	255	HNQ	C9-C5	-3.95	1.32	1.42
2	B	255	HNQ	C1-C9	-3.64	1.31	1.43
2	A	255	HNQ	C1-C9	-3.37	1.32	1.43
2	B	255	HNQ	C6-N2	-3.03	1.26	1.32
2	B	255	HNQ	O1-N1	-2.99	1.15	1.35
2	B	255	HNQ	C3-C4	-2.62	1.32	1.37
2	B	255	HNQ	C8-C9	-2.56	1.37	1.42
2	B	255	HNQ	C3-C2	-2.03	1.35	1.38

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	255	HNQ	C1-C9-C5	4.73	119.80	116.73
2	A	255	HNQ	C1-C9-C5	3.63	119.09	116.73
2	B	255	HNQ	C3-C4-C5	-2.06	117.80	120.11
2	B	255	HNQ	O2-N1-C1	-2.03	115.55	119.03

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	B	255	HNQ	C2-C1-N1-O2
2	B	255	HNQ	C9-C1-N1-O2
2	A	255	HNQ	C2-C1-N1-O2
2	A	255	HNQ	C9-C1-N1-O2

There are no ring outliers.

2 monomers are involved in 12 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	255	HNQ	6	0
2	B	255	HNQ	6	0

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	256/256 (100%)	-0.40	2 (0%) 82 85	8, 19, 34, 64	4 (1%)
1	B	256/256 (100%)	-0.24	2 (0%) 82 85	13, 22, 38, 63	3 (1%)
All	All	512/512 (100%)	-0.32	4 (0%) 82 85	8, 20, 36, 64	7 (1%)

All (4) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	-1	LEU	3.4
1	B	135	GLY	3.1
1	A	137	SER	2.1
1	A	-1	LEU	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	HNQ	A	255	14/14	0.75	0.21	29,34,38,39	14

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	HNQ	B	255	14/14	0.76	0.20	26,29,34,38	14

6.5 Other polymers [i](#)

There are no such residues in this entry.