



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 08:07 AM UTC

PDB ID : 3R2J / pdb_00003r2j
Title : Crystal Structure of PnC1 from *L. infantum* in complex with nicotinate
Authors : Gazanion, E.; Garcia, D.; Guichou, J.-F.; Labesse, G.; Sereno, D.; Vergnes, B.
Deposited on : 2011-03-14
Resolution : 2.68 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

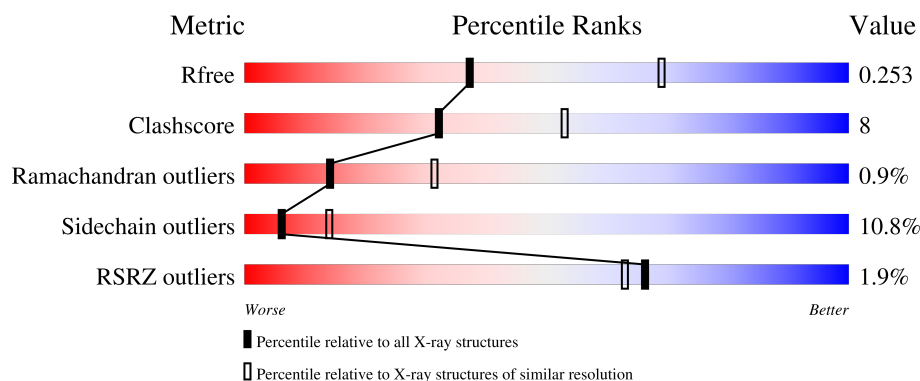
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.68 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	5070 (2.70-2.66)
Clashscore	190562	5409 (2.70-2.66)
Ramachandran outliers	187476	5324 (2.70-2.66)
Sidechain outliers	187428	5324 (2.70-2.66)
RSRZ outliers	180081	5070 (2.70-2.66)

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	227	0.2% 69% 18% 12%
1	B	227	2% 65% 18% 5% 12%
1	C	227	0.2% 67% 16% 13%
1	D	227	2% 68% 15% 12%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 6060 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 Alpha/beta-hydrolase-like protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	199	Total	C	N	O	S	0	0	0
			1469	925	257	280	7			
1	B	200	Total	C	N	O	S	0	0	0
			1485	937	259	282	7			
1	C	198	Total	C	N	O	S	0	0	0
			1471	928	257	279	7			
1	D	199	Total	C	N	O	S	0	0	0
			1474	930	257	280	7			

There are 88 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	-8	MET	-	expression tag	UNP A4HRG8
A	-7	ALA	-	expression tag	UNP A4HRG8
A	-6	HIS	-	expression tag	UNP A4HRG8
A	-5	HIS	-	expression tag	UNP A4HRG8
A	-4	HIS	-	expression tag	UNP A4HRG8
A	-3	HIS	-	expression tag	UNP A4HRG8
A	-2	HIS	-	expression tag	UNP A4HRG8
A	-1	HIS	-	expression tag	UNP A4HRG8
A	0	VAL	-	expression tag	UNP A4HRG8
A	1	GLY	-	expression tag	UNP A4HRG8
A	2	THR	-	expression tag	UNP A4HRG8
A	3	GLY	-	expression tag	UNP A4HRG8
A	4	SER	-	expression tag	UNP A4HRG8
A	5	ASN	-	expression tag	UNP A4HRG8
A	6	ASP	-	expression tag	UNP A4HRG8
A	7	ASP	-	expression tag	UNP A4HRG8
A	8	ASP	-	expression tag	UNP A4HRG8
A	9	ASP	-	expression tag	UNP A4HRG8
A	10	LYS	-	expression tag	UNP A4HRG8
A	11	SER	-	expression tag	UNP A4HRG8
A	12	PRO	-	expression tag	UNP A4HRG8

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Chain	Residue	Modelled	Actual	Comment	Reference
A	13	ASP	-	expression tag	UNP A4HRG8
B	-8	MET	-	expression tag	UNP A4HRG8
B	-7	ALA	-	expression tag	UNP A4HRG8
B	-6	HIS	-	expression tag	UNP A4HRG8
B	-5	HIS	-	expression tag	UNP A4HRG8
B	-4	HIS	-	expression tag	UNP A4HRG8
B	-3	HIS	-	expression tag	UNP A4HRG8
B	-2	HIS	-	expression tag	UNP A4HRG8
B	-1	HIS	-	expression tag	UNP A4HRG8
B	0	VAL	-	expression tag	UNP A4HRG8
B	1	GLY	-	expression tag	UNP A4HRG8
B	2	THR	-	expression tag	UNP A4HRG8
B	3	GLY	-	expression tag	UNP A4HRG8
B	4	SER	-	expression tag	UNP A4HRG8
B	5	ASN	-	expression tag	UNP A4HRG8
B	6	ASP	-	expression tag	UNP A4HRG8
B	7	ASP	-	expression tag	UNP A4HRG8
B	8	ASP	-	expression tag	UNP A4HRG8
B	9	ASP	-	expression tag	UNP A4HRG8
B	10	LYS	-	expression tag	UNP A4HRG8
B	11	SER	-	expression tag	UNP A4HRG8
B	12	PRO	-	expression tag	UNP A4HRG8
B	13	ASP	-	expression tag	UNP A4HRG8
C	-8	MET	-	expression tag	UNP A4HRG8
C	-7	ALA	-	expression tag	UNP A4HRG8
C	-6	HIS	-	expression tag	UNP A4HRG8
C	-5	HIS	-	expression tag	UNP A4HRG8
C	-4	HIS	-	expression tag	UNP A4HRG8
C	-3	HIS	-	expression tag	UNP A4HRG8
C	-2	HIS	-	expression tag	UNP A4HRG8
C	-1	HIS	-	expression tag	UNP A4HRG8
C	0	VAL	-	expression tag	UNP A4HRG8
C	1	GLY	-	expression tag	UNP A4HRG8
C	2	THR	-	expression tag	UNP A4HRG8
C	3	GLY	-	expression tag	UNP A4HRG8
C	4	SER	-	expression tag	UNP A4HRG8
C	5	ASN	-	expression tag	UNP A4HRG8
C	6	ASP	-	expression tag	UNP A4HRG8
C	7	ASP	-	expression tag	UNP A4HRG8
C	8	ASP	-	expression tag	UNP A4HRG8
C	9	ASP	-	expression tag	UNP A4HRG8
C	10	LYS	-	expression tag	UNP A4HRG8

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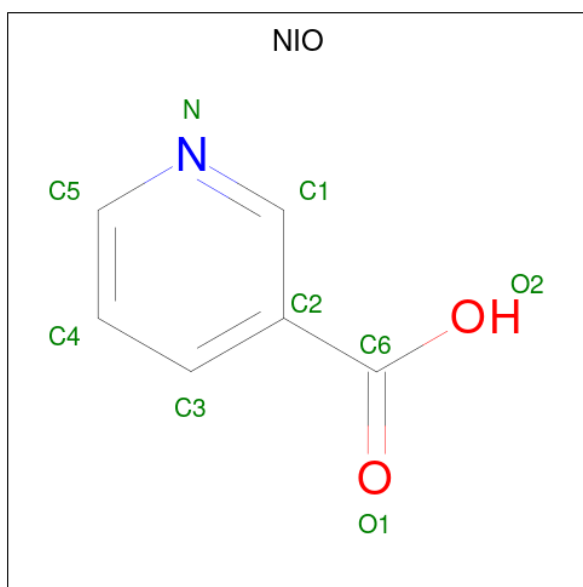
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Chain	Residue	Modelled	Actual	Comment	Reference
C	11	SER	-	expression tag	UNP A4HRG8
C	12	PRO	-	expression tag	UNP A4HRG8
C	13	ASP	-	expression tag	UNP A4HRG8
D	-8	MET	-	expression tag	UNP A4HRG8
D	-7	ALA	-	expression tag	UNP A4HRG8
D	-6	HIS	-	expression tag	UNP A4HRG8
D	-5	HIS	-	expression tag	UNP A4HRG8
D	-4	HIS	-	expression tag	UNP A4HRG8
D	-3	HIS	-	expression tag	UNP A4HRG8
D	-2	HIS	-	expression tag	UNP A4HRG8
D	-1	HIS	-	expression tag	UNP A4HRG8
D	0	VAL	-	expression tag	UNP A4HRG8
D	1	GLY	-	expression tag	UNP A4HRG8
D	2	THR	-	expression tag	UNP A4HRG8
D	3	GLY	-	expression tag	UNP A4HRG8
D	4	SER	-	expression tag	UNP A4HRG8
D	5	ASN	-	expression tag	UNP A4HRG8
D	6	ASP	-	expression tag	UNP A4HRG8
D	7	ASP	-	expression tag	UNP A4HRG8
D	8	ASP	-	expression tag	UNP A4HRG8
D	9	ASP	-	expression tag	UNP A4HRG8
D	10	LYS	-	expression tag	UNP A4HRG8
D	11	SER	-	expression tag	UNP A4HRG8
D	12	PRO	-	expression tag	UNP A4HRG8
D	13	ASP	-	expression tag	UNP A4HRG8

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

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
2	A	1	Total Zn 1 1	0	0
2	B	1	Total Zn 1 1	0	0
2	C	1	Total Zn 1 1	0	0
2	D	1	Total Zn 1 1	0	0

- Molecule 3 is NICOTINIC ACID (CCD ID: NIO) (formula: C₆H₅NO₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			9	6	1	2		
3	B	1	Total	C	N	O	0	0
			9	6	1	2		
3	C	1	Total	C	N	O	0	0
			9	6	1	2		
3	D	1	Total	C	N	O	0	0
			9	6	1	2		

- Molecule 4 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	1	Total	Cl	0	0
			1	1		
4	D	1	Total	Cl	0	0
			1	1		

- Molecule 5 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	27	Total	O	0	0
			27	27		
5	B	35	Total	O	0	0
			35	35		
5	C	31	Total	O	0	0
			31	31		

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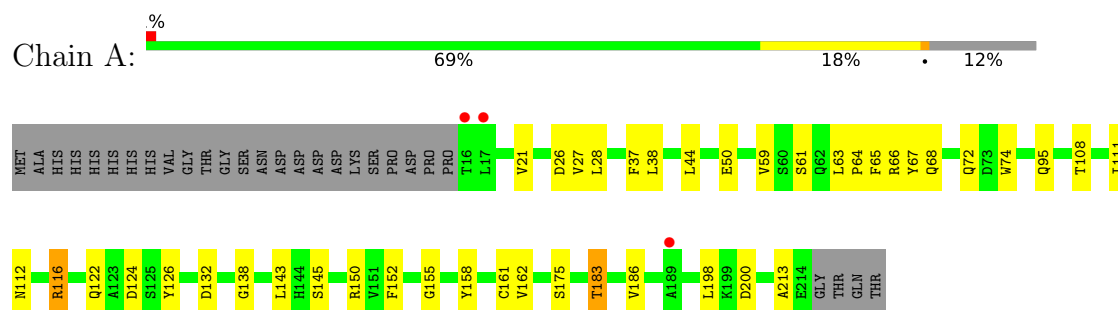
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	D	26	Total	O	0	0
			26	26		

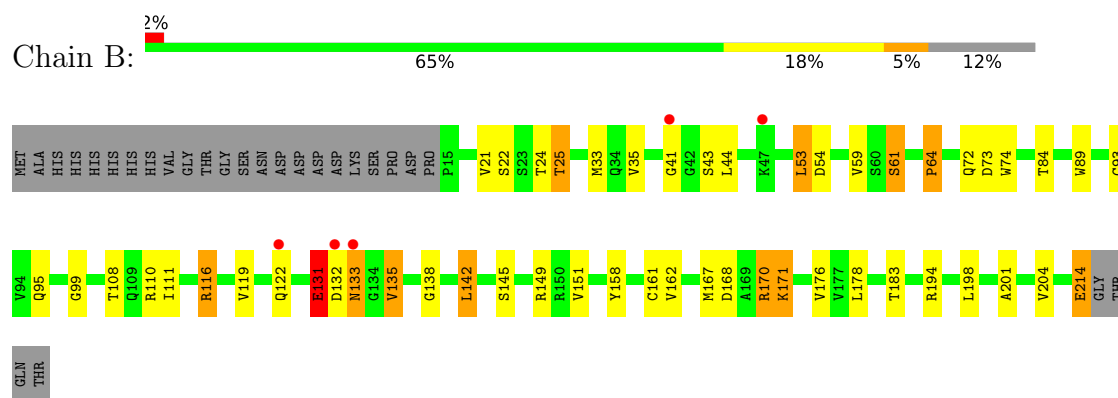
3 Residue-property plots [i](#)

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.

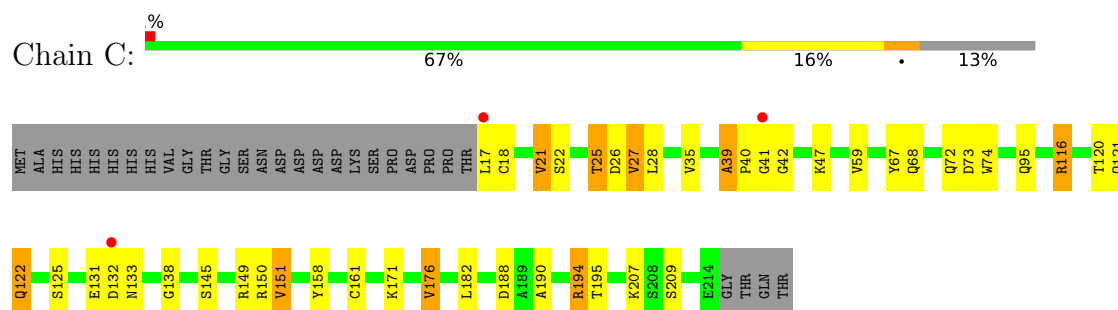
- Molecule 1: Alpha/beta-hydrolase-like protein



- Molecule 1: Alpha/beta-hydrolase-like protein

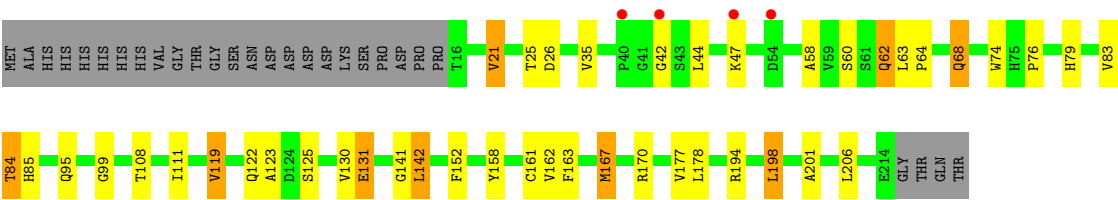


- Molecule 1: Alpha/beta-hydrolase-like protein



- Molecule 1: Alpha/beta-hydrolase-like protein





4 Data and refinement statistics

Property	Value	Source
Space group	P 4 21 2	Depositor
Cell constants a, b, c, α , β , γ	123.39Å 123.39Å 114.99Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	57.25 – 2.68 57.25 – 2.68	Depositor EDS
% Data completeness (in resolution range)	98.6 (57.25-2.68) 98.5 (57.25-2.68)	Depositor EDS
R_{merge}	0.11	Depositor
R_{sym}	0.10	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.64 (at 2.65Å)	Xtrriage
Refinement program	REFMAC 5.5.0102	Depositor
R, R_{free}	0.214 , 0.298 (Not available) , 0.253	Depositor DCC
R_{free} test set	1335 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	32.7	Xtrriage
Anisotropy	0.051	Xtrriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.32 , 33.9	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtrriage
Estimated twinning fraction	No twinning to report.	Xtrriage
F_o, F_c correlation	0.92	EDS
Total number of atoms	6060	wwPDB-VP
Average B, all atoms (Å ²)	28.0	wwPDB-VP

Xtrriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 32.02 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 1.0064e-03. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

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: NIO, CL, 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	0.56	0/1500	0.91	0/2046
1	B	0.61	0/1517	0.97	2/2068 (0.1%)
1	C	0.59	1/1502 (0.1%)	0.97	5/2047 (0.2%)
1	D	0.61	0/1505	0.93	1/2052 (0.0%)
All	All	0.59	1/6024 (0.0%)	0.94	8/8213 (0.1%)

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	21	VAL	CA-CB	5.08	1.59	1.53

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	40	PRO	N-CA-C	7.25	124.55	113.75
1	C	176	VAL	N-CA-C	5.82	116.50	108.12
1	B	41	GLY	N-CA-C	-5.71	104.77	112.14
1	C	73	ASP	N-CA-C	-5.52	101.88	110.10
1	D	123	ALA	N-CA-C	5.28	117.98	108.48
1	C	39	ALA	CA-C-N	5.19	125.23	119.32
1	C	39	ALA	C-N-CA	5.19	125.23	119.32
1	B	61	SER	N-CA-C	5.02	116.44	111.07

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	1469	0	1419	23	0
1	B	1485	0	1452	27	0
1	C	1471	0	1437	21	0
1	D	1474	0	1438	26	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
2	D	1	0	0	0	0
3	A	9	0	4	1	0
3	B	9	0	4	1	0
3	C	9	0	4	1	0
3	D	9	0	4	1	0
4	B	1	0	0	0	0
4	D	1	0	0	0	0
5	A	27	0	0	1	0
5	B	35	0	0	0	0
5	C	31	0	0	0	0
5	D	26	0	0	0	0
All	All	6060	0	5762	93	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 (93) 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:D:167:MET:HE1	1:D:198:LEU:HD12	1.71	0.71
1:B:108:THR:HA	1:B:111:ILE:HD12	1.72	0.70
1:D:161:CYS:HB2	3:D:311:NIO:O1	1.91	0.70
1:D:167:MET:CE	1:D:198:LEU:HD12	2.24	0.67
1:A:108:THR:HA	1:A:111:ILE:HD12	1.77	0.66
1:A:161:CYS:HB2	3:A:311:NIO:O2	1.96	0.65
1:D:170:ARG:HD3	1:D:201:ALA:O	1.97	0.64
1:A:124:ASP:O	1:A:132:ASP:HB2	1.98	0.63
1:D:125:SER:HB2	1:D:131:GLU:HA	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:74:TRP:HD1	1:D:119:VAL:HG23	1.65	0.62
1:D:108:THR:HA	1:D:111:ILE:HD12	1.81	0.62
1:D:68:GLN:HB3	1:D:111:ILE:HA	1.81	0.62
1:A:150:ARG:HB3	1:A:175:SER:HB2	1.83	0.61
1:B:132:ASP:HB3	1:B:135:VAL:HG21	1.83	0.61
1:A:150:ARG:CB	1:A:175:SER:HB2	2.32	0.60
1:C:161:CYS:HB2	3:C:311:NIO:O2	2.02	0.60
1:B:72:GLN:OE1	1:B:116:ARG:NH2	2.30	0.60
1:C:27:VAL:HG22	1:C:67:TYR:HB3	1.85	0.58
1:D:84:THR:HG23	1:D:85:HIS:CD2	2.41	0.56
1:C:120:THR:HB	1:C:122:GLN:OE1	2.05	0.56
1:C:28:LEU:HB3	1:C:68:GLN:HG2	1.88	0.55
1:B:168:ASP:OD1	1:B:171:LYS:CE	2.55	0.55
1:A:26:ASP:HB3	1:A:152:PHE:HE1	1.72	0.55
1:A:138:GLY:HA3	1:B:142:LEU:HD13	1.89	0.55
1:C:145:SER:HB2	1:D:141:GLY:HA3	1.87	0.55
1:B:168:ASP:OD1	1:B:171:LYS:HE3	2.06	0.55
1:A:65:PHE:HE2	1:A:152:PHE:CD1	2.25	0.55
1:B:132:ASP:HB3	1:B:135:VAL:CG2	2.37	0.55
1:C:158:TYR:OH	1:C:195:THR:OG1	2.18	0.54
1:B:142:LEU:C	1:B:142:LEU:HD12	2.33	0.54
1:B:170:ARG:HD3	1:B:201:ALA:O	2.09	0.53
1:C:39:ALA:O	1:C:42:GLY:HA3	2.10	0.51
1:A:74:TRP:CD1	1:A:95:GLN:HG2	2.45	0.51
1:C:74:TRP:CG	1:C:116:ARG:HG2	2.46	0.50
1:A:28:LEU:HB3	1:A:68:GLN:HG2	1.94	0.50
1:C:207:LYS:HD2	1:C:209:SER:OG	2.12	0.50
1:D:58:ALA:O	1:D:62:GLN:HB2	2.13	0.49
1:B:73:ASP:O	1:B:93:CYS:HB3	2.13	0.49
1:D:21:VAL:HG13	1:D:63:LEU:HD22	1.95	0.48
1:A:37:PHE:HA	1:A:44:LEU:O	2.14	0.48
1:B:161:CYS:HB2	3:B:311:NIO:O2	2.13	0.48
1:B:64:PRO:HA	1:B:110:ARG:HH22	1.79	0.47
1:B:132:ASP:O	1:B:133:ASN:CB	2.63	0.47
1:D:21:VAL:HG11	1:D:63:LEU:HD13	1.97	0.46
1:A:67:TYR:CZ	1:A:112:ASN:HB2	2.50	0.46
1:B:35:VAL:HB	1:B:99:GLY:HA2	1.97	0.46
1:A:155:GLY:O	1:A:183:THR:HG22	2.16	0.46
1:C:125:SER:HB2	1:C:131:GLU:HA	1.98	0.45
1:A:158:TYR:HA	1:A:162:VAL:HB	1.99	0.45
1:C:26:ASP:OD1	1:C:150:ARG:HB3	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:MET:HE1	1:D:198:LEU:HA	1.97	0.45
1:A:59:VAL:HG13	1:A:63:LEU:HD12	1.99	0.45
1:B:158:TYR:HA	1:B:162:VAL:HB	1.99	0.45
1:C:72:GLN:OE1	1:C:116:ARG:NH2	2.49	0.45
1:B:44:LEU:HD21	1:B:89:TRP:CE3	2.52	0.45
1:C:151:VAL:HG23	1:C:176:VAL:HG22	1.98	0.45
1:A:63:LEU:HA	1:A:64:PRO:HD3	1.71	0.44
1:B:21:VAL:O	1:B:214:GLU:HG2	2.17	0.44
1:C:138:GLY:HA3	1:D:142:LEU:HD13	1.99	0.44
1:B:132:ASP:O	1:B:133:ASN:HB2	2.17	0.44
1:D:142:LEU:C	1:D:142:LEU:HD12	2.43	0.44
1:C:190:ALA:O	1:C:194:ARG:HB2	2.18	0.44
1:A:61:SER:HB3	5:A:407:HOH:O	2.18	0.43
1:A:26:ASP:OD1	1:A:150:ARG:HG2	2.19	0.43
1:C:39:ALA:C	1:C:41:GLY:HA3	2.44	0.42
1:D:163:PHE:CE1	1:D:198:LEU:HD13	2.54	0.42
1:C:25:THR:HG23	1:C:149:ARG:HB2	2.01	0.42
1:D:74:TRP:CD1	1:D:95:GLN:HG2	2.54	0.42
1:C:122:GLN:H	1:C:122:GLN:CD	2.28	0.42
1:B:74:TRP:CD1	1:B:95:GLN:HG2	2.54	0.42
1:A:74:TRP:CG	1:A:116:ARG:HG2	2.54	0.42
1:B:131:GLU:HG3	1:B:132:ASP:N	2.35	0.42
1:D:125:SER:CB	1:D:131:GLU:HA	2.49	0.42
1:A:126:TYR:O	1:A:161:CYS:HA	2.20	0.41
1:B:170:ARG:HG2	1:B:176:VAL:CG2	2.50	0.41
1:D:60:SER:OG	1:D:68:GLN:NE2	2.53	0.41
1:B:53:LEU:O	1:B:54:ASP:C	2.63	0.41
1:B:158:TYR:CD1	1:B:183:THR:HG21	2.56	0.41
1:D:35:VAL:HB	1:D:99:GLY:HA2	2.03	0.41
1:B:168:ASP:HA	1:B:171:LYS:HE2	2.03	0.41
1:A:27:VAL:HG11	1:A:143:LEU:HD22	2.02	0.41
1:D:152:PHE:HA	1:D:177:VAL:O	2.20	0.41
1:D:158:TYR:HA	1:D:162:VAL:HB	2.02	0.41
1:A:72:GLN:OE1	1:A:116:ARG:NH2	2.46	0.41
1:C:22:SER:OG	1:C:25:THR:HB	2.21	0.41
1:D:21:VAL:HA	1:D:26:ASP:OD2	2.21	0.41
1:D:21:VAL:HG22	1:D:64:PRO:HD2	2.02	0.40
1:D:76:PRO:HD2	1:D:79:HIS:HD2	1.86	0.40
1:B:33:MET:HE3	1:B:53:LEU:HD13	2.02	0.40
1:B:22:SER:HB3	1:B:25:THR:HG22	2.04	0.40
1:A:145:SER:OG	1:B:138:GLY:HA2	2.22	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:74:TRP:CD1	1:C:95:GLN:HG2	2.56	0.40
1:C:131:GLU:C	1:C:133:ASN:H	2.29	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	197/227 (87%)	190 (96%)	6 (3%)	1 (0%)	24	45
1	B	198/227 (87%)	181 (91%)	14 (7%)	3 (2%)	8	19
1	C	196/227 (86%)	185 (94%)	9 (5%)	2 (1%)	12	28
1	D	197/227 (87%)	182 (92%)	14 (7%)	1 (0%)	24	45
All	All	788/908 (87%)	738 (94%)	43 (6%)	7 (1%)	14	31

All (7) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	133	ASN
1	C	18	CYS
1	C	132	ASP
1	D	42	GLY
1	A	213	ALA
1	B	64	PRO
1	B	131	GLU

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	153/180 (85%)	143 (94%)	10 (6%)	15	34
1	B	157/180 (87%)	133 (85%)	24 (15%)	3	6
1	C	155/180 (86%)	140 (90%)	15 (10%)	8	17
1	D	155/180 (86%)	137 (88%)	18 (12%)	5	12
All	All	620/720 (86%)	553 (89%)	67 (11%)	6	14

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

Mol	Chain	Res	Type
1	A	21	VAL
1	A	38	LEU
1	A	50	GLU
1	A	66	ARG
1	A	116	ARG
1	A	122	GLN
1	A	183	THR
1	A	186	VAL
1	A	198	LEU
1	A	200	ASP
1	B	24	THR
1	B	25	THR
1	B	43	SER
1	B	53	LEU
1	B	59	VAL
1	B	61	SER
1	B	84	THR
1	B	116	ARG
1	B	119	VAL
1	B	122	GLN
1	B	131	GLU
1	B	135	VAL
1	B	142	LEU
1	B	145	SER
1	B	149	ARG
1	B	151	VAL
1	B	167	MET
1	B	170	ARG
1	B	171	LYS
1	B	178	LEU

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Mol	Chain	Res	Type
1	B	194	ARG
1	B	198	LEU
1	B	204	VAL
1	B	214	GLU
1	C	17	LEU
1	C	21	VAL
1	C	25	THR
1	C	27	VAL
1	C	35	VAL
1	C	47	LYS
1	C	59	VAL
1	C	116	ARG
1	C	121	GLN
1	C	122	GLN
1	C	151	VAL
1	C	171	LYS
1	C	182	LEU
1	C	188	ASP
1	C	194	ARG
1	D	21	VAL
1	D	25	THR
1	D	44	LEU
1	D	47	LYS
1	D	62	GLN
1	D	68	GLN
1	D	83	VAL
1	D	84	THR
1	D	119	VAL
1	D	122	GLN
1	D	130	VAL
1	D	131	GLU
1	D	142	LEU
1	D	167	MET
1	D	178	LEU
1	D	194	ARG
1	D	198	LEU
1	D	206	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	62	GLN

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Mol	Chain	Res	Type
1	A	101	GLN
1	B	85	HIS
1	B	133	ASN
1	B	144	HIS
1	C	101	GLN
1	C	121	GLN
1	C	122	GLN
1	C	144	HIS
1	D	68	GLN
1	D	85	HIS
1	D	107	HIS

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 10 ligands modelled in this entry, 6 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
3	NIO	C	311	2	9,9,9	1.02	0	11,11,11	1.33	2 (18%)
3	NIO	D	311	2	9,9,9	1.36	1 (11%)	11,11,11	1.30	2 (18%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
3	NIO	B	311	2	9,9,9	1.01	0	11,11,11	1.32	2 (18%)
3	NIO	A	311	2	9,9,9	1.03	1 (11%)	11,11,11	1.37	2 (18%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
3	NIO	C	311	2	-	0/4/4/4	0/1/1/1
3	NIO	D	311	2	-	4/4/4/4	0/1/1/1
3	NIO	B	311	2	-	4/4/4/4	0/1/1/1
3	NIO	A	311	2	-	0/4/4/4	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	D	311	NIO	C2-C6	3.34	1.56	1.49
3	A	311	NIO	C2-C6	2.19	1.54	1.49

All (8) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	311	NIO	C5-N-C1	2.81	121.77	116.85
3	D	311	NIO	C5-N-C1	2.77	121.71	116.85
3	B	311	NIO	C5-N-C1	2.40	121.06	116.85
3	A	311	NIO	C4-C3-C2	-2.30	118.10	120.36
3	A	311	NIO	C5-N-C1	2.30	120.88	116.85
3	D	311	NIO	O2-C6-C2	2.10	120.23	114.84
3	C	311	NIO	C2-C1-N	-2.08	120.41	123.50
3	B	311	NIO	C2-C1-N	-2.07	120.42	123.50

There are no chirality outliers.

All (8) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	311	NIO	C1-C2-C6-O1
3	B	311	NIO	C1-C2-C6-O2
3	B	311	NIO	C3-C2-C6-O1
3	B	311	NIO	C3-C2-C6-O2

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Mol	Chain	Res	Type	Atoms
3	D	311	NIO	C3-C2-C6-O2
3	D	311	NIO	C3-C2-C6-O1
3	D	311	NIO	C1-C2-C6-O2
3	D	311	NIO	C1-C2-C6-O1

There are no ring outliers.

4 monomers are involved in 4 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	311	NIO	1	0
3	D	311	NIO	1	0
3	B	311	NIO	1	0
3	A	311	NIO	1	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	199/227 (87%)	0.09	3 (1%) 72 69	13, 28, 53, 67	6 (3%)
1	B	200/227 (88%)	0.14	5 (2%) 58 54	13, 29, 46, 56	9 (4%)
1	C	198/227 (87%)	-0.03	3 (1%) 72 69	14, 26, 46, 61	6 (3%)
1	D	199/227 (87%)	0.01	4 (2%) 65 61	11, 26, 43, 51	11 (5%)
All	All	796/908 (87%)	0.05	15 (1%) 66 63	11, 27, 47, 67	32 (4%)

All (15) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	189	ALA	6.2
1	B	132	ASP	3.7
1	C	17	LEU	3.3
1	A	16	THR	3.1
1	C	41	GLY	3.1
1	D	42	GLY	2.9
1	D	47	LYS	2.4
1	B	47	LYS	2.3
1	B	133	ASN	2.2
1	B	41	GLY	2.2
1	D	54	ASP	2.2
1	A	17	LEU	2.1
1	D	40	PRO	2.1
1	C	132	ASP	2.1
1	B	122	GLN	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
3	NIO	B	311	9/9	0.95	0.09	22,23,26,26	0
3	NIO	D	311	9/9	0.95	0.10	26,27,31,31	0
3	NIO	A	311	9/9	0.97	0.07	24,26,27,28	0
3	NIO	C	311	9/9	0.98	0.06	13,16,17,18	0
2	ZN	B	301	1/1	0.98	0.03	30,30,30,30	0
4	CL	D	321	1/1	0.98	0.08	27,27,27,27	0
2	ZN	D	301	1/1	0.99	0.02	27,27,27,27	0
2	ZN	A	301	1/1	0.99	0.03	19,19,19,19	0
4	CL	B	321	1/1	0.99	0.10	30,30,30,30	0
2	ZN	C	301	1/1	0.99	0.04	23,23,23,23	0

6.5 Other polymers [i](#)

There are no such residues in this entry.