



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 10, 2026 – 09:41 AM UTC

PDB ID : 3EPV / pdb_00003epv
Title : X-ray Structure of the Metal-sensor CnrX in both the Apo- and Copper-bound Forms
Authors : Pompidor, G.; Maillard, A.P.; Girard, E.; Gambarelli, S.; Kahn, R.; Coves, J.
Deposited on : 2008-09-30
Resolution : 1.74 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

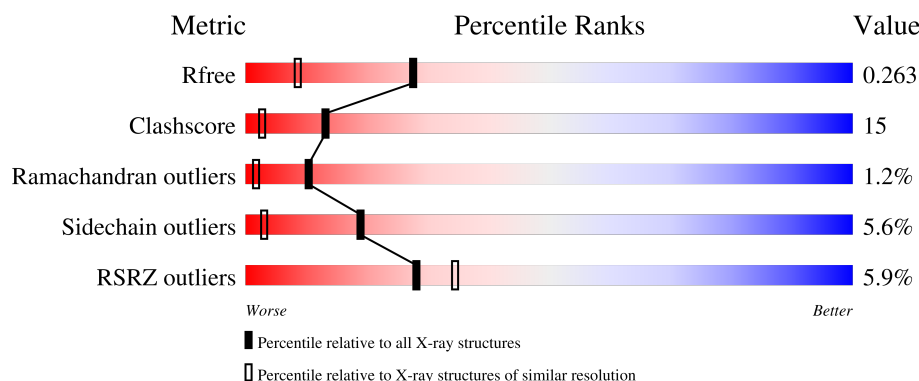
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.74 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	1187 (1.74-1.74)
Clashscore	190562	1207 (1.74-1.74)
Ramachandran outliers	187476	1200 (1.74-1.74)
Sidechain outliers	187428	1200 (1.74-1.74)
RSRZ outliers	180081	1188 (1.74-1.74)

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	109	3% 67% 25% 5% .
1	B	109	2% 64% 30% . .
1	C	109	3% 74% 20% . .
1	D	109	16% 59% 28% 9% 5%

2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 3940 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 Nickel and cobalt resistance protein cnrR.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	105	Total ?	C	N	O	Se	0	3	1	
			839 1	518	161	157	2				
1	B	109	Total	C	N	O	Se	0	3	0	
			887	548	170	167	2				
1	C	106	Total	C	N	O	Se	0	3	0	
			873	544	167	159	3				
1	D	109	Total	C	N	O	Se	0	4	0	
			897	554	174	167	2				

- Molecule 2 is COPPER (II) ION (CCD ID: CU) (formula: Cu).

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

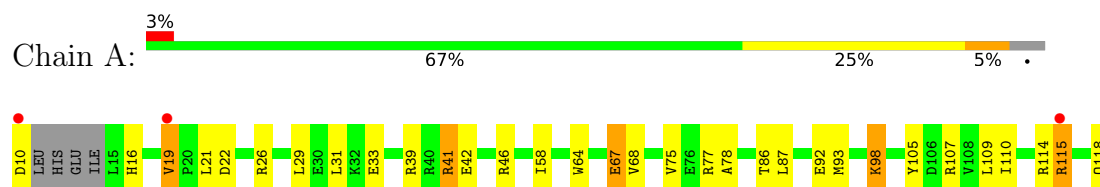
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	109	Total	O	0	0
			109	109		
3	B	121	Total	O	0	0
			121	121		
3	C	127	Total	O	0	0
			127	127		
3	D	84	Total	O	0	0
			84	84		

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: Nickel and cobalt resistance protein *cnrR*



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	31.94Å 77.89Å 93.20Å 90.00° 90.17° 90.00°	Depositor
Resolution (Å)	40.00 – 1.74 40.00 – 1.74	Depositor EDS
% Data completeness (in resolution range)	97.5 (40.00-1.74) 97.5 (40.00-1.74)	Depositor EDS
R_{merge}	0.04	Depositor
R_{sym}	0.04	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.70 (at 1.74Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.196 , 0.259 (Not available) , 0.263	Depositor DCC
R_{free} test set	2294 reflections (4.91%)	wwPDB-VP
Wilson B-factor (Å ²)	23.1	Xtriage
Anisotropy	0.171	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 49.6	EDS
L-test for twinning ²	$\langle L \rangle = 0.40$, $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	0.217 for h,-k,-l	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3940	wwPDB-VP
Average B, all atoms (Å ²)	26.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.66% 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: CU

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	1.86	14/870 (1.6%)	1.58	8/1171 (0.7%)
1	B	1.91	11/909 (1.2%)	1.65	14/1224 (1.1%)
1	C	1.75	8/897 (0.9%)	1.46	5/1208 (0.4%)
1	D	1.78	14/921 (1.5%)	1.65	17/1238 (1.4%)
All	All	1.82	47/3597 (1.3%)	1.59	44/4841 (0.9%)

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	2
1	D	0	2
All	All	0	5

All (47) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	104	ALA	CA-CB	-10.87	1.36	1.53
1	B	30	GLU	N-CA	8.84	1.57	1.46
1	B	15	LEU	CA-C	8.37	1.64	1.52
1	B	78	ALA	CA-CB	7.80	1.65	1.53
1	C	80	GLY	N-CA	7.26	1.54	1.45
1	C	54	LEU	C-O	6.87	1.32	1.24
1	C	95	ALA	CA-CB	-6.85	1.41	1.53
1	A	86	THR	N-CA	6.83	1.54	1.46
1	A	109	LEU	C-O	6.82	1.31	1.24
1	A	78	ALA	CA-CB	-6.73	1.42	1.53
1	A	67	GLU	CG-CD	6.59	1.68	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	34	ASP	CA-C	6.32	1.59	1.52
1	A	64	TRP	C-O	6.26	1.30	1.23
1	A	110	ILE	CA-CB	6.20	1.62	1.54
1	A	68	VAL	CA-CB	6.10	1.62	1.54
1	D	19	VAL	CA-C	6.10	1.59	1.52
1	A	19	VAL	CA-CB	5.93	1.61	1.54
1	B	86	THR	C-O	-5.88	1.17	1.24
1	B	83	GLN	N-CA	-5.83	1.39	1.46
1	D	71	ALA	CA-CB	-5.74	1.44	1.53
1	B	88	VAL	C-O	-5.74	1.17	1.24
1	C	79	ALA	N-CA	-5.73	1.39	1.46
1	A	67	GLU	CD-OE2	5.69	1.36	1.25
1	D	63	ALA	CA-CB	5.68	1.63	1.53
1	A	92	GLU	N-CA	-5.68	1.39	1.46
1	B	37	ALA	N-CA	5.59	1.53	1.46
1	D	105	TYR	N-CA	5.57	1.52	1.46
1	A	98	LYS	N-CA	5.50	1.52	1.45
1	D	49	ALA	CA-CB	-5.48	1.44	1.53
1	D	64	TRP	CA-C	5.47	1.59	1.53
1	B	49	ALA	CA-CB	-5.46	1.44	1.53
1	D	68	VAL	CA-CB	5.46	1.61	1.54
1	D	78	ALA	C-O	5.44	1.30	1.24
1	D	113	LEU	C-O	-5.44	1.17	1.24
1	C	101	HIS	CA-C	5.43	1.60	1.52
1	B	83	GLN	CA-C	5.42	1.59	1.52
1	C	52	GLY	N-CA	5.36	1.53	1.45
1	C	30	GLU	N-CA	5.34	1.52	1.46
1	A	58	ILE	C-O	5.22	1.30	1.24
1	D	82	LEU	N-CA	-5.21	1.40	1.46
1	D	58	ILE	CA-C	5.18	1.59	1.52
1	A	41	ARG	C-O	5.16	1.30	1.24
1	C	95	ALA	N-CA	5.09	1.52	1.46
1	D	87	LEU	C-O	-5.07	1.18	1.24
1	B	76	GLU	N-CA	5.05	1.52	1.46
1	A	75	VAL	C-O	5.03	1.30	1.24
1	B	84	ARG	CZ-NH2	-5.01	1.26	1.33

All (44) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	19	VAL	CA-C-N	11.77	134.55	119.84
1	D	19	VAL	C-N-CA	11.77	134.55	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	15	LEU	N-CA-C	11.70	128.72	112.45
1	B	84	ARG	NE-CZ-NH2	-10.71	109.56	119.20
1	B	35	ALA	N-CA-C	-7.94	102.71	111.36
1	D	34	ASP	N-CA-C	7.23	125.43	113.50
1	D	19	VAL	N-CA-C	6.91	123.80	108.88
1	C	18	ALA	N-CA-C	6.87	122.62	112.94
1	A	107	ARG	NE-CZ-NH2	-6.78	113.10	119.20
1	B	84	ARG	NE-CZ-NH1	6.36	127.86	121.50
1	A	46	ARG	NE-CZ-NH1	6.03	127.53	121.50
1	D	46	ARG	NE-CZ-NH2	-5.99	113.81	119.20
1	A	67	GLU	CB-CG-CD	5.98	122.77	112.60
1	D	32	LYS	N-CA-C	-5.96	105.85	113.01
1	D	68	VAL	N-CA-C	5.95	116.69	110.62
1	A	19	VAL	CA-C-N	-5.93	113.83	119.76
1	A	19	VAL	C-N-CA	-5.93	113.83	119.76
1	B	82	LEU	CB-CG-CD1	-5.93	92.92	110.70
1	A	67	GLU	N-CA-C	-5.92	104.91	111.36
1	C	19	VAL	N-CA-CB	5.89	119.46	111.21
1	B	15	LEU	CA-C-N	5.78	132.58	121.54
1	B	15	LEU	C-N-CA	5.78	132.58	121.54
1	B	77	ARG	N-CA-C	-5.64	105.22	111.36
1	C	31	LEU	N-CA-C	-5.64	105.22	111.36
1	B	84	ARG	CG-CD-NE	-5.59	99.71	112.00
1	D	31	LEU	N-CA-C	5.53	119.75	111.96
1	B	65	SER	CA-C-N	5.47	125.56	119.32
1	B	65	SER	C-N-CA	5.47	125.56	119.32
1	A	67	GLU	N-CA-CB	5.45	118.22	110.16
1	D	18	ALA	N-CA-C	5.40	119.87	113.28
1	C	17	GLU	N-CA-C	5.36	116.81	111.07
1	D	105	TYR	CA-C-N	5.36	127.46	120.28
1	D	105	TYR	C-N-CA	5.36	127.46	120.28
1	D	19	VAL	CB-CA-C	-5.35	101.63	111.36
1	D	115	ARG	N-CA-C	-5.31	105.49	111.28
1	A	107	ARG	NE-CZ-NH1	5.24	126.74	121.50
1	B	48	ARG	CA-C-N	5.11	127.09	120.44
1	B	48	ARG	C-N-CA	5.11	127.09	120.44
1	D	98	LYS	CA-C-O	-5.08	114.95	120.69
1	B	50	ALA	N-CA-C	5.07	116.50	111.07
1	D	20	PRO	CA-C-N	5.05	130.80	121.70
1	D	20	PRO	C-N-CA	5.05	130.80	121.70
1	C	56	ASP	CB-CA-C	-5.05	102.93	110.90
1	D	22	ASP	N-CA-CB	5.02	118.58	110.85

There are no chirality outliers.

All (5) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	10	ASP	Peptide
1	B	15	LEU	Peptide
1	B	17	GLU	Peptide
1	D	19	VAL	Peptide
1	D	21	LEU	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	839	0	854	19	0
1	B	887	0	885	26	0
1	C	873	0	891	16	0
1	D	897	0	906	45	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	109	0	0	8	1
3	B	121	0	0	5	1
3	C	127	0	0	6	2
3	D	84	0	0	3	0
All	All	3940	0	3536	106	2

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 15.

All (106) 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:19:VAL:HG12	3:A:170:HOH:O	1.46	1.15
1:B:19:VAL:HG21	3:B:307:HOH:O	1.44	1.14
1:D:29:LEU:O	1:D:93[B]:MSE:HE1	1.60	1.01
1:A:29:LEU:HD13	1:A:93[B]:MSE:HE3	1.43	0.99
1:D:34:ASP:H	1:D:35:ALA:HB3	1.24	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:45:THR:HA	1:D:48:ARG:HD2	1.45	0.97
1:D:35:ALA:O	1:D:37:ALA:N	1.97	0.97
1:A:29:LEU:HD13	1:A:93[B]:MSE:CE	2.05	0.86
1:D:31:LEU:HD13	1:D:32:LYS:H	1.40	0.86
1:D:32:LYS:HB2	3:D:179:HOH:O	1.74	0.85
1:D:45:THR:HA	1:D:48:ARG:CD	2.11	0.81
1:B:14:ILE:O	1:B:18:ALA:HB2	1.82	0.79
1:B:30:GLU:OE2	3:B:306:HOH:O	2.01	0.77
1:A:16:HIS:CE1	1:A:33:GLU:OE2	2.38	0.77
1:C:115:ARG:NE	1:C:115:ARG:HA	1.99	0.77
1:C:115:ARG:HA	1:C:115:ARG:HE	1.51	0.76
1:D:35:ALA:O	1:D:36:PHE:C	2.28	0.76
1:B:39:ARG:O	1:B:42:GLU:HG2	1.87	0.75
1:B:16:HIS:O	1:B:17:GLU:C	2.30	0.74
1:D:19:VAL:HG23	1:D:21:LEU:HD12	1.70	0.74
1:C:16:HIS:HE1	1:C:93[B]:MSE:HE2	1.52	0.73
1:D:34:ASP:N	1:D:35:ALA:HB3	2.01	0.73
1:D:24:ASN:O	1:D:28:ILE:HD13	1.91	0.71
1:C:15:LEU:O	3:C:192:HOH:O	2.09	0.70
1:C:18:ALA:N	3:C:192:HOH:O	2.25	0.70
1:C:28[B]:ILE:HD12	3:C:248:HOH:O	1.93	0.69
1:B:111[B]:ASP:OD1	3:B:249:HOH:O	2.12	0.67
1:C:28[B]:ILE:CD1	3:C:248:HOH:O	2.43	0.67
1:D:31:LEU:HG	3:D:183:HOH:O	1.94	0.67
1:D:31:LEU:HD13	1:D:32:LYS:N	2.08	0.67
1:D:31:LEU:C	1:D:31:LEU:HD22	2.20	0.66
1:C:40:ARG:NH1	1:C:82:LEU:HD11	2.09	0.66
1:D:32:LYS:O	1:D:35:ALA:HB1	1.96	0.65
1:D:45:THR:O	1:D:48:ARG:HG2	1.98	0.64
1:B:43:ILE:HG21	1:B:82:LEU:HD23	1.80	0.63
1:D:48:ARG:HG2	1:D:49:ALA:N	2.14	0.62
1:A:19:VAL:CG1	3:A:170:HOH:O	2.22	0.61
1:D:19:VAL:CG2	1:D:21:LEU:HD12	2.31	0.61
1:A:29:LEU:HD22	1:A:93[B]:MSE:SE	2.51	0.59
1:C:114:ARG:O	1:C:115:ARG:HD2	2.03	0.58
1:D:28:ILE:HD12	1:D:28:ILE:N	2.18	0.58
1:D:29:LEU:O	1:D:33:GLU:HB2	2.03	0.57
1:A:22:ASP:OD1	1:A:98:LYS:NZ	2.24	0.57
1:D:28:ILE:N	1:D:28:ILE:CD1	2.66	0.57
1:B:114:ARG:NH2	3:B:311:HOH:O	2.34	0.57
1:B:87:LEU:O	1:B:90:VAL:HG22	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:10:ASP:HA	1:D:13:GLU:HG3	1.87	0.56
1:A:19:VAL:HG12	1:A:19:VAL:O	2.05	0.55
1:D:31:LEU:CD1	1:D:32:LYS:HG3	2.36	0.55
1:B:15:LEU:O	1:B:18:ALA:HB3	2.06	0.54
1:B:22:ASP:OD2	1:B:98:LYS:NZ	2.37	0.54
1:D:29:LEU:C	1:D:93[B]:MSE:HE1	2.32	0.54
1:B:89:HIS:CE1	1:B:93[B]:MSE:SE	3.11	0.54
1:D:29:LEU:HD23	3:D:171:HOH:O	2.08	0.54
1:D:21:LEU:HD22	1:D:26:ARG:HB2	1.91	0.52
1:B:12[B]:HIS:CD2	1:B:86:THR:HG23	2.44	0.52
1:C:53:LYS:NZ	3:C:188:HOH:O	2.43	0.52
1:A:42:GLU:OE1	3:A:228:HOH:O	2.19	0.51
1:B:12[B]:HIS:CE1	1:B:90:VAL:HG13	2.46	0.51
1:C:38:GLN:O	1:C:42:GLU:CD	2.54	0.51
1:D:31:LEU:HD13	1:D:32:LYS:HG3	1.93	0.51
1:D:19:VAL:CG2	1:D:21:LEU:CD1	2.89	0.51
1:A:114:ARG:HB3	1:A:115:ARG:HH21	1.75	0.50
1:B:79:ALA:HB2	3:B:299:HOH:O	2.12	0.50
1:A:29:LEU:HB3	1:A:93[B]:MSE:HE1	1.94	0.50
1:C:114:ARG:O	1:C:115:ARG:HB2	2.11	0.50
1:A:87[A]:LEU:HG	3:A:154:HOH:O	2.10	0.49
1:D:30[B]:GLU:HA	1:D:33:GLU:HB3	1.95	0.49
1:D:48:ARG:HG2	1:D:49:ALA:H	1.77	0.49
1:B:33:GLU:OE1	1:B:93[B]:MSE:HE2	2.13	0.48
1:D:22:ASP:OD2	1:D:101:HIS:HE1	1.96	0.48
1:D:32:LYS:O	1:D:35:ALA:CB	2.61	0.47
1:D:31:LEU:O	1:D:34:ASP:OD2	2.33	0.47
1:C:16:HIS:C	3:C:192:HOH:O	2.57	0.46
1:A:21:LEU:HD11	1:A:93[B]:MSE:CE	2.46	0.46
1:A:39:ARG:NH1	3:A:187:HOH:O	2.49	0.46
1:B:19:VAL:CG2	1:B:20:PRO:HD2	2.45	0.46
1:B:15:LEU:HA	1:B:18:ALA:CB	2.46	0.46
1:D:21:LEU:N	1:D:25:GLU:OE1	2.47	0.46
1:A:115:ARG:HE	1:A:115:ARG:CA	2.30	0.44
1:A:42:GLU:HB2	3:A:228:HOH:O	2.18	0.44
1:D:26:ARG:O	1:D:26:ARG:HG3	2.16	0.44
1:A:19:VAL:HG11	1:A:105:TYR:HD1	1.83	0.44
1:A:26:ARG:NH2	3:A:167:HOH:O	2.49	0.44
1:B:10:ASP:N	1:B:13:GLU:HG3	2.32	0.44
1:D:29:LEU:O	1:D:33:GLU:CB	2.66	0.43
1:C:89:HIS:CE1	1:C:93[B]:MSE:SE	3.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:41:ARG:HD2	3:A:132:HOH:O	2.17	0.43
1:D:19:VAL:HG21	1:D:21:LEU:HD11	2.00	0.43
1:B:12[A]:HIS:CE1	1:B:33:GLU:OE2	2.72	0.43
1:B:12[B]:HIS:NE2	1:B:86:THR:HA	2.34	0.42
1:B:19:VAL:HG23	1:B:20:PRO:HD2	2.01	0.42
1:B:17:GLU:OE2	1:B:17:GLU:HA	2.19	0.42
1:D:20:PRO:HA	1:D:21:LEU:HB2	2.00	0.42
1:C:40:ARG:HH11	1:C:82:LEU:HD11	1.80	0.42
1:D:21:LEU:HD22	1:D:26:ARG:HA	2.01	0.42
1:D:38:GLN:O	1:D:42:GLU:HG3	2.20	0.42
1:B:12[B]:HIS:CE1	1:B:89:HIS:HB3	2.55	0.41
1:D:31:LEU:HD22	1:D:31:LEU:O	2.20	0.41
1:D:31:LEU:C	1:D:31:LEU:CD2	2.88	0.41
1:D:32:LYS:C	1:D:35:ALA:CB	2.94	0.40
1:C:115:ARG:NE	1:C:115:ARG:CA	2.78	0.40
1:D:48:ARG:CG	1:D:49:ALA:N	2.82	0.40
1:D:57:ALA:HA	1:D:60:LYS:HE2	2.04	0.40
1:B:51:ASN:HD22	1:B:51:ASN:HA	1.78	0.40

All (2) 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)
3:A:128:HOH:O	3:C:235:HOH:O[2_555]	1.88	0.32
3:B:209:HOH:O	3:C:241:HOH:O[2_555]	2.06	0.14

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	106/109 (97%)	105 (99%)	1 (1%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	B	110/109 (101%)	106 (96%)	3 (3%)	1 (1%)	14	3
1	C	108/109 (99%)	106 (98%)	2 (2%)	0	100	100
1	D	111/109 (102%)	102 (92%)	5 (4%)	4 (4%)	2	0
All	All	435/436 (100%)	419 (96%)	11 (2%)	5 (1%)	10	2

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	B	16	HIS
1	D	36	PHE
1	D	35	ALA
1	D	20	PRO
1	D	21	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	86/86 (100%)	81 (94%)	5 (6%)	18	3
1	B	90/86 (105%)	88 (98%)	2 (2%)	45	22
1	C	89/86 (104%)	86 (97%)	3 (3%)	32	10
1	D	91/86 (106%)	81 (89%)	10 (11%)	6	0
All	All	356/344 (104%)	336 (94%)	20 (6%)	19	3

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	31	LEU
1	A	67	GLU
1	A	77	ARG
1	A	115	ARG
1	A	118	GLN
1	B	17	GLU

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Mol	Chain	Res	Type
1	B	82	LEU
1	C	42	GLU
1	C	60	LYS
1	C	115	ARG
1	D	10	ASP
1	D	22	ASP
1	D	28	ILE
1	D	29	LEU
1	D	30[A]	GLU
1	D	30[B]	GLU
1	D	31	LEU
1	D	33	GLU
1	D	44	GLU
1	D	99	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (9) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	118	GLN
1	B	51	ASN
1	B	83	GLN
1	C	16	HIS
1	C	83	GLN
1	C	89	HIS
1	D	16	HIS
1	D	51	ASN
1	D	118	GLN

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

Of 3 ligands modelled in this entry, 3 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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	104/109 (95%)	0.16	3 (2%) 53 62	10, 21, 36, 42	2 (1%)
1	B	108/109 (99%)	0.09	2 (1%) 66 73	13, 21, 39, 48	2 (1%)
1	C	105/109 (96%)	0.12	3 (2%) 53 62	8, 20, 40, 47	2 (1%)
1	D	108/109 (99%)	0.75	17 (15%) 5 6	11, 24, 52, 56	3 (2%)
All	All	425/436 (97%)	0.28	25 (5%) 28 34	8, 21, 45, 56	9 (2%)

All (25) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	31	LEU	6.0
1	D	20	PRO	6.0
1	D	19	VAL	5.6
1	D	18	ALA	4.2
1	D	41	ARG	3.7
1	D	30[A]	GLU	3.2
1	D	10	ASP	3.1
1	D	34	ASP	3.1
1	D	21	LEU	3.0
1	C	10	ASP	2.8
1	D	16	HIS	2.7
1	D	28	ILE	2.7
1	D	29	LEU	2.6
1	A	19	VAL	2.6
1	D	11	LEU	2.5
1	D	35	ALA	2.4
1	A	10	ASP	2.3
1	D	22	ASP	2.3
1	D	15	LEU	2.2
1	D	32	LYS	2.2
1	C	42	GLU	2.2

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Mol	Chain	Res	Type	RSRZ
1	C	16	HIS	2.2
1	A	115	ARG	2.1
1	B	16	HIS	2.1
1	B	10	ASP	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	CU	B	3	1/1	0.91	0.19	33,33,33,33	1
2	CU	C	2	1/1	0.98	0.04	35,35,35,35	1
2	CU	A	1	1/1	0.99	0.05	30,30,30,30	1

6.5 Other polymers [i](#)

There are no such residues in this entry.