



wwPDB X-ray Structure Validation Summary Report ⓘ

Mar 9, 2026 – 09:21 AM UTC

PDB ID : 3DP8 / pdb_00003dp8
Title : Structural characterization of a putative endogenous metal chelator in the periplasmic nickel transporter NikA (nickel butane-1,2,4-tricarboxylate form)
Authors : Cherrier, M.V.; Cavazza, C.; Bochot, C.; Lemaire, D.; Fontecilla-Camps, J.C.
Deposited on : 2008-07-07
Resolution : 2.50 Å(reported)

This is a wwPDB X-ray Structure Validation Summary 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

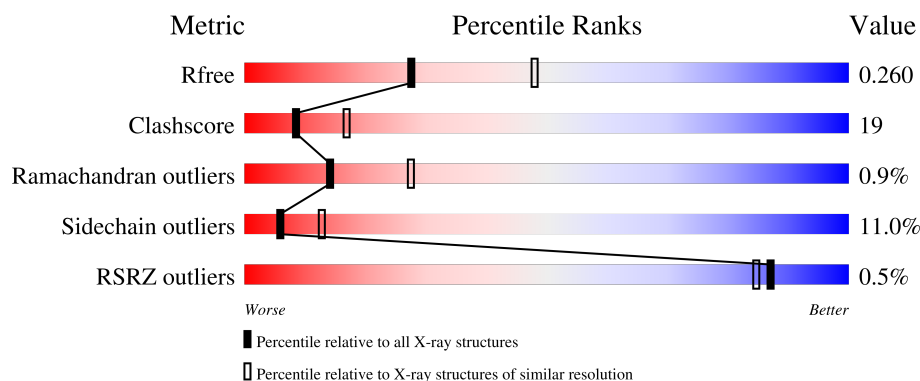
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.50 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	5829 (2.50-2.50)
Clashscore	190562	6492 (2.50-2.50)
Ramachandran outliers	187476	6378 (2.50-2.50)
Sidechain outliers	187428	6380 (2.50-2.50)
RSRZ outliers	180081	5833 (2.50-2.50)

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	502	% 64% 29% 5% ..
1	B	502	66% 27% 5% ..
1	C	502	% 61% 32%

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
3	ACT	A	507	-	-	X	-
3	ACT	B	507	-	-	X	-
3	ACT	C	504	-	X	X	-
7	GOL	A	514	-	-	X	-
7	GOL	B	513	-	-	X	-
7	GOL	B	515	-	-	X	-

2 Entry composition

There are 8 unique types of molecules in this entry. The entry contains 12491 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-binding periplasmic protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	498	Total	C	N	O	S	0	15	0
			4019	2582	672	755	10			
1	B	497	Total	C	N	O	S	6	18	0
			4055	2609	680	755	11			
1	C	496	Total	C	N	O	S	0	11	0
			4006	2570	673	751	12			

- Molecule 2 is NICKEL (II) ION (CCD ID: NI) (formula: Ni).

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

- Molecule 3 is ACETATE ION (CCD ID: ACT) (formula: C₂H₃O₂).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	A	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	B	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		
3	C	1	Total	C	O	0	0
			4	2	2		

- Molecule 4 is SULFATE ION (CCD ID: SO4) (formula: O₄S).

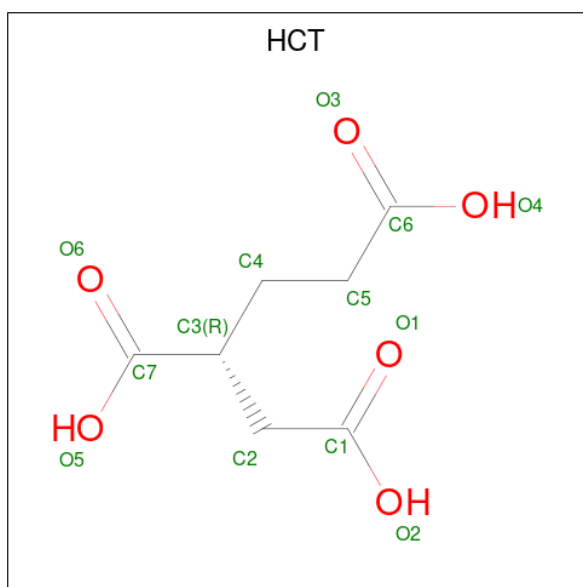


Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	O	S	0	0
			5	4	1		

- Molecule 5 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

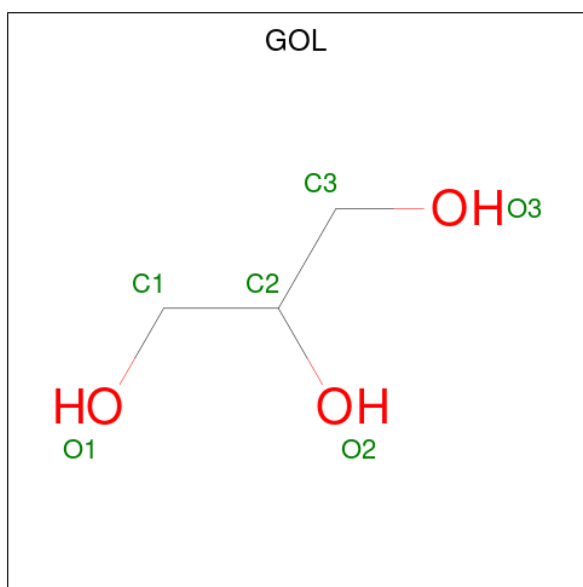
Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	2	Total	Cl	0	0
			2	2		
5	B	3	Total	Cl	0	0
			3	3		
5	C	2	Total	Cl	0	0
			2	2		

- Molecule 6 is (2R)-butane-1,2,4-tricarboxylic acid (CCD ID: HCT) (formula: C₇H₁₀O₆).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
6	A	1	Total	C	O	0	0
			13	7	6		
6	B	1	Total	C	O	0	0
			13	7	6		
6	C	1	Total	C	O	0	0
			13	7	6		

- Molecule 7 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		

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Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	A	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		
7	B	1	Total	C	O	0	0
			6	3	3		

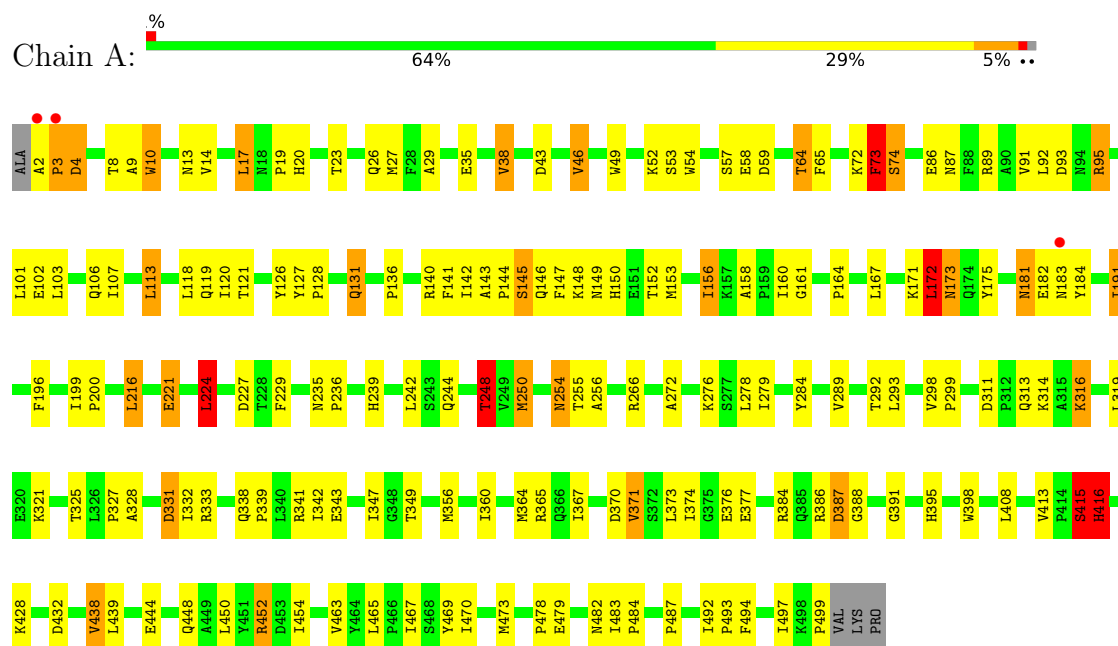
- Molecule 8 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
8	A	100	Total	O	0	0
			100	100		
8	B	110	Total	O	0	0
			110	110		
8	C	55	Total	O	0	0
			55	55		

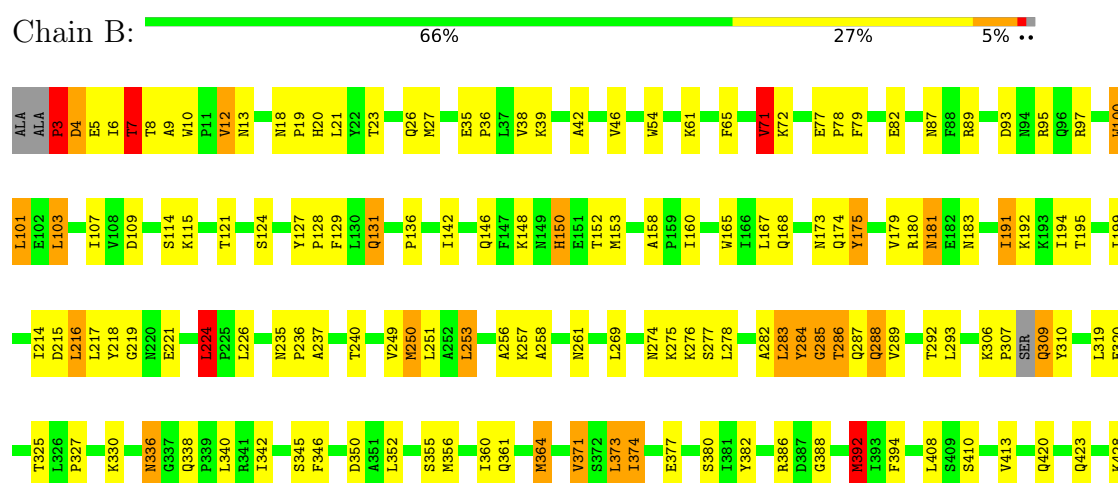
3 Residue-property plots [i](#)

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-binding periplasmic protein

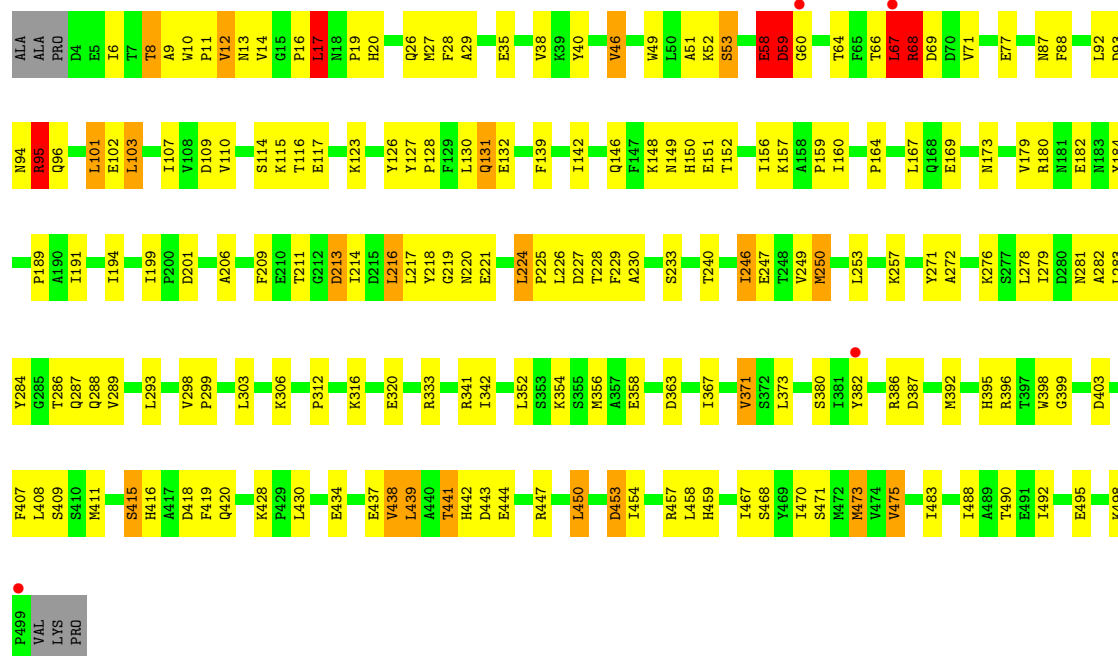


• Molecule 1: Nickel-binding periplasmic protein





• Molecule 1: Nickel-binding periplasmic protein



4 Data and refinement statistics

Property	Value	Source
Space group	P 62	Depositor
Cell constants a, b, c, α , β , γ	158.57Å 158.57Å 134.94Å 90.00° 90.00° 120.00°	Depositor
Resolution (Å)	20.00 – 2.50 20.00 – 2.50	Depositor EDS
% Data completeness (in resolution range)	99.5 (20.00-2.50) 99.5 (20.00-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	0.05	Depositor
$\langle I/\sigma(I) \rangle$ ¹	6.20 (at 2.50Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.199 , 0.270 0.194 , 0.260	Depositor DCC
R_{free} test set	1707 reflections (2.56%)	wwPDB-VP
Wilson B-factor (Å ²)	54.2	Xtriage
Anisotropy	0.117	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 35.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.025 for h,-h-k,-l	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	12491	wwPDB-VP
Average B, all atoms (Å ²)	51.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.36% 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: ACT, SO4, GOL, HCT, NI, CL

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	1.09	2/4167 (0.0%)	1.20	22/5676 (0.4%)
1	B	1.09	3/4212 (0.1%)	1.21	20/5729 (0.3%)
1	C	1.01	3/4139 (0.1%)	1.13	17/5634 (0.3%)
All	All	1.07	8/12518 (0.1%)	1.18	59/17039 (0.3%)

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	3
1	B	0	3
1	C	0	4
All	All	0	10

The worst 5 of 8 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	249	VAL	CA-CB	7.97	1.64	1.54
1	B	257	LYS	C-O	-6.09	1.17	1.24
1	A	465	LEU	CA-C	5.36	1.58	1.52
1	A	492	ILE	CA-C	5.16	1.56	1.52
1	C	471	SER	CA-C	-5.12	1.46	1.52

The worst 5 of 59 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	73	PHE	N-CA-C	-13.84	90.73	110.24
1	B	4	ASP	N-CA-C	9.39	130.80	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	2	ALA	CA-C-N	-9.20	110.06	119.99
1	A	2	ALA	C-N-CA	-9.20	110.06	119.99
1	A	199	ILE	CA-C-N	7.91	127.98	119.28

There are no chirality outliers.

5 of 10 planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	172	LEU	Peptide
1	A	415	SER	Peptide
1	A	73	PHE	Peptide
1	B	215	ASP	Peptide
1	B	3	PRO	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	4019	0	4002	148	0
1	B	4055	0	4060	160	0
1	C	4006	0	3975	157	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
2	C	1	0	0	0	0
3	A	16	0	12	3	0
3	B	16	0	12	16	0
3	C	12	0	9	3	0
4	A	5	0	0	0	0
5	A	2	0	0	0	0
5	B	3	0	0	1	0
5	C	2	0	0	0	0
6	A	13	0	6	1	0
6	B	13	0	7	0	0
6	C	13	0	6	0	0
7	A	24	0	32	12	0
7	B	24	0	32	9	0
8	A	100	0	0	14	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	B	110	0	0	10	0
8	C	55	0	0	5	0
All	All	12491	0	12153	462	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 19.

The worst 5 of 462 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:95:ARG:HG3	1:A:95:ARG:HH11	1.09	1.11
1:C:226:LEU:CD2	1:C:473[B]:MET:HE1	1.80	1.10
1:C:67:LEU:HB3	1:C:68:ARG:HB2	1.35	1.08
1:A:4:ASP:HA	8:A:607:HOH:O	1.53	1.07
1:A:92:LEU:HD22	1:A:95:ARG:HH12	1.23	1.03

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	511/502 (102%)	473 (93%)	33 (6%)	5 (1%)	12	24
1	B	510/502 (102%)	478 (94%)	30 (6%)	2 (0%)	30	49
1	C	505/502 (101%)	467 (92%)	31 (6%)	7 (1%)	9	17
All	All	1526/1506 (101%)	1418 (93%)	94 (6%)	14 (1%)	14	27

5 of 14 Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	C	67	LEU

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Mol	Chain	Res	Type
1	A	74	SER
1	C	59	ASP
1	C	282	ALA
1	A	113	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	435/425 (102%)	384 (88%)	51 (12%)	5	11
1	B	440/425 (104%)	397 (90%)	43 (10%)	7	16
1	C	432/425 (102%)	380 (88%)	52 (12%)	5	10
All	All	1307/1275 (102%)	1161 (89%)	146 (11%)	6	12

5 of 146 residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	C	167	LEU
1	C	490	THR
1	C	213	ASP
1	C	341	ARG
1	A	452	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. 5 of 48 such sidechains are listed below:

Mol	Chain	Res	Type
1	B	420	GLN
1	C	87	ASN
1	B	448	GLN
1	C	20	HIS
1	C	149	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 ⓘ

Of 33 ligands modelled in this entry, 10 are monoatomic - leaving 23 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	ACT	C	504	-	3,3,3	1.68	1 (33%)	3,3,3	3.87	2 (66%)
7	GOL	A	514	-	5,5,5	0.43	0	5,5,5	0.41	0
3	ACT	A	504	-	3,3,3	0.94	0	3,3,3	0.69	0
3	ACT	A	506	-	3,3,3	0.78	0	3,3,3	1.49	0
7	GOL	A	513	-	5,5,5	0.45	0	5,5,5	0.62	0
3	ACT	C	505	-	3,3,3	0.88	0	3,3,3	1.83	2 (66%)
3	ACT	B	504	-	3,3,3	0.83	0	3,3,3	1.21	0
7	GOL	B	512	-	5,5,5	0.40	0	5,5,5	0.55	0
7	GOL	A	515	-	5,5,5	0.45	0	5,5,5	0.36	0
3	ACT	B	507	-	3,3,3	0.97	0	3,3,3	0.34	0
6	HCT	B	511	2	12,12,12	2.78	3 (25%)	14,15,15	2.97	6 (42%)
3	ACT	B	505	-	3,3,3	0.99	0	3,3,3	1.15	0
4	SO4	A	508	-	4,4,4	0.25	0	6,6,6	0.37	0
7	GOL	B	513	-	5,5,5	0.26	0	5,5,5	0.85	0
6	HCT	A	511	2	12,12,12	1.94	3 (25%)	14,15,15	2.64	6 (42%)
3	ACT	A	507	-	3,3,3	0.82	0	3,3,3	1.49	0

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
6	HCT	C	509	2	12,12,12	2.07	2 (16%)	14,15,15	2.41	2 (14%)
7	GOL	B	514	-	5,5,5	0.33	0	5,5,5	0.35	0
7	GOL	B	515	-	5,5,5	0.61	0	5,5,5	0.97	0
7	GOL	A	512	-	5,5,5	0.29	0	5,5,5	0.51	0
3	ACT	B	506	-	3,3,3	0.86	0	3,3,3	1.36	0
3	ACT	C	506	-	3,3,3	1.13	0	3,3,3	0.75	0
3	ACT	A	505	-	3,3,3	0.91	0	3,3,3	1.18	0

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
6	HCT	B	511	2	-	4/13/13/13	-
7	GOL	A	514	-	-	2/4/4/4	-
6	HCT	C	509	2	-	7/13/13/13	-
7	GOL	B	514	-	-	4/4/4/4	-
7	GOL	B	515	-	-	3/4/4/4	-
7	GOL	A	512	-	-	2/4/4/4	-
7	GOL	B	513	-	-	4/4/4/4	-
7	GOL	B	512	-	-	2/4/4/4	-
7	GOL	A	513	-	-	0/4/4/4	-
6	HCT	A	511	2	-	5/13/13/13	-
7	GOL	A	515	-	-	1/4/4/4	-

The worst 5 of 9 bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	B	511	HCT	C2-C1	5.62	1.65	1.51
6	B	511	HCT	C2-C3	5.24	1.64	1.53
6	C	509	HCT	C2-C1	4.44	1.62	1.51
6	B	511	HCT	C5-C6	4.36	1.60	1.50
6	C	509	HCT	C2-C3	3.86	1.61	1.53

The worst 5 of 18 bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	C	509	HCT	C3-C2-C1	6.73	129.14	113.92
6	B	511	HCT	C3-C2-C1	6.72	129.11	113.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	A	511	HCT	C3-C2-C1	5.90	127.25	113.92
3	C	504	ACT	OXT-C-O	-5.55	101.43	122.03
6	B	511	HCT	C5-C4-C3	5.49	123.19	113.45

There are no chirality outliers.

5 of 34 torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
6	B	511	HCT	C1-C2-C3-C4
6	B	511	HCT	C1-C2-C3-C7
6	C	509	HCT	C1-C2-C3-C7
7	A	512	GOL	O1-C1-C2-C3
7	B	512	GOL	O1-C1-C2-O2

There are no ring outliers.

11 monomers are involved in 44 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	C	504	ACT	3	0
7	A	514	GOL	10	0
3	A	506	ACT	1	0
7	A	513	GOL	1	0
3	B	504	ACT	1	0
3	B	507	ACT	15	0
7	B	513	GOL	4	0
6	A	511	HCT	1	0
3	A	507	ACT	2	0
7	B	515	GOL	5	0
7	A	512	GOL	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	498/502 (99%)	-0.33	3 (0%) 85 83	20, 46, 66, 76	15 (3%)
1	B	497/502 (99%)	-0.41	0 100 100	20, 44, 63, 83	19 (3%)
1	C	496/502 (98%)	-0.05	4 (0%) 82 80	24, 59, 87, 99	12 (2%)
All	All	1491/1506 (99%)	-0.26	7 (0%) 87 85	20, 48, 79, 99	46 (3%)

The worst 5 of 7 RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	C	382	TYR	4.9
1	C	67	LEU	4.0
1	A	3	PRO	2.9
1	A	183	ASN	2.6
1	C	60	GLY	2.6

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	ACT	A	505	4/4	0.48	0.39	45,45,45,46	4
3	ACT	B	506	4/4	0.51	0.23	41,43,43,43	4
7	GOL	A	512	6/6	0.53	0.26	57,59,61,63	6
7	GOL	B	514	6/6	0.58	0.31	51,52,53,55	6
3	ACT	A	507	4/4	0.60	0.21	48,49,49,50	4
7	GOL	A	515	6/6	0.62	0.20	51,54,55,55	6
3	ACT	B	504	4/4	0.66	0.28	41,41,41,42	4
3	ACT	A	506	4/4	0.68	0.23	57,58,58,58	4
7	GOL	B	515	6/6	0.69	0.20	29,40,42,42	6
7	GOL	B	512	6/6	0.70	0.31	46,49,50,51	6
3	ACT	C	505	4/4	0.71	0.32	40,40,40,40	4
7	GOL	A	514	6/6	0.71	0.22	39,42,44,45	6
5	CL	B	510	1/1	0.71	0.35	50,50,50,50	1
3	ACT	C	506	4/4	0.72	0.22	34,34,35,35	4
7	GOL	A	513	6/6	0.77	0.35	45,49,50,51	6
7	GOL	B	513	6/6	0.79	0.20	28,30,31,33	6
5	CL	A	510	1/1	0.85	0.09	90,90,90,90	0
4	SO4	A	508	5/5	0.85	0.16	47,48,52,52	5
3	ACT	C	504	4/4	0.87	0.16	37,38,38,39	0
6	HCT	C	509	13/13	0.88	0.11	48,58,65,67	0
3	ACT	B	505	4/4	0.88	0.09	65,66,66,66	0
3	ACT	B	507	4/4	0.88	0.11	36,37,37,37	4
3	ACT	A	504	4/4	0.90	0.11	66,66,66,66	0
5	CL	B	508	1/1	0.90	0.36	44,44,44,44	1
6	HCT	A	511	13/13	0.93	0.09	33,53,61,61	0
6	HCT	B	511	13/13	0.94	0.08	35,47,52,53	0
5	CL	C	508	1/1	0.97	0.04	58,58,58,58	0
2	NI	A	503	1/1	0.97	0.05	78,78,78,78	0
2	NI	C	503	1/1	0.97	0.04	66,66,66,66	0
5	CL	A	509	1/1	0.97	0.13	61,61,61,61	0
5	CL	C	507	1/1	0.98	0.15	57,57,57,57	0
2	NI	B	503	1/1	0.99	0.03	53,53,53,53	0
5	CL	B	509	1/1	0.99	0.04	40,40,40,40	0

6.5 Other polymers ⓘ

There are no such residues in this entry.