



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 14, 2026 – 02:17 PM UTC

PDB ID : 7WRU / pdb_00007wru
Title : Crystal structure of the apo chicken glutamyl-tRNA synthetase 1 (EARS1)
Authors : Chung, S.; Cho, Y.
Deposited on : 2022-01-27
Resolution : 2.50 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
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

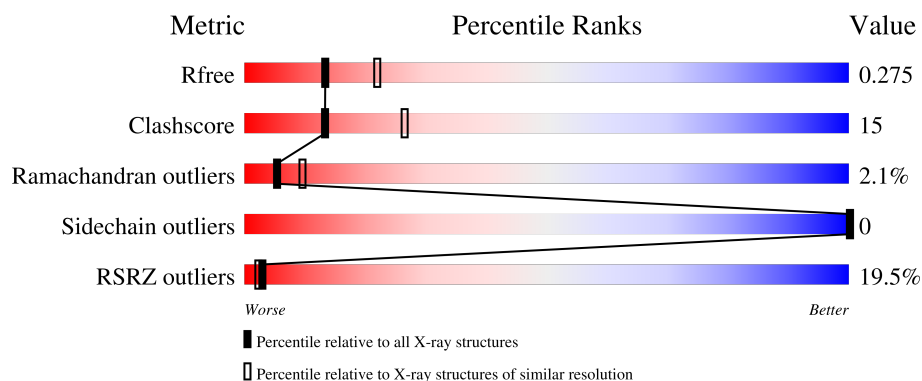
1 Overall quality at a glance

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	531	18% 67% 24% • 7%

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 4005 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 Glutamyl-tRNA synthetase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	493	Total	C	N	O	S	0	0	0
			4000	2544	691	740	25			

- Molecule 2 is MERCURY (II) ION (CCD ID: HG) (formula: Hg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
2	A	2	Total	Hg	0	0
			2	2		

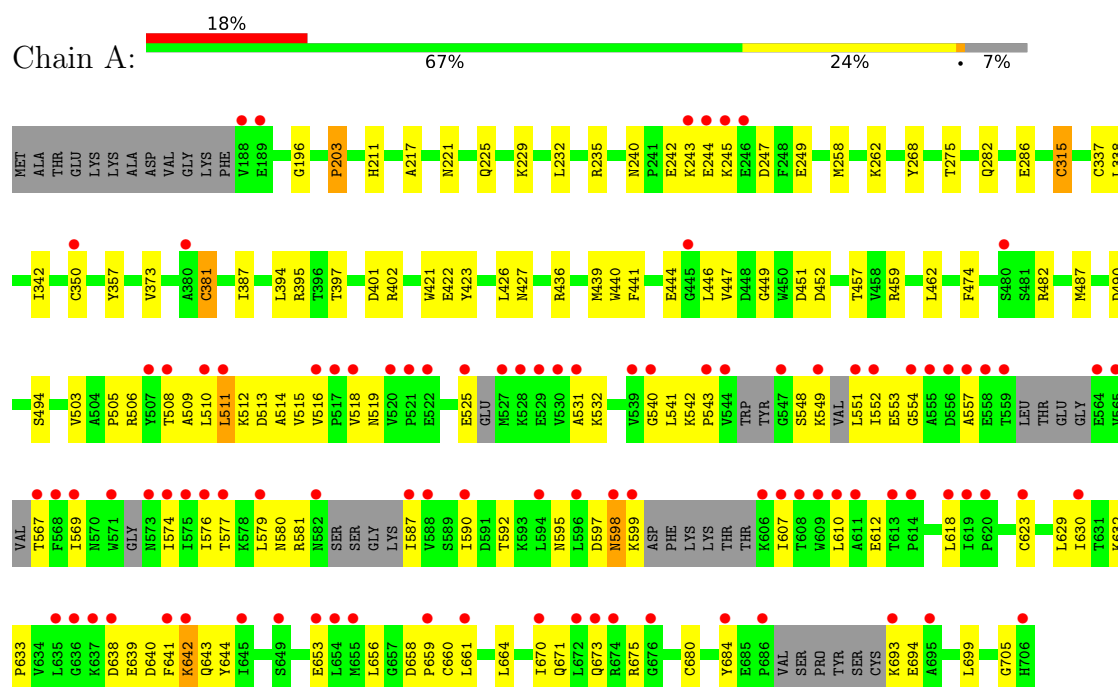
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	3	Total	O	0	0
			3	3		

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: Glutamyl-tRNA synthetase



4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α , β , γ	89.04Å 41.76Å 92.19Å 90.00° 100.20° 90.00°	Depositor
Resolution (Å)	45.36 – 2.50 45.36 – 2.50	Depositor EDS
% Data completeness (in resolution range)	98.5 (45.36-2.50) 98.4 (45.36-2.50)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.46 (at 2.51Å)	Xtriage
Refinement program	PHENIX 1.14-3260_1069	Depositor
R, R_{free}	0.224 , 0.270 0.235 , 0.275	Depositor DCC
R_{free} test set	1159 reflections (4.90%)	wwPDB-VP
Wilson B-factor (Å ²)	33.2	Xtriage
Anisotropy	0.764	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.31 , 48.7	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.018 for l,-k,h	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	4005	wwPDB-VP
Average B, all atoms (Å ²)	54.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.51% 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: HG

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	0.49	3/4084 (0.1%)	0.66	0/5513

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

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	337	CYS	CB-SG	7.95	2.07	1.81
1	A	381	CYS	CB-SG	7.13	2.04	1.81
1	A	315	CYS	CB-SG	6.54	2.02	1.81

There are no bond angle outliers.

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	580	ASN	Peptide

5.2 Too-close contacts [i](#)

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	4000	0	3979	118	0
2	A	2	0	0	0	0
3	A	3	0	0	0	0
All	All	4005	0	3979	118	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 15.

All (118) 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:315:CYS:CB	1:A:315:CYS:SG	2.02	1.47
1:A:381:CYS:SG	1:A:381:CYS:CB	2.04	1.45
1:A:574:ILE:HD11	1:A:592:THR:HG21	1.38	1.04
1:A:511:LEU:HD23	1:A:514:ALA:H	1.36	0.91
1:A:436:ARG:HH11	1:A:439:MET:HE1	1.45	0.81
1:A:397:THR:HG22	1:A:422:GLU:OE1	1.80	0.80
1:A:397:THR:HG22	1:A:422:GLU:CD	2.10	0.76
1:A:511:LEU:CD2	1:A:514:ALA:H	1.98	0.76
1:A:511:LEU:HG	1:A:512:LYS:H	1.51	0.75
1:A:542:LYS:NZ	1:A:660:CYS:SG	2.57	0.74
1:A:357:TYR:HD1	1:A:373:VAL:HG22	1.52	0.73
1:A:511:LEU:CD2	1:A:514:ALA:N	2.51	0.73
1:A:514:ALA:O	1:A:554:GLY:N	2.23	0.71
1:A:551:LEU:HD21	1:A:612:GLU:HB2	1.72	0.70
1:A:610:LEU:HD13	1:A:618:LEU:HD13	1.75	0.68
1:A:511:LEU:HD22	1:A:514:ALA:HB3	1.79	0.65
1:A:441:PHE:HZ	1:A:630:ILE:HD11	1.61	0.65
1:A:511:LEU:CG	1:A:512:LYS:H	2.10	0.64
1:A:350:CYS:SG	1:A:402:ARG:HA	2.37	0.64
1:A:639:GLU:OE1	1:A:644:TYR:OH	2.15	0.62
1:A:275:THR:HG21	1:A:387:ILE:HD11	1.82	0.62
1:A:597:ASP:O	1:A:598:ASN:HB2	2.00	0.61
1:A:447:VAL:HG13	1:A:452:ASP:CB	2.32	0.60
1:A:664:LEU:HD13	1:A:680:CYS:HB2	1.83	0.60
1:A:436:ARG:NH1	1:A:439:MET:HE1	2.14	0.60
1:A:506:ARG:HD2	1:A:671:GLN:OE1	2.03	0.59
1:A:664:LEU:HD11	1:A:670:ILE:HD13	1.83	0.58
1:A:515:VAL:HA	1:A:553:GLU:HA	1.85	0.58
1:A:440:TRP:CD1	1:A:642:LYS:HZ1	2.21	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:474:PHE:HZ	1:A:487:MET:HE3	1.68	0.58
1:A:680:CYS:HA	1:A:699:LEU:HD23	1.86	0.58
1:A:249:GLU:OE2	1:A:268:TYR:OH	2.20	0.57
1:A:282:GLN:O	1:A:286:GLU:HG3	2.05	0.57
1:A:505:PRO:HB3	1:A:532:LYS:HD3	1.86	0.57
1:A:490:ASP:HB3	1:A:705:GLY:HA2	1.84	0.57
1:A:357:TYR:CD1	1:A:373:VAL:HG22	2.39	0.56
1:A:640:ASP:OD1	1:A:642:LYS:HG3	2.05	0.56
1:A:577:THR:H	1:A:592:THR:HA	1.71	0.56
1:A:240:ASN:OD1	1:A:242:GLU:HG3	2.07	0.55
1:A:509:ALA:O	1:A:675:ARG:NH1	2.39	0.55
1:A:511:LEU:HD23	1:A:513:ASP:N	2.21	0.54
1:A:551:LEU:N	1:A:610:LEU:O	2.41	0.54
1:A:395:ARG:NH1	1:A:422:GLU:OE1	2.41	0.54
1:A:641:PHE:C	1:A:643:GLN:H	2.17	0.53
1:A:659:PRO:C	1:A:661:LEU:H	2.17	0.53
1:A:401:ASP:HB2	1:A:402:ARG:NH2	2.24	0.53
1:A:587:ILE:HG21	1:A:590:ILE:HD11	1.93	0.51
1:A:641:PHE:O	1:A:643:GLN:N	2.44	0.51
1:A:632:LYS:HE3	1:A:644:TYR:CE1	2.45	0.51
1:A:510:LEU:O	1:A:656:LEU:N	2.43	0.51
1:A:441:PHE:CD1	1:A:629:LEU:HD13	2.46	0.50
1:A:579:LEU:HG	1:A:581:ARG:HD3	1.92	0.50
1:A:518:VAL:HG21	1:A:552:ILE:HG23	1.92	0.50
1:A:474:PHE:CZ	1:A:487:MET:HE3	2.46	0.50
1:A:543:PRO:HD2	1:A:660:CYS:SG	2.51	0.50
1:A:618:LEU:HD23	1:A:659:PRO:HG3	1.93	0.50
1:A:576:ILE:HD12	1:A:590:ILE:HG21	1.94	0.49
1:A:630:ILE:HD12	1:A:641:PHE:HB2	1.93	0.49
1:A:211:HIS:HA	1:A:457:THR:HA	1.93	0.49
1:A:574:ILE:HD11	1:A:592:THR:CG2	2.27	0.49
1:A:531:ALA:HA	1:A:541:LEU:HG	1.95	0.49
1:A:632:LYS:HE3	1:A:644:TYR:CZ	2.48	0.49
1:A:574:ILE:CD1	1:A:592:THR:HG21	2.25	0.49
1:A:422:GLU:HG2	1:A:482:ARG:CZ	2.42	0.48
1:A:196:GLY:HA2	1:A:229:LYS:O	2.14	0.48
1:A:446:LEU:H	1:A:446:LEU:HD12	1.78	0.48
1:A:508:THR:HB	1:A:673:GLN:OE1	2.12	0.48
1:A:569:ILE:HD12	1:A:607:ILE:O	2.13	0.48
1:A:511:LEU:CD2	1:A:513:ASP:H	2.26	0.48
1:A:506:ARG:HD3	1:A:671:GLN:HB3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:240:ASN:HB3	1:A:244:GLU:OE2	2.14	0.48
1:A:338:LEU:HB3	1:A:357:TYR:HB2	1.96	0.47
1:A:511:LEU:HD22	1:A:514:ALA:CB	2.44	0.47
1:A:245:LYS:HB2	1:A:247:ASP:OD1	2.13	0.47
1:A:511:LEU:CG	1:A:512:LYS:N	2.78	0.47
1:A:217:ALA:O	1:A:221:ASN:ND2	2.49	0.46
1:A:548:SER:O	1:A:549:LYS:HG2	2.15	0.46
1:A:567:THR:OG1	1:A:599:LYS:HD2	2.16	0.46
1:A:579:LEU:H	1:A:579:LEU:HD23	1.81	0.46
1:A:511:LEU:CD2	1:A:513:ASP:N	2.79	0.45
1:A:518:VAL:O	1:A:549:LYS:HA	2.16	0.45
1:A:693:LYS:HB3	1:A:694:GLU:H	1.47	0.45
1:A:394:LEU:HA	1:A:421:TRP:O	2.16	0.45
1:A:447:VAL:HG21	1:A:629:LEU:HD11	1.99	0.45
1:A:440:TRP:CE2	1:A:444:GLU:HG3	2.52	0.45
1:A:516:VAL:HG11	1:A:590:ILE:HD12	1.99	0.44
1:A:540:GLY:C	1:A:541:LEU:HD12	2.43	0.44
1:A:490:ASP:O	1:A:494:SER:OG	2.30	0.44
1:A:509:ALA:O	1:A:510:LEU:HD13	2.18	0.43
1:A:598:ASN:HB3	1:A:599:LYS:H	1.61	0.43
1:A:217:ALA:HB2	1:A:423:TYR:OH	2.19	0.43
1:A:548:SER:C	1:A:549:LYS:HG2	2.43	0.43
1:A:576:ILE:HA	1:A:592:THR:CB	2.49	0.43
1:A:511:LEU:HD23	1:A:514:ALA:N	2.10	0.43
1:A:525:GLU:OE1	1:A:525:GLU:N	2.51	0.43
1:A:658:ASP:O	1:A:661:LEU:HB2	2.18	0.43
1:A:258:MET:HE2	1:A:462:LEU:HD12	2.01	0.43
1:A:519:ASN:O	1:A:592:THR:HG22	2.19	0.43
1:A:242:GLU:HB2	1:A:243:LYS:H	1.73	0.42
1:A:262:LYS:HA	1:A:262:LYS:HD2	1.83	0.42
1:A:395:ARG:HH11	1:A:397:THR:HA	1.84	0.42
1:A:436:ARG:HA	1:A:436:ARG:HD3	1.67	0.42
1:A:427:ASN:O	1:A:487:MET:N	2.43	0.42
1:A:659:PRO:C	1:A:661:LEU:N	2.78	0.41
1:A:447:VAL:HG12	1:A:449:GLY:H	1.85	0.41
1:A:623:CYS:SG	1:A:653:GLU:OE2	2.62	0.41
1:A:664:LEU:HD23	1:A:664:LEU:HA	1.75	0.41
1:A:511:LEU:O	1:A:656:LEU:HD12	2.20	0.41
1:A:203:PRO:HA	1:A:235:ARG:O	2.20	0.41
1:A:512:LYS:HE2	1:A:512:LYS:HB3	1.89	0.41
1:A:519:ASN:HD21	1:A:549:LYS:HZ2	1.68	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:VAL:HG13	1:A:452:ASP:HB2	2.03	0.40
1:A:451:ASP:HB2	1:A:459:ARG:HB3	2.02	0.40
1:A:511:LEU:H	1:A:553:GLU:CD	2.30	0.40
1:A:519:ASN:HD21	1:A:549:LYS:NZ	2.19	0.40
1:A:684:TYR:OH	1:A:694:GLU:OE2	2.33	0.40
1:A:225:GLN:NE2	1:A:232:LEU:HB3	2.35	0.40
1:A:426:LEU:HD23	1:A:426:LEU:HA	1.97	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	473/531 (89%)	438 (93%)	25 (5%)	10 (2%)	5 9

All (10) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	203	PRO
1	A	598	ASN
1	A	557	ALA
1	A	595	ASN
1	A	633	PRO
1	A	642	LYS
1	A	511	LEU
1	A	638	ASP
1	A	503	VAL
1	A	342	ILE

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	440/472 (93%)	440 (100%)	0	100	100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (10) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	222	GLN
1	A	285	GLN
1	A	298	GLN
1	A	334	GLN
1	A	478	GLN
1	A	486	ASN
1	A	519	ASN
1	A	582	ASN
1	A	625	ASN
1	A	651	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 2 ligands modelled in this entry, 2 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	493/531 (92%)	0.80	96 (19%) 3 2	16, 48, 103, 113	0

All (96) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	579	LEU	5.3
1	A	565	VAL	4.7
1	A	574	ILE	4.7
1	A	588	VAL	4.5
1	A	686	PRO	4.5
1	A	557	ALA	4.4
1	A	551	LEU	4.4
1	A	590	ILE	4.1
1	A	599	LYS	4.1
1	A	635	LEU	4.0
1	A	610	LEU	3.9
1	A	569	ILE	3.9
1	A	350	CYS	3.8
1	A	188	VAL	3.8
1	A	516	VAL	3.6
1	A	609	TRP	3.6
1	A	577	THR	3.6
1	A	520	VAL	3.5
1	A	552	ILE	3.5
1	A	571	TRP	3.4
1	A	606	LYS	3.4
1	A	596	LEU	3.4
1	A	620	PRO	3.4
1	A	547	GLY	3.4
1	A	706	HIS	3.3
1	A	243	LYS	3.2
1	A	623	CYS	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	654	LEU	3.2
1	A	555	ALA	3.1
1	A	594	LEU	3.1
1	A	608	THR	3.1
1	A	244	GLU	3.1
1	A	517	PRO	3.1
1	A	607	ILE	3.1
1	A	531	ALA	3.0
1	A	641	PHE	3.0
1	A	582	ASN	3.0
1	A	576	ILE	3.0
1	A	693	LYS	3.0
1	A	575	ILE	3.0
1	A	189	GLU	2.9
1	A	518	VAL	2.9
1	A	567	THR	2.8
1	A	645	ILE	2.8
1	A	649	SER	2.7
1	A	619	ILE	2.7
1	A	525	GLU	2.7
1	A	564	GLU	2.7
1	A	508	THR	2.6
1	A	653	GLU	2.6
1	A	245	LYS	2.6
1	A	568	PHE	2.6
1	A	480	SER	2.6
1	A	613	THR	2.6
1	A	510	LEU	2.5
1	A	636	GLY	2.5
1	A	507	TYR	2.5
1	A	587	ILE	2.4
1	A	511	LEU	2.4
1	A	528	LYS	2.4
1	A	672	LEU	2.4
1	A	530	VAL	2.4
1	A	380	ALA	2.4
1	A	549	LYS	2.4
1	A	521	PRO	2.3
1	A	246	GLU	2.3
1	A	529	GLU	2.3
1	A	676	GLY	2.3
1	A	618	LEU	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	527	MET	2.3
1	A	637	LYS	2.3
1	A	445	GLY	2.3
1	A	522	GLU	2.3
1	A	655	MET	2.2
1	A	695	ALA	2.2
1	A	544	VAL	2.2
1	A	614	PRO	2.2
1	A	659	PRO	2.2
1	A	598	ASN	2.2
1	A	556	ASP	2.2
1	A	543	PRO	2.2
1	A	559	THR	2.2
1	A	638	ASP	2.2
1	A	573	ASN	2.1
1	A	670	ILE	2.1
1	A	674	ARG	2.1
1	A	539	VAL	2.1
1	A	673	GLN	2.1
1	A	611	ALA	2.1
1	A	558	GLU	2.1
1	A	661	LEU	2.0
1	A	540	GLY	2.0
1	A	554	GLY	2.0
1	A	684	TYR	2.0
1	A	642	LYS	2.0
1	A	630	ILE	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	HG	A	2002	1/1	0.85	0.22	147,147,147,147	0
2	HG	A	2001	1/1	0.91	0.19	176,176,176,176	0

6.5 Other polymers [i](#)

There are no such residues in this entry.