



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 6, 2026 – 06:50 PM UTC

PDB ID : 2CUZ / pdb_00002cuz
Title : Glutamyl-tRNA synthetase from *Thermus thermophilus* in complex with L-glutamate
Authors : Sekine, S.; Yokoyama, S.; RIKEN Structural Genomics/Proteomics Initiative (RSGI)
Deposited on : 2005-05-31
Resolution : 1.98 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

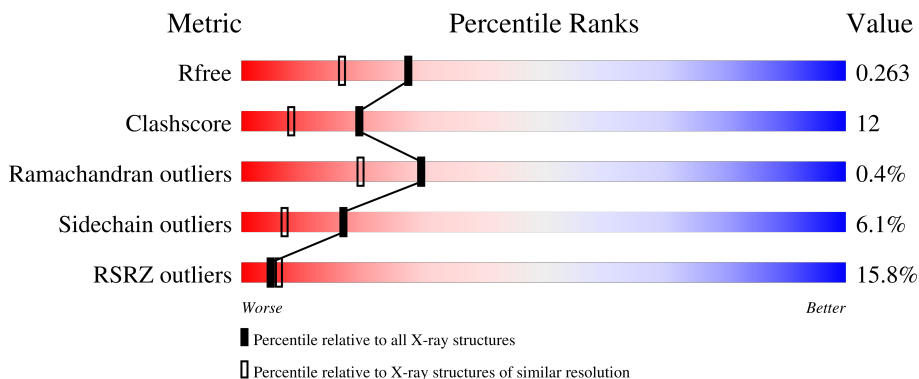
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.98 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	1506 (1.98-1.98)
Clashscore	190562	1534 (1.98-1.98)
Ramachandran outliers	187476	1518 (1.98-1.98)
Sidechain outliers	187428	1518 (1.98-1.98)
RSRZ outliers	180081	1506 (1.98-1.98)

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	468	

2 Entry composition [i](#)

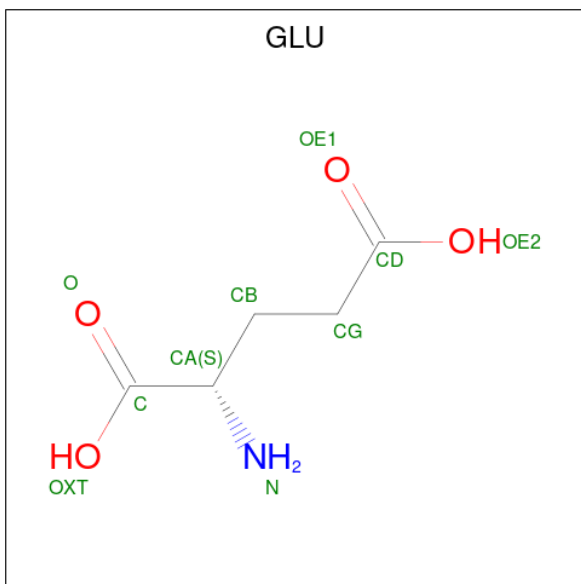
There are 3 unique types of molecules in this entry. The entry contains 3974 atoms, of which 0 are hydrogens and 0 are deuteriums.

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
			Total	C	N	O	S			
1	A	468	3814	2443	676	687	8	0	0	0

- Molecule 2 is GLUTAMIC ACID (CCD ID: GLU) (formula: C₅H₉NO₄).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
			Total	C	N	O		
2	A	1	10	5	1	4	0	0

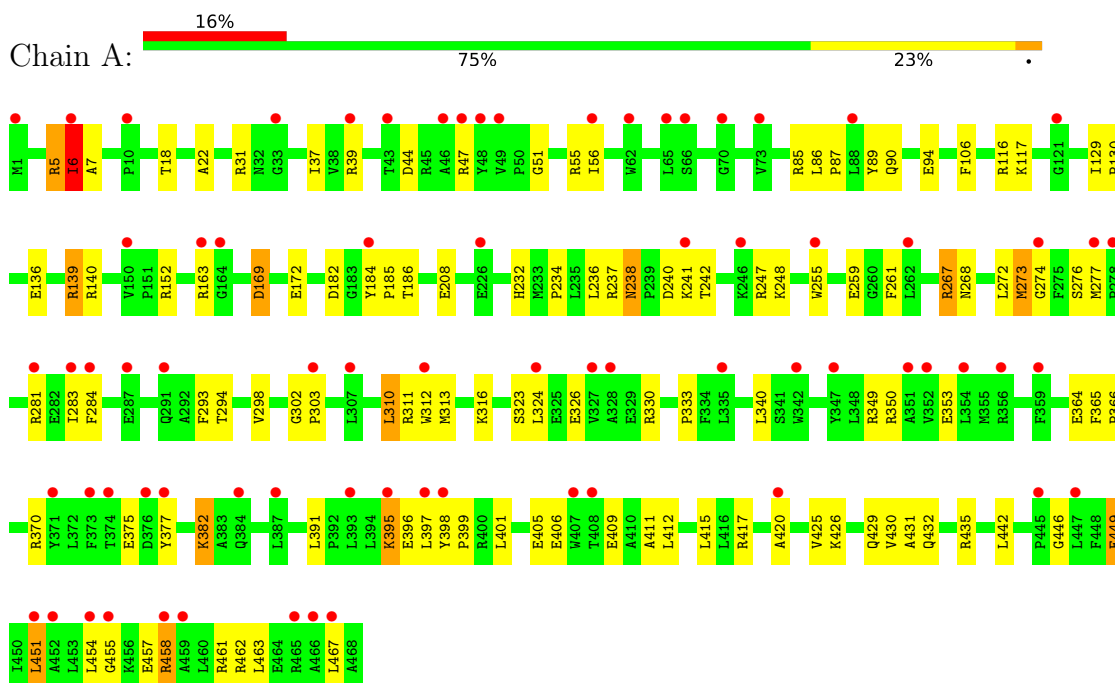
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	150	Total	O	0	0
			150	150		

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 i

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.15Å 84.04Å 83.66Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 1.98 19.95 – 1.98	Depositor EDS
% Data completeness (in resolution range)	98.6 (19.95-1.98) 98.5 (19.95-1.98)	Depositor EDS
R_{merge}	0.06	Depositor
R_{sym}	0.06	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.97 (at 1.95Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.228 , 0.263 0.230 , 0.263	Depositor DCC
R_{free} test set	2113 reflections (5.01%)	wwPDB-VP
Wilson B-factor (Å ²)	43.2	Xtriage
Anisotropy	0.093	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.27 , 27.4	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.32$	Xtriage
Estimated twinning fraction	0.019 for -h,l,k 0.019 for -k,-h,-l 0.023 for l,-k,h 0.007 for l,h,k 0.007 for k,l,h	Xtriage
F_o, F_c correlation	0.94	EDS
Total number of atoms	3974	wwPDB-VP
Average B, all atoms (Å ²)	50.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.77% 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](#)

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	0.67	0/3910	0.99	13/5293 (0.2%)

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	302	GLY	CA-C-N	7.11	126.87	119.76
1	A	302	GLY	C-N-CA	7.11	126.87	119.76
1	A	6	ILE	N-CA-C	-6.97	98.44	108.48
1	A	237	ARG	N-CA-C	6.88	120.72	109.85
1	A	293	PHE	N-CA-C	6.45	119.73	110.24
1	A	169	ASP	N-CA-C	-6.22	99.88	109.76
1	A	186	THR	N-CA-C	-6.20	101.29	110.46
1	A	106	PHE	N-CA-C	6.13	120.46	112.92
1	A	430	VAL	N-CA-C	-5.87	106.76	111.81
1	A	417	ARG	N-CA-C	-5.81	104.86	111.07
1	A	129	ILE	N-CA-C	-5.77	103.66	108.63
1	A	431	ALA	N-CA-C	5.75	117.22	111.07
1	A	238	ASN	N-CA-C	-5.75	101.68	110.07

There are no chirality outliers.

There are no planarity outliers.

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	3814	0	3818	89	0
2	A	10	0	5	0	0
3	A	150	0	0	4	0
All	All	3974	0	3823	89	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 12.

All (89) 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:238:ASN:HD22	1:A:242:THR:HG23	1.23	0.99
1:A:458:ARG:HE	1:A:458:ARG:H	1.04	0.96
1:A:457:GLU:H	1:A:458:ARG:HH21	1.04	0.94
1:A:240:ASP:OD2	1:A:242:THR:HG22	1.68	0.93
1:A:457:GLU:N	1:A:458:ARG:HH21	1.74	0.84
1:A:6:ILE:HD12	1:A:22:ALA:HB2	1.59	0.83
1:A:458:ARG:H	1:A:458:ARG:NE	1.78	0.81
1:A:457:GLU:H	1:A:458:ARG:NH2	1.81	0.77
1:A:139:ARG:HH11	1:A:139:ARG:HB3	1.49	0.76
1:A:6:ILE:HD11	1:A:18:THR:HG22	1.65	0.76
1:A:454:LEU:HD22	1:A:454:LEU:H	1.51	0.75
1:A:458:ARG:HE	1:A:458:ARG:N	1.84	0.74
1:A:56:ILE:HG13	3:A:1071:HOH:O	1.90	0.72
1:A:238:ASN:HD22	1:A:242:THR:CG2	1.99	0.71
1:A:6:ILE:HD11	1:A:18:THR:CG2	2.23	0.69
1:A:324:LEU:HD13	1:A:349:ARG:NH2	2.09	0.68
1:A:412:LEU:HD13	1:A:451:LEU:HD13	1.74	0.68
1:A:234:PRO:HB2	1:A:303:PRO:HD3	1.76	0.66
1:A:454:LEU:O	1:A:458:ARG:HD2	1.99	0.63
1:A:426:LYS:H	1:A:429:GLN:NE2	1.96	0.63
1:A:312:TRP:CZ2	1:A:316:LYS:HD2	2.35	0.62
1:A:365:PHE:HB3	1:A:366:PRO:HD3	1.81	0.62
1:A:323:SER:OG	1:A:326:GLU:HG3	1.99	0.61
1:A:169:ASP:O	1:A:172:GLU:HG3	2.00	0.60
1:A:391:LEU:HD22	1:A:467:LEU:HD23	1.83	0.60
1:A:340:LEU:HD21	1:A:370:ARG:NH1	2.16	0.60
1:A:377:TYR:OH	1:A:462:ARG:HD3	2.02	0.59
1:A:398:TYR:HB3	1:A:399:PRO:HD3	1.83	0.59
1:A:272:LEU:HD11	1:A:313:MET:HE1	1.85	0.57
1:A:90:GLN:O	1:A:94:GLU:HG3	2.04	0.56
1:A:382:LYS:HB2	1:A:382:LYS:NZ	2.21	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:ARG:CZ	1:A:281:ARG:HB3	2.36	0.56
1:A:261:PHE:CE2	1:A:310:LEU:HD13	2.41	0.55
1:A:311:ARG:NH2	1:A:364:GLU:OE2	2.40	0.55
1:A:116:ARG:HH12	1:A:117:LYS:HE3	1.73	0.54
1:A:455:GLY:HA3	1:A:458:ARG:NH1	2.22	0.54
1:A:324:LEU:HD22	1:A:349:ARG:HG3	1.89	0.54
1:A:396:GLU:O	1:A:399:PRO:HD2	2.09	0.52
1:A:240:ASP:O	1:A:241:LYS:HB2	2.11	0.51
1:A:397:LEU:HG	1:A:401:LEU:HD13	1.93	0.51
1:A:454:LEU:HD22	1:A:454:LEU:N	2.23	0.51
1:A:116:ARG:NH1	1:A:117:LYS:HE3	2.27	0.49
1:A:277:MET:HE2	1:A:284:PHE:CG	2.47	0.49
1:A:324:LEU:HD11	1:A:353:GLU:HB2	1.94	0.49
1:A:454:LEU:H	1:A:454:LEU:CD2	2.23	0.49
1:A:89:TYR:CD2	1:A:185:PRO:HG3	2.48	0.49
1:A:56:ILE:CG1	3:A:1071:HOH:O	2.56	0.49
1:A:182:ASP:OD2	1:A:184:TYR:HB2	2.13	0.49
1:A:273:MET:HE2	1:A:273:MET:HA	1.95	0.49
1:A:391:LEU:HD22	1:A:467:LEU:CD2	2.43	0.48
1:A:277:MET:CE	1:A:281:ARG:HH12	2.26	0.48
1:A:409:GLU:CD	1:A:449:GLU:HG3	2.39	0.47
1:A:426:LYS:HB2	1:A:429:GLN:HE21	1.81	0.46
1:A:44:ASP:OD1	1:A:47:ARG:HG3	2.16	0.46
1:A:420:ALA:HB1	1:A:425:VAL:O	2.16	0.45
1:A:86:LEU:N	1:A:87:PRO:CD	2.78	0.45
1:A:163:ARG:NH1	1:A:232:HIS:O	2.42	0.45
1:A:324:LEU:O	1:A:324:LEU:HD23	2.15	0.45
1:A:274:GLY:O	1:A:298:VAL:HG13	2.17	0.45
1:A:139:ARG:HH11	1:A:139:ARG:CB	2.25	0.44
1:A:281:ARG:HB3	1:A:281:ARG:NH1	2.33	0.44
1:A:412:LEU:HD13	1:A:451:LEU:HB3	1.99	0.44
1:A:163:ARG:HH11	1:A:163:ARG:HG3	1.82	0.44
1:A:208:GLU:H	1:A:208:GLU:CD	2.25	0.44
1:A:395:LYS:HG2	1:A:467:LEU:HD22	2.00	0.44
1:A:406:GLU:OE1	1:A:411:ALA:HB2	2.18	0.44
1:A:281:ARG:HH11	1:A:281:ARG:HG2	1.81	0.44
1:A:5:ARG:HB3	1:A:37:ILE:CG1	2.48	0.43
1:A:391:LEU:CD2	1:A:467:LEU:HD23	2.48	0.43
1:A:406:GLU:CD	1:A:411:ALA:HB2	2.43	0.43
1:A:51:GLY:O	1:A:55:ARG:HG3	2.19	0.43
1:A:281:ARG:NH1	1:A:284:PHE:HB3	2.33	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:281:ARG:HH11	1:A:281:ARG:CG	2.32	0.42
1:A:274:GLY:O	1:A:298:VAL:HA	2.19	0.42
1:A:330:ARG:O	1:A:333:PRO:HD2	2.20	0.42
1:A:136:GLU:O	1:A:140:ARG:HG3	2.20	0.41
1:A:281:ARG:CZ	1:A:281:ARG:CB	2.98	0.41
1:A:238:ASN:ND2	1:A:242:THR:HG23	2.08	0.41
1:A:272:LEU:CD1	1:A:313:MET:HE1	2.50	0.41
1:A:255:TRP:CZ2	1:A:259:GLU:HG3	2.55	0.41
1:A:435:ARG:HD2	1:A:442:LEU:HA	2.03	0.41
1:A:432:GLN:OE1	1:A:435:ARG:NH2	2.50	0.41
1:A:5:ARG:HB3	1:A:37:ILE:HG12	2.02	0.40
1:A:283:ILE:HD13	1:A:313:MET:HE2	2.03	0.40
1:A:5:ARG:HD2	3:A:1001:HOH:O	2.21	0.40
1:A:268:ASN:HD22	1:A:268:ASN:C	2.28	0.40
1:A:375:GLU:CD	1:A:462:ARG:HH21	2.30	0.40
1:A:267:ARG:HD3	3:A:1067:HOH:O	2.20	0.40
1:A:7:ALA:HA	1:A:39:ARG:O	2.22	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	466/468 (100%)	456 (98%)	8 (2%)	2 (0%)	30 20

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	273	MET
1	A	446	GLY

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	393/393 (100%)	369 (94%)	24 (6%)	17 7

All (24) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	5	ARG
1	A	6	ILE
1	A	31	ARG
1	A	85	ARG
1	A	130	PRO
1	A	139	ARG
1	A	152	ARG
1	A	236	LEU
1	A	247	ARG
1	A	248	LYS
1	A	267	ARG
1	A	276	SER
1	A	294	THR
1	A	310	LEU
1	A	350	ARG
1	A	382	LYS
1	A	395	LYS
1	A	405	GLU
1	A	415	LEU
1	A	449	GLU
1	A	451	LEU
1	A	458	ARG
1	A	461	ARG
1	A	463	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (4) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	170	ASN

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Mol	Chain	Res	Type
1	A	196	HIS
1	A	238	ASN
1	A	429	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 [i](#)

1 ligand is 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	GLU	A	501	-	8,9,9	1.12	0	8,11,11	0.77	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
2	GLU	A	501	-	-	0/9/9/9	-

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 [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

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	468/468 (100%)	1.01	74 (15%) 5 6	28, 47, 76, 91	0

All (74) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	451	LEU	8.2
1	A	274	GLY	7.1
1	A	335	LEU	6.9
1	A	447	LEU	5.9
1	A	121	GLY	4.9
1	A	184	TYR	4.6
1	A	327	VAL	4.4
1	A	359	PHE	4.4
1	A	46	ALA	4.2
1	A	65	LEU	4.1
1	A	342	TRP	4.0
1	A	454	LEU	4.0
1	A	328	ALA	3.9
1	A	408	THR	3.9
1	A	241	LYS	3.8
1	A	284	PHE	3.8
1	A	351	ALA	3.8
1	A	56	ILE	3.6
1	A	48	TYR	3.5
1	A	278	PRO	3.5
1	A	466	ALA	3.4
1	A	150	VAL	3.3
1	A	420	ALA	3.3
1	A	467	LEU	3.3
1	A	393	LEU	3.2
1	A	88	LEU	3.2
1	A	287	GLU	3.2

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Mol	Chain	Res	Type	RSRZ
1	A	398	TYR	3.1
1	A	387	LEU	3.1
1	A	407	TRP	3.0
1	A	459	ALA	3.0
1	A	262	LEU	3.0
1	A	312	TRP	3.0
1	A	458	ARG	2.9
1	A	6	ILE	2.8
1	A	324	LEU	2.8
1	A	281	ARG	2.8
1	A	49	VAL	2.7
1	A	291	GLN	2.7
1	A	62	TRP	2.6
1	A	66	SER	2.6
1	A	47	ARG	2.6
1	A	10	PRO	2.6
1	A	1	MET	2.6
1	A	371	TYR	2.6
1	A	452	ALA	2.5
1	A	395	LYS	2.5
1	A	307	LEU	2.5
1	A	465	ARG	2.5
1	A	354	LEU	2.4
1	A	397	LEU	2.4
1	A	303	PRO	2.4
1	A	376	ASP	2.4
1	A	43	THR	2.4
1	A	164	GLY	2.4
1	A	277	MET	2.3
1	A	70	GLY	2.3
1	A	455	GLY	2.3
1	A	384	GLN	2.3
1	A	377	TYR	2.3
1	A	246	LYS	2.3
1	A	373	PHE	2.2
1	A	226	GLU	2.2
1	A	283	ILE	2.1
1	A	33	GLY	2.1
1	A	163	ARG	2.1
1	A	374	THR	2.1
1	A	352	VAL	2.1
1	A	356	ARG	2.1

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Mol	Chain	Res	Type	RSRZ
1	A	347	TYR	2.0
1	A	73	VAL	2.0
1	A	255	TRP	2.0
1	A	445	PRO	2.0
1	A	39	ARG	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(\AA^2)	Q<0.9
2	GLU	A	501	10/10	0.72	0.16	48,64,73,76	0

6.5 Other polymers [i](#)

There are no such residues in this entry.