



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 8, 2026 – 05:10 PM UTC

PDB ID : 8WIA / pdb_00008wia
Title : Crystal structure of E. coli ThrS catalytic domain mutant G463S
Authors : Qiao, H.; Wang, Z.; Wang, J.; Fang, P.
Deposited on : 2023-09-24
Resolution : 1.96 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

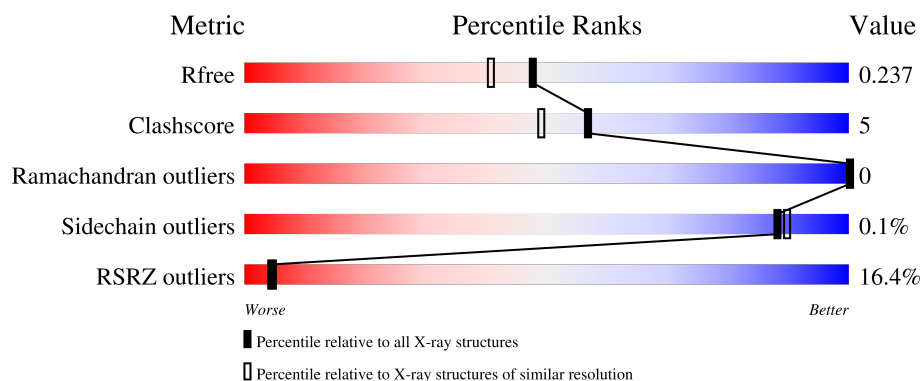
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.96 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	3494 (1.96-1.96)
Clashscore	190562	3612 (1.96-1.96)
Ramachandran outliers	187476	3587 (1.96-1.96)
Sidechain outliers	187428	3587 (1.96-1.96)
RSRZ outliers	180081	3495 (1.96-1.96)

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	410	17% 88% 10% .
1	B	410	15% 84% 13% .

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 7126 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 Threonine-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	402	Total	C	N	O	S	0	1	0
			3285	2077	574	610	24			
1	B	399	Total	C	N	O	S	0	1	0
			3265	2061	577	604	23			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	MET	-	initiating methionine	UNP A0A8S7FUD7
A	463	SER	GLY	engineered mutation	UNP A0A8S7FUD7
A	643	LEU	-	expression tag	UNP A0A8S7FUD7
A	644	GLU	-	expression tag	UNP A0A8S7FUD7
A	645	HIS	-	expression tag	UNP A0A8S7FUD7
A	646	HIS	-	expression tag	UNP A0A8S7FUD7
A	647	HIS	-	expression tag	UNP A0A8S7FUD7
A	648	HIS	-	expression tag	UNP A0A8S7FUD7
A	649	HIS	-	expression tag	UNP A0A8S7FUD7
A	650	HIS	-	expression tag	UNP A0A8S7FUD7
B	241	MET	-	initiating methionine	UNP A0A8S7FUD7
B	463	SER	GLY	engineered mutation	UNP A0A8S7FUD7
B	643	LEU	-	expression tag	UNP A0A8S7FUD7
B	644	GLU	-	expression tag	UNP A0A8S7FUD7
B	645	HIS	-	expression tag	UNP A0A8S7FUD7
B	646	HIS	-	expression tag	UNP A0A8S7FUD7
B	647	HIS	-	expression tag	UNP A0A8S7FUD7
B	648	HIS	-	expression tag	UNP A0A8S7FUD7
B	649	HIS	-	expression tag	UNP A0A8S7FUD7
B	650	HIS	-	expression tag	UNP A0A8S7FUD7

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

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

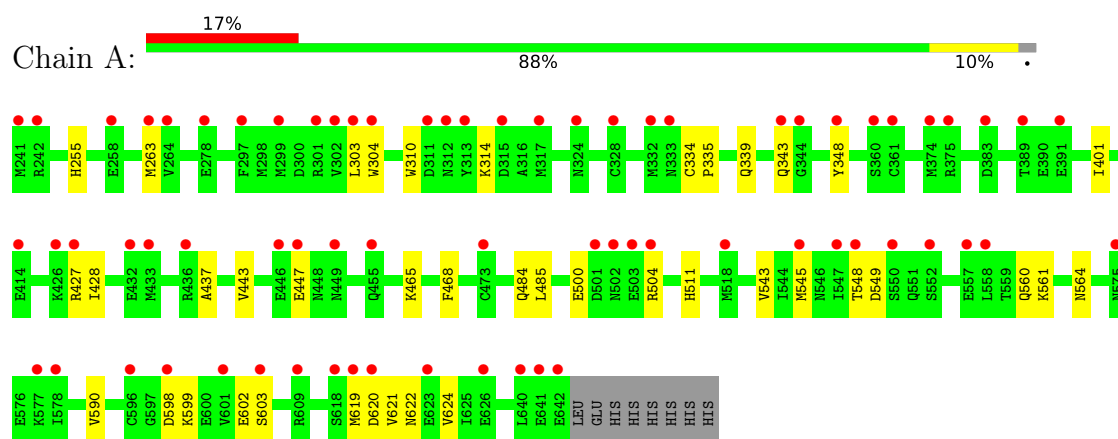
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	273	Total 273	O 273	0	0
3	B	301	Total 301	O 301	0	0

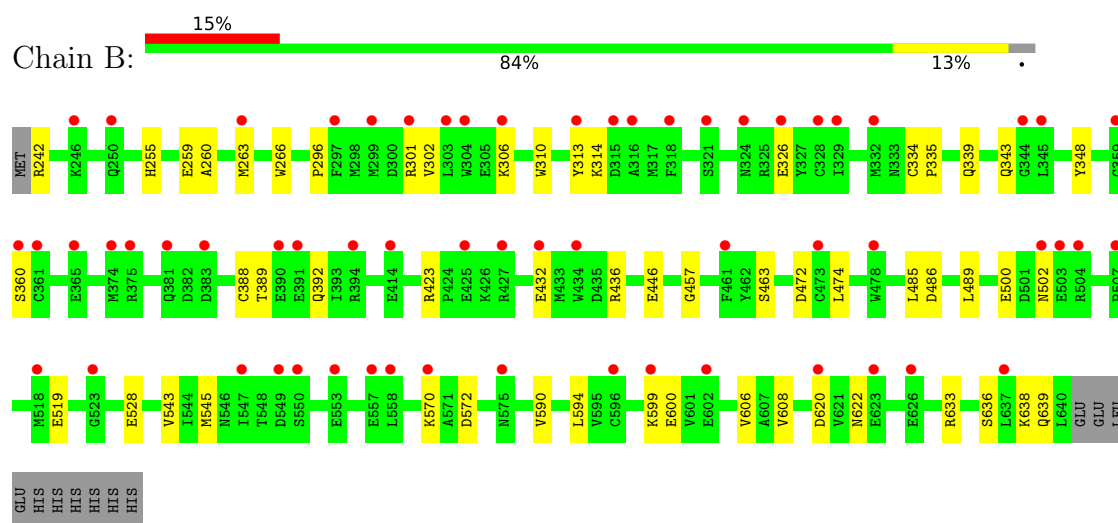
3 Residue-property plots [i](#)

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: Threonine-tRNA ligase



• Molecule 1: Threonine-tRNA ligase



4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	90.96Å 107.41Å 112.79Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	42.18 – 1.96 42.18 – 1.96	Depositor EDS
% Data completeness (in resolution range)	97.1 (42.18-1.96) 97.1 (42.18-1.96)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.27 (at 1.95Å)	Xtriage
Refinement program	PHENIX (1.20.1_4487: ???)	Depositor
R, R_{free}	0.212 , 0.237 0.213 , 0.237	Depositor DCC
R_{free} test set	3848 reflections (4.80%)	wwPDB-VP
Wilson B-factor (Å ²)	34.5	Xtriage
Anisotropy	0.535	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.28 , 48.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.50$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.005 for -h,l,k	Xtriage
F_o, F_c correlation	0.95	EDS
Total number of atoms	7126	wwPDB-VP
Average B, all atoms (Å ²)	37.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.30% 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: 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	0.10	0/3357	0.28	0/4521
1	B	0.09	0/3336	0.27	0/4492
All	All	0.10	0/6693	0.27	0/9013

There are no bond length outliers.

There are no bond angle outliers.

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	3285	0	3204	25	0
1	B	3265	0	3195	38	0
2	A	1	0	0	0	0
2	B	1	0	0	0	0
3	A	273	0	0	1	0
3	B	301	0	0	6	0
All	All	7126	0	6399	59	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 5.

All (59) 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:B:633:ARG:HD3	3:B:981:HOH:O	1.60	1.01
1:B:360:SER:HB2	3:B:1042:HOH:O	1.94	0.65
1:B:639:GLN:CB	3:B:1026:HOH:O	2.44	0.65
1:A:484:GLN:HB2	1:A:511:HIS:HB2	1.82	0.61
1:B:348:TYR:CZ	1:B:500:GLU:HG3	2.36	0.60
1:A:465:LYS:HB3	1:A:484:GLN:HG2	1.84	0.59
1:A:561:LYS:NZ	1:A:622:ASN:OD1	2.37	0.58
1:A:619:MET:HE2	1:A:624:VAL:HG22	1.87	0.57
1:B:389:THR:H	1:B:392:GLN:NE2	2.03	0.56
1:A:263:MET:HB3	1:B:296:PRO:HB3	1.87	0.55
1:A:620:ASP:OD1	1:A:621:VAL:N	2.40	0.55
1:A:599:LYS:O	1:A:603:SER:OG	2.20	0.54
1:B:260:ALA:HB1	1:B:263:MET:HE3	1.90	0.54
1:B:301:ARG:NH1	1:B:326:GLU:OE1	2.42	0.52
1:A:310:TRP:O	1:A:314:LYS:HB3	2.10	0.52
1:A:543:VAL:HG23	1:A:590:VAL:HG11	1.91	0.52
1:B:334:CYS:HB2	1:B:335:PRO:HD3	1.91	0.51
1:A:334:CYS:HB2	1:A:335:PRO:HD3	1.92	0.50
1:B:335:PRO:O	1:B:339:GLN:HG2	2.11	0.50
1:B:594:LEU:HD22	1:B:608:VAL:HG22	1.93	0.49
1:B:389:THR:H	1:B:392:GLN:HE21	1.59	0.48
1:A:348:TYR:CZ	1:A:500:GLU:HG3	2.49	0.48
1:B:446:GLU:OE2	3:B:802:HOH:O	2.20	0.48
1:A:255:HIS:ND1	1:B:343:GLN:HG3	2.29	0.47
1:B:310:TRP:O	1:B:314:LYS:HB2	2.14	0.47
1:B:570:LYS:HB3	1:B:570:LYS:HE2	1.64	0.47
1:B:594:LEU:HB3	1:B:606:VAL:HG21	1.96	0.47
1:A:504:ARG:NH1	3:A:810:HOH:O	2.48	0.46
1:B:543:VAL:HG23	1:B:590:VAL:HG11	1.97	0.46
1:A:335:PRO:O	1:A:339:GLN:HG2	2.15	0.46
1:B:313:TYR:OH	3:B:801:HOH:O	2.20	0.46
1:B:636:SER:OG	1:B:638:LYS:O	2.34	0.46
1:A:437:ALA:HA	1:A:485:LEU:HD23	1.97	0.45
1:B:472:ASP:HB2	1:B:528:GLU:OE1	2.16	0.45
1:A:427:ARG:HG2	1:A:428:ILE:N	2.31	0.45
1:A:560:GLN:HE21	1:A:564:ASN:ND2	2.15	0.45
1:B:242:ARG:N	3:B:813:HOH:O	2.49	0.45
1:B:242:ARG:HD2	1:B:474:LEU:HD11	1.99	0.45
1:B:620:ASP:OD1	1:B:622:ASN:N	2.49	0.44
1:B:301:ARG:HD2	1:B:310:TRP:CZ2	2.53	0.44
1:A:401:ILE:HD12	1:A:468:PHE:HZ	1.83	0.43

Continued on next page...

Continued from previous page...

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:TRP:CZ3	1:A:335:PRO:HG2	2.53	0.43
1:B:348:TYR:CE2	1:B:500:GLU:HG3	2.54	0.43
1:B:266:TRP:HZ2	1:B:519:GLU:HG3	1.84	0.43
1:B:432:GLU:O	1:B:436[B]:ARG:HG3	2.19	0.43
1:A:545:MET:HE2	1:A:545:MET:HB3	1.95	0.43
1:A:548:THR:OG1	1:A:549:ASP:N	2.52	0.43
1:B:263:MET:HE3	1:B:263:MET:HB2	1.90	0.42
1:B:302:VAL:O	1:B:306:LYS:HG3	2.20	0.42
1:B:463:SER:HB2	1:B:485:LEU:O	2.19	0.42
1:B:545:MET:HG2	1:B:572:ASP:HB3	2.01	0.42
1:A:598:ASP:O	1:A:602:GLU:HG3	2.20	0.41
1:B:486:ASP:OD2	1:B:489:LEU:HB2	2.20	0.41
1:A:343:GLN:HG3	1:B:255:HIS:CG	2.55	0.41
1:A:443:VAL:O	1:A:447:GLU:HG3	2.20	0.41
1:B:423:ARG:O	1:B:457:GLY:HA2	2.21	0.41
1:B:599:LYS:NZ	1:B:600:GLU:OE2	2.31	0.41
1:A:303:LEU:HD13	1:B:259:GLU:HG2	2.02	0.40
1:B:388:CYS:HB2	1:B:392:GLN:HE21	1.86	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	401/410 (98%)	399 (100%)	2 (0%)	0	100	100
1	B	398/410 (97%)	397 (100%)	1 (0%)	0	100	100
All	All	799/820 (97%)	796 (100%)	3 (0%)	0	100	100

There are no Ramachandran outliers to report.

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	356/366 (97%)	356 (100%)	0	100	100
1	B	354/366 (97%)	353 (100%)	1 (0%)	86	87
All	All	710/732 (97%)	709 (100%)	1 (0%)	88	90

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	B	502	ASN

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	250	GLN
1	A	449	ASN
1	A	560	GLN
1	A	564	ASN
1	B	392	GLN
1	B	479	GLN
1	B	484	GLN
1	B	502	ASN
1	B	630	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](#)

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 [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	402/410 (98%)	1.09	70 (17%) 4 4	17, 30, 38, 57	288 (71%)
1	B	399/410 (97%)	1.05	61 (15%) 5 6	19, 29, 37, 61	283 (70%)
All	All	801/820 (97%)	1.07	131 (16%) 4 5	17, 29, 38, 61	571 (71%)

All (131) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	313	TYR	7.2
1	B	332	MET	7.0
1	A	620	ASP	6.7
1	A	383	ASP	6.1
1	A	241	MET	5.6
1	B	313	TYR	5.3
1	B	328	CYS	5.1
1	B	297	PHE	4.8
1	B	361	CYS	4.7
1	B	303	LEU	4.4
1	B	575	ASN	4.3
1	B	360	SER	4.2
1	A	332	MET	4.2
1	A	449	ASN	4.1
1	B	383	ASP	4.1
1	A	361	CYS	4.1
1	A	548	THR	4.0
1	A	258	GLU	4.0
1	B	390	GLU	3.9
1	B	427	ARG	3.8
1	A	311	ASP	3.8
1	B	461	PHE	3.8
1	B	315	ASP	3.7
1	A	642	GLU	3.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	641	GLU	3.7
1	B	473	CYS	3.7
1	B	553	GLU	3.6
1	B	549	ASP	3.5
1	A	598	ASP	3.5
1	A	263	MET	3.5
1	A	303	LEU	3.4
1	B	550	SER	3.3
1	A	432	GLU	3.2
1	A	619	MET	3.2
1	B	478	TRP	3.2
1	A	504	ARG	3.2
1	B	432	GLU	3.2
1	B	318	PHE	3.1
1	B	620	ASP	3.1
1	A	501	ASP	3.1
1	B	304	TRP	3.1
1	B	434	TRP	3.0
1	A	575	ASN	3.0
1	A	317	MET	3.0
1	B	503	GLU	3.0
1	A	547	ILE	3.0
1	A	640	LEU	2.9
1	A	596	CYS	2.9
1	A	312	ASN	2.8
1	B	637	LEU	2.8
1	B	326	GLU	2.8
1	A	391	GLU	2.8
1	B	602	GLU	2.8
1	A	297[A]	PHE	2.7
1	B	557	GLU	2.7
1	A	618	SER	2.7
1	B	321	SER	2.7
1	A	264	VAL	2.7
1	A	348	TYR	2.7
1	A	360	SER	2.7
1	A	552	SER	2.7
1	A	446	GLU	2.7
1	B	414	GLU	2.7
1	A	518	MET	2.7
1	A	503	GLU	2.7
1	B	391	GLU	2.7

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	299	MET	2.6
1	A	447	GLU	2.6
1	A	304	TRP	2.6
1	B	345	LEU	2.6
1	B	263	MET	2.6
1	A	557	GLU	2.6
1	A	623	GLU	2.6
1	B	623	GLU	2.6
1	A	550	SER	2.6
1	B	518	MET	2.5
1	B	299	MET	2.5
1	B	324	ASN	2.5
1	B	504	ARG	2.5
1	B	365	GLU	2.5
1	A	545	MET	2.5
1	B	375	ARG	2.4
1	A	302	VAL	2.4
1	A	626	GLU	2.4
1	A	426	LYS	2.4
1	A	502	ASN	2.4
1	B	381	GLN	2.4
1	B	502	ASN	2.4
1	B	306	LYS	2.4
1	A	578	ILE	2.3
1	B	547	ILE	2.3
1	A	433	MET	2.3
1	B	359	GLY	2.3
1	A	375	ARG	2.3
1	B	596	CYS	2.3
1	B	374	MET	2.3
1	A	577	LYS	2.3
1	B	344	GLY	2.3
1	A	242	ARG	2.3
1	A	473	CYS	2.3
1	A	558	LEU	2.3
1	A	389	THR	2.3
1	B	316	ALA	2.3
1	B	626	GLU	2.3
1	B	250	GLN	2.3
1	B	425	GLU	2.2
1	A	601	VAL	2.2
1	B	558	LEU	2.2

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	RSRZ
1	A	603	SER	2.2
1	A	436	ARG	2.2
1	A	609	ARG	2.2
1	B	301	ARG	2.2
1	B	394	ARG	2.2
1	A	278	GLU	2.2
1	A	315	ASP	2.2
1	A	374	MET	2.2
1	A	344	GLY	2.1
1	B	246	LYS	2.1
1	B	599	LYS	2.1
1	B	523	GLY	2.1
1	A	328	CYS	2.1
1	B	507	PRO	2.1
1	A	455	GLN	2.1
1	A	301	ARG	2.1
1	A	414	GLU	2.0
1	A	324	ASN	2.0
1	A	333	ASN	2.0
1	B	570	LYS	2.0
1	B	329	ILE	2.0
1	A	343	GLN	2.0
1	A	427	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.

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
-----	------	-------	-----	-------	------	-----	-----------------------------	-------

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	ZN	A	701	1/1	0.87	0.10	38,38,38,38	1
2	ZN	B	701	1/1	0.91	0.09	37,37,37,37	1

6.5 Other polymers [i](#)

There are no such residues in this entry.