



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 12, 2026 – 04:12 PM UTC

PDB ID : 4NCX / pdb_00004ncx
Title : Crystal Structure of Prolyl-tRNA synthetase (ProRS, Proline-tRNA ligase)
from Plasmodium falciparum 3D7
Authors : Seattle Structural Genomics Center for Infectious Disease (SSGCID)
Deposited on : 2013-10-25
Resolution : 1.85 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

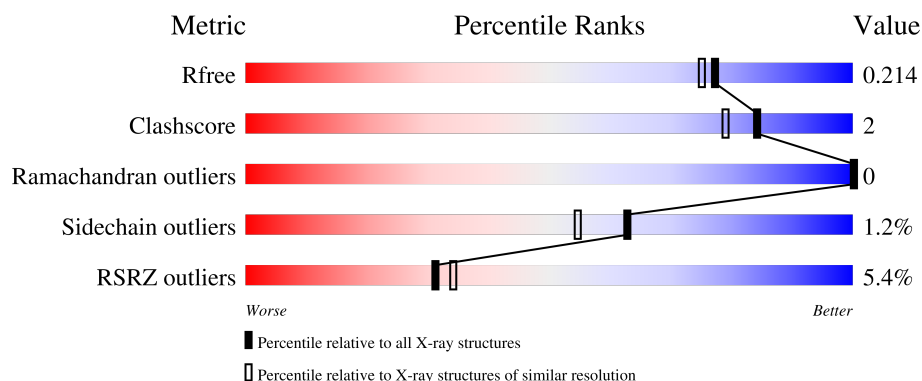
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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	3428 (1.86-1.86)
Clashscore	190562	3579 (1.86-1.86)
Ramachandran outliers	187476	3553 (1.86-1.86)
Sidechain outliers	187428	3553 (1.86-1.86)
RSRZ outliers	180081	3429 (1.86-1.86)

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	506	6% 82% 6% 11%
1	B	506	4% 81% • 14%

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 7861 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 Proline-tRNA ligase.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	449	Total	C	N	O	S	0	6	0
			3650	2347	607	675	21			
1	B	433	Total	C	N	O	S	0	9	0
			3563	2295	591	656	21			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	MET	-	expression tag	UNP Q8I5R7
A	242	ALA	-	expression tag	UNP Q8I5R7
A	243	HIS	-	expression tag	UNP Q8I5R7
A	244	HIS	-	expression tag	UNP Q8I5R7
A	245	HIS	-	expression tag	UNP Q8I5R7
A	246	HIS	-	expression tag	UNP Q8I5R7
A	247	HIS	-	expression tag	UNP Q8I5R7
A	248	HIS	-	expression tag	UNP Q8I5R7
B	241	MET	-	expression tag	UNP Q8I5R7
B	242	ALA	-	expression tag	UNP Q8I5R7
B	243	HIS	-	expression tag	UNP Q8I5R7
B	244	HIS	-	expression tag	UNP Q8I5R7
B	245	HIS	-	expression tag	UNP Q8I5R7
B	246	HIS	-	expression tag	UNP Q8I5R7
B	247	HIS	-	expression tag	UNP Q8I5R7
B	248	HIS	-	expression tag	UNP Q8I5R7

- Molecule 2 is 1,2-ETHANEDIOL (CCD ID: EDO) (formula: C₂H₆O₂).



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

- Molecule 3 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

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

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	318	Total	O	0	8
			326	326		

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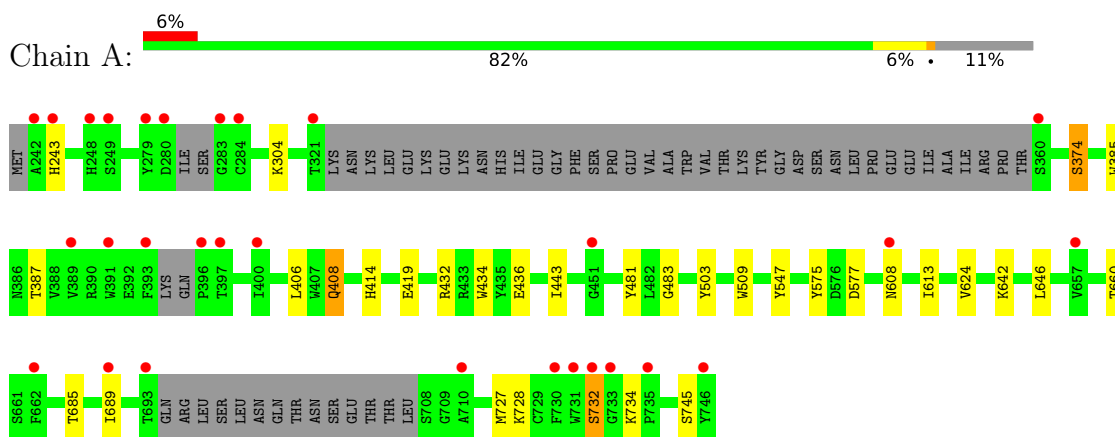
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Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	B	286	Total 295	O 295	0	9

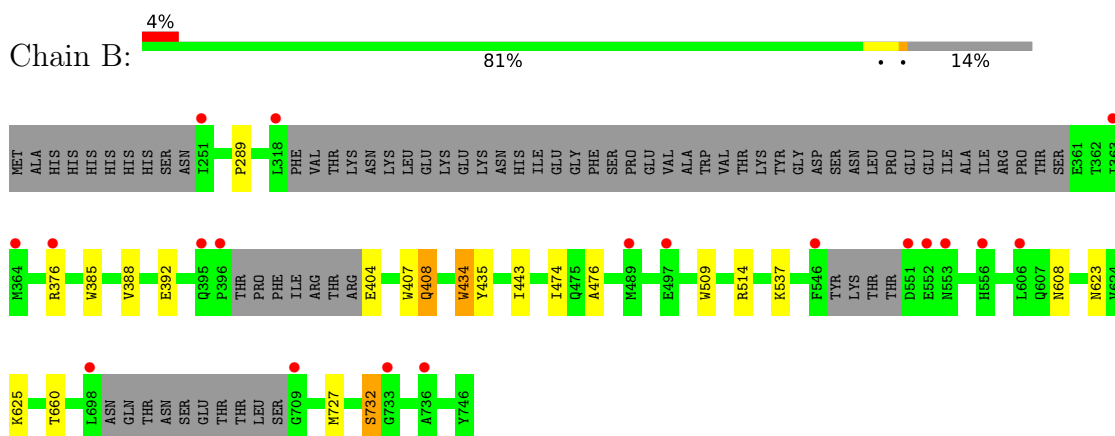
3 Residue-property plots [i](#)

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: Proline-tRNA ligase



• Molecule 1: Proline-tRNA ligase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	147.96Å 91.38Å 110.84Å 90.00° 129.48° 90.00°	Depositor
Resolution (Å)	46.46 – 1.85 46.46 – 1.85	Depositor EDS
% Data completeness (in resolution range)	99.5 (46.46-1.85) 99.5 (46.46-1.85)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	3.12 (at 1.86Å)	Xtriage
Refinement program	REFMAC	Depositor
R, R_{free}	0.169 , 0.206 0.178 , 0.214	Depositor DCC
R_{free} test set	4832 reflections (4.98%)	wwPDB-VP
Wilson B-factor (Å ²)	24.8	Xtriage
Anisotropy	0.286	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.36 , 55.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.49$, $\langle L^2 \rangle = 0.33$	Xtriage
Estimated twinning fraction	0.014 for h,-k,-h-l	Xtriage
F_o, F_c correlation	0.96	EDS
Total number of atoms	7861	wwPDB-VP
Average B, all atoms (Å ²)	33.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.74% 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: EDO, 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	0.85	0/3742	0.90	2/5071 (0.0%)
1	B	0.82	0/3656	0.87	3/4947 (0.1%)
All	All	0.83	0/7398	0.88	5/10018 (0.0%)

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	B	0	1

There are no bond length outliers.

All (5) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	732	SER	N-CA-C	6.36	121.11	113.23
1	A	243	HIS	N-CA-C	5.74	118.88	109.76
1	B	434	TRP	CA-CB-CG	5.39	123.83	113.60
1	A	732	SER	N-CA-C	5.25	116.69	110.97
1	B	408	GLN	N-CA-CB	-5.15	101.87	110.83

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	732	SER	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	3650	0	3523	18	0
1	B	3563	0	3456	11	1
2	A	16	0	24	5	0
2	B	8	0	12	0	0
3	A	2	0	0	1	0
3	B	1	0	0	0	0
4	A	326	0	0	8	1
4	B	295	0	0	2	0
All	All	7861	0	7015	33	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 2.

All (33) 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:376[A]:ARG:HD2	4:B:1095:HOH:O	1.64	0.97
1:A:642:LYS:O	1:A:646:LEU:HD13	1.82	0.79
1:A:660:THR:HG23	1:A:727:MET:HE1	1.76	0.66
1:A:503:TYR:OH	4:A:1059:HOH:O	2.12	0.65
1:A:414:HIS:HD1	1:A:419:GLU:HG2	1.68	0.58
1:A:304:LYS:NZ	4:A:1112:HOH:O	2.39	0.55
2:A:803:EDO:H21	4:A:934:HOH:O	2.09	0.53
1:A:387:THR:HG22	1:A:406:LEU:HD22	1.91	0.52
1:A:414:HIS:ND1	1:A:419:GLU:HG2	2.25	0.52
3:A:806:CL:CL	4:A:1098[A]:HOH:O	2.56	0.52
1:B:388:VAL:HG23	1:B:407:TRP:HZ3	1.74	0.51
1:B:404:GLU:CD	4:B:1107:HOH:O	2.54	0.50
1:B:660:THR:HB	1:B:727:MET:HE1	1.94	0.49
1:A:432:ARG:O	1:A:436[A]:GLU:HG3	2.14	0.48
2:A:804:EDO:H12	1:B:537:LYS:HE2	1.97	0.47
1:A:374:SER:HB3	4:A:1168:HOH:O	2.14	0.47
1:B:435:TYR:CZ	1:B:476:ALA:HB1	2.50	0.46
1:B:608:ASN:O	1:B:625:LYS:NZ	2.46	0.46
2:A:804:EDO:H21	4:A:915:HOH:O	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:547:TYR:HE1	4:A:1100:HOH:O	1.99	0.45
1:A:727:MET:HE3	1:A:728:LYS:H	1.82	0.44
1:A:613:ILE:HD12	1:A:624:VAL:HG21	2.00	0.43
2:A:803:EDO:C2	4:A:934:HOH:O	2.65	0.43
1:B:385:TRP:CZ3	1:B:408:GLN:HB2	2.54	0.42
1:A:732:SER:OG	1:A:734:LYS:N	2.47	0.42
2:A:804:EDO:H22	1:B:289:PRO:C	2.44	0.42
1:A:443:ILE:C	1:A:443:ILE:HD12	2.45	0.42
1:A:385:TRP:CE3	1:A:408:GLN:HB3	2.56	0.41
1:A:481:TYR:CZ	1:A:483:GLY:HA2	2.56	0.41
1:B:474:ILE:HD11	1:B:514:ARG:HD3	2.03	0.41
1:A:575:TYR:CZ	1:A:577:ASP:HB3	2.55	0.41
1:A:685:THR:O	1:A:689:ILE:HG12	2.21	0.41
1:B:443:ILE:HD12	1:B:443:ILE:C	2.46	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)
1:B:392:GLU:O	1:B:392:GLU:O[2_555]	1.17	1.03
4:A:1033:HOH:O	4:A:1033:HOH:O[2_555]	2.16	0.04

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	445/506 (88%)	437 (98%)	8 (2%)	0	100	100
1	B	432/506 (85%)	421 (98%)	11 (2%)	0	100	100
All	All	877/1012 (87%)	858 (98%)	19 (2%)	0	100	100

There are no Ramachandran outliers to report.

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	394/460 (86%)	388 (98%)	6 (2%)	57	47
1	B	383/460 (83%)	380 (99%)	3 (1%)	73	67
All	All	777/920 (84%)	768 (99%)	9 (1%)	63	55

All (9) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	374	SER
1	A	408	GLN
1	A	434	TRP
1	A	509	TRP
1	A	608	ASN
1	A	745	SER
1	B	434	TRP
1	B	509	TRP
1	B	623	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (13) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	408	GLN
1	A	498	ASN
1	A	506	GLN
1	A	588	ASN
1	A	609	ASN
1	B	310	ASN
1	B	383	ASN
1	B	408	GLN
1	B	485	ASN
1	B	570	GLN
1	B	609	ASN
1	B	623	ASN
1	B	667	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 9 ligands modelled in this entry, 3 are monoatomic - leaving 6 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	$\# Z > 2$
2	EDO	B	801	-	3,3,3	0.35	0	2,2,2	0.38	0
2	EDO	A	804	-	3,3,3	0.54	0	2,2,2	0.89	0
2	EDO	A	803	-	3,3,3	0.37	0	2,2,2	0.26	0
2	EDO	A	801	-	3,3,3	0.48	0	2,2,2	0.20	0
2	EDO	A	802	-	3,3,3	0.34	0	2,2,2	0.79	0
2	EDO	B	802	-	3,3,3	0.43	0	2,2,2	0.67	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	EDO	B	801	-	-	0/1/1/1	-
2	EDO	A	804	-	-	1/1/1/1	-
2	EDO	A	803	-	-	1/1/1/1	-
2	EDO	A	801	-	-	1/1/1/1	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	EDO	A	802	-	-	1/1/1/1	-
2	EDO	B	802	-	-	0/1/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (4) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	A	802	EDO	O1-C1-C2-O2
2	A	803	EDO	O1-C1-C2-O2
2	A	804	EDO	O1-C1-C2-O2
2	A	801	EDO	O1-C1-C2-O2

There are no ring outliers.

2 monomers are involved in 5 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	804	EDO	3	0
2	A	803	EDO	2	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

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	449/506 (88%)	0.19	29 (6%)	25	27	8, 29, 61, 79	6 (1%)
1	B	433/506 (85%)	0.12	19 (4%)	39	42	9, 31, 55, 91	9 (2%)
All	All	882/1012 (87%)	0.15	48 (5%)	31	34	8, 30, 59, 91	15 (1%)

All (48) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	363	ILE	5.9
1	A	393	PHE	5.4
1	A	279	TYR	5.0
1	A	242	ALA	5.0
1	A	396	PRO	4.6
1	B	251	ILE	4.4
1	A	321	THR	4.2
1	A	662	PHE	4.0
1	B	698	LEU	4.0
1	A	391	TRP	3.9
1	B	551	ASP	3.7
1	B	709	GLY	3.6
1	A	280	ASP	3.4
1	B	376[A]	ARG	3.2
1	B	733	GLY	3.1
1	B	318	LEU	3.1
1	A	735	PRO	3.1
1	B	606	LEU	3.0
1	A	243	HIS	2.9
1	A	389	VAL	2.9
1	A	608	ASN	2.8
1	A	248	HIS	2.8
1	A	730	PHE	2.7
1	B	552	GLU	2.7

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Mol	Chain	Res	Type	RSRZ
1	A	746	TYR	2.7
1	A	283	GLY	2.6
1	A	284	CYS	2.6
1	A	733	GLY	2.5
1	A	710	ALA	2.5
1	B	396	PRO	2.5
1	A	400	ILE	2.4
1	A	657	VAL	2.3
1	A	360	SER	2.3
1	A	732	SER	2.3
1	B	497	GLU	2.3
1	A	397	THR	2.3
1	A	693	THR	2.3
1	A	249	SER	2.2
1	B	546	PHE	2.2
1	A	451	GLY	2.2
1	B	489	MET	2.2
1	B	364	MET	2.1
1	B	556	HIS	2.1
1	B	736	ALA	2.1
1	A	731	TRP	2.1
1	B	553	ASN	2.1
1	B	395	GLN	2.0
1	A	689	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	EDO	A	802	4/4	0.87	0.14	33,34,41,46	0
2	EDO	B	802	4/4	0.87	0.13	42,45,45,49	0
2	EDO	A	803	4/4	0.90	0.14	29,30,36,40	0
2	EDO	A	804	4/4	0.91	0.22	32,41,42,43	0
3	CL	B	803	1/1	0.95	0.08	42,42,42,42	0
3	CL	A	805	1/1	0.97	0.05	27,27,27,27	0
2	EDO	A	801	4/4	0.97	0.06	26,28,29,29	0
3	CL	A	806	1/1	0.98	0.09	46,46,46,46	0
2	EDO	B	801	4/4	0.98	0.05	20,23,24,25	0

6.5 Other polymers [i](#)

There are no such residues in this entry.