



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 19, 2021 – 10:03 AM EDT

PDB ID : 7LVO
Title : Cryptococcus neoformans GAR synthetase
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Deposited on : 2021-02-26
Resolution : 2.00 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 following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix) : 1.13
EDS : 2.23.1
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac : 5.8.0158
CCP4 : 7.0.044 (Gargrove)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.23.1

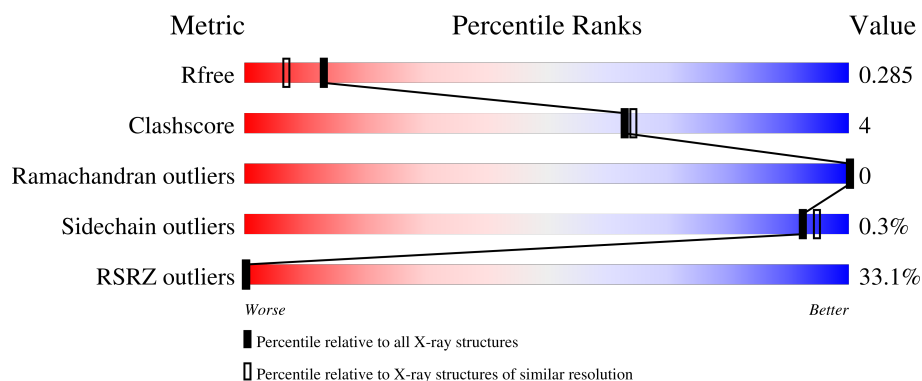
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.00 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}	130704	8085 (2.00-2.00)
Clashscore	141614	9178 (2.00-2.00)
Ramachandran outliers	138981	9054 (2.00-2.00)
Sidechain outliers	138945	9053 (2.00-2.00)
RSRZ outliers	127900	7900 (2.00-2.00)

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	476	<div> <div>30%</div> <div>82%</div> <div>9%</div> <div>9%</div> </div>

2 Entry composition

There are 3 unique types of molecules in this entry. The entry contains 6186 atoms, of which 2817 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.

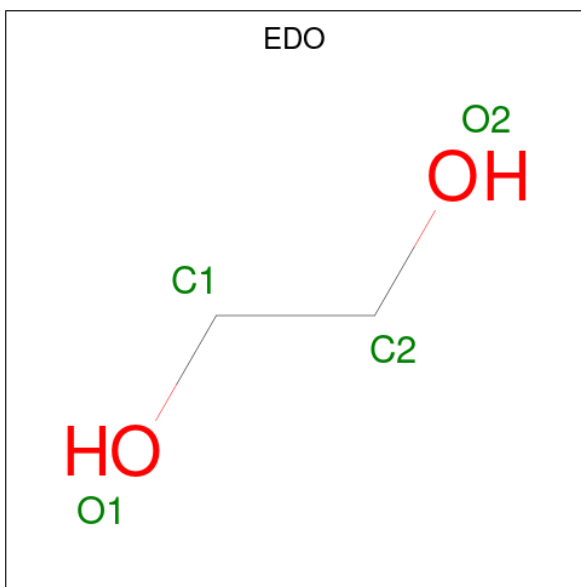
- Molecule 1 is a protein called phosphoribosyl-glycinamide (GAR) synthetase.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
			Total	C	H	N	O	S			
1	A	435	6053	2071	2799	546	621	16	0	0	0

There are 24 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1	MET	-	initiating methionine	UNP J9VYP5
A	2	HIS	-	expression tag	UNP J9VYP5
A	3	HIS	-	expression tag	UNP J9VYP5
A	4	HIS	-	expression tag	UNP J9VYP5
A	5	HIS	-	expression tag	UNP J9VYP5
A	6	HIS	-	expression tag	UNP J9VYP5
A	7	HIS	-	expression tag	UNP J9VYP5
A	8	SER	-	expression tag	UNP J9VYP5
A	9	SER	-	expression tag	UNP J9VYP5
A	10	GLY	-	expression tag	UNP J9VYP5
A	11	VAL	-	expression tag	UNP J9VYP5
A	12	ASP	-	expression tag	UNP J9VYP5
A	13	LEU	-	expression tag	UNP J9VYP5
A	14	GLY	-	expression tag	UNP J9VYP5
A	15	THR	-	expression tag	UNP J9VYP5
A	16	GLU	-	expression tag	UNP J9VYP5
A	17	ASN	-	expression tag	UNP J9VYP5
A	18	LEU	-	expression tag	UNP J9VYP5
A	19	TYR	-	expression tag	UNP J9VYP5
A	20	PHE	-	expression tag	UNP J9VYP5
A	21	GLN	-	expression tag	UNP J9VYP5
A	22	SER	-	expression tag	UNP J9VYP5
A	23	ASN	-	expression tag	UNP J9VYP5
A	24	ALA	-	expression tag	UNP J9VYP5

- Molecule 2 is 1,2-ETHANEDIOL (three-letter code: EDO) (formula: C₂H₆O₂).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		
2	A	1	Total	C	H	O	0	0
			10	2	6	2		

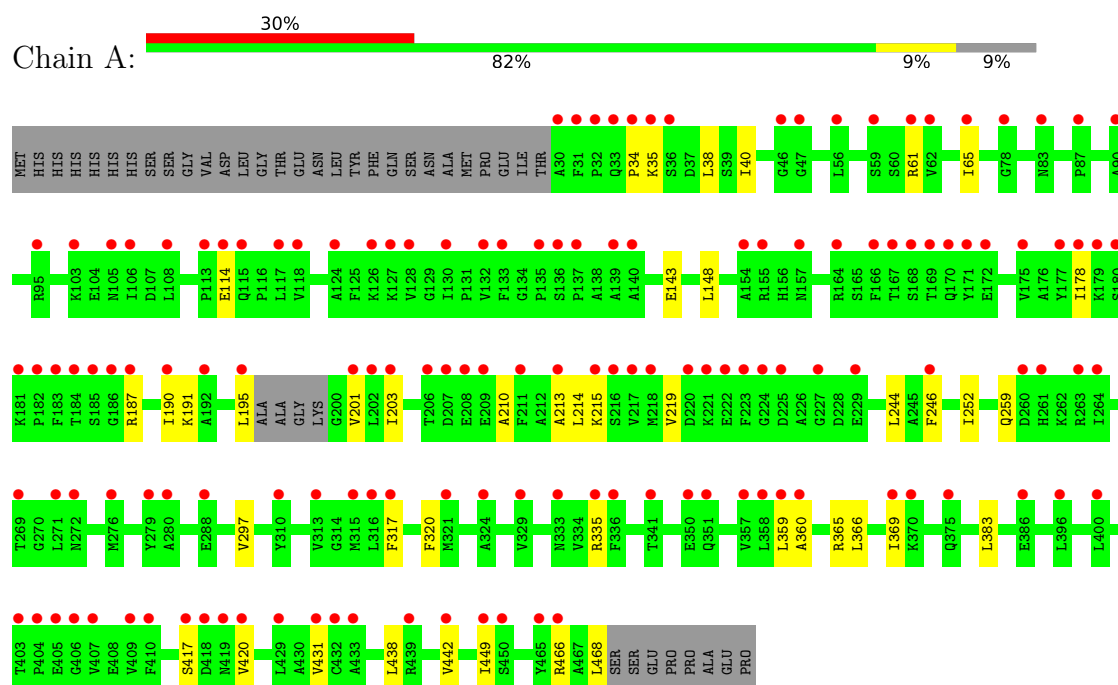
- Molecule 3 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	103	Total	O	0	0
			103	103		

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: phosphoribosyl-glycinamide (GAR) synthetase



4 Data and refinement statistics

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α , β , γ	87.10Å 76.49Å 74.97Å 90.00° 107.57° 90.00°	Depositor
Resolution (Å)	38.24 – 2.00 38.24 – 2.00	Depositor EDS
% Data completeness (in resolution range)	97.5 (38.24-2.00) 97.6 (38.24-2.00)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.67 (at 2.00Å)	Xtriage
Refinement program	PHENIX 1.19.2_4158	Depositor
R, R_{free}	0.242 , 0.285 0.240 , 0.285	Depositor DCC
R_{free} test set	3172 reflections (10.20%)	wwPDB-VP
Wilson B-factor (Å ²)	30.4	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.41 , 45.1	EDS
L-test for twinning ²	$\langle L \rangle = 0.51$, $\langle L^2 \rangle = 0.34$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6186	wwPDB-VP
Average B, all atoms (Å ²)	36.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 11.37% 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: EDO

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	0.29	0/3322	0.48	0/4507

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 [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	3254	2799	3260	28	0
2	A	12	18	18	0	0
3	A	103	0	0	1	0
All	All	3369	2817	3278	28	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 4.

All (28) 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:360:ALA:CB	1:A:369:ILE:HD13	2.23	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:114:GLU:OE2	1:A:195:LEU:HD22	1.98	0.63
1:A:431:VAL:HG21	1:A:449:ILE:HD13	1.83	0.59
1:A:34:PRO:HB2	1:A:61:ARG:NH1	2.18	0.58
1:A:383:LEU:HD11	1:A:449:ILE:HD12	1.86	0.57
1:A:215:LYS:HG3	1:A:219:VAL:HB	1.85	0.57
1:A:259:GLN:NE2	1:A:466:ARG:HH12	2.03	0.55
1:A:190:ILE:HD12	1:A:213:ALA:HB3	1.89	0.55
1:A:360:ALA:HB3	1:A:369:ILE:HD13	1.88	0.54
1:A:417:SER:O	1:A:420:VAL:HG12	2.08	0.53
1:A:438:LEU:O	1:A:442:VAL:HG23	2.14	0.48
1:A:178:ILE:HD13	1:A:210:ALA:HB1	1.96	0.47
1:A:187:ARG:HH21	1:A:203:ILE:HG22	1.78	0.47
1:A:178:ILE:CD1	1:A:214:LEU:HD11	2.45	0.46
1:A:187:ARG:NH2	1:A:203:ILE:HG22	2.30	0.46
1:A:178:ILE:HD12	1:A:214:LEU:HD11	1.96	0.46
1:A:191:LYS:HG2	1:A:201:VAL:HG22	1.98	0.45
1:A:297:VAL:HG21	1:A:320:PHE:HE2	1.82	0.45
1:A:246:PHE:O	1:A:252:ILE:HA	2.18	0.44
1:A:35:LYS:HB2	3:A:642:HOH:O	2.17	0.43
1:A:148:LEU:HD23	1:A:148:LEU:C	2.38	0.43
1:A:438:LEU:HG	1:A:468:LEU:HD21	2.01	0.43
1:A:34:PRO:C	1:A:61:ARG:HH12	2.22	0.42
1:A:40:ILE:HB	1:A:65:ILE:HD13	2.02	0.41
1:A:38:LEU:HD13	1:A:359:LEU:HD11	2.01	0.41
1:A:143:GLU:OE2	1:A:335:ARG:NH2	2.54	0.41
1:A:244:LEU:HD11	1:A:317:PHE:CE2	2.56	0.40
1:A:366:LEU:HD12	1:A:369:ILE:HD11	2.03	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	431/476 (90%)	410 (95%)	21 (5%)	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	343/377 (91%)	342 (100%)	1 (0%)	92	95

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

Mol	Chain	Res	Type
1	A	365	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

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 monosaccharides in this entry.

5.6 Ligand geometry [i](#)

3 ligands are 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	EDO	A	503	-	3,3,3	0.46	0	2,2,2	0.32	0
2	EDO	A	501	-	3,3,3	0.45	0	2,2,2	0.30	0
2	EDO	A	502	-	3,3,3	0.48	0	2,2,2	0.27	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	A	503	-	-	0/1/1/1	-
2	EDO	A	501	-	-	0/1/1/1	-
2	EDO	A	502	-	-	0/1/1/1	-

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	435/476 (91%)	1.80	144 (33%) 0 0	20, 32, 61, 82	0

All (144) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	465	TYR	11.7
1	A	418	ASP	10.3
1	A	419	ASN	8.9
1	A	168	SER	8.0
1	A	179	LYS	7.3
1	A	175	VAL	7.1
1	A	184	THR	6.9
1	A	216	SER	6.4
1	A	185	SER	6.1
1	A	208	GLU	5.9
1	A	169	THR	5.6
1	A	140	ALA	5.3
1	A	202	LEU	5.3
1	A	32	PRO	4.8
1	A	375	GLN	4.4
1	A	195	LEU	4.4
1	A	466	ARG	4.3
1	A	190	ILE	4.0
1	A	350	GLU	3.9
1	A	183	PHE	3.9
1	A	172	GLU	3.9
1	A	225	ASP	3.8
1	A	215	LYS	3.8
1	A	217	VAL	3.8
1	A	211	PHE	3.7
1	A	223	PHE	3.7
1	A	264	ILE	3.7

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Mol	Chain	Res	Type	RSRZ
1	A	34	PRO	3.7
1	A	90	ALA	3.6
1	A	417	SER	3.6
1	A	30	ALA	3.5
1	A	222	GLU	3.5
1	A	269	THR	3.5
1	A	181	LYS	3.5
1	A	400	LEU	3.4
1	A	115	GLN	3.4
1	A	170	GLN	3.4
1	A	272	ASN	3.4
1	A	127	LYS	3.4
1	A	370	LYS	3.3
1	A	35	LYS	3.3
1	A	224	GLY	3.3
1	A	213	ALA	3.2
1	A	220	ASP	3.2
1	A	46	GLY	3.2
1	A	357	VAL	3.2
1	A	47	GLY	3.2
1	A	358	LEU	3.1
1	A	359	LEU	3.1
1	A	218	MET	3.1
1	A	166	PHE	3.1
1	A	31	PHE	3.1
1	A	95	ARG	3.1
1	A	263	ARG	3.0
1	A	206	THR	3.0
1	A	157	ASN	3.0
1	A	420	VAL	3.0
1	A	33	GLN	3.0
1	A	409	VAL	2.9
1	A	155	ARG	2.9
1	A	317	PHE	2.9
1	A	167	THR	2.9
1	A	221	LYS	2.9
1	A	61	ARG	2.9
1	A	336	PHE	2.9
1	A	62	VAL	2.8
1	A	405	GLU	2.8
1	A	310	TYR	2.8
1	A	442	VAL	2.8

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Mol	Chain	Res	Type	RSRZ
1	A	449	ILE	2.8
1	A	171	TYR	2.8
1	A	128	VAL	2.8
1	A	132	VAL	2.8
1	A	406	GLY	2.7
1	A	133	PHE	2.7
1	A	124	ALA	2.7
1	A	329	VAL	2.7
1	A	78	GLY	2.7
1	A	201	VAL	2.7
1	A	360	ALA	2.6
1	A	288	GLU	2.6
1	A	271	LEU	2.6
1	A	429	LEU	2.6
1	A	324	ALA	2.6
1	A	433	ALA	2.6
1	A	351	GLN	2.6
1	A	209	GLU	2.5
1	A	177	TYR	2.5
1	A	404	PRO	2.5
1	A	65	ILE	2.5
1	A	450	SER	2.5
1	A	87	PRO	2.5
1	A	316	LEU	2.4
1	A	246	PHE	2.4
1	A	130	ILE	2.4
1	A	369	ILE	2.4
1	A	36	SER	2.4
1	A	164	ARG	2.4
1	A	154	ALA	2.4
1	A	315	MET	2.4
1	A	403	THR	2.4
1	A	386	GLU	2.4
1	A	341	THR	2.4
1	A	105	ASN	2.3
1	A	439	ARG	2.3
1	A	137	PRO	2.3
1	A	192	ALA	2.3
1	A	186	GLY	2.3
1	A	135	PRO	2.3
1	A	136	SER	2.3
1	A	279	TYR	2.3

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Mol	Chain	Res	Type	RSRZ
1	A	178	ILE	2.3
1	A	182	PRO	2.2
1	A	203	ILE	2.2
1	A	139	ALA	2.2
1	A	396	LEU	2.2
1	A	431	VAL	2.2
1	A	103	LYS	2.2
1	A	227	GLY	2.2
1	A	114	GLU	2.2
1	A	313	VAL	2.2
1	A	59	SER	2.2
1	A	187	ARG	2.2
1	A	407	VAL	2.2
1	A	113	PRO	2.2
1	A	56	LEU	2.1
1	A	118	VAL	2.1
1	A	410	PHE	2.1
1	A	321	MET	2.1
1	A	333	ASN	2.1
1	A	83	ASN	2.1
1	A	106	ILE	2.1
1	A	126	LYS	2.1
1	A	276	MET	2.1
1	A	229	GLU	2.1
1	A	260	ASP	2.1
1	A	261	HIS	2.1
1	A	180	SER	2.0
1	A	108	LEU	2.0
1	A	207	ASP	2.0
1	A	432	CYS	2.0
1	A	335	ARG	2.0
1	A	117	LEU	2.0
1	A	280	ALA	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 monosaccharides 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	EDO	A	502	4/4	0.48	0.28	18,18,46,46	0
2	EDO	A	503	4/4	0.73	0.20	18,18,63,63	0
2	EDO	A	501	4/4	0.77	0.26	16,16,36,36	0

6.5 Other polymers [i](#)

There are no such residues in this entry.